
VisTrails Documentation

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NYU Poly

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Part I

User's Guide

PRELIMINARY PAGES

1.1 Preface

Welcome to the *VisTrails User's Guide*. This book has been updated for version 2.1 of the VisTrails software.

VisTrails is a new scientific workflow management system developed at the University of Utah that provides support for data exploration and visualization. For an engineer or scientist, generating and evaluating hypotheses is an interactive process. With each change, a different, albeit related, workflow is created. VisTrails was designed to manage these rapidly-evolving workflows. By automatically managing the data, metadata, and the data exploration process, VisTrails allows you to focus on the task at hand and relieves you from tedious and time-consuming tasks involved in organizing vast volumes of data. VisTrails provides infrastructure that can be combined with and enhance existing visualization and workflow systems.

VisTrails is an open-source software system. You can contribute to VisTrails by sharing bug reports, bug fixes, and suggestions with the VisTrails community. The easiest way to get started is to sign up for the VisTrails Users mailing list. Instructions for doing this can be found on the VisTrails web site: www.vistrails.org.

This book is divided into four parts. The first part, [Getting started](#), provides instructions on how to download and install the VisTrails software, and introduces you to its user interface. The second and longest part, “Learning VisTrails by Example,” consists of a number of tutorial chapters that guide you, step by step, through the features of VisTrails. We encourage you to try out these examples for yourself as you read this book. The third part provides information on additional features and packages. The fourth and final part is the “Developer’s Guide” and is intended for programmers who wish to add new features, packages, and modules to VisTrails.

We hope that you will find VisTrails to be a useful tool towards automating and streamlining your workflows, leading to faster discoveries and deeper insight.

For your convenience, the html version of this manual is also available at <http://www.vistrails.org/usersguide>.

About the figures: VisTrails works across multiple platforms, and the screenshots shown in this manual reflect this. Hence, some of the images in this book may vary slightly from what you see on your system, depending on the look and feel of your platform.

1.1.1 Acknowledgements

VisTrails research and development has been funded the Department of Energy SciDAC (VACET and SDM centers), the National Science Foundation (grants IIS-0746500, CNS-0751152, IIS-0713637, OCE-0424602, IIS-0534628, CNS-0514485, IIS-0513692, CNS-0524096, CCF-0401498, OISE-0405402, CCF-0528201, CNS-0551724), and IBM Faculty Awards (2005, 2006, 2007, and 2008).

AN INTRODUCTION TO VISTRAILS

2.1 What Is VisTrails?

VisTrails is a new system that provides data and process management support for exploratory computational tasks. It combines features of both workflow and visualization systems. Similar to workflow systems, it allows the combination of loosely-coupled resources, specialized libraries, and grid and Web services. Similar to some visualization systems, it provides a mechanism for parameter exploration and comparison of different results. But unlike these other systems, VisTrails was designed to manage *exploratory processes* in which computational tasks evolve over time as a user iteratively formulates and tests hypotheses. A key distinguishing feature of VisTrails is its comprehensive provenance infrastructure that maintains detailed history information about the steps followed in the course of an exploratory task. VisTrails leverages this information to provide novel operations and user interfaces that streamline this process.

2.1.1 Important Features

One of our main uses for VisTrails has been exploratory visualization, but the system is much more general and provides many other features, such as:

- *Flexible Provenance Architecture.* VisTrails transparently tracks changes made to workflows, including all the steps followed in the exploration. The system can optionally track run-time information about the execution of workflows (*e.g.*, who executed a module, on which machine, elapsed time *etc.*). VisTrails also provides a flexible annotation framework whereby you can specify application-specific provenance information.
- *Querying and Re-using History.* The provenance information is stored in a structured way. You have a choice of using a relational database (such as MySQL or IBM DB2) or XML files in the file system. The system provides flexible and intuitive query interfaces through which you can explore and reuse provenance information. You can formulate simple keyword-based and selection queries (*e.g.*, find a visualization created by a given user) as well as structured queries (*e.g.*, find visualizations that apply simplification before an isosurface computation for irregular grid data sets).
- *Support for collaborative exploration.* The system can be configured with a database backend that can be used as a shared repository. It also provides a synchronization facility that allows multiple users to collaborate asynchronously and in a disconnected fashion—you can check in and check out changes, akin to a version control system (*e.g.*, SVN: <http://subversion.tigris.org>).
- *Extensibility.* VisTrails provides a very simple plugin functionality that can be used to dynamically add packages and libraries. Neither changes to the user interface nor re-compilation of the system are necessary. Because VisTrails is written in Python, the integration of Python-wrapped libraries is straightforward. For example, a single line in the VisTrails start-up file is needed to import all of VTK's classes.
- *Scalable Derivation of Data Products and Parameter Exploration.* VisTrails supports a series of operations for the simultaneous generation of multiple data products, including an interface that allows you to specify sets of values for different parameters in a workflow. The results of a parameter exploration can be displayed side by side in the VisTrails Spreadsheet for easy comparison.

- *Task Creation by Analogy*. Analogies are supported as first-class operations to guide semi-automated changes to multiple workflows, without requiring you to directly manipulate or edit the workflow specifications.

2.1.2 Obtaining the software

Visit <http://www.vistrails.org> to access the VisTrails community website. Here you will find information including instructions for obtaining the software, online documentation, video tutorials, and pointers to papers and presentations.

VisTrails is available as open source; it is released under the GPL 2.0 license. The pre-compiled versions for Windows and Mac OS X come with an installer and include a number of packages, including VTK, matplotlib, and Image Magick. Additional packages, including packages written by users, are also available (*e.g.*, ITK, Matlab, Metro). Developers can easily add new packages using the VisTrails plugin infrastructure.

2.2 Getting Started

The VisTrails system is distributed both as source code and pre-built binaries, and instructions for obtaining either can be found at our website: <http://www.vistrails.org>. Because the system is written in Python using a Qt interface, it can be run on most architectures that support these two components, even if a pre-built binary is not available for your system. Section *Installation* provides instructions to guide you through installation procedures, and Section *Quick Start* gives a quick orientation and serves as a springboard for exploring the different features of VisTrails.

2.2.1 Installation

There are two types of VisTrails installations. The first is a binary installation that lets you use VisTrails by running the precompiled executable. The second is a full source code installation that requires you to install and compile VisTrails and all of its dependencies. Of the two types of installations, the binary version is much easier, and we encourage first-time users to use this option whenever possible. Precompiled binaries are currently available for Microsoft Windows (XP and Vista) and Mac OS X (10.5.x or higher). To obtain either a binary or source copy of VisTrails, please see our website: <http://www.vistrails.org>.

Installing VisTrails on Windows XP/Vista

To install VisTrails on Windows, download the installation bundle for Windows from the VisTrails website: <http://www.vistrails.org>. Unzip the file using the decompression program of your choice, then double-click the executable to begin installation (Figure *Installation wizard for Microsoft Windows XP/Vista*). Follow the prompts in the installation wizard to complete the installation process.

Installing VisTrails on Mac OS X

To install VisTrails on Mac OS X, download the installation bundle for Mac from the VisTrails website: <http://www.vistrails.org>. The precompiled binary currently only supports Mac OS X 10.5.x or higher. The disk image should be mounted automatically (Figure *Installing VisTrails on Mac OS X*). Once the disk image is mounted, drag the VisTrails folder to the Applications folder to install the software.

Installing VisTrails on Ubuntu Linux

Although not a binary installation *per se*, installing VisTrails on Ubuntu Linux is nonetheless quite straightforward. VisTrails now interfaces with “apt” directly via a Python API. This allows dynamic installation of necessary packages.

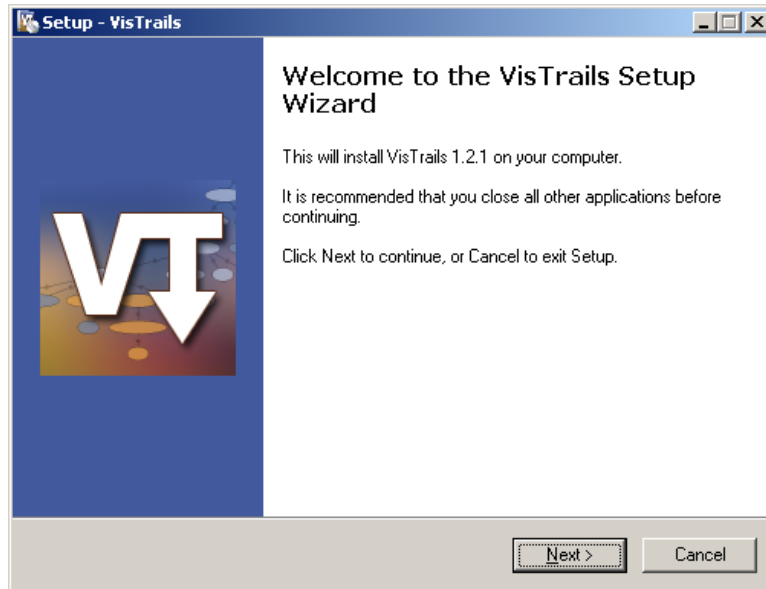


Fig. 2.1: Installation wizard for Microsoft Windows XP/Vista.

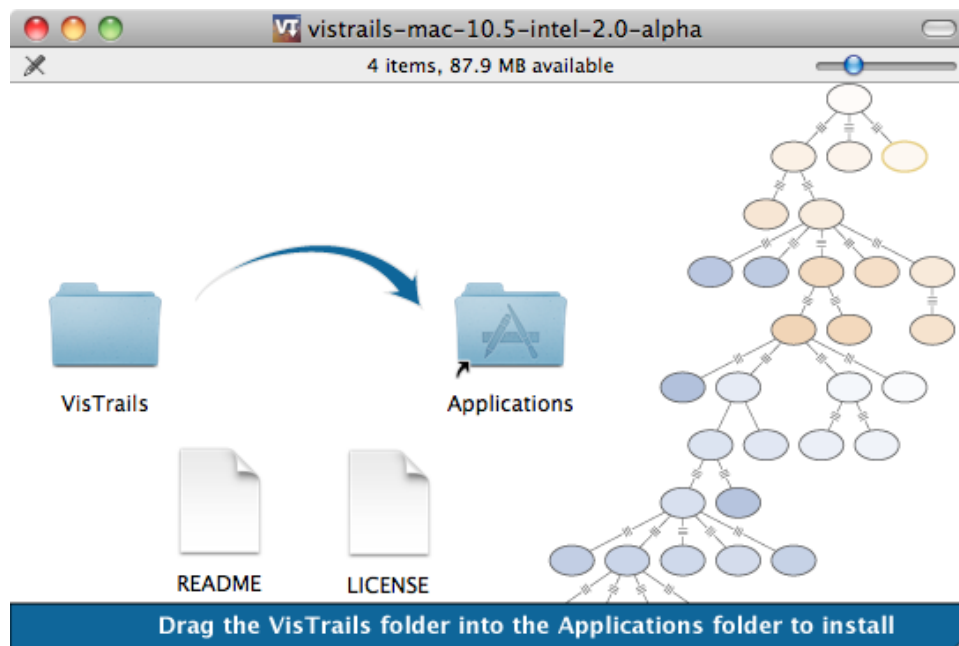


Fig. 2.2: Installing VisTrails on Mac OS X.

As a result, you do not need to manually install any of the dependent packages. Just download the VisTrails source code and execute it with:

```
python vistrails/run.py
```

and VisTrails should detect all necessary software and, if necessary, ask for your permission to install it.

Installing VisTrails from source

Installing VisTrails from source code is a non-trivial task. Rather than listing full compilation instructions in this manual, we instead provide a list of software packages upon which VisTrails is dependent, and refer you to the VisTrails website for additional details.

- Python 2.6 or higher
- Qt 4.4 or higher
- PyQt4
- SciPy
- VTK (needed to run the examples in this book)

There may also be additional dependencies, depending on which optional features of VisTrails you plan to use.

Please refer to http://www.vistrails.org/index.php/Mac_Intel_Instructions for more details.

2.2.2 Quick Start

On Windows and Mac OS X, you can launch VisTrails by double-clicking on the VisTrails application icon. In general, however, it is possible to start VisTrails on any system by navigating to the directory where the file `run.py` is located (usually the root directory of your installation) and executing the command:

```
python run.py
```

Depending on a number of factors, it can take a few seconds for the system to start up. As VisTrails loads, you may see some messages that detail the packages being loaded and initialized. This is normal operation, but if the system fails to load, these messages will provide information that may help you understand why.

2.2.3 Installing additional packages

VisTrails releases come with a number of packages already installed. In addition to these, you can write your own packages or install packages from third-party developers. To do that, just drop the Python module (single file) or package (i.e. directory) in `$HOME/.vistrails/userpackages/` (VisTrails should automatically create this folder on the first run).

You can then enable and disable standard or user packages from the preferences dialog, under the module packages tab.

2.2.4 The Vistrails Builder Window

After everything has loaded, you will see the VisTrails Builder window as shown in Figure *VisTrails Builder Window*. If you have enabled the VisTrails Spreadsheet (Packages → VisTrails Spreadsheet → Show Spreadsheet), you will also see a second window like that in Figure *VisTrails Spreadsheet Window*. Note that if the spreadsheet window is not visible, it will open upon execution of a workflow that uses it.

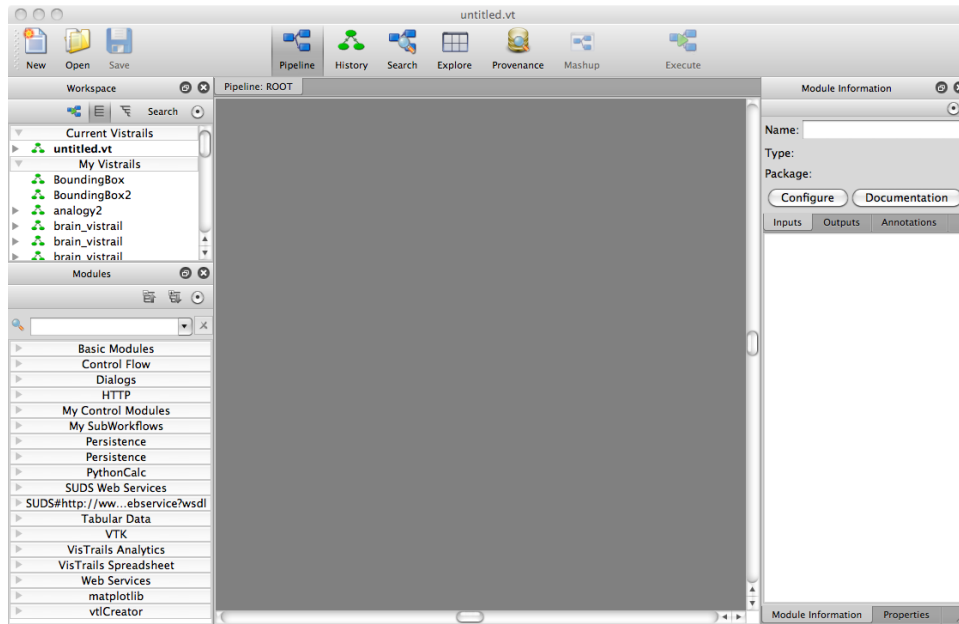


Fig. 2.3: VisTrails Builder Window

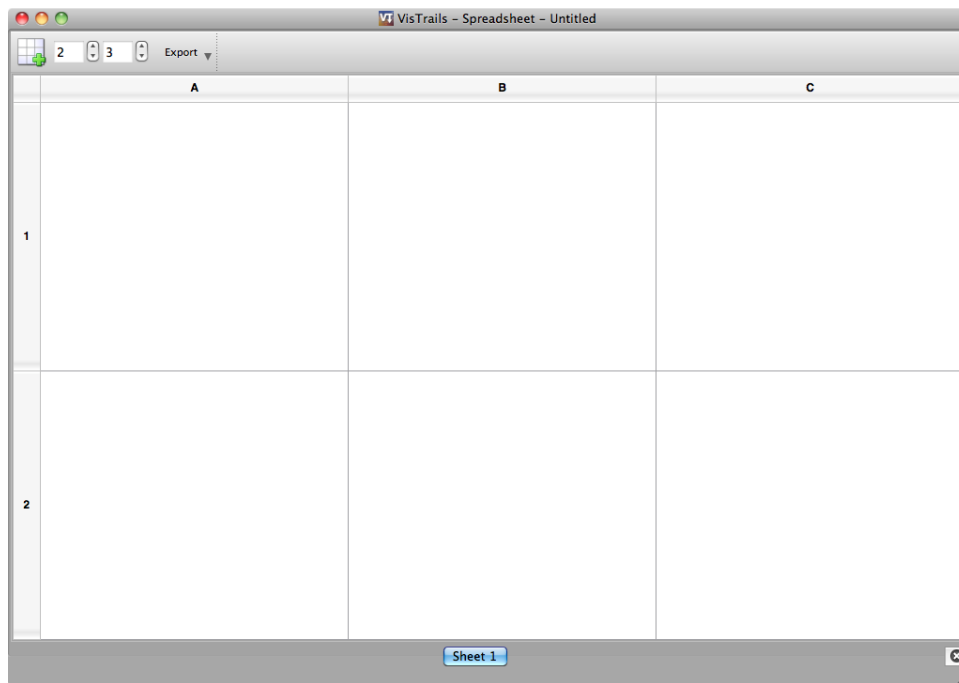


Fig. 2.4: VisTrails Spreadsheet Window

The VisTrails Toolbar



Fig. 2.5: VisTrails Toolbar

The VisTrails toolbar both allows you to execute the current workflow or function, and switch between various modes. A brief description of each member of the toolbar follows:

Pipeline This view shows the current workflow. See Chapter *Creating and Modifying Workflows* for information about creating a workflow.

History This view shows different versions of the workflow(s) as it has progressed over time. See Chapter *Interacting with the Version Tree*.

Search Use this mode to search for modules or subpipeline within the current version, the current vistrail, or all vistrails. See Chapter *Querying the Version Tree*.

Explore This option allows you to select one or more parameter(s) for which a set of values is created. The workflow is then executed once for each value in the set and displayed in the spreadsheet for comparison purposes. See Chapter *Parameter Exploration*.

Provenance The `Provenance` mode shows the user a given vistrail's execution history. When a particular execution is selected, its pipeline view with modules colored according to its associated execution result is shown. See Chapter *Provenance Browser*.

Mashup The `Mashup` mode allows you to create a small application that allows you to explore different values for a selected set of parameters. See Chapter *Mashups* for more information.

Execute `Execute` will either execute the current pipeline when the `Pipeline`, `History`, or `Provenance` views are selected, or perform the search or exploration when in `Search` or `Exploration` mode. This button is disabled for `Mashup` mode, or when there is not a current workflow to execute.

The `New`, `Open`, and `Save` buttons will create, open, and save a vistrail, as expected.

Palettes and Associated Views

Palettes

As you can see, the builder window has a center widget with a palette on each side. There are a number of views (listed in the 4th group of the views menu) that when made visible, will be opened in these palettes. In this section, we will discuss how the views are arranged.

Notice that when VisTrails first launches the builder window, both palettes contain two views. The left palette is split so both views are visible, whereas the right palette uses tabs to display one view at a time. By default, additional views will be shown in the right, and lower left panels when they are made visible. To make a view visible, either switch to a mode that requires it, or select it from the views menu. For example, the `Mashup` mode will add the `Mashup Pipeline` and `Mashups Inspector` views to the panels. When the mode is changed from `Mashup`, these two views will be removed (hidden).

Buttons

Notice that there is a button with a pin icon in the upper right corner of each view (see Figure *Buttons - Close, Detach, and Pin*). If you don't want a view to disappear when you change modes, make sure it is pinned. When the pin points up, it is unpinned and the view is likely to disappear when you change modes.

The other two buttons, the one with the ‘X’ and the one with the rectangular outlines (see Figure *Buttons - Close, Detach, and Pin*), will either close the view, or undock the view, depending on which one you push. Alternatively, you may undock a view by clicking on the view’s title bar and pulling it out of the palette. The view can then either remain in its own window, or can be docked by placing it in either palette.

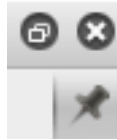


Fig. 2.6: Buttons - Close, Detach, and Pin

View Locations

The following table gives the view that is visible in each palette for each of the main views/modes:

	Lower Left Palette	Right Palette
Pipeline	Modules	Module Information
History	Modules	Properties
Explore	Explore Properties	Set Methods
Provenance	Modules	Log Details
Mashup	Mashups Inspector	Mashup Pipeline

Notice that the `Workspace`, `Diff Properties`, and `Vistrail Variables` views are not in the table. That is because, the `Workspace` view is always visible, the `Diff Properties` view opens in the right palette when a visual diff is performed in the `History` view, and the `Vistrail Variables` view is opened from the `Views` menu. Note: with the `Vistrail Variables` view especially, if you don’t want it to disappear, you should make sure it is pinned.

The Center Widget

The center widget is somewhat larger than the side panels as it is intended to be the main workspace. It displays the following views: `Pipeline`, `History`, `Search-query and results`, `Visual Diff results`, `Explore`, `Provenance`, and `Mashup`. By default, one view is shown. To open an additional view, type `CTRL-t` to create a new tab. The new tab starts out in the `Pipeline` view, but you are free to change it to any of the other views. Note that the tabs from only one vistrail are displayed at a time. When you switch to a different vistrail, the other vistrail’s set of open tabs are displayed.

If you would like to see views from more than one vistrail at a time, you may do this by right-clicking on the vistrail (listed in `Current Vistrails` of the `Workspace` view), and selecting the option to open in a new window. The side palettes will stay with the original window, but can be moved to the current window by selecting `Dock Palettes` from the `Views` menu.

If you would like to see multiple views from the same vistrail, double-click the title of the view to detach it. It is not possible to reattach the view, so once you are finished with the detached view, you may close it. If you would like the view to be reattached, you should close it and open it again in a new tab.

2.2.5 Manipulating VisTrails Files

To open a VisTrails file, or *vistrail*, you can either click the `Open` button in the toolbar or select `Open` from the `File` menu. This brings up a standard file dialog where you can select a vistrail to open. Vistrails are identified by the `.vt` file extension. Alternatively, if the vistrail is listed under *My Vistrails* in the `Workspace Panel`, double clicking its name will open it. When a vistrail is opened, it is listed in the `Workspace` (upper left panel) under *Current Vistrails*. Since only one open vistrail is displayed at a time, the `Workspace` allows you to select which one to display. Vistrails

can also be stored in a database, enabling a central repository for workflows. See Chapter *Connecting to a Database* for more details about this feature.

To close a vistrail, you can either choose the `Close` option from the `File` menu or type `Ctrl-w`. If the vistrail has not been saved, you will be asked if you wish to save your work. To save a vistrail, there is both a button and a menu item in the `File` menu. If you would like to save the vistrail with a different name or in a different location, you can use the `Save As` option.

2.2.6 VisTrails Basics

In general, a *workflow* is a way to structure a complex computational process that may involve a variety of different resources and services. Instead of trying to keep track of multiple programs, scripts, and their dependencies, workflows abstract the details of computations and dependencies into a graph consisting of computational *modules* and *connections* between these modules.

The `Pipeline` button on the VisTrails toolbar accesses VisTrails' interface for building workflows. Similar to many existing workflow systems, it allows you to interactively create workflows using an extensible library of modules and a connection protocol that helps you determine how to connect modules. To add a module to a workflow, simply drag the module's name from the list of available modules to the workflow canvas. Each module has a set of input and output ports, and outputs from one module can be connected to inputs of another module, provided that the types match. For more information on building workflows in VisTrails, see Chapter *Creating and Modifying Workflows*.

In addition to VisTrails' *Pipeline* interface for manipulating individual workflows, the *History* interface (accessed through the `History` button on the toolbar) contains a number of features that function on a collection of workflows. A *vistrail* is a collection of related workflows. As you explore different computational approaches or visualization techniques, a workflow may evolve in a lot of directions. VisTrails captures all of these changes automatically and transparently. Thus, you can revisit a previous version of a workflow and modify it without worrying about saving intermediate versions. This history is displayed by the VisTrails Version Tree, and different ways of interacting with this tree are discussed in Chapter *Interacting with the Version Tree*.

With a collection of workflows, one of the necessary tasks is to search for specific workflows. VisTrails' search functionality is accessed by clicking the `Query` button on the toolbar. The criteria for these searches may vary from finding workflows modified within a specific time frame to finding workflows that contain a specific module. Because of the version history that VisTrails captures, these tasks are natural to implement and query. VisTrails has two methods for querying workflows, a simple text-based query language and a query-by-example canvas that lets you build exactly the workflow structure you are looking for. Both of these techniques are described in Chapter *Querying the Version Tree*.

The `Exploration` button allows you to explore workflows by running the same workflow with different parameters. Parameter Exploration provides an intuitive interface for computing workflows with parameters that vary in multiple dimensions. When coupled with the VisTrails Spreadsheet, parameter exploration allows you to quickly compare results and discover optimal parameter settings. See Chapter *Parameter Exploration* for specific information on using Parameter Exploration.

2.2.7 VisTrails Interaction

Workflow Execution

The `Execute` button on the toolbar serves as the “play” button for each of the modes described above. In both the `Builder` and `Version Tree` modes, it executes the current workflow. In `Query` mode, it executes the query, and in `Parameter Exploration` mode, it executes the workflow for each of the possible parameter settings.

When a workflow is executed, the module color is determined as follows:

- lilac: module was not executed

- yellow: module is currently being executed
- green: module was successfully executed
- orange: module was cached
- red: module execution failed

A popup is shown when executing workflows from the pipeline or history view. The popup shows overall progress, the type of module being executed, and a cancel button. Pressing cancel will show a dialog where you can choose to abort or continue the execution. Note that the cancel button may appear frozen while a module is being executed. This is due to limitations in python.

Note

VisTrails caches by default, so after a workflow is executed, if none of its parameters change, it won't be executed again.

If a workflow reads a file using the basic module File, VisTrails does check whether the file was modified since the last run. It does so by keeping a signature that is based on the modification time of the file. And if the file was modified, the File module and all downstream modules (the ones which depend on File) will be executed.

If you do not want VisTrails to cache executions, you can turn off caching: go to Menu Edit → Preferences and in the General Configuration tab, change Cache execution results to Never.

If you would like your input and output data to be versioned, you can use the Persistence package.

Additional Interactions

From the `Edit` menu, `Undo` and `Redo` function in the standard way, but note that these actions are implicitly switching between different versions of a workflow. Thus, you will notice that as you undo or redo a change to a workflow, the selected version in the version tree changes.

For all modes except Parameter Exploration, the center pane of VisTrails is a canvas where you can manipulate the current workflow, version tree, or query. The buttons on the right side of the toolbar allow you to change the default behavior of the primary mouse button (the left button for most multiple button mice) within this canvas. You can choose the behavior to select items in the scene, pan around the scene, or zoom in and out of the scene by selecting the given button. In addition, if you are using a 3-button mouse, the right button will zoom, and the middle button will pan. To use the zoom functionality, click and drag up to zoom out and drag down to zoom in.

Note

Pressing `Ctrl-R` will recenter the window.

LEARNING VISTRAILS BY EXAMPLE

3.1 Creating and Modifying Workflows

3.1.1 Working with Modules

In VisTrails, modules are represented by a rectangle in the `Pipeline` view of the Builder. The name of the module is shown in bold letters in the middle of the rectangle. The input and output ports for the module are denoted by small squares on the top and bottom of the module, respectively. Modules are connected together to define the dataflow using curved black lines that go from output to input ports between modules. Each module may also have adjustable parameters that can be viewed when a module is selected. Modules can be connected, disconnected, added, and deleted from a workflow.

As a running example in this chapter, we will make some changes to the “`vtk_book_3rd_p189.vt`” vistrail, included in the “examples” folder of the VisTrails installation.

Try it now!

Open the “`vtk_book_3rd_p189.vt`” vistrail, either by selecting `File` → `Open` from the menu, or by clicking the `Open` button on the toolbar. After opening this vistrail, select the version labeled `final`, then click on the `Pipeline` toolbar button to enter workflow editing mode.

3.1.2 Adding and Deleting Modules

A list of available modules is displayed hierarchically in the `Modules` container on the left side of the VisTrails Builder (Figure *The main VisTrails Pipeline...*). A core set of basic modules is always distributed with the VisTrails system. Other packages, such as VTK, are also distributed, but are not necessary for VisTrails and thus can be disabled on startup (see Chapter *Writing VisTrails Packages*). Note, however, that the VTK module *is* required for most of the examples in this book. Depending on the number of packages imported on startup, the number of modules to select from can be difficult to navigate. Thus, a simple search box is provided at the top of the container to narrow the displayed results. To add a module to the workflow, simply drag the text from the `Module` container to the workflow canvas.

Modules and connections may be selected in multiple ways and are denoted by a yellow highlight. Besides directly left clicking on the object, a box selection is available by left clicking and dragging over the modules and connections in the canvas. Multiple selection can be performed with the box selection as well as by right clicking on multiple objects with the ‘Shift’ key pressed.

There are several ways to manipulate selected modules in the workflow canvas. Moving them is performed by dragging a selected module using the left mouse button. Deleting selected modules is performed by pressing the ‘Delete’ key.

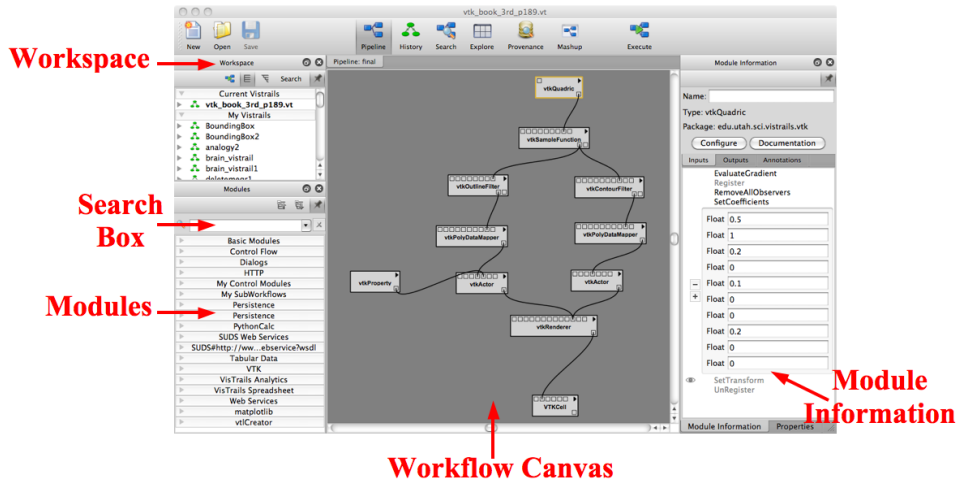


Fig. 3.1: The main VisTrails Pipeline user interface. The major components are labeled.

The modules and connections can also be copied and pasted using the Edit menu, or with ‘Ctrl-C’ and ‘Ctrl-V’, respectively.

Try it now!

Let’s replace the `vtkQuadric` module in our example with a `vtkCylinder` module instead. To do this, first type “`vtkCylinder`” into the search box of the Module container. As the letters are typed, the list filters the available modules to match the query. Select this module and drag the text onto an empty space in the canvas (see Figure *The `vtkCylinder` module is added to the canvas*). Then, select the `vtkQuadric` module in the canvas and press the ‘Delete’ key. This removes the module along with any connections it has (see Figure *The `vtkQuadric` module is deleted*).

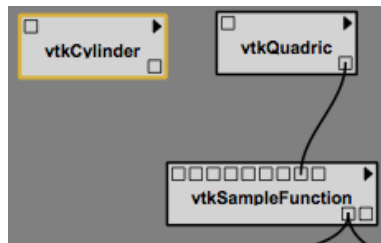


Fig. 3.2: The `vtkCylinder` module is added to the canvas.

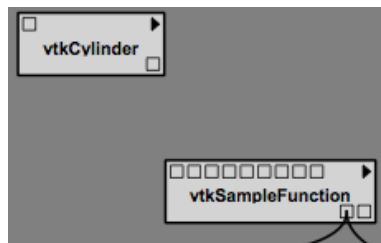


Fig. 3.3: The `vtkQuadric` module is deleted.

3.1.3 Connecting Modules

Modules are connected in VisTrails through the input and output ports at the top and bottom of the module, respectively. By hovering the mouse over the box that defines a port, the name and data type are shown in a small tooltip. To connect two ports from different modules, start by left clicking inside one port, then dragging the mouse to the other. The connection line will automatically snap to the ports in a module that have a matching datatype. Since multiple ports may match, hovering the mouse over the port to confirm the desired match may be necessary. Once a suitable match is found, releasing the left mouse button will create the connection. Note, a connection will only be made if the input and output port's data types match. To disconnect a connection between modules, the line between the modules can be selected and deleted with the 'Delete' key.

Try it now!

To connect the `vtkCylinder` module to the `vtkSampleFunction` module, place the cursor over the only output port on the `vtkCylinder` module, located on the bottom right. A tooltip should appear that reads "Output port self (`vtkCylinder`).". Left click on the port and drag the mouse over the `vtkSampleFunction` module. The connection should snap to the fourth input port from the left. Hovering the mouse over this port shows a tooltip that reads "Input port SetImplicitFunction (`vtkImplicitFunction`).". Release the mouse button to complete the connection between these two modules (see Figure *The connection replaced*). To check for a valid dataflow, execute the workflow by pressing the `Execute` button on the toolbar, and see if the results appear in the spreadsheet.

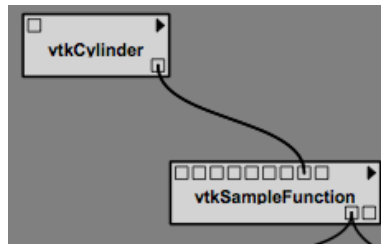


Fig. 3.4: The connection replaced.

If the ports are not directly compatible, VisTrails may automatically insert a conversion module between the two ports. If such a module is about to be used, VisTrails will display the connection you are drawing with a dotted line (see Figure *Automatic conversion*).

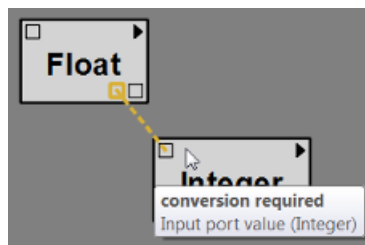


Fig. 3.5: Insertion of a conversion module

3.1.4 Changing Module Parameters

The parameters for a module can be accessed in the `Module Information` tab located on the right side of the Builder window. When a module on the canvas is selected, the corresponding module information is displayed. The

Inputs, Outputs, and Annotations tabs can be selected to set parameters within the respective categories. To set a parameter, simply click on its name to reveal its input box and enter the desired value. Notice that a – and + button appears to the left of the input box. The – button removes the corresponding input box and the + button adds one. This allows you to experiment with different values, but only the values in the last box are used in the final result.

Try it now!

To perform a parameter change, select the `vtkCylinder` module in the canvas. Select `SetRadius`, enter 0.25 into the text box and press the ‘Enter’ key. By executing the workflow, the modified visualization appears in the spreadsheet. Figures *The module methods...* and *The results...* show the interface and results of the parameter explorations.

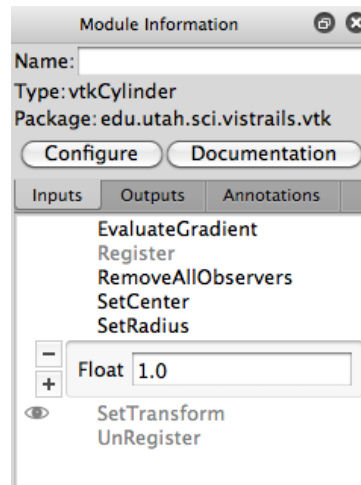


Fig. 3.6: The module methods interface is shown with a change of the `SetRadius` parameter to 1.0.

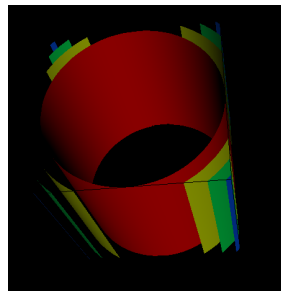


Fig. 3.7: The results of the changes are displayed on execution.

3.1.5 Using Global Variables

VisTrails supports the use of global variables, which allows the user to create a variable which can be used anywhere within the vistrail. So, if you create a variable of type `String`, you can assign that variable to any port of type `String`. This is done by opening the `Vistrail Variables` view, creating a variable, and then dragging it to the desired port.

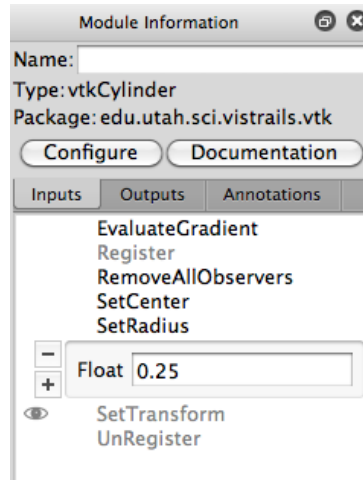


Fig. 3.8: The module methods interface is shown with a change of the `SetRadius` parameter to 0.25.

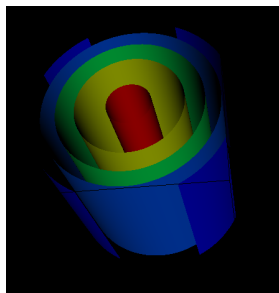


Fig. 3.9: The results of the changes are displayed on execution.

Try it now!

Open `vtk_http.vt` and go to the Pipeline view of the Fran Cut Smoothed version. Select Views → Vistrail Variables. Select the String module from Basic Modules, drag it over to the Vistrail Variables tab, and drop it (see Figure *Create a Variable...*). Name it 'Filename1' and assign it the following value: '`http://www.sci.utah.edu/~cscheid/stuff/vtkdata-5.0.2.zip`'. Click on String, which is just below Filename1 in the Vistrail Variables tab. Drag it over and drop it in the port of the DownloadFile (as shown in Figure *Assign a Variable...*). The variable should be assigned and the port should be filled in with yellow. (Open result)

To delete a global variable, simply click on the 'X' button that appears to the right of its name. This will remove the variable, but if any ports are assigned to it, they need to be disconnected. You can do this by right-clicking on the port and selecting `Disconnect Vistrail Variables` (see Figure *Disconnect a Variable...*).

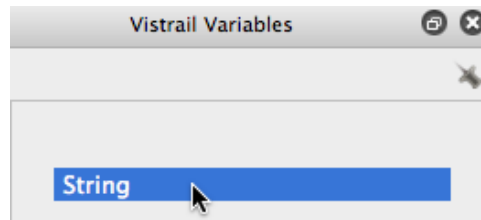


Fig. 3.10: Create a Variable - Drag the String module and drop it in the Vistrail Variables tab to create a global variable.

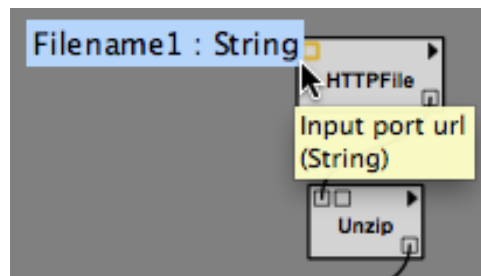


Fig. 3.11: Assign a Variable - Drag the type from just below the Global Variables name on the Vistrail Variables tab. Drop it on a port to set the variable.

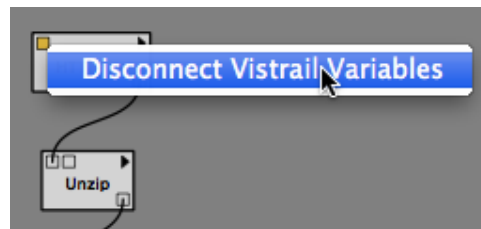


Fig. 3.12: Disconnect a Variable - To disconnect a global variable, right click on the assigned port and select `Disconnect Vistrail Variables`.

3.1.6 Configuring Module Labels

To give the module a custom name, enter it in the `Module Information` tab's `Name` box. The module's name will be displayed with the original module name (type) displayed in parenthesis below it.

3.1.7 Configuring Module Ports

For convenience, all the inputs and outputs of a module are not always shown in the canvas as ports. The ports that are shown by default are defined with the method signatures of a package. A full list of ports is available on the `Module Information` panel, which is displayed on the right by default. There, module ports can be enabled/disabled by clicking in the left margin next to the port name in the `Inputs` or `Outputs` tabs (see Figure [Enabling the GetRadius port from the Module Information tab](#)). When enabled, an eye icon will appear to the left of the port name.

Try it now!

As an example of configuring a module port, select the `vtkCylinder` module in the canvas, select `Outputs` from the `Module Information` tab, and click in the left margin next to `GetRadius` (see Figure [Enabling the GetRadius port from the Module Information tab](#)). A new circle port should appear on the module. Next, add a new `StandardOutput` module from the basic modules and connect the output port for `GetRadius` to the input port of `StandardOutput`. Upon execution, the value `0.25` is now output to the console. Figure [The vtkCylinder module...](#) shows the new workflow.

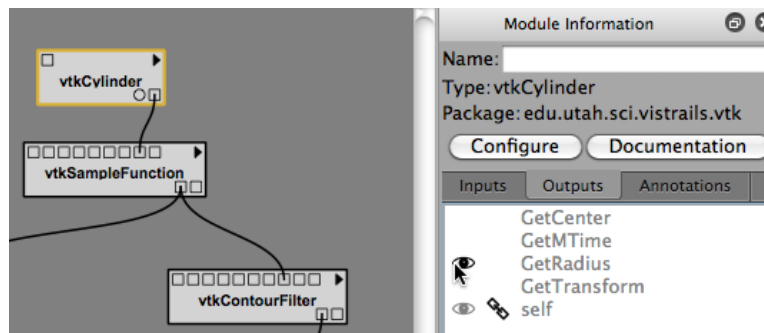


Fig. 3.13: Enabling the `GetRadius` port from the `Module Information` tab.

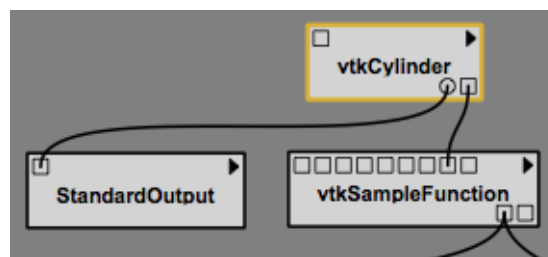


Fig. 3.14: The `vtkCylinder` module is configured to show an additional `GetRadius` port, which is then connected to a `StandardOutput` module.

3.1.8 Basic Modules

In addition to the modules provided by external libraries, VisTrails provides a few basic modules for convenience and to facilitate the coupling of multiple packages in one workflow. These modules mostly consist of basic data types in

Python and some manipulators for them. In addition, file manipulation modules are provided to read files from disk and write files to disk.

PythonSource

Because not every Python operation can be represented as a module, the `PythonSource` module is provided to allow you to write Python statements to be executed as part of a workflow. By pressing ‘Ctrl-E’ when a `PythonSource` module is selected in the canvas, a configuration window is opened. This window allows you to specify custom input and output ports as well as directly enter Python source to be executed in the workflow.

Note

Sometimes it is useful to view the source code that is contained in the `PythonSource` module when working with other modules. Since the `PythonSource` configuration window will disappear when you select a new module, a `Show read-only window` button can be used to open a read-only window of the `PythonSource`’s configuration, which will remain open until it is closed.

Try it now!

To demonstrate a `PythonSource` module, we will output the center of the cylinder using Python instead of the `StandardOutput` module. First, add a `PythonSource` module to the canvas and remove the `StandardOutput` module. Select the `PythonSource` module and press ‘Ctrl-E’ to edit the configuration. In the newly opened configuration window, create a new input port named “radius” of type `Float`. Next, in the source window enter:

```
print radius
```

then select OK to close the window. Finally, connect the `GetRadius` output of the `vtkCylinder` module to the new input port of `PythonSource`. Upon execution, the radius of the cylinder is printed to the console as before. Figure A *PythonSource module can be used to directly insert scripts into the workflow* shows the new workflow together with the `PythonSource` configuration window.

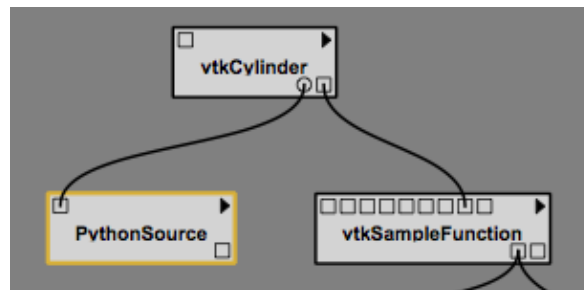


Fig. 3.15: A `PythonSource` module can be used to directly insert scripts into the workflow.

Accessing `vtkObjects` in `PythonSource` When using a `PythonSource` module, users will often rely on their knowledge of VTK to interact with VTK modules. It is important to realize that a VTK module is really a wrapping of a `vtkObject`. The real `vtkObject` is called `vtkInstance`, meaning the `vtkObject` of a module called ‘dataset’ is called ‘dataset.vtkInstance’ (see figure *Accessing `vtkObjects`...*).

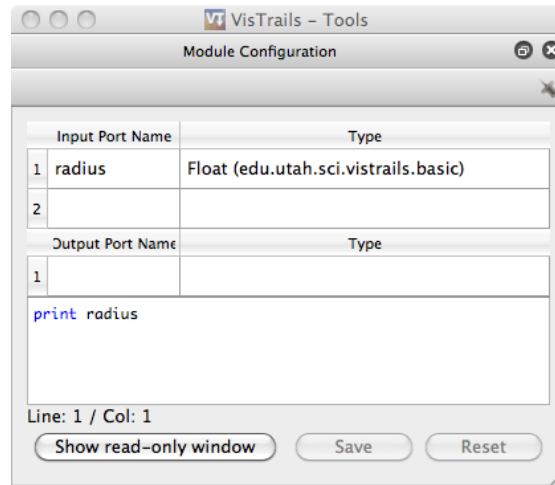


Fig. 3.16: The configuration window for `PythonSource` allows multiple input and output ports to be specified along with the Python code that is to be executed.

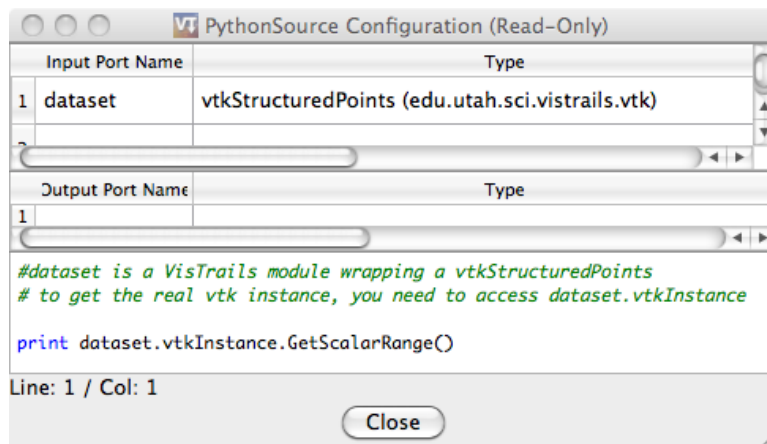


Fig. 3.17: Accessing `vtkObjects` - The `vtkObject` of a VTK module, 'dataset', is accessed with 'dataset.vtkInstance'.

3.2 Groups and Subworkflows

3.2.1 Grouping Modules

As the number of modules in a pipeline increases, the pipeline can grow quite large and cumbersome. This also makes the pipeline more difficult to understand and maintain. With any large system, it can be helpful to cluster related pieces together and represent them as a single unit. This idea, called *encapsulation*, is commonly used in computer programming as a way of controlling complexity. VisTrails likewise supports the grouping of multiple modules together so that they can be treated as a single module. This “group” module can be thought of as a monolithic entity that performs all the same functions as its individual parts, but shields its inner details from everyone else. As such, a group module inherits all the input and output ports of the modules inside it, but only displays those ports that have connections to another module outside of the group. To borrow another term from programming languages, these visible ports might be considered the *public interface* of the group module.

Multiple modules are grouped together by first selecting them, and then choosing the Group option from the Edit menu. Alternatively, you can use the keyboard shortcut ‘Ctrl-G’.

An example may clarify how this works.

Try it now!

Open `vtk_book_3rd_p189.vt`. Select the `vtkOutlineFilter`, `vtkPolyDataMapper`, `vtkProperty`, and `vtkActor` modules on the left side of the pipeline, as shown in Figure *Box selection of four modules*. Type ‘Ctrl-G’ to group these modules. Notice how the pipeline changes, as shown in Figure *The modules represented as a single group module*. Since the label “Group” isn’t very descriptive, you can change this by selecting the Group module, and entering a name in the Name box of the Module Information panel. Type a more descriptive name, such as “BoundingBox,” into the text field and click OK. The new label is reflected in the pipeline (Figure *Renaming the group*).



Fig. 3.18: Box selection of four modules.

Just as any number of modules may be clustered into a group, any number of groups may be combined with other groups or modules to form still larger groups. This is done in the same way as described above.

Further, the contents of the groups or combinations of groups are revealed through the Show Pipeline option. First select the group module in the pipeline and then select Show Pipeline from the Workflow menu. The

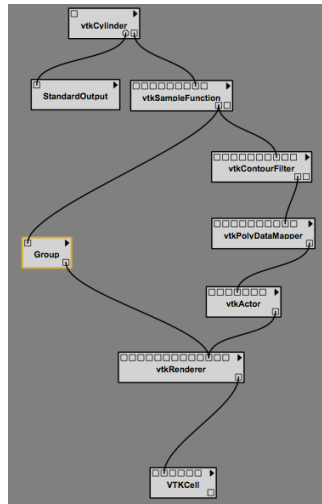


Fig. 3.19: The modules represented as a single group module.

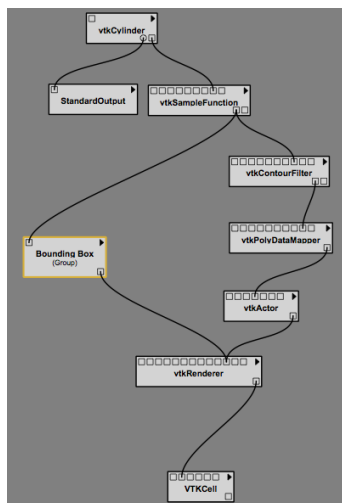


Fig. 3.20: Renaming the group.

group's contents will be shown in a new tab. If there is a group within a group, selecting the interior group module and then selecting `Show Pipeline` will show the interior group's pipeline in an additional tab.

In addition to viewing the group's contents, any group may be also un-grouped; that is, restored to its individual modules. This is done by selecting the group module in the pipeline, and then choosing the `Edit → Ungroup` menu option or by pressing 'Ctrl-Shift-G'. A group's pipeline may not be used to ungroup interior groups, however. The tabs opened by the `Show Pipeline` command are read only.

3.2.2 Subworkflows and Group Modules

A subworkflow is similar to a group, but has some differences. Here, we will explain the differences to make it easier to understand which one to use when:

- A subworkflow is a VisTrail, and a history of changes to a subworkflow is kept, whereas a group is part of a vistrail. So, if you copy and paste a group, the pasted group won't necessarily be linked to the group's history.
- When a subworkflow is created, it is listed in the `My Subworkflows` portion of the `Modules` panel. It is saved and will be accessible from any vistrail. A group, on the other hand can be named and copied and pasted within a file, or even across files. However, it will not be placed in the modules panel.
- Subworkflows can be edited and saved without needing to ungroup and regroup the modules. To edit anything within a group, it first needs to be ungrouped, and then regrouped.

3.2.3 Subworkflows

To create a subworkflow, select the modules to include and select `Create Subworkflow` from the `Workflow` menu. See Figure *Creating a subworkflow*. You will be prompted to name the subworkflow. The subworkflow will appear in the modules list under `My Subworkflows`. Groups can be converted to subworkflows by selecting the `Convert to Subworkflow` option.

To edit a subworkflow, select a module of the corresponding subworkflow and select `Edit Subworkflow` from the `Workflow` menu. This will open the subworkflow's file. If you make changes to the subworkflow and save them, the modules that correspond to the old subworkflow will be marked with a '!', meaning that it is not the latest version. To upgrade to the latest version, either select the triangle in the module's upper right corner and choose `Upgrade Module`, or delete the old module and replace it with a new one. See Figure *Upgrading a subworkflow module that had been edited*.

Importing and Exporting Subworkflows

Since subworkflows are saved locally, the `Import Subworkflow` and `Export Subworkflow` options can be used for sharing. For example, to add a subworkflow from an open VisTrail to your local list of `My Subworkflows` modules, you would select the subworkflow and select `Import Subworkflow` from the `Workflows` menu. Alternatively, you can save any number of subworkflows to a package by dragging the subworkflow modules to the canvas, selecting them, selecting `Export Subworkflow`, and following the prompts to name/create the appropriate folders/files. The subworkflows will be exported to a folder which can be added to the `userpackages` directory. The package should contain a `__init__.py`, and an `init.py` file. The importing of the individual subworkflows will be handled in the `init.py` file. See the *Writing Vistrails Packages* chapter of the *Developer's Guide* for more information on packages.

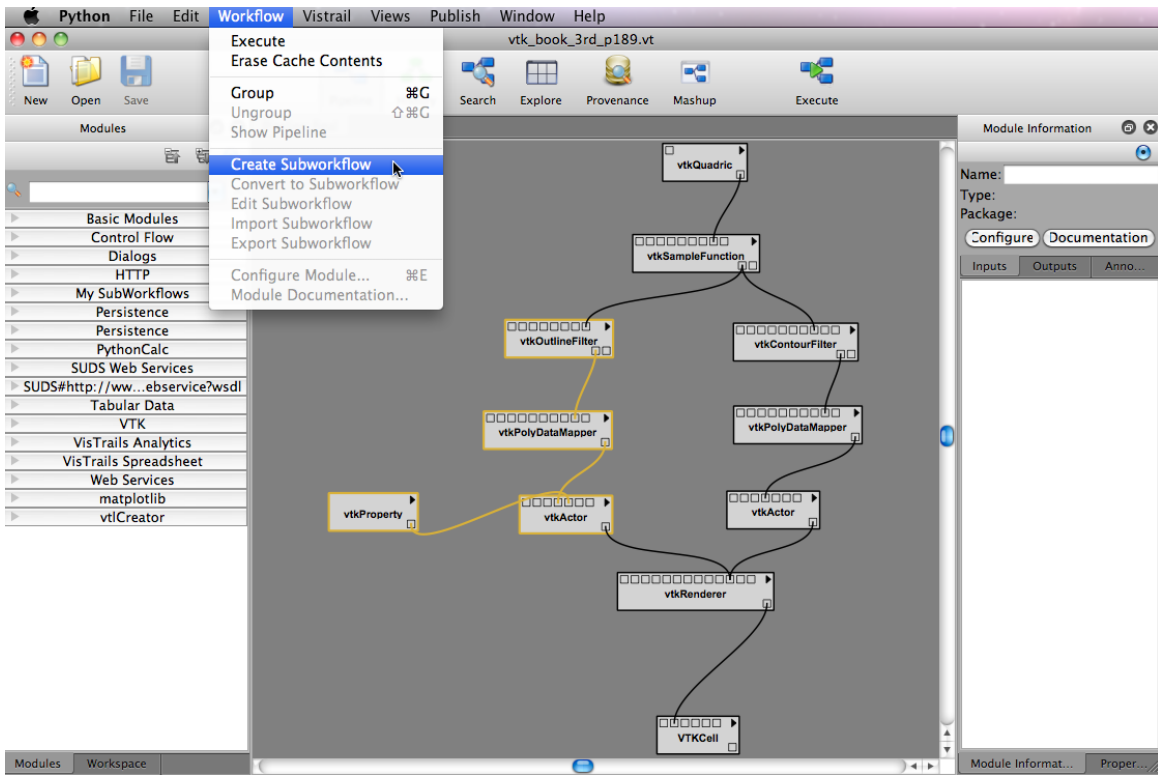


Fig. 3.21: Creating a subworkflow.

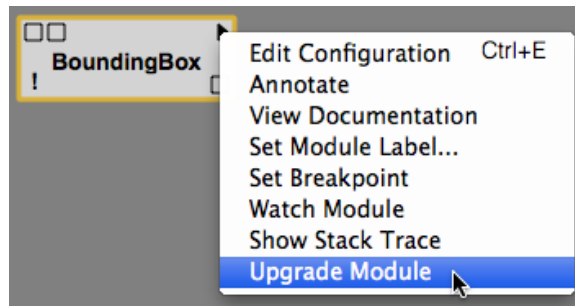


Fig. 3.22: Upgrading a subworkflow module that has been edited.

3.3 Interacting with the Version Tree

3.3.1 Version Tree View

The `History` button on the VisTrails toolbar lets users interact with a workflow history. It consists of a tree view in the center and the `Properties` tool container on the right for querying and managing version properties (see Figure *In History mode, you can examine...*). Versions are displayed as ellipses in the tree view where the root of the tree is displayed at the top of the view. The nodes of the tree correspond to a version of a workflow while an edge between two nodes indicates that one was derived from the other.

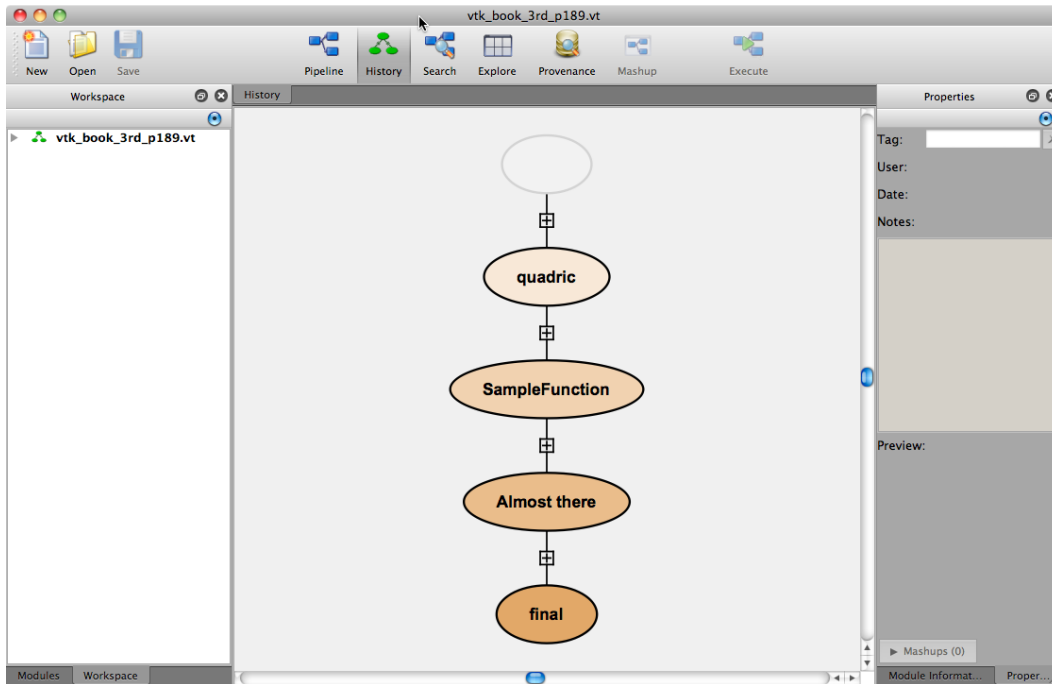


Fig. 3.23: In `History` mode, you can examine and annotate different versions of a workflow.

The nodes are displayed as colored ellipses, and are either blue or orange. A blue color denotes that the corresponding version was created by the current user while orange nodes were created by other users. The brightness of each node indicates how recently a version was created; brighter nodes were created more recently than dimmer ones. Each node may also have a *tag* that describes the version, and this tag is displayed as a text label in the center of the ellipse of the corresponding version.

The nodes are connected by a solid line if the child node is a direct descendent of the parent node; that is, if you have made only a single change from the older version to the newer version. By default, only nodes that: are leaves, have more than one child node, are specially tagged (see Section *Adding and Deleting Tags*), or are current version will be displayed. To save space, other nodes will be “collapsed,” or hidden from view. Collapsed nodes are marked by the appearance of a small expansion button along an edge connecting two nodes. Clicking this button expands the version tree to reveal the hidden versions (Figure *To conserve space...*). The tree expansion is smoothly animated to help you maintain context from one view to the next. Clicking the button a second time collapses the nodes once again. Because most non-trivial changes to a workflow take more than one action, most edges in a the version tree will be shown with these expansion buttons.

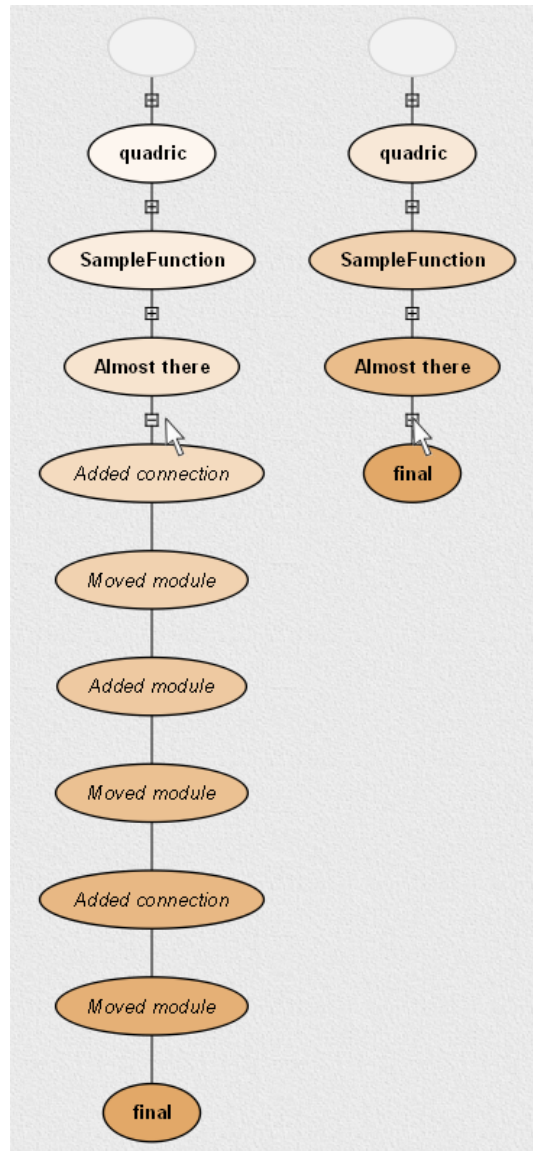


Fig. 3.24: To conserve space, linear sequences of non-tagged nodes may be hidden from view. They can be restored by clicking on the expansion button, which resembles a plus sign (+) inside a small box.

Try it now!

To see an example of a version tree, load the example vistrail `vtk_book_3rd_p189.vt`. All versions will be shown in orange unless your username happens to be “emanuele.” Recall that this tree displays the structure of changes to a workflow, so let’s make some changes to see their effect on the version history. In the History view, select the node tagged `Almost there`, and then click on the Pipeline button to switch to a view of the workflow. Select a connection and delete it. Now, switch back to the History view, and notice that there is a new child node connected to `Almost there`. In addition, the line connecting the new node to its parent is solid, indicating that only a single change has been made. If we delete more connections, an expansion button would appear (Figures *All versions created...*, *Deleting a connection...*, and *More iterations...*).

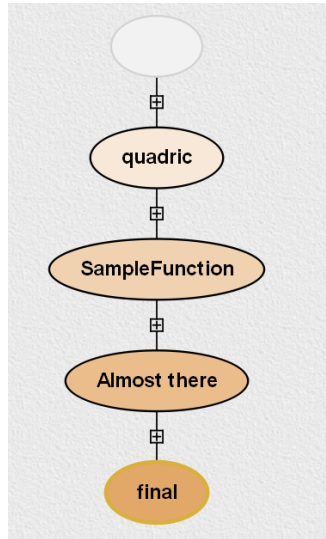


Fig. 3.25: All versions created by other users are shown in orange.

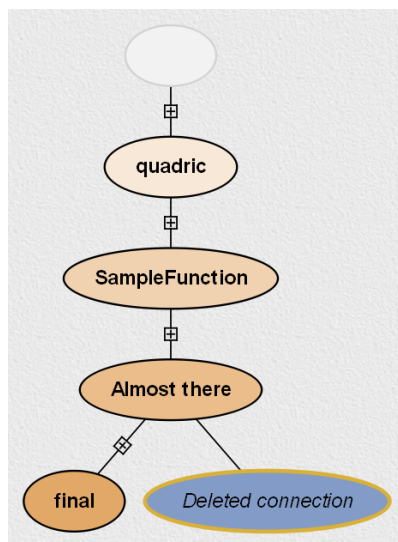


Fig. 3.26: Deleting a connection results in a blue version connected by a solid line.

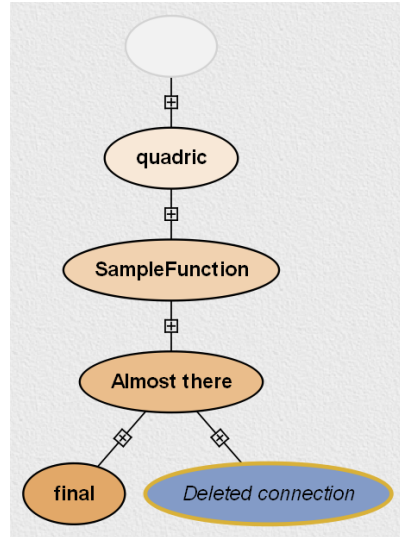


Fig. 3.27: More interactions on this version cause additional versions to be created. To save space, these intermediate nodes are hidden, and an expansion button appears on the edge between the current node and the last tagged node.

3.3.2 Adding and Deleting Tags

As noted above, only certain nodes, including specially tagged ones, are shown by default in the version tree. To tag a version, simply click inside a selected node and type some meaningful text. The tag is created when you either click outside the node or press ‘Enter’. If you would like to change the tag’s text, click inside the node again and modify the text as before. (Alternately, you can also create and modify tags using the `Tag` text field in the `Properties` panel.)

Note that deleting all of the text in the tag field effectively deletes the tag. A second way to delete a tag is to click the ‘X’ button to the right of the text box. Removing a tag from a node may cause it to not be displayed in the default version tree view if it doesn’t satisfy any of the other criteria for display.

3.3.3 Upgrading Versions

As module packages are continuously updated, with new versions being released periodically, VisTrails is set up to automatically incorporate module upgrades into existing workflows before they are executed. In other words, VisTrails upgrades the current vistrail’s current version after the `execute` button is pressed, but prior to execution. When this happens, a new version is created in the version tree and tagged ‘Upgrade’. You are then free to rename this version if desired.

After an upgrade, you will not be able to select the original version because the focus is passed to the upgraded version. However, if you right-click on the original version and select ‘Display raw pipeline’, this version will keep the focus, which allows you to see its pipeline by pressing the `Pipeline` button on the toolbar. See figure *Original Pipeline....*

Finally, although VisTrails tags the new version with ‘Upgrade’ by default, some users prefer the original version’s name to be transferred to the upgraded version. VisTrails will do this if you: select `Preferences` from the `VisTrails` menu, select the `Expert Configuration` tab, and change the `migrateTags` value to ‘True’.

3.3.4 Adding Version Annotations

In addition to the tag field, the `Properties` panel displays information about the user who created the selected version and when that version was created. Also, the `Notes` field which allows users to store notes or annotations related to a version. As with tags, adding notes to a version is as easy as selecting the desired version and modifying

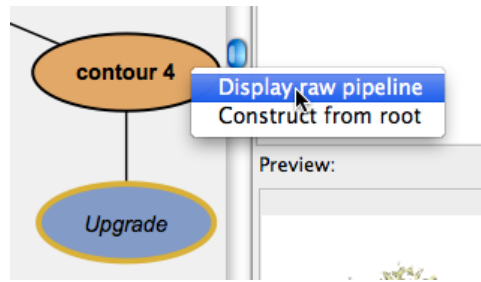


Fig. 3.28: Original Pipeline - This figure shows how to view the original pipeline after an upgrade has occurred.

the text field. Notes are automatically saved when you save the vistrail file. Finally, a thumbnail is displayed in the preview portion of the panel if the version has been successfully executed.

3.3.5 Navigating Versions

Clicking on nodes in the version tree is not the only way to navigate different versions of a workflow; you can also use Undo (Ctrl-z) and Redo (Ctrl-Shift-z). Because the version tree captures all changes to a workflow, undo and redo not only revert or reinstate changes to a workflow, but also change the currently selected version in the version tree. More precisely, undoing a change in a workflow is exactly the same as selecting the parent of the current node in the version tree. Note that because the current version is always shown in the version tree, undo and redo provide an effective way to navigate between two nodes whose intermediate versions might be currently hidden from view.

3.3.6 Comparing Versions

While selecting versions in the History view and using the Pipeline view to examine each version is extremely useful, this approach can be cumbersome when trying to compare two different versions. To help with such a comparison, VisTrails provides a Version Difference mechanism for quickly comparing two versions. This is done by dragging one version and dropping it onto another, after which a Visual Diff tab will open (see Figure A *Visual Diff showing the difference...*).

In the new tab, the difference is displayed in a manner that is very similar to the pipeline view, but modules and connections are colored based on similarity. Dark gray indicates those modules and connections that are shared between the two versions; orange and blue show modules and connections that exist in one workflow and not the other; and light gray modules are those where parameters between the two versions differ. The Legend, which is displayed in the Diff Properties panel on the right, will remind you of these color correspondences. If the Diff Properties panel is not visible on the right, you may enable it by selecting Diff Properties under the View menu. This panel also shows the differences in parameters for light gray colored modules that are selected.

Try it now!

To try out this feature, open the `lung.vt` example vistrail, and click the History button. Within the version tree, click and drag the `z-space` version to the `textureMapper` version. After the diff appears, select View → Diff Properties (if the Diff Properties panel is not visible), and then click on the `vtkRenderer` module to see the parameter differences. We can see that one of the changes from `z-space` to `textureMapper` was to add a black background. Figure A *Visual Diff showing the difference...* shows the result of this comparison.

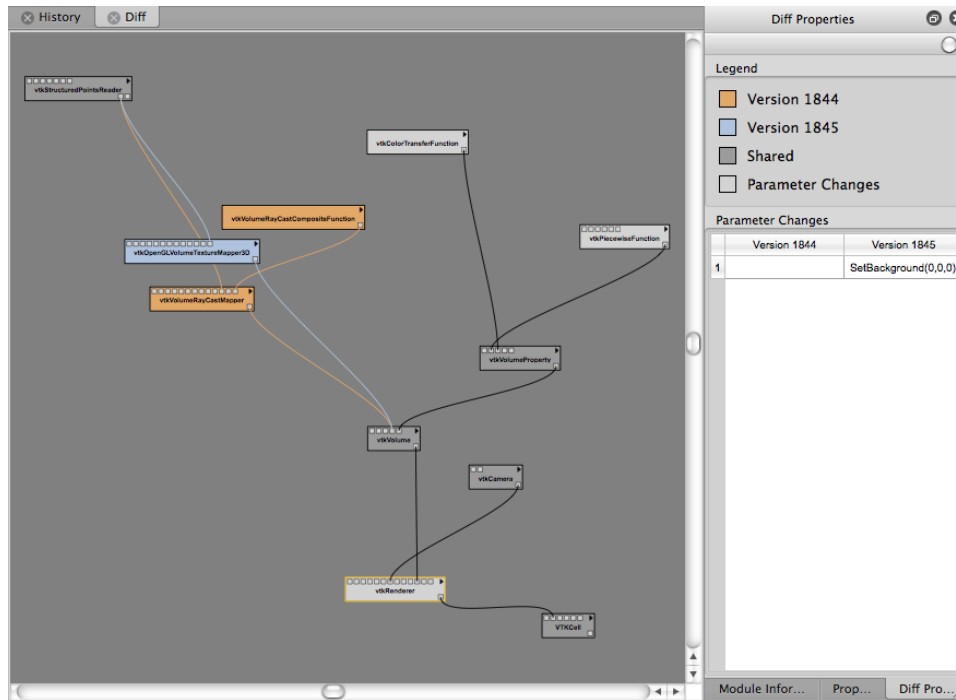


Fig. 3.29: A Visual Diff showing the difference between version z-space and version textureMapper.

3.4 Merging Two Version Trees

One of the benefits of having a version tree is that branching allows users to work on multiple workflows within the same file. This is especially useful when workflows are similar or when one workflow provides output for another. However, if a user creates two different workflows in two different files and decides he/she wants them to be part of the same file/history, VisTrails allows file merging.

To merge two files:

- Open both files
- Select one of the files you would like to be merged.
- Place your mouse over the `Merge With` arrow from the Edit menu. A list of open files should appear.
- Select the file that you would like to join with the current (previously selected) file.

The history trees of both files should now be joined and placed in a new file.

3.4.1 Example

3.5 Querying the Version Tree

VisTrails is designed for manipulating collections of workflows, and an integral part of this design is the ability to quickly search through these collections. VisTrails provides two methods for querying vistrails and workflows. The first is a Query by Example interface which allows you to build query workflows and search for those with similar structures and parameters. The second is a textual interface with a straightforward syntax. For each interface, the results are *visual*: each matching version is highlighted in the History view, and if the query involves specific workflow characteristics, any matching entities are also highlighted in the Pipeline view for the current version.

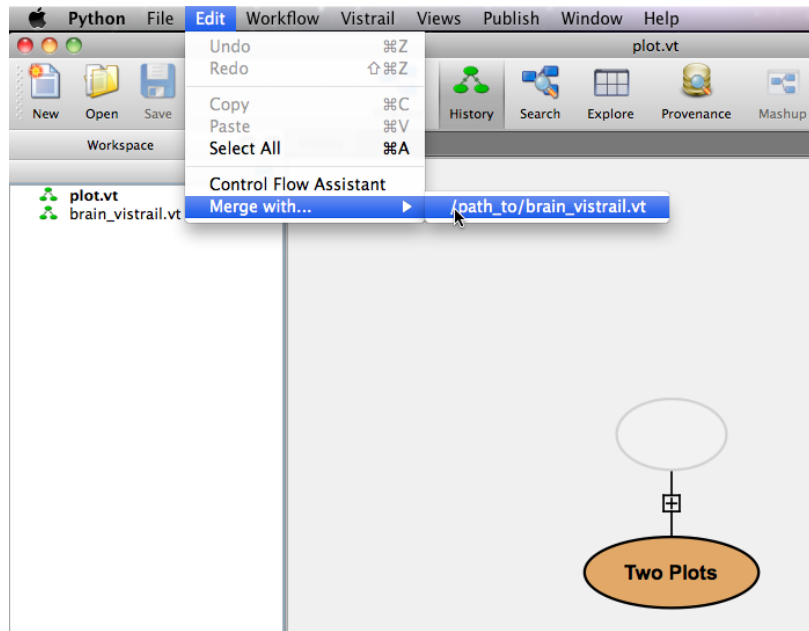


Fig. 3.30: Merging two vistrails.

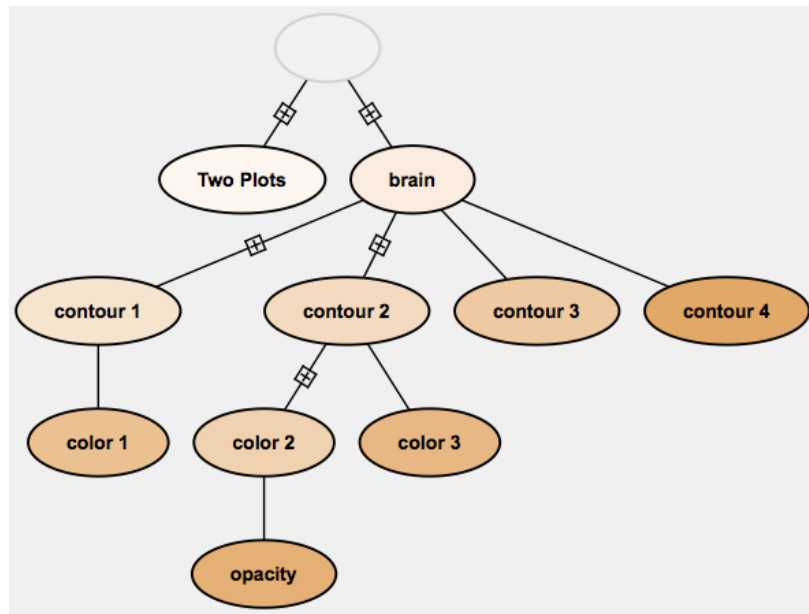


Fig. 3.31: The resultant history tree.

3.5.1 Query By Example

One of the problems faced when trying to query a collection of workflows is the fact that structure is important. Suppose that you want to find only workflows where two modules are used in sequence. Instead of trying to translate this into a text-based syntax, it is easier to construct this relationship visually. VisTrails provides such an interface which mirrors the Pipeline view, allowing you to construct a (partial) workflow to serve as the search criteria.

To use the Query by Example interface, click on the Search button on the toolbar. This view is extremely similar to the Pipeline view and pipelines can be built in a similar manner. Just like the Pipeline view, modules are added by dragging them from the list on the left side of the window, connections are added by clicking and dragging from a port on one module to a corresponding port on another module. Setting module parameters in this view will narrow the search to matching modules whose parameters fall within the specified range of values. Figure *Example pipeline in Search mode* shows an example pipeline that has been built in the query builder.

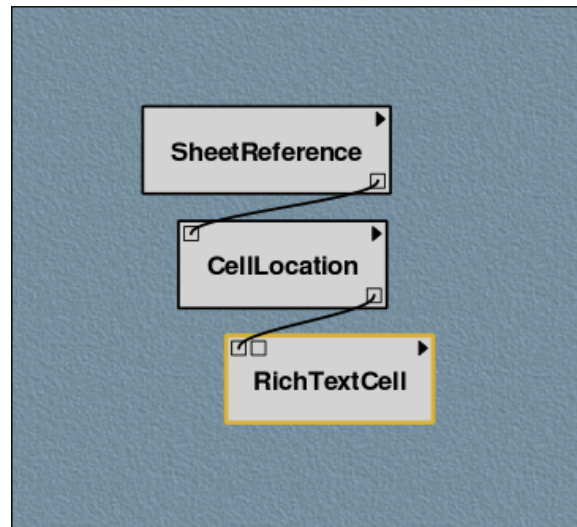


Fig. 3.32: Example pipeline in Search mode.

The next step is to decide whether to search the Current Vistrail, Current Workflow, or all Open Vistrails. The results of the first option are displayed on a version tree as well as in the Workspace panel. Non-matching versions in the version tree will be grayed out while matching versions will be displayed in the tree as normal. In contrast, the Workspace panel will display matching results and omit versions with no matches. Double-clicking a version from the Workspace's results will bring up the associated pipeline with matching modules highlighted. See Figures *Workspace...* and *Pipeline...*

The remaining two options are Current Workflow and Open Vistrails. The Current Workflow option is the simplest and will display the pipeline with matching modules highlighted. The Open Vistrails option will put all of its results in the Workspace panel, listing open vistrails with their matching versions. From here, double-clicking on a vistrail will bring up a version tree which emphasizes matching versions, or double-clicking on a version will bring up the associated pipeline with matching modules highlighted.

After constructing a pipeline and selecting the appropriate search option, click the Execute button to begin the query. This button will be available as long as the query window is not empty. However, you may need to press the Back to Search button to return to the query window to re-execute.

Note

You may leave the Query either through use of the toolbar or by pressing the Edit button. However, the search results will persist until the search is cleared (press Clear Search), returning the workspace to its normal form.

Try it now!

Let's practice making a simple query. Open the `offscreen.vt` example vistrail. Click on the Search button to enter Search mode. Create a query like the one shown in Figure *Example pipeline in Search mode* by dragging the modules SheetReference, CellLocation, and RichTextCell onto the Search canvas. (These modules can be found under the "VisTrails Spreadsheet" header in the Modules panel.) Connect the input and output ports of the modules as shown, then click the Execute button to perform the query. VisTrails will automatically switch to the History view, with all matching versions highlighted (Figure *History...*). Notice that the query results are also displayed in the Workspace tab. Double-click on the html version in the workspace to open the results in the pipeline view.

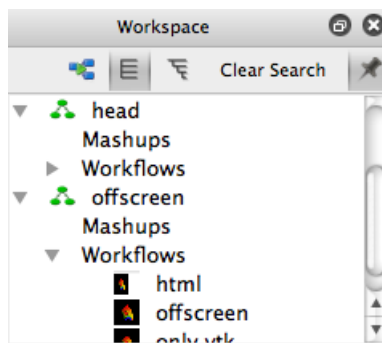


Fig. 3.33: Workspace - The query results displayed in the workspace.

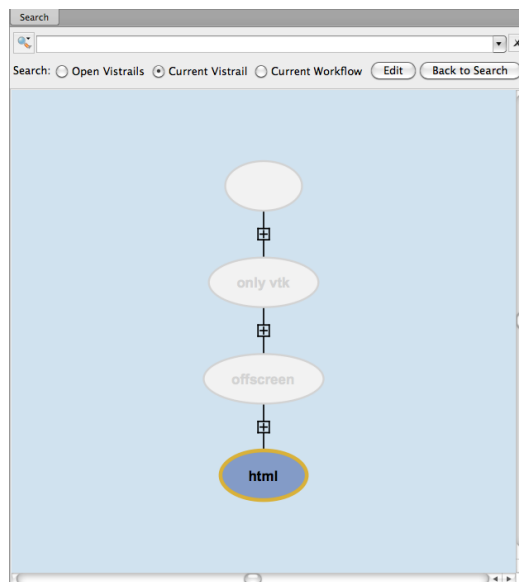


Fig. 3.34: History - Search results in the History view.

Note that Query by Example provides the capability to iteratively refine searches by adding more criteria. For example,

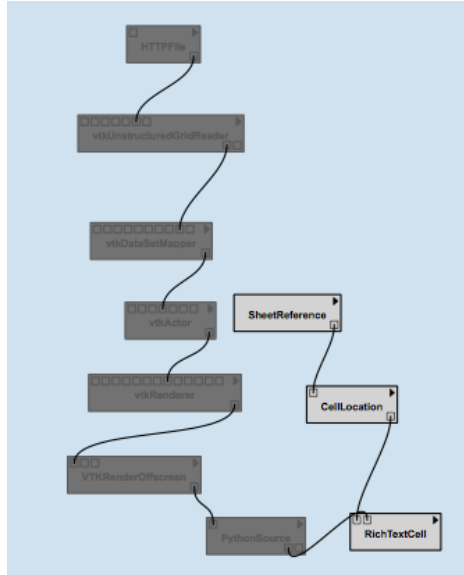


Fig. 3.35: Pipeline - The results in the Pipeline view.

if you were interested in workflows that contain a certain module, you may find that such a query returns too many results. You could then refine the query to find only those workflows where the given module has a parameter with a specific value. This is done by specifying parameter values in the `Inputs` panel on the right side of the window.

3.5.2 Textual Queries

There are many ways to search for versions in the version tree using textual queries, but they all rely on a simple text box for input. Begin a search by selecting `Search` on the toolbar. The search box is at the top of the center panel and has a magnifying glass icon next to it. If you enter query text, VisTrails will attempt to match logical categories, but if your query is more specific, VisTrails has special syntax to markup the query. To execute a query, simply press the ‘Enter’ key after typing your query.

Table 3.1: Syntax for querying specific information using textual queries.

Search Type	Syntax
User name	<code>user: <i>user name</i></code>
Annotation	<code>notes: <i>phrase</i></code>
Tag	<code>name: <i>version tag</i></code>
Any	<code>any: match user/notes/name (the default)</code>
Module	<code>module: <i>module name</i></code>
Date	<code>before: <i>date</i> <i>relative time</i></code>
	<code>after: <i>date</i> <i>relative time</i></code>

Note

Since we allow regular expressions in our search box, question marks are treated as meta-characters. Thus, searching for `??` returns everything and `abc??` will return everything containing `abc`. You need to use `\\?` instead to search for `??`. So the search for `???` would be `\\?\\?`.

Table *Syntax for querying specific information using textual queries*. lists the different ways to markup a query. Note that you can search by user name to see which changes a particular user has made, and also by date to see which changes were made in a specific time frame. When searching by date, you can search for all changes before or after a given date or an amount of time relative to the present. If searching for changes before or after a specific date, the date can be entered in a variety of formats. The simplest is ‘*day month year*,’ but if the year is omitted, the current year is used. The month may be specified by either its full name or an abbreviation. For example, ‘*before: 18 November 2004*’ and ‘*after: 20 Dec*’ are both valid queries. If searching by relative time, you can prepend the amount of time relative to the present including the units to ‘*ago*’. An example of this type of query is ‘*after: 30 minutes ago*’. The available units are seconds, minutes, hours, days, months, or years.

You can concatenate simple search statements to create a compound query to search across different criteria or for a specific range. For example, to search for workflows whose tag includes ‘*brain*’ and were created by the user ‘*johnsmith*’, the query would be ‘*name: brain user: johnsmith*’. To search for all workflows created between April 1 and June 1, the query would be ‘*after: April 1 before: June 1*’.

Try it now!

Open the `terminator.vt` example file, and enter Search mode. Let’s look for all workflows that were created after November 24, 2010. In the search box in the Search panel, type ‘*after: 24 nov 2010*’ and press ‘Enter’. The expected result is shown in Figure *Results of a query to find any changes made after November 24, 2010*.

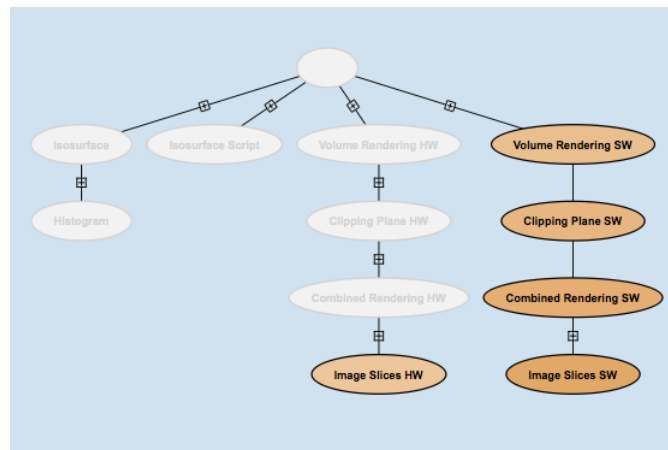


Fig. 3.36: Results of a query to find any changes made after November 24, 2010.

In addition, VisTrails keeps track of the most recent textual queries, and repeating or clearing these queries can be accomplished by selecting the recent query from the dropdown menu attached to the search box. Finally, the ‘X’ button next to the search box will reset the query.

Refining the Results

While in the Search view, you can select two different ways of viewing search results. The magnifying glass icon to the left of the textual search box contains a dropdown menu with two options: “Search” and “Refine” (Figure *Clicking the button to the left...*). The first displays results by simply highlighting the matching nodes while the second condenses the tree to show only the versions that match. For large vistrails, this second method can help you determine relationships between the matching versions more easily.

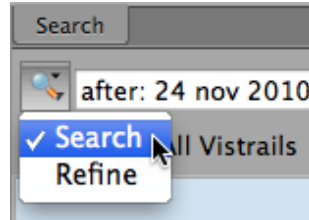


Fig. 3.37: Clicking the button to the left of the query text box accesses a dropdown menu.

3.6 Spreadsheet

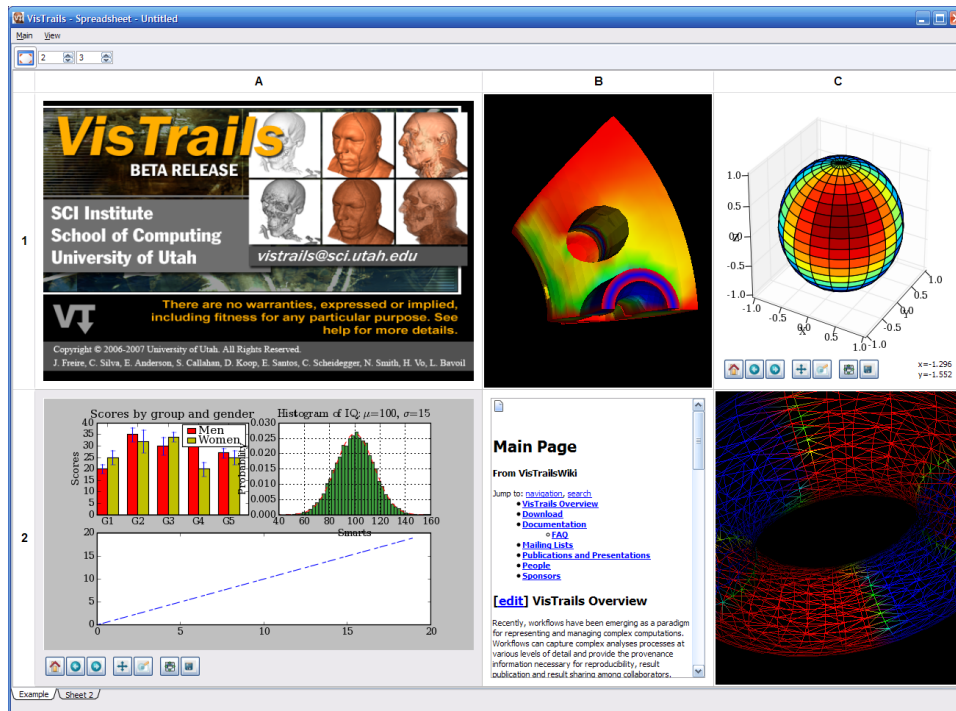


Fig. 3.38: The VisTrails Spreadsheet.

As described in Section *Comparing Versions*, VisTrails has a powerful built-in mechanism to compare workflows. However, this comparison shows changes in the *design* of the workflows, and we are often also interested in differences in the *results* of workflows. The VisTrails Spreadsheet provides a simple, flexible, and extensible interface to display and compare results from workflows. Coupled with the version differences, users can explore the evolution of their workflows.

The Spreadsheet package is installed with VisTrails by default, and it can display a variety of data ranging from VTK renderings to webpages without additional configuration. To view the spreadsheet if it is hidden, select Packages → Spreadsheet → Show Spreadsheet.

3.6.1 The Spreadsheet Layout

As should be expected, the VisTrails Spreadsheet consists of one or more sheets, each with a customizable number of rows and columns.

Custom Layout Options

To modify the layout for the active sheet, you can change both the number of rows and columns and resize individual cells. The number of rows is controlled by the left spinner in the toolbar and the number of columns by the right spinner. To resize a given row or column, click and drag on one edge of the row or column header. In addition, you can resize an individual cell by moving the mouse to lower-right corner of the cell until the cursor changes and clicking and dragging to the desired size (see Figure *Different states of a spreadsheet cell (d)*). Note that this will affect the entire layout, compressing or expanding rows and columns to generate or fill space for the resized cell.

To adjust the default number of rows and columns in the spreadsheet: select `preferences` from the `VisTrails` menu, select `spreadsheet` from the `Enabled Packages` portion of the `Module Packages` tab, press the `Configure` button, and adjust the values as for `rowCount` and `colCount` as desired.

Multiple Spreadsheets

VisTrails supports the use of multiple spreadsheets which can be added, docked, ordered and deleted. Sheets are added either by clicking the `New Sheet` button in the `Spreadsheet` toolbar or choosing the menu item with the same name from the `Main` menu. Each of these sheets can optionally be displayed as a dock widget separated from the main spreadsheet window by dragging its tab name out of the tab bar at the bottom of the spreadsheet, allowing multiple spreadsheets to be visible at the same time. To dock a sheet back to the main window, drag it back to the tab bar or double-click on its title bar. Similarly, sheets are ordered by dragging sheet names to desired locations within the tab bar. Finally, a sheet can be deleted by clicking the 'X' button in the lower-right corner or choosing the `Delete Sheet` menu item.

3.6.2 Sending Output to the Spreadsheet

Users may send results to the spreadsheet by using a spreadsheet cell. Upon inspecting the `VisTrails Spreadsheet` package (in the list of packages, to the left of the pipeline builder), one can see there are built-in cells for different kinds of data, e.g., `RichTextCell` to display HTML and plain text.

By default, an unoccupied cell on the active sheet will be chosen to display the result. However, you can specify in the pipeline exactly where a spreadsheet cell will be placed by using `CellLocation` and `SheetReference`. `CellLocation` specifies the location (row and column) of a cell when connecting to a spreadsheet cell (`VTKCell`, `ImageViewerCell`, ...). Similarly, a `SheetReference` module (when connecting to a `CellLocation`) will specify which sheet the cell will be put on given its name, minimum row size and minimum column size. There is an example of this in [examples/vtk.vt](#) (select the `Cell Location` version).

Advanced Cell Options

The user can define new cell types to display application-specific data. For example, we have developed `VtkCell`, `MplFigureCell`, and `OpenGLCell`. It is possible to display pretty much anything on the Spreadsheet!

Examples of writing cell modules can be found in: `RichTextCell`: `packages/spreadsheet/widgets/richtext/richtext.py`
`VTK`: `packages/vtk/vtkcell.py`

Here is the summary of some requirements on a cell widget:

1. It must be a Qt widget. It should inherit from `spreadsheet_cell.QCellWidget` in the spreadsheet package. Although any Qt Widget would work, certain features such as animation will not be available (without rewriting it).
2. It must re-implement the `updateContents()` function to take a set of inputs (usually coming from input ports of a wrapper Module) and display on the cells. VisTrails uses this function to update/reuse cells on the spreadsheet when new data comes in.

- It needs a wrapper VisTrails Module (inherited from `basic_widgets.SpreadsheetCell` of the spreadsheet package). Inside the `compute()` method of this module, it may call `self.display(CellWidgetType, (inputs))` to trigger the display event on the spreadsheet.

3.6.3 Interacting with the Spreadsheet

Currently, there are two operating modes in the Spreadsheet: Interactive Mode and Editing Mode. Interactive Mode allows users to view and interact with the spreadsheet cells, while Editing Mode provides operations for manipulating cells. The modes can be toggled via the `View` menu or their corresponding keyboard shortcuts ('Ctrl-Shift-I') and ('Ctrl-Shift-E').

Interactive Mode

In Interactive Mode, users can interact directly with the viewer for an individual cell, interact with multiple cells at once, or change the layout of the sheet. Because cells can differ in their contents, interacting with a cell changes based on the type of data displayed. For example, in a cell displaying VTK data (a `VTKCell`), a user can rotate, pan, and zoom in or out using the mouse.

In a sheet, a cell can be both *active* and *selected*. There can only be one active cell, and that cell is highlighted by a yellow or grey border. Clicking on any cell will make it active. This active cell will respond to keyboard shortcuts as well as mouse input. In contrast to the active cell, one or more cells can be selected, and the active cell need not be selected. To select multiple cells, either click on a row or column heading to toggle selection or 'Ctrl'-click to add or remove a cell from the group of selected cells. The backgrounds of selected cells are highlighted using a platform-dependent selection color. See Figure *Different states of a spreadsheet cell...* for examples of the different cell states.

Depending on the cell type, additional controls may appear in the toolbar when a cell is activated. These controls affect only the active cell, and change for different cell types. As shown by Figure *Different states of a spreadsheet cell (d)*, a cell optimized for rendering 2D images (a `ImageViewerCell`) adds controls for resizing, flipping, and rotating the image in the active cell.

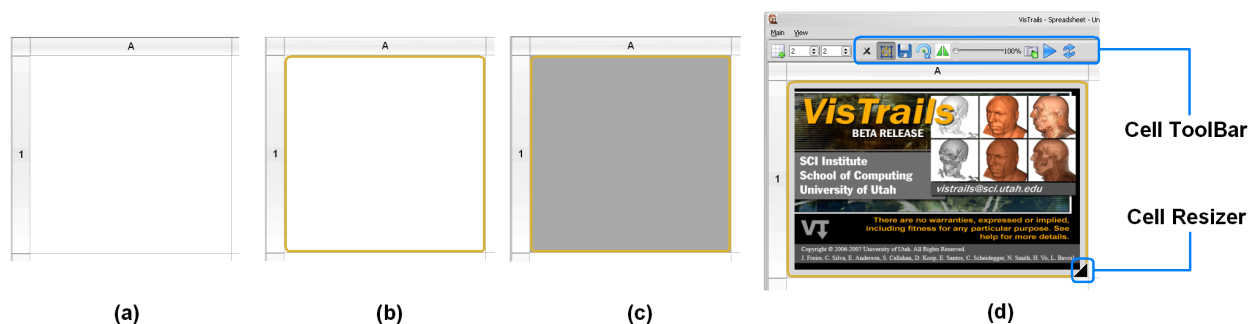


Fig. 3.39: Different states of a spreadsheet cell. (a) inactive and unselected, (b) active and unselected, (c) active and selected, (d) an active cell with its toolbar and resizer.

The Camera

Spreadsheet cells that display VTK data typically are associated with a `vtkRenderer`, which is associated with a `vtkCamera`. If the camera is not assigned in the workflow, a default one is created. If the rendered geometry is not visible

in the window, pressing ‘r’ will invoke the renderer’s `ResetCamera()` command, which centers the geometry. Also, pressing ‘i’ will initiate interactions with interactive vtk objects.

Arranging Cells

As described in Section *Custom Layout Options*, cells can be resized by either resizing rows, columns, or an individual cell. In addition to resizing, a row or column can be moved by clicking on its header and dragging it along the header bar to the desired position. See Section *Editing Mode* for instructions on moving a specific cell to a different location.

Synchronizing Cells

Often, when a group of cells all display results from similar workflows, it is useful to interact with all of these cells at the same time. For example, for a group of `VTKCells`, it is instructive to rotate or zoom in on multiple cells at once and compare the results. For this reason, if a group of cells is selected, mouse and keyboard events for a single cell of the selection are propagated to each of the other selected cells. Currently, this feature only works for `VTKCells`, but we plan to add this to other cell types as well. An example of this functionality is shown in Figure *When selecting all cells...*

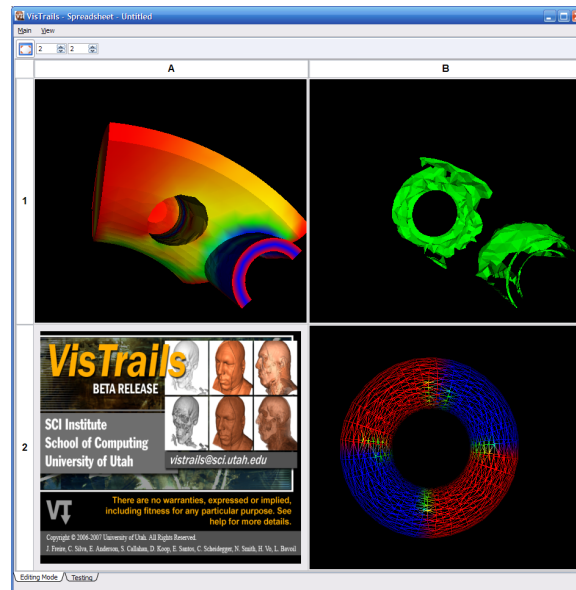


Fig. 3.40: When selecting all cells, interacting with one VTK cell (A1) causes the other two VTK cells (B1 and B2) to change their camera to the same position.

Editing Mode

Recall that Editing Mode can be entered either by accessing the `View` menu or by keying ‘`Ctrl-Shift-E`’. Editing Mode provides more operations to layout and organize spreadsheet cells. In this mode, the view for each cell is frozen and overlaid with additional information and controls (see Figure *The spreadsheet in editing mode...*). The top of the overlay displays information about which vistrail, version, and type of execution were used to generate the cell. The bottom piece of the overlay contains a variety of controls to manipulate the cell depending on its state.

Cells can be moved or copied to different locations on the spreadsheet by clicking and dragging the appropriate icons (`Move` or `Copy`) for a given cell to its desired location. To move a cell to a location on a different sheet, drag the icon over the target sheet tab to bring that sheet into focus first and then drop it at the desired location. If you move a cell to

an already-occupied cell, the contents of the two cells will be swapped. See Figure *The spreadsheet in editing mode...* for an example of swapping two cells.

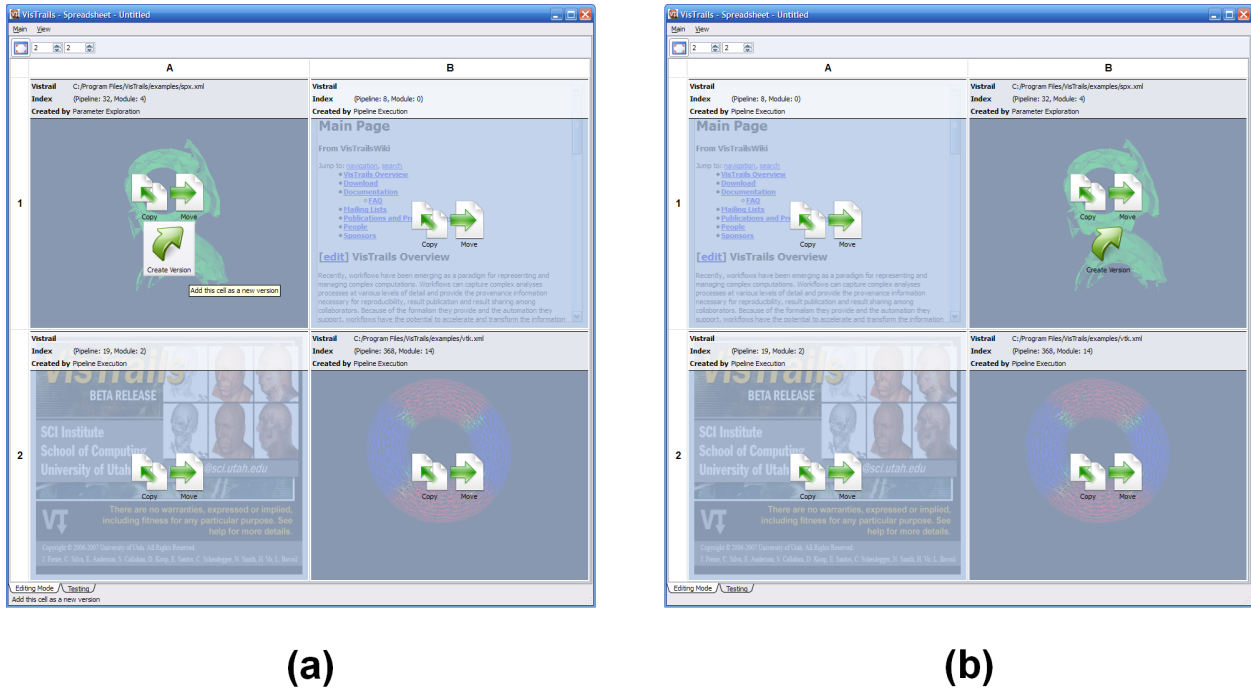


Fig. 3.41: The spreadsheet in Editing Mode. (a) All cell widgets are replaced with an information widget (b) Two cells are swapped after drag and drop the ‘Move’ icon from A1 to B1.

Clicking the `Locate Version` icon will highlight the node in the version tree (in the `History` view) from which the visualization in that cell was generated. The next two icons, `Create Analogy` and `Apply Analogy`, help with creating visualizations by analogy. Please refer to Chapter *Using Analogies to Update Workflows* for information about this feature.

If a cell was generated via parameter exploration (see Chapter *Parameter Exploration*), the `Create Version` button will be available to save the workflow that generated the result back to the vistrail. Clicking this button modifies the vistrail from which the cell was generated by adding a new version with the designated parameter settings. Thus, if you go back to the `History` mode of the VisTrails Builder for that vistrail, you will find that a new version has been added to the version tree.

3.6.4 Launching a Web Browser

It is sometimes difficult to view web pages within a spreadsheet cell due to limited space. It may therefore be desirable to launch a web browser from within the spreadsheet cell. While this functionality is not provided by VisTrails, here are some possible solutions:

1. You can use parameter exploration to generate multiple sheets so you might have an exploration that opens each page in a new sheet. Use the third column/dimension in the exploration interface to have a parameter span sheets.
2. The spreadsheet is extensible so you can write a custom spreadsheet cell widget that has a button or label with the desired link (a `QLabel` with `openExternalLinks` set to `True`, for example).

3. You can tweak the existing RichTextCell by adding the line “self.browser.setOpenExternalLinks(True)” at line 63 of the source file “vistrails/packages/spreadsheet/widgets/richtext/richtext.py”. Then, if your workflow creates a file with html markup text like “VisTrails” connected to a RichTextCell, clicking on the rendered link in the cell will open it in a web browser. You need to add the aforementioned line to the source to let Qt know that you want the link opened externally; by default, it will just issue an event that isn’t processed.

3.6.5 Saving a Spreadsheet

Warning: This is currently an experimental feature and as such is not robust. If you rename or move the vistrails used by the saved spreadsheet, the spreadsheet will not load correctly.

Because spreadsheets can include several workflow executions or parameter explorations, it is helpful to be able to save the layout of the current spreadsheet. To save a spreadsheet, simply choose the *Save* menu item from the *Main* menu, and complete the dialog. After saving a spreadsheet, you can reopen it using the *Open* menu item. A whole sheet can also be saved by selecting *Export* (either from the menu or from the toolbar).

Saving a Spreadsheet Image

To save an image from the spreadsheet, click on the image’s cell to make it active. Then select the camera on the toolbar to take a snapshot. The system will prompt you for the location and file name where it should be saved. The other icons can be used for saving multiple images that can be used for generating an animation on demand.

3.7 Tabular data package

The *tabledata* package provides facilities to load and manipulate data in table formats.

It provides modules to read tables from CSV files and numpy arrays (including plain binary files) and extract or convert columns.

Try it Now!

This example shows how to use *tabledata* together with *matplotlib* to visualize trip data from [NYC Citibike’s open data](#).

Note that you can find the completed example here: [bikes.vt](#).

Start by dragging the following modules to the canvas:

- `DownloadFile` (from the *URL* package)
- `CSVFile` (under *read/csv*)
- `TableCell`
- **Two `ExtractColumn` modules**
- `StringToDates` (under *convert/dates*)
- `MplLinePlot` from the *matplotlib* package
- `MplFigure` from the *matplotlib* package
- `MplFigureCell` from the *matplotlib* package

Connect the modules as shown in Figure *The pipeline for the Bikes example*.

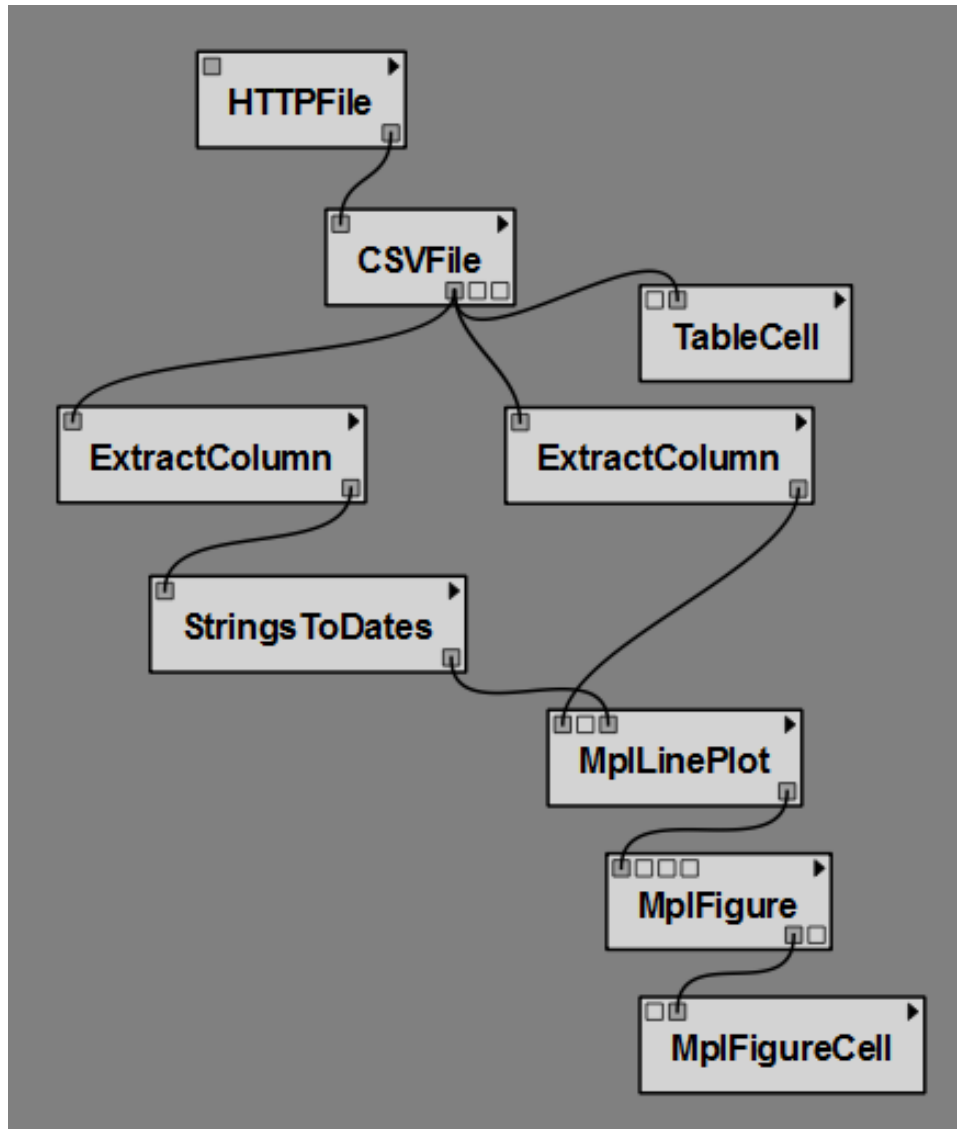


Fig. 3.42: The pipeline for the Bikes example

Next Step!

Set the ‘url’ input of DownloadFile to `http://www.vistrails.org/download/download.php?type=DATA&id=citih`. Make sure ‘header_present’ is checked on CSVFile. Set the ‘column_name’ parameters on both ExtractColumn modules to Date (for the one on the left) and Miles traveled today (midnight to 11:59 pm) (for the one on the right). Alternatively, you can set column_index to 0 and 3. The workflow is now ready. On execution, you will see a graphical view of the CSV file as a table, and a line plot showing the variations of the total distance traveled daily.

3.8 Using Analogies to Update Workflows

In Chapter *Interacting with the Version Tree*, we saw how the provenance data maintained by VisTrails allows you to compare different versions of a workflow. In Chapter *Querying the Version Tree*, you learned how this same provenance information forms the basis of an elegant Query by Example mechanism, letting you find all versions of a workflow that match a given arrangement of modules. In this chapter, we will see yet another benefit of the VisTrails provenance architecture. Through a process we call *visualization by analogy*, you can reuse pipeline information to create new visualizations semi-automatically without directly editing the workflow.

3.8.1 Visualization by Analogy

The main idea behind visualization by analogy is as follows. Given two versions of a workflow (called the “source” and “target” versions, respectively), VisTrails can automatically find the differences between them and apply those differences to another (potentially unrelated) workflow. This powerful feature lets you create a new visualization without having to add or remove modules to/from the pipeline. VisTrails takes care of these details for you behind the scenes.

There are two distinct user interfaces for constructing visualizations by analogy. In the first, you set up the analogy in the Visual Diff window. In the second, you interact with the Spreadsheet. Both ways are logically equivalent, and which method you use will be largely a matter of personal preference.

Before explaining either approach, however, let’s first set up the vistrail that we’ll be using as a running example in this chapter.

Try it now!

Open the `vtk_http.vt` vistrail, located in the examples directory of the VisTrails distribution. If the `tetra mesh contour` version is not selected, go to the History view and select it. This will be our “source” workflow. Execute this workflow, and take a look at the resultant visualization in the Spreadsheet.

We will now create our “target” workflow. Switch to the Pipeline view and add a new module, `vtkSmoothPolyDataFilter` between the `vtkContourFilter` and `vtkDataSetMapper` modules. Your modified pipeline should resemble the one shown in Figure *Modified pipeline for use in our example*.

Next, let’s adjust some of the parameters for the new module. Select the `vtkSmoothPolyDataFilter` module. In the Module Information panel, select `SetNumberOfIterations` and type 20 in the input box. Then, select `SetRelaxationFactor` enter 0.5. Now, execute this workflow, and compare the two results in the Spreadsheet.

Return to the History view, and give your new version a meaningful tag such as `smoothed` (Figure *Corresponding version tree*). Finally, select the `Fran Cut` version and execute it too. Your spreadsheet should now resemble the one shown in Figure *Analogy example...*

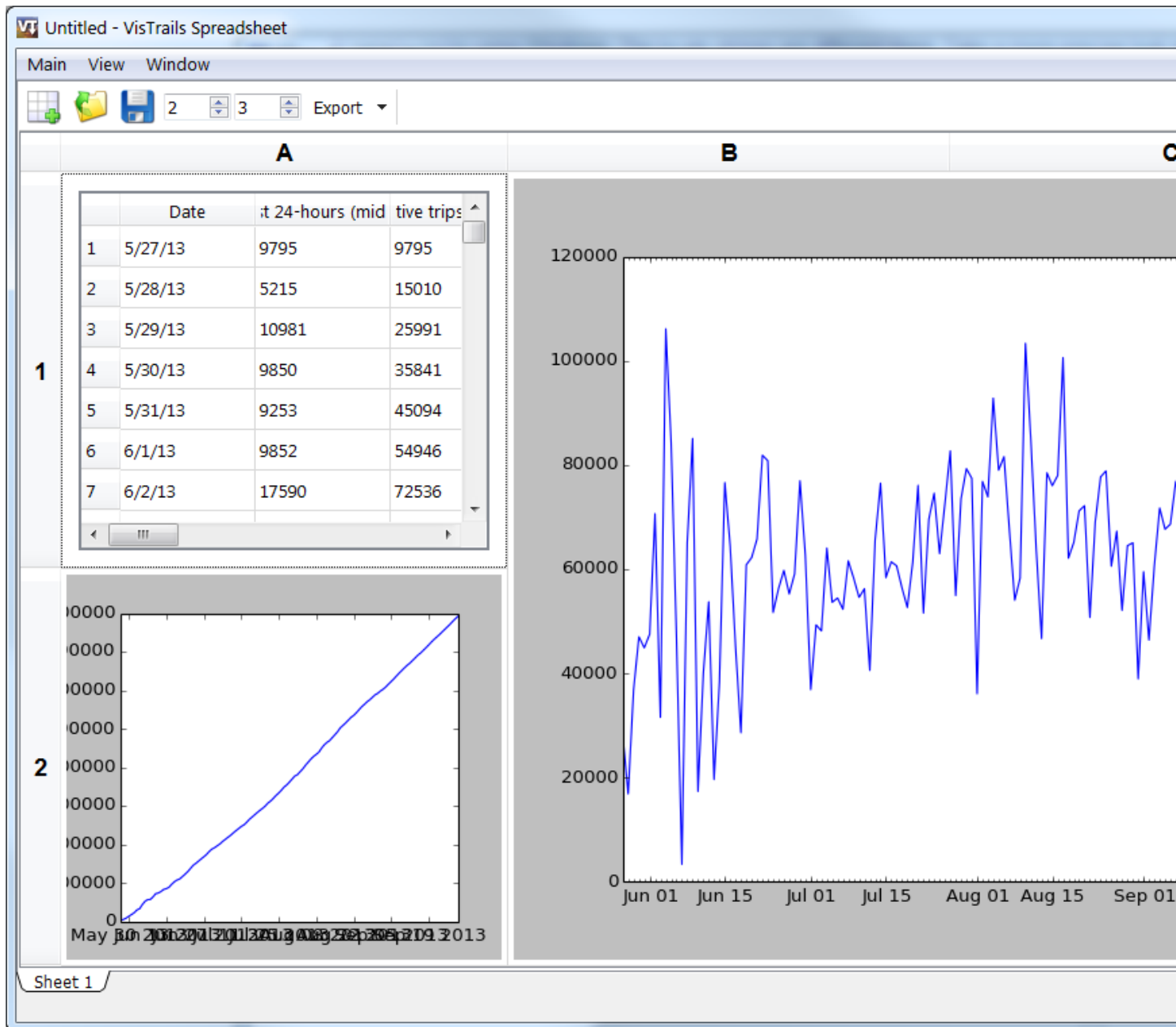


Fig. 3.43: The result in the VisTrails Spreadsheet

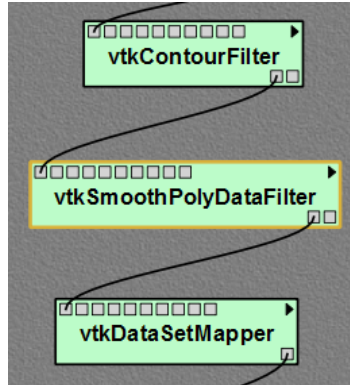


Fig. 3.44: Modified pipeline for use in our example.

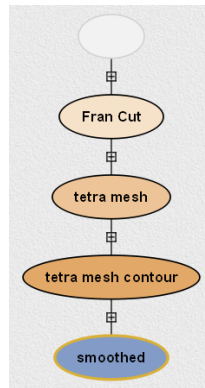


Fig. 3.45: Corresponding version tree.

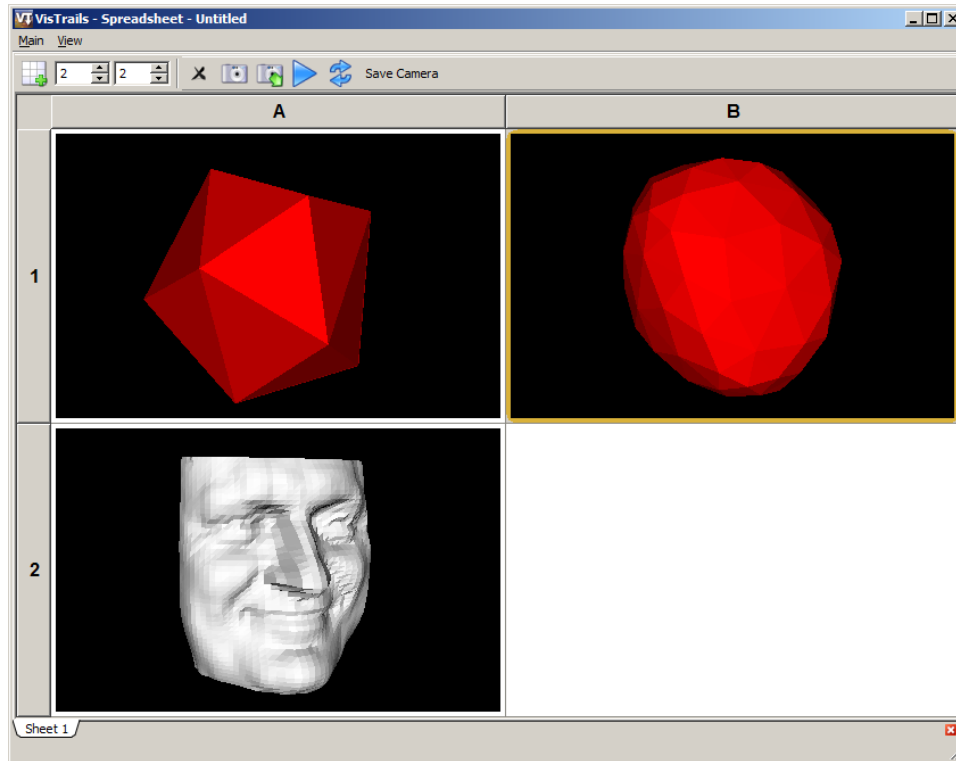


Fig. 3.46: Analogy example - (top left) Original tetrahedral mesh model. (top right) Smoothed tetrahedral mesh. (bottom left) “Fran Cut” model.

3.8.2 Using the Visual Diff Window

By creating an analogy, you’re telling VisTrails to analyze and store the differences between the “source” and “target” versions of a workflow. Then when you apply that analogy to another (perhaps completely different) version of the workflow, VisTrails attempts to make similar types of changes to this other workflow.

One way to create an analogy is to run a `Visual Diff` between the “source” and “target” workflows. Recall from Chapter *Interacting with the Version Tree* that to perform a `Visual Diff` between two versions of a workflow, you need to drag the icon for one version atop the icon for the other. However, in the case of analogies, the sequence is important. In order for the analogy to work correctly, the icon for the *source* version of the workflow must be dragged atop the icon for the *target* version (not vice versa).

In the toolbar of the `Diff Properties` window, there is a button whose tooltip is labeled `Create Analogy` (Figure *Click the Create Analogy button...*). Clicking the `Create Analogy` will open up a dialog that lets you give this analogy a descriptive name. Once the analogy has a name, you can then apply it to any version of the workflow. This is done by returning to the `History` view, and selecting then right-clicking the version you want to apply the analogy to. A menu will appear, showing you a list of available analogies. Choose the one you want, and VisTrails will attempt to apply the selected analogy to this version of the workflow.

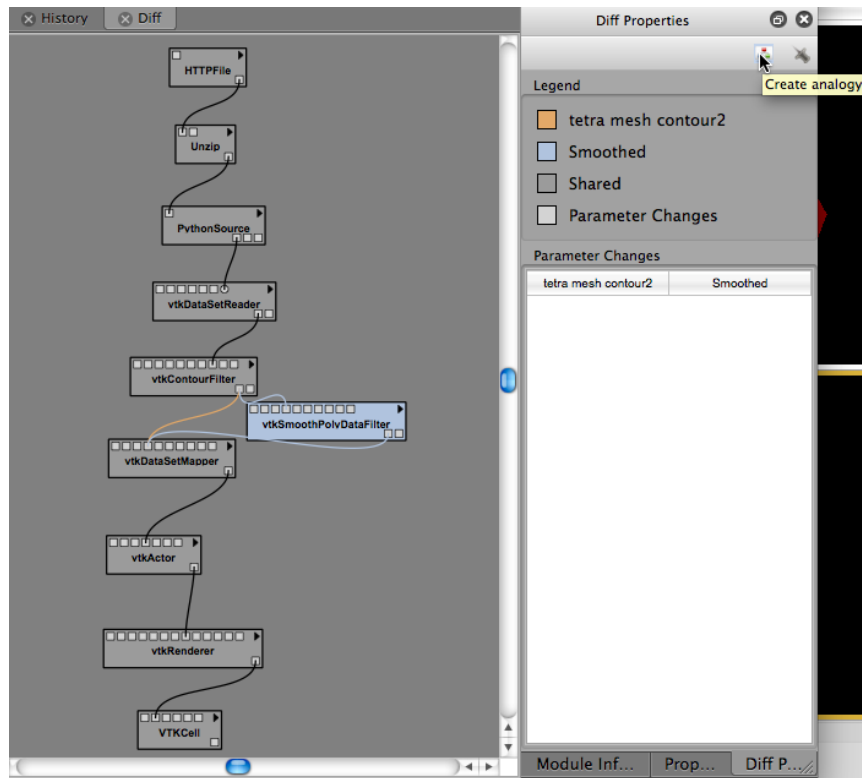


Fig. 3.47: Click the Create Analogy button in the Diff Properties window to create a named analogy.

Try it now!

In the History view, drag the tetra mesh contour icon (the “source” version) atop the smoothed icon (the “target” version). A Visual Diff window will open. Click the Create Analogy button in the toolbar and then choose a name for this analogy, for example “SmoothFilter.” Close the Visual Diff window. Select the Fran Cut icon in the History view so that it is highlighted, then right-click to access the Perform analogy menu. Choose the name of the analogy you just made (Figure [Access the Perform analogy menu by right-clicking...](#)). A new version icon will appear as a child of the current icon. Select the new icon, and click Execute to run this new version of the workflow. The resulting visualization will appear in the Spreadsheet (Figure [Result of applying a smoothing analogy to a different workflow](#)).

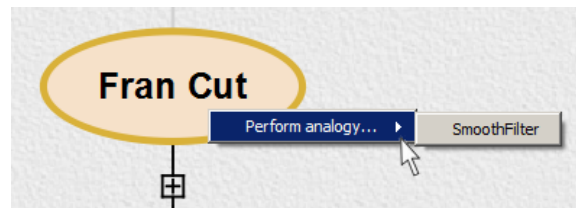


Fig. 3.48: Access the Perform analogy menu by right-clicking on a selected icon in the version tree.

3.8.3 Using the Spreadsheet

You can also create and apply analogies directly in the Spreadsheet, without the use of the Visual Diff window. The Spreadsheet uses a simple “drag and drop” interface to manipulate analogies, and many users find it simpler to

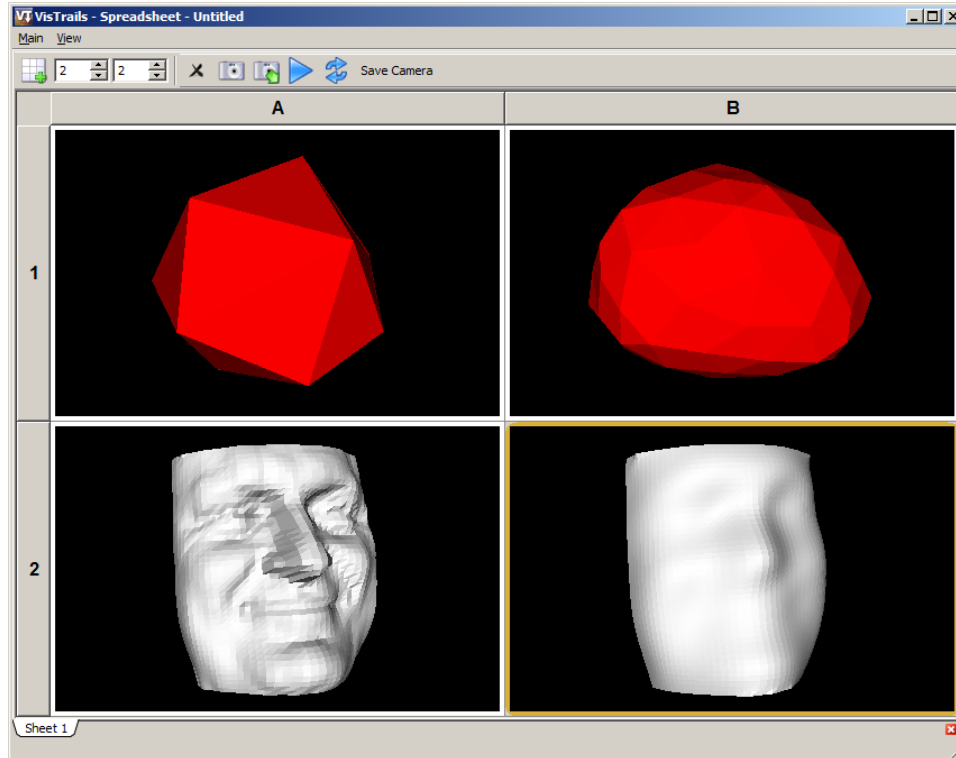


Fig. 3.49: Result of applying a smoothing analogy to a different workflow.

work with than the method described above. The drawback is that the Spreadsheet does not allow you to name your analogies like the `Visual Diff` window does.

The Spreadsheet must be in Editing Mode in order to use analogies. Please refer to Chapter *Spreadsheet* for more information about the Spreadsheet’s modes. Identify the two cells representing the “source” and “target” visualizations for which you wish to create an analogy. Drag the `Create Analogy` icon *from* the “source” *to* the “target.” This creates an analogy that you can use to apply changes to other workflows. To apply an analogy to another version, drag the `Apply Analogy` icon *from* the cell containing a visualization to which you want to apply the analogy, *to* an empty cell. A new version of the workflow will be created, and rendered in the designated cell.

The following example illustrates how to use analogies within the Spreadsheet. If you completed the previous “Try it now!” exercise, first clear the cell containing the smoothed version of the `Fran Cut` model, so that it won’t interfere with the present example. The Spreadsheet should again resemble Figure *Analogy example...*

Try it now!

Switch to the Spreadsheet’s Editing Mode by hitting ‘Ctrl-Shift-E.’ Create the analogy by dragging the `Create Analogy` icon from the top-left cell over to the top-right cell (Figure *Drag the Create Analogy icon from the source cell...*). Next, apply this analogy to the `Fran Cut` model by dragging the `Apply Analogy` icon from the bottom-left cell over to the bottom-right cell (Figure *Drag the Apply Analogy icon from the cell you wish to modify...*). Hit ‘Ctrl-Shift-I’ to return to Interactive Mode, and see the result of your analogy. It should resemble the output of the first example, as shown in Figure *Result of applying a smoothing analogy...*

Regardless of whether you use the `Visual Diff` interface or the Spreadsheet interface to create your analogy, the end result is the same. To verify this, you can inspect the `Pipeline` view for the newly created version of the workflow. All the module(s) necessary to implement the analogy’s behavior are automatically inserted by VisTrails at the correct locations in the pipeline.

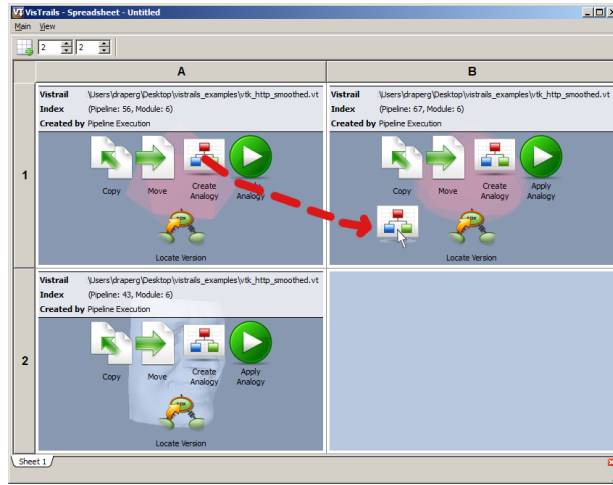


Fig. 3.50: Drag the Create Analogy icon from the “source” cell to the “target” cell to create an analogy.

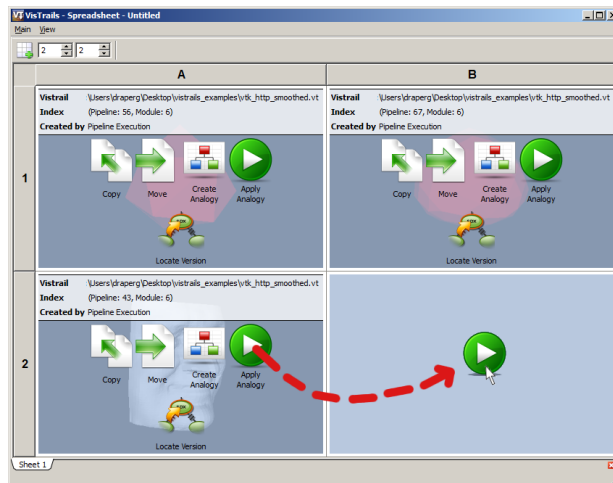


Fig. 3.51: Drag the Apply Analogy icon from the cell you wish to modify to an empty cell.

3.8.4 Notes

Creating visualizations by analogy is a relatively new feature of VisTrails, and as such is not yet fully mature. Although it works well for the examples presented herein, our algorithm may fail to create intuitive visualizations on other pipelines. Furthermore, it is not yet possible to save an analogy, nor apply an analogy to a vistrail other than the one in which it was created. Please contact the VisTrails development team with any bug reports and/or suggestions.

3.9 Parameter Exploration

While exploring workflows, one critical task is tweaking parameter values to improve simulations or visualizations. VisTrails contains an integrated parameter exploration interface that lets you thoroughly explore the parameter space and quickly identify the desired settings. By binding parameters to a range of values, you can generate a collection of results without having to tediously edit the workflow.

VisTrails Parameter Exploration is Spreadsheet-aware, so you can map the intermediate results from explorations into cells of the Spreadsheet. Because the Spreadsheet provides a multi-view interface that makes efficient use of screen space, you can quickly compare the results of different parameter settings. The changes in parameters can be displayed across rows, columns, and sheets. In addition, parameters can be explored across timesteps, and then displayed in the Spreadsheet as animations. This could be used, for example, to show how pathological tissues and tumors are affected by radiation treatment in a series of scans.

3.9.1 Creating a Parameter Exploration

To access VisTrails Parameter Exploration for the currently-active workflow, click on the `Exploration` button in the VisTrails toolbar.

The `Parameter Exploration` view starts out with a blank central canvas wherein exploration parameters can be set up. On the right side of the window, there are a variety of panels that control aspects of the exploration.

The `Set Methods` panel contains the list of parameters that can be explored, the `Annotated Pipeline` panel displays the workflow to be explored and helps resolve ambiguities for parameter settings, and the `Spreadsheet Virtual Cell` aids users in laying out exploration results in the spreadsheet.

To add parameters to an exploration, simply drag the corresponding method from the `Set Methods` panel to the center canvas. To reduce clutter, this panel only shows the methods for which parameters were assigned values in the `Pipeline` view. See Chapter [Creating and Modifying Workflows](#) for instructions on adding methods and parameters to a module.

After dragging a method to the exploration canvas, you can, for each parameter, set the collection of values to be explored and the direction in which to explore (Figure [Setting values for parameter exploration](#)). By default, intermediate parameter values are set via linear interpolation. We will discuss other options later.

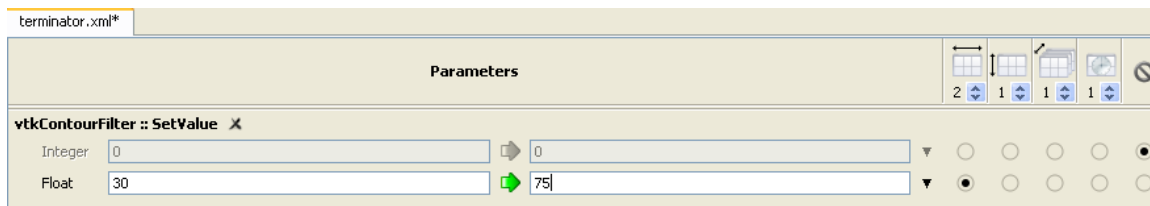
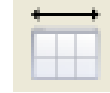
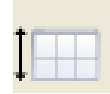





Fig. 3.52: Setting values for parameter exploration.

The five column headings in the upper-right corner of the main canvas control how the results of the parameter exploration will be displayed in the Spreadsheet. From left to right, the five controls determine:

	exploration in the 'x' direction
	exploration in the 'y' direction
	exploration in the 'z' direction
	exploration in time
	none; do not vary this parameter

The spinner beneath each of these icons lets you control the number of parameter values to be explored in that direction. For each parameter, you must select one of the radio buttons corresponding to a direction of exploration ('x', 'y', 'z', time, or none). Note that choosing the final column disables exploration for that parameter.

To run a parameter exploration, click the `Execute` button in the VisTrails toolbar or select `Execute` from the `Workflow` menu.

We now reinforce the above discussion with three examples, motivated by the problem of finding isosurfaces for medical imaging. In the examples that follow, we'll look at determining the interfaces between different types of tissue captured by CT scans.

Try it now!

To begin, load the `terminator.vt` vistrail, select the "Isosurface" node in the version tree, and switch to parameter exploration. From the `Pipeline Methods` panel, click and drag the `SetValue` method of the `vtkContourFilter` module to the center canvas.

We'd like to compare different values for the isosurfaces so change the start and end values of the "Float" parameter to "30" and "75". Since side-by-side visualization will look better on most monitors, select the radio button below the 'x' dimension control, and increase the value of the control to 2 (see Figure *Setting values for parameter exploration*). Execute the exploration and switch to the Spreadsheet to view the results. They should match Figure *Parameter Exploration of two isovalues...* (Open result)

Next Step!

While these two isovalues show interesting features, we may wish to examine other intermediate isosurfaces. To do so, switch back to the main VisTrails window and increase the number of results to generate in the 'x' direction to four. VisTrails will calculate the intermediate values via linear interpolation, and your execution of this new exploration should match Figure *Parameter Exploration of four isovalues...* (Open result)

In our next example, we demonstrate how multiple parameter values can be explored simultaneously. We will use both X and Y exploration directions to change the values of two parameters at the same time in the same spreadsheet.

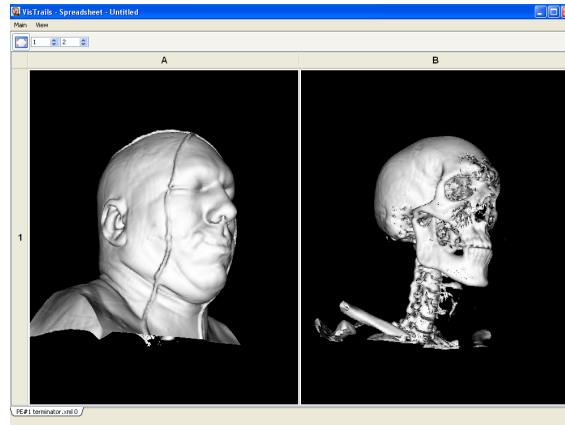


Fig. 3.53: Parameter Exploration of two isovalues as displayed in the Spreadsheet.

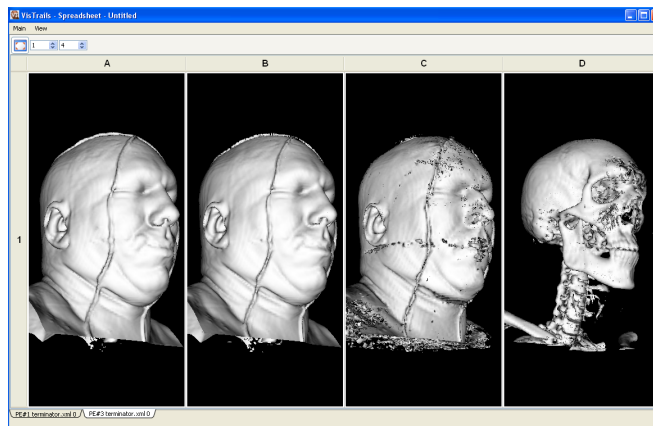


Fig. 3.54: Parameter Exploration of four isovalues as displayed in the Spreadsheet.

Try it now!

In the `terminator.vt` example vistrail, make sure you're working with the "Isosurface" version of the workflow, then go to the Pipeline view. Add the module `vtkImageResample` to the pipeline, and insert it between `vtkStructuredPointsReader` and `vtkContourFilter`, connecting the output of the reader to input of the resampler and the output of the resampler to the input of the contour filter as shown in Figure *Inserting a `vtkImageResample` module...* Finally, select the `vtkImageResample` module and set the `SetAxisMagnificationFactor` to 0 and 0.2. See Chapter *Creating and Modifying Workflows* for reminders on how to accomplish these tasks. After modifying the workflow, switch back to the Exploration view. Inside the Set Methods panel, select the `SetValue` method from the `vtkContourFilter` module, and drag it to the center canvas. Also select the `SetAxisMagnificationFactor` method from the `vtkImageResample` module and drag it to the canvas. Set the values as in the previous example, and set the range of the "Float" parameter of "SetAxisMagnificationFactor" to start at 0.2 and end at 1.0. Also, set the magnification factor to vary over the 'y' direction. Finally, set the exploration to generate 16 results, four in the 'x' direction, and four in the 'y' direction. Your exploration setup should match Figure *Setting up parameter exploration*, and after executing, you should see a result that resembles Figure *Resulting spreadsheet*. Notice that the isosurface changes from left to right while the images have less artifacts as the magnification factor approaches 1.0 from top to bottom. ([Open result](#))

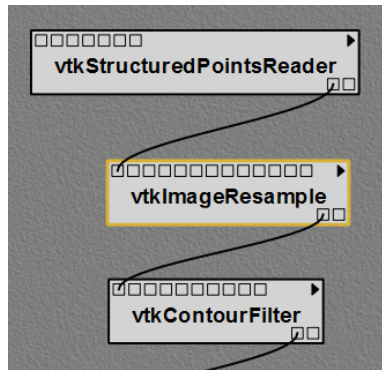


Fig. 3.55: Inserting a `vtkImageResample` module into the "terminator.vt" example pipeline.

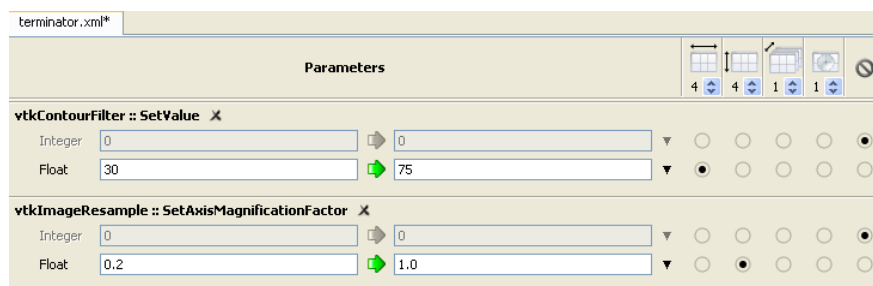


Fig. 3.56: Setting up parameter exploration.

Our third example shows how to create an animation by exploring parameter values in *time*, rather than in 'X' or 'Y'.

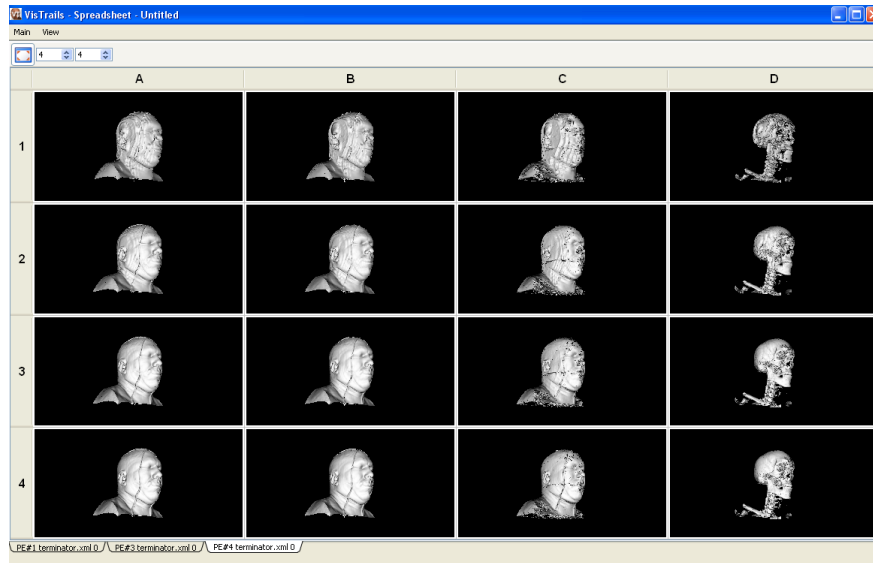


Fig. 3.57: Resulting spreadsheet.
Using parameter exploration with two parameters.

Try it now!

To create an animation, we'll use the same `terminator` example (make sure that you have the "Isosurface" version selected). Follow the same steps as in the first example, but this time, use the range from 30 to 80 and select "time" as the dimension to explore, setting the number of results to generate to 7. See Figure [Setting up parameter exploration](#) to check your settings. After executing, the Spreadsheet will show a *single cell*, but if you select that cell, you will be able to click the `Play` button in the toolbar. You should see an animation where each frame is the result of choosing a different isovalue. A sample frame is displayed in Figure [One frame from the resulting animation](#). (Open result)

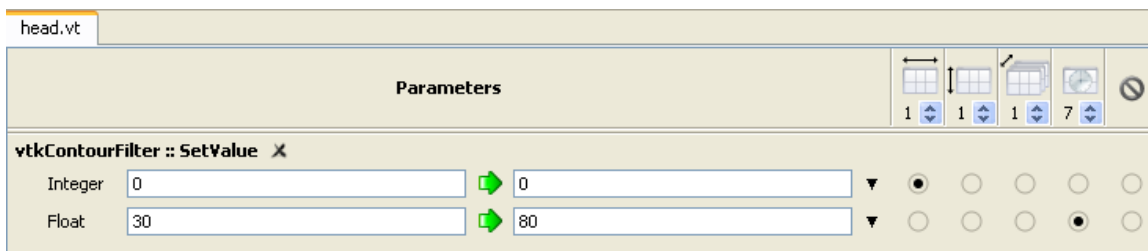


Fig. 3.58: Setting up parameter exploration.

3.9.2 Alternatives to Linear Interpolation

In each of the examples above, we used linear interpolation to vary the parameter values in 'X' and 'Y' and time. However, linear interpolation is only one of three methods for exploring a range of parameter values. The other two are to iterate through a simple list of values, or use a user-defined function. You can choose the desired method from the drop-down menu on the right side of the parameter input field (Figure [Choose from linear interpolation, list, or user-defined function](#)). For linear interpolation, the starting and ending values must be specified; for a list, the entire comma-separated list must be specified, and for a user-defined function, a Python function must be specified. For the list and user-defined functions, you can access an editor via the '...' button. (See Figure [Editors for lists of values](#) for

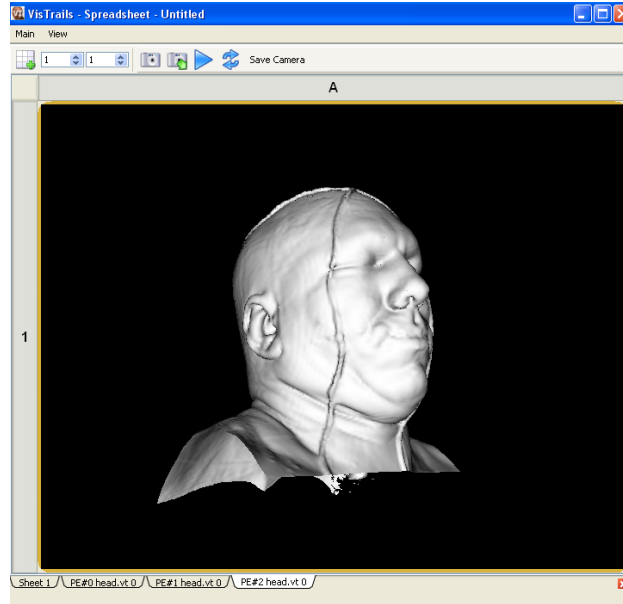


Fig. 3.59: One frame from the resulting animation.

examples of the list editor and Python editor widgets.) As an alternative to the list editor, you can manually enter a list using Python notation; for example, `[30, 36, 45, 75]`. As before, to set the direction in which to explore a given parameter, simply select the radio button in the column for the specified direction.

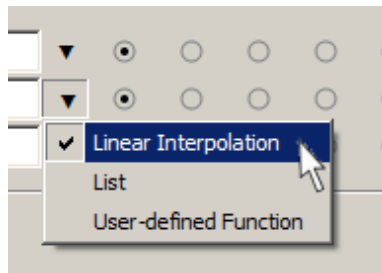


Fig. 3.60: Choose from linear interpolation, list, or user-defined function.

In both the `Set Methods` and `Annotated Pipeline` panels, you may see numbered red circles. See Figure *The panels of the Parameter Exploration window...* for an example of what this looks like. These circles appear when there is more than one module of a given type in a workflow. For each type satisfying this criteria, the instances are numbered and displayed so that you can identify which part of the pipeline a module in the `Set Methods` panel corresponds to.

3.9.3 Saving Parameter Explorations

New parameter explorations are saved automatically when they are executed. The *inspector (below)* has buttons for moving back and forward through the history of parameter explorations. Explorations can be tagged with a name, which will make them visible in the workspace view.

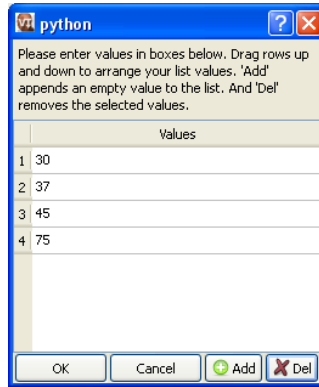


Fig. 3.61: Editors for lists of values.

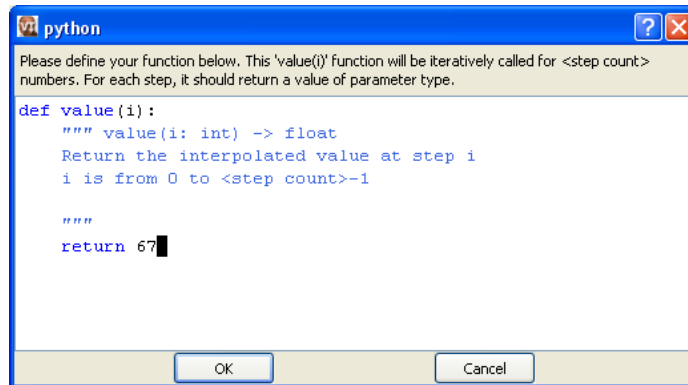
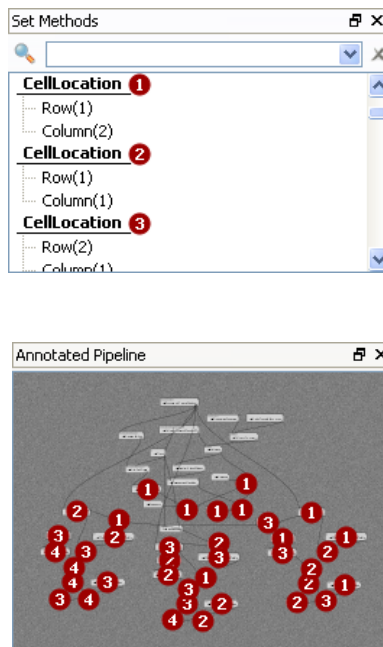


Fig. 3.62: Editors for user-defined functions.



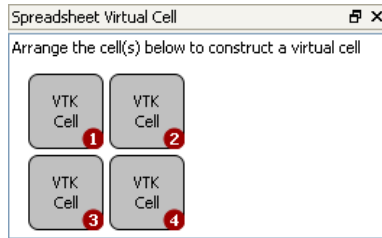


Fig. 3.63: The panels of the Parameter Exploration window. Set Methods (Top) will appear in the right panel and the others will be on the left. The numbered red circles in the Annotated Pipeline (Middle) distinguish duplicate modules, and the cells in the Spreadsheet Virtual Cell (Bottom) determine the layout for spreadsheet results.

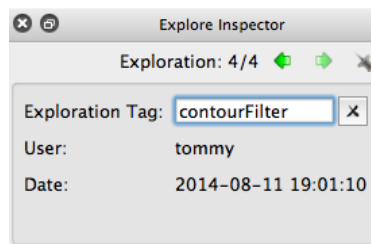


Fig. 3.64: The parameter exploration inspector

3.9.4 “Virtual Cell” Layout

As stated earlier, the Spreadsheet provides integrated support for parameter explorations. Each of the directions of exploration corresponds to a visual dimension in the spreadsheet: the ‘x’ direction corresponds to columns; the ‘y’ direction to rows; the ‘z’ direction to sheets; and time to animations. However, when a workflow already outputs to more than one cell, you can layout the group of cells as it will be replicated during the exploration. For example, given a workflow with two output cells and an exploration for three parameter values in the ‘x’ direction, the resulting spreadsheet could be 1×6 or 2×3 . The Spreadsheet Virtual Cell panel controls the layout of the pattern. Drag and drop cells to position them. See Figures *The panels of the Parameter Exploration window (Bottom)* and *Results of the Virtual Cell arrangement* for an example.

3.10 Provenance Browser

The Provenance Browser allows you to browse through all executions performed on a vistrail. When the Provenance mode is selected, executions are displayed in the Log Details panel on the right (see figure *Provenance Browser*). Selecting an execution from the Log Details panel will display the pipeline with modules colored according to their execution results. Alternatively, this pipeline is displayed by double-clicking on the execution in the Workspace panel. Executions in the Workspace panel are displayed under the version to which they belong and are made visible or invisible by toggling the panel’s executions button. Notice that only executions that belong to tagged versions are displayed in the Workspace, but all executions are displayed in the Log Details.

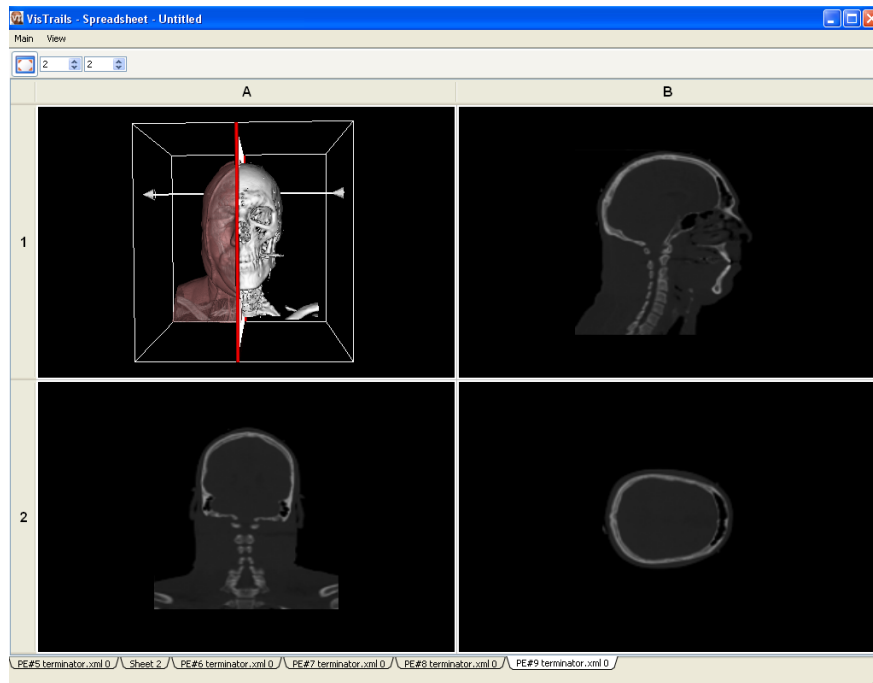


Fig. 3.65: Results of the Virtual Cell arrangement.

3.11 Mashups

3.11.1 Creating Parameter Aliases

If you would like to be able to explore different values for a specific parameter, you will need to create an alias by double-clicking the parameter in the `Parameter Aliases` section. After naming the alias, you can select the alias in the `Mashup` tab (center panel), and configure the alias by selecting the `Display Widget` type and setting `Default` values.

Notice that a pipeline can have multiple modules of the same type or name, making it difficult to differentiate between them. These modules are each assigned a number, with the numbers in the `Annotated Pipeline` section corresponding to the numbers in the `Parameter Aliases` section, making it possible to set an alias for the desired module without much confusion. See figure [Numbered Modules...](#)

Finally, not all modules in the `Annotated Pipeline` will show up in the `Parameter Aliases` section. Only modules whose parameters have been set in the pipeline will appear.

3.11.2 Configuring Parameter Aliases

As mentioned in section [Creating Parameter Aliases](#), aliases are configured in the center panel (the `Mashup` tab). This is pretty simple, so here are the steps:

1. Select the alias you wish to configure from the top box in the `Aliases` tab. The name and position of the selected alias should be displayed below. Both of these can be changed by editing the `Name` and/or `Order` values.
2. Next select the type of widget to display. The choices are `combobox`, `slider`, and `numeric stepper`. The `combobox` will allow you to enter specific values, whereas the `numeric stepper` and `slider` will allow you to scroll through a range of values.

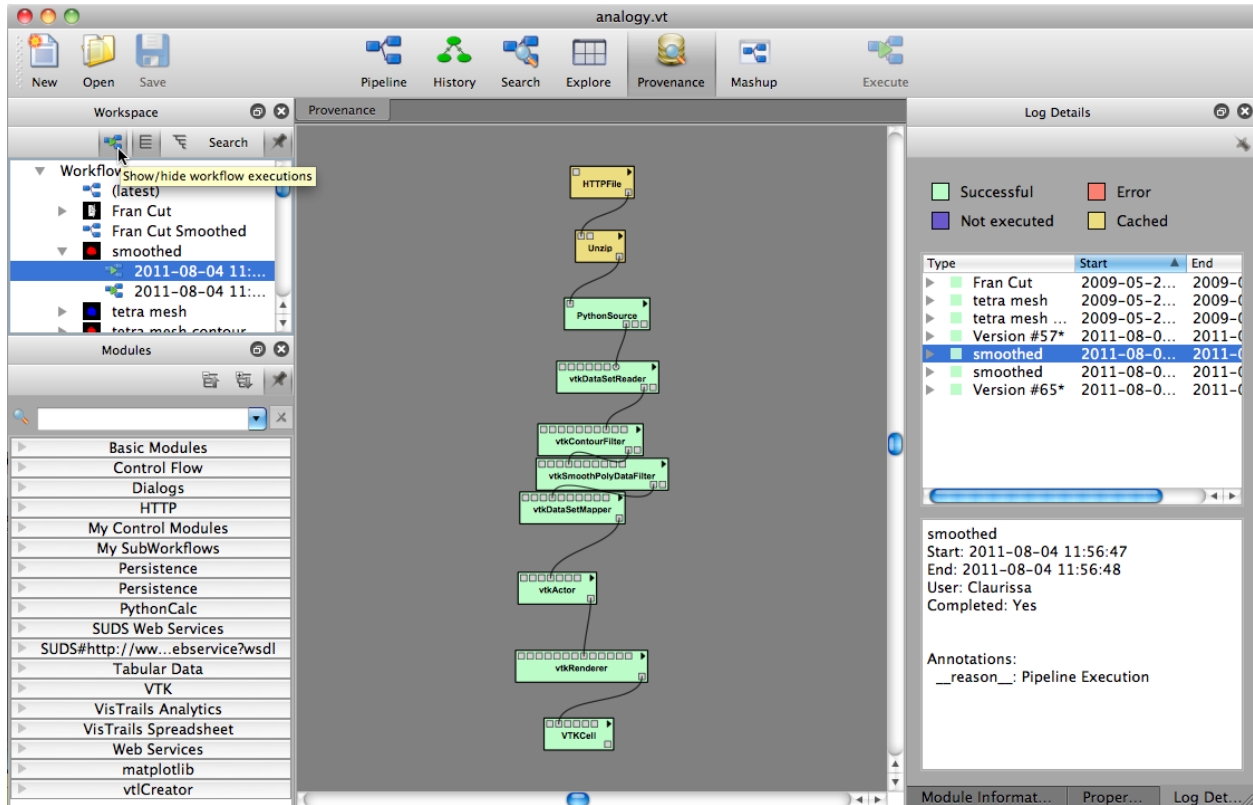


Fig. 3.66: Provenance Browser - *Left*: The *Workspace* has a button to enable/disable executions. When enabled, executions of each tagged version in the *vistrail* will appear when each respective version is expanded. *Right*: The *Provenance* Browser keeps track of all executions whether they belong to tagged versions or not. When selected, the color coded execution pipeline will appear in the center panel.

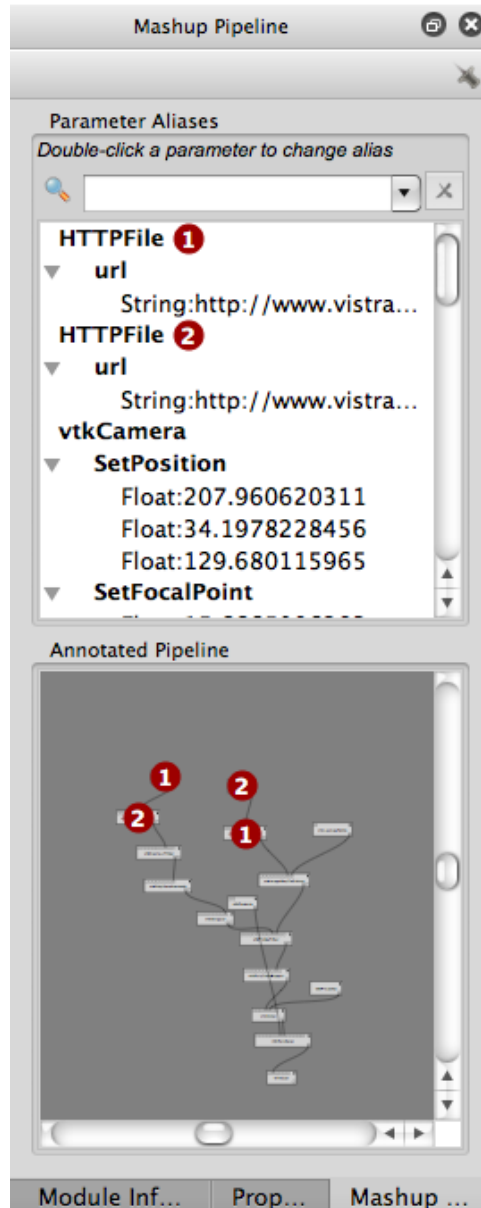


Fig. 3.67: Numbered Modules - The DownloadFile modules 1 and 2 appear in the annotated pipeline and in the parameter aliases. The annotated pipeline also, numbers the vtkDataSetReader modules (which appear below the respective HTTPFile modules in the pipeline). Their parameters have not been exposed to the mashup, so they do not appear in the Parameter Aliases section.

3. Set the Min Val, Max Val, and Step Size (for slider and numeric stepper only).
4. Set the Default Value. The default value should already be set based on the value it was given in the pipeline, but you are allowed to change it here if desired.
5. Enter suggested values. If you have a set of values to suggest to the user through the Mashups interface, you should add them to the values list. You can do this by either clicking the . . . button and adding the appropriate values, or by entering the values in the Values List box in list format.
6. Finally, you may delete an alias with the Delete Alias button.

After configuring the necessary aliases, press Preview to interact with your mashup and to ensure its proper functionality.

3.11.3 Saving a Mashup

Mashups are added to the VisTrail when you press the keep button. However, this changes the VisTrail, but does not save it. To fully save your mashup, you should both press the Keep button and save the VisTrail.

3.11.4 Managing Multiple Mashups

The Mashups Inspector allows you to both rename a mashup, and easily switch between existing mashups.

3.11.5 A Simple Example

Try it now!

- Open `brain_vistrail.vt`
- Choose `Save As` and rename the file if you do not want to overwrite the original.
- Select the “contour 3” version
- Press execute to ensure any necessary upgrades are made
- Select Mashup from the toolbar.
- In the Mashup Pipeline tab, look under `vtkProperty` → `SetOpacity` and double-click on `Float`.
- Enter “Opacity” in the `Set Parameter` box that pops up, then click `OK`. See figure *Creating the Opacity Alias*.
- Under `vtkRenderer` → `SetBackgroundWidget`, double-click on `Color` and enter “Background” as the alias. See figure *Creating the Background Alias*.
- In the center panel, select the `Opacity` alias.
- Change the display widget to `numericstepper`.
- Set the `Min Val`, `Max Val`, and `Step Size` to 0, 1, and 0.1 respectively.
- Set the `Values List` to [0.3, 0.5]. See figure *Configuring the Opacity Alias*.
- Select the `Background` alias and make sure the display widget is a `combobox`.
- Select `Preview`. See figure *The resulting mashup*.
- Select `Tag`, `No`, and then enter “one” as the new tag name.
- Save the file. (Open result)

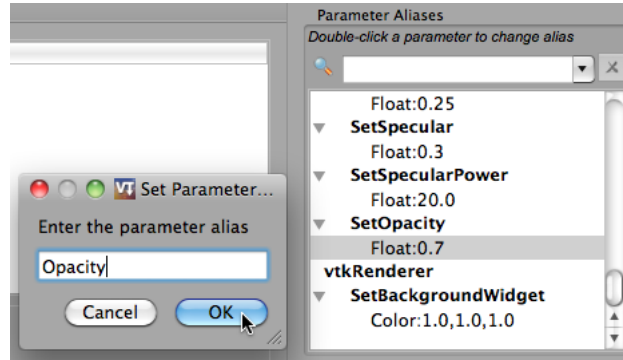


Fig. 3.68: Creating the Opacity Alias.

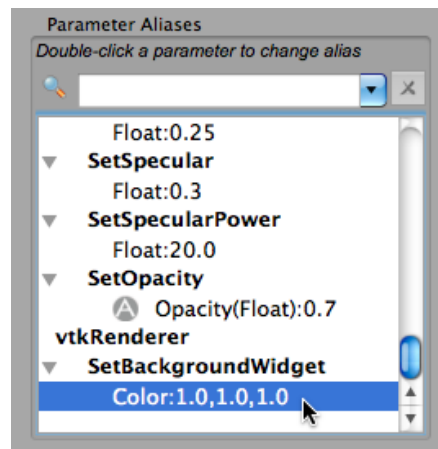


Fig. 3.69: Creating the Background Alias.

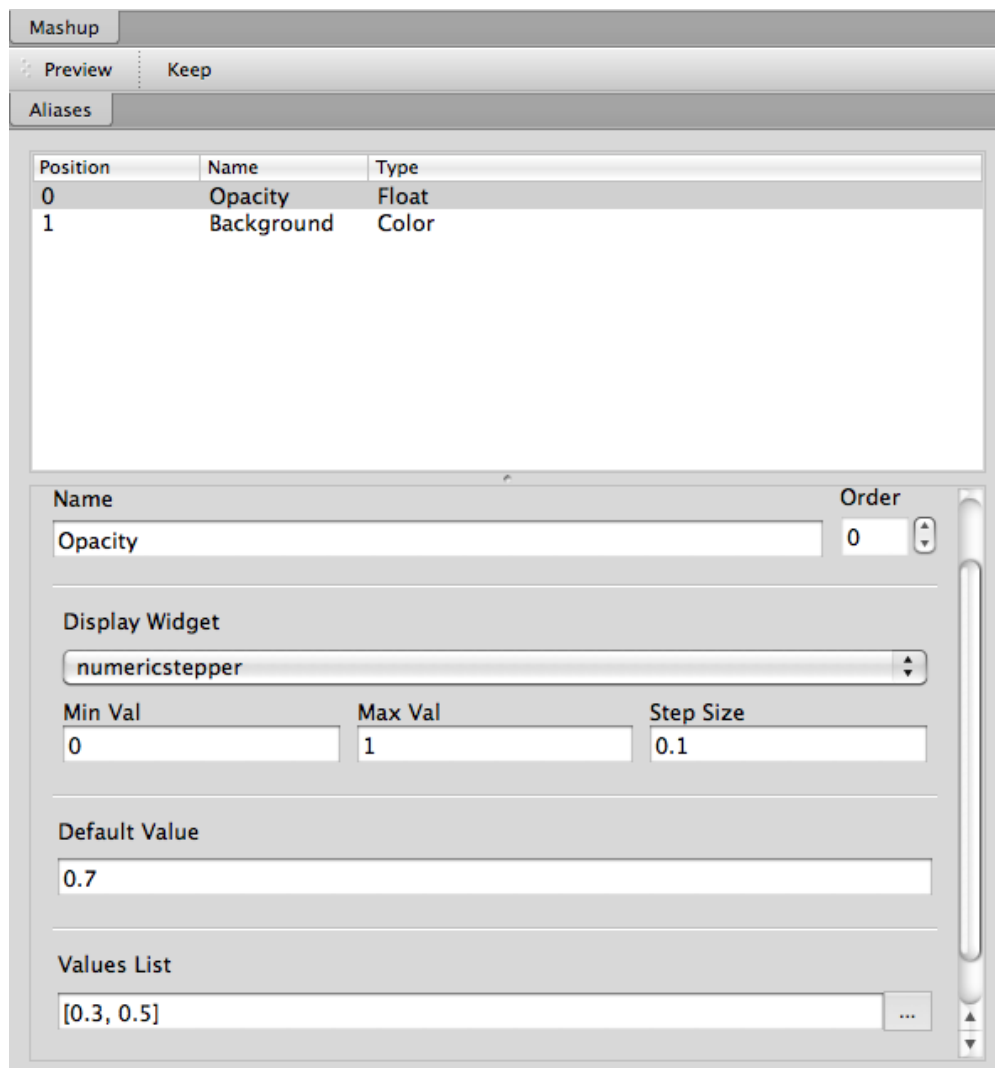


Fig. 3.70: Configuring the `Opacity` alias.

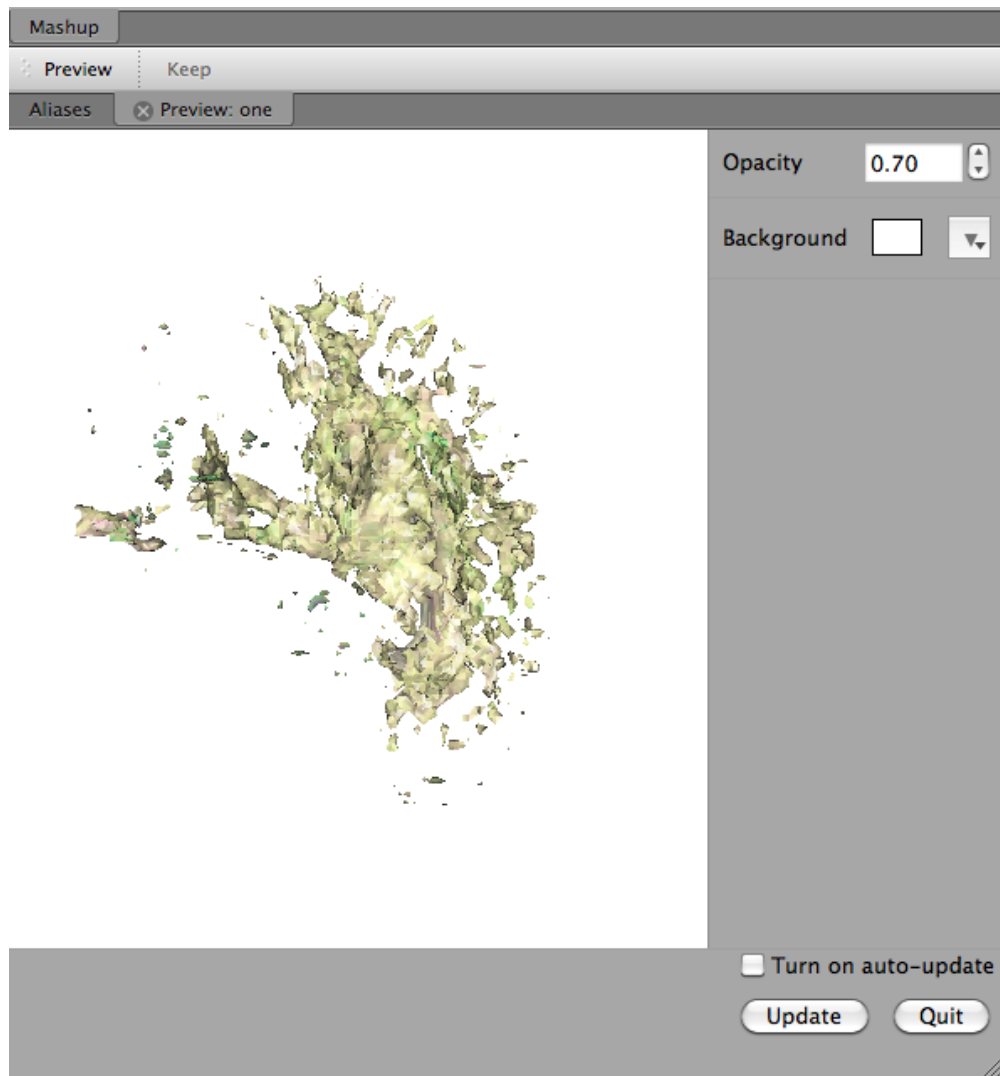


Fig. 3.71: The resulting mashup.

3.12 Module Descriptions and Examples

3.12.1 VisTrails VTK modules

Most VTK modules in VisTrails represents VTK classes. Inputs and outputs are based on class methods. A warning, in VTK it is sometimes important to call input methods in the correct order. This order is not preserved in the parameter list in VisTrails, but will still be used during execution. Method names may differ in VisTrails:

- Most Set/Get prefixes have been removed.
- SetXToY-style methods are reduced to single SetX names with a list selection.
- Methods without parameters are replaced by booleans (that need to be set to True).
- VTK6's SetInputData-style names are used even for VTK5.

Although most VTK modules in VisTrails would be familiar to vtk users, or at least in the vtk documentation, there are a few modules that VisTrails introduces. They are used as follows:

- **PythonSource** - Although a PythonSource is in the Basic Modules list rather than VTK, it is mentioned here for convenience. This module allows you write python statements to be executed as part of the workflow. See Section *PythonSource* for more information.
- **VTKCell** - VTKCell is a VisTrails module that can display a vtkRenderWindow inside a cell. Simply pass it a vtkRenderer and any additional optional inputs, and it will display the results in the spreadsheet.
- **VTKRenderOffscreen** - Takes the output of a vtkRenderer and produces a PNG image of size width X height. Default values of width and height are 512. The output can then be written to a file using a FileSink.
- **vtkInspectors: vtkDataArrayInspector, vtkDataSetAttributesInspector, vtkDataSetInspector, vtkPolyDataInspector** - These inspectors were created to allow easy access to information that is not otherwise exposed by module ports, but would be accessible through vtk objects. This information includes: normals, scalars, tensors, and vectors as well as statistical information such as bounds, center, length, max, min. Looking at the output ports of these inspectors gives an idea of the information available.
- **vtkInteractionHandler** - The vtkInteractionHandler is used when a callback function is needed. To setup this handler:
 - Connect the Observer input port to the output port of the object that needs the callback function.
 - Connect the SharedData input port to the modules that would be passed as parameters to the callback function. Multiple modules can be connected (see terminator.vt - Images Slices SW).
 - Connect the output port to the VTKCell.
 - Select configure to write the callback function.
 - * Name the function after the event that initiates it, but replace 'Event' with 'Handler'. If the function should be called when a StartInteractionEvent occurs, the function should be named `startInteractionHandler`.
 - * The function should take the parameters observer, and shareddata.
 - * Add the contents of the function.

There are a number of examples that use the vtkInteractionHandler. If there is any confusion, comparing the callback/interaction handler portions of the .py and .vt files in the `vtk_examples/GUI` directory is helpful.

Accessing vtkObjects in vtkInteractionHandler VtkObjects passed to the vtkInteractionHandler are VisTrails modules. The vtkObject within that module is called a vtkInstance and is accessed by calling `myModule.vtkInstance`. See Section *PythonSource* for more information.

- **vtkScaledTransferFunction** - Allows you to add a transfer function through the use of an interactive widget. See `head.vt` - volume rendering or `terminator.vt` for example usage.

3.12.2 Modules and Corresponding Examples

Here we provide a list of the `.vt` files in the examples directory that use the following modules:

Warning, this list is out-of-date and some examples may have been removed.

- **AreaFilter:** `triangle_area.vt`
- **CellLocation:** `offscreen.vt`, `terminator.vt`, `vtk.vt`
- **ConcatenateString:** `KEGG_SearchEntities_webservice.vt`
- **Cross:** `triangle_area.vt`
- **fetchData:** `structure_or_id_webservice.vt`, `protein_visualization.vt`
- **FileSink:** `offscreen.vt` - `offscreen`
- **Filter:** `triangle_area.vt`
- **If:** `structure_or_id_webservice.vt`, `protein_visualization.vt`
- **ImageViewerCell:** `r_stats.vt`
- **List:** `triangle_area.vt`
- **Map:** `triangle_area.vt`
- **MplFigure:** `plot.vt`, `terminator.vt` - Histogram, `triangle_area.vt`, `vtk.vt` - Three Cells
- **MplFigureCell:** `plot.vt`, `terminator.vt` - Histogram, `triangle_area.vt`, `vtk.vt` - Three Cells
- **MplPlot:** `plot.vt`, `terminator.vt` - Histogram, `triangle_area.vt`, `vtk.vt` - Three Cells
- **PythonCalc:** `ProbeWithPointWidget.vt`, `officeTube.vt`
- **PythonSource:** `infovis.vt`, `noaa_webservices.vt`, `offscreen.vt`, `KEGG_SearchEntities_webservice.vt`, `chebi_webservice.vt`, `EMBOSS_webservices.vt`, `structure_or_id_webservice.vt`, `vtk_http.vt`, `protein_visualization.vt`, `terminator.vt`, `triangle_area.vt`
- **RichTextCell:** `noaa_webservices.vt`, `offscreen.vt`, `KEGG_SearchEntities_webservice.vt`, `chebi_webservice.vt`, `EMBOSS_webservices.vt`, `protein_visualization.vt`
- **RPNGFigure:** `r_stats.vt`
- **RReadCSV:** `r_stats.vt`
- **Rsource:** `r_stats.vt`
- **SheetReference:** `offscreen.vt`, `vtk.vt`
- **StandardOutput:** `r_stats.vt`, `triangle_area.vt`
- **Tuple:** `marching.vt`, `ProbingWithPlaneWidget.vt`, `TransformWithBoxWidget.vt`, `BandContourTerrain.vt`, `probeComb.vt`, `ImplicitPlaneWidget.vt`, `BuildUGrid.vt`, `ProbeWithPointWidget.vt`, `VolumeRenderWithBoxWidget.vt`, `PerlinTerrain.vt`
- **Untuple:** `probeComb.vt`, `BandContourTerrain.vt`
- **vtk3DSImporter:** `flamingo.vt`
- **vtkAppendPolyData:** `vtk.vt` - Implicit Plane Clipper, `xyPlot.vt`, `TransformWithBoxWidget.vt`, `probeComb.vt`, `ImplicitPlaneWidget.vt`, `warpComb.vt`

- **vtkAssembly:** assembly.vt
- **vtkAxes:** textOrigin.vt
- **vtkBandedPolyDataContourFilter:** BandContourTerrain.vt
- **vtkBMPReader:** Tplane.vt, imageWarp.vt, GenerateTextureCoords.vt
- **vtkBoxWidget:** TransformWithBoxWidget.vt, VolumeRenderWithBoxWidget.vt, cone.vt - 6
- **vtkBYUReader:** cubeAxes.vt, ClipCow.vt
- **vtkCastToConcrete:** ExtractUGrid.vt
- **vtkCellArray:** constrainedDelaunay.vt, Arrays.vt, CreateStrip.vt
- **vtkClipPolyData:** terminator.vt, vtk.vt - Implicit Plane Clipper, ImplicitPlaneWidget.vt, ClipCow.vt
- **vtkColorTransferFunction:** lung.vt, SimpleRayCast.vt, mummy.xml - volume rendering, SimpleTextureMap2D.vt, VolumeRenderWithBoxWidget.vt
- **vtkCone:** iceCream.vt
- **vtkConeSource:** vtk_book_3rd_p193.vt, vtk.vt - Implicit Plane Clipper, TransformWithBoxWidget.vt, Cone.vt, ImplicitPlaneWidget.vt, ProbeWithPointWidget.vt, assembly.vt
- **vtkConnectivityFilter:** ExtractUGrid.vt, pointToCellData.vt
- **vtkContourFilter:** brain_vistrail.vt, spx.vt, vtk_http.vt, marching.vt, head.vt - alias, mummy.xml - Isosurface, terminator.vt, pointToCellData.vt, triangle_area.vt - CalculateArea, Medical1.vt, hello.vt, VisQuad.vt, probeComb.vt, vtk_book_3rd_p189.vt, Medical2.vt, iceCream.vt, Contours2D.vt, Medical3.vt, PerlinTerrain.vt, ColorIsosurface.vt, PseudoVolumeRendering.vt
- **vtkCubeAxesActor2D:** cubeAxes.vt
- **vtkCubeSource:** assembly.vt, marching.vt
- **vtkCutter:** ClipCow.vt, CutCombustor.vt, PseudoVolumeRendering.vt
- **vtkCylinderSource:** assembly.vt, cylinder.vt
- **vtkDataArrayInspector:** CutCombustor.vt, officeTube.vt
- **vtkDataSetAttributesInspector:** officeTube.vt, CutCombustor.vt
- **vtkDataSetInspector:** ProbingWithPlaneWidget.vt, StreamlinesWithLineWidget.vt, CutCombustor.vt, officeTube.vt, TextureThreshold.vt, BandContourTerrain.vt, probeComb.vt, ProbeWithPointWidget.vt, rainbow.vt, streamSurface.vt, warpComb.vt
- **vtkDataSetMapper:** offscreen.vt, spx.vt, structure_or_id_webservice.vt, vtk_http.vt, SubsampleGrid.vt, TextureThreshold.vt, imageWarp.vt, protein_visualization.vt, head.vt - alias, mummy.xml - Isosurface, terminator.vt - Histogram, pointToCellData.vt, ExtractUGrid.vt, ExtractGeometry.vt, vtk.vt, BuildUGrid.vt, GenerateTextureCoords.vt
- **vtkDataSetReader:** brain_vistrail.vt, vtk_http.vt, triangle_area.vt, ExtractUGrid.vt, vtk.vt
- **vtkDecimatePro:** smoothFran.vt
- **vtkDelaunay2D:** constrainedDelaunay.vt, faultLines.vt
- **vtkDelaunay3D:** GenerateTextureCoords.vt
- **vtkDEMReader:** BandContourTerrain.vt
- **vtkDoubleArray:** Arrays.vt
- **vtkExtractEdges:** constrainedDelaunay.vt, marching.vt

- **vtkExtractGeometry:** ExtractGeometry.vt
- **vtkExtractGrid:** SubsampleGrid.vt, PseudoVolumeRendering.vt - vtkPlane
- **vtkExtractUnstructuredGrid:** ExtractUGrid.vt
- **vtkExtractVOI:** Contours2D.vt
- **vtkFloatArray:** Arrays.vt, BuildUGrid.vt, marching.vt
- **vtkFollower:** textOrigin.vt
- **vtkGeometryFilter:** ExtractUGrid.vt, pointToCellData.vt
- **vtkGlyph3D:** vtk_book_3rd_p193.vt, marching.vt, vtk.vt - Implicit Plane Clipper, TransformWithBoxWidget.vt, ImplicitPlaneWidget.vt, ProbeWithPointWidget.vt, spikeF.vt
- **vtkGraphLayoutView:** infovis.vt
- **vtkHexahedron:** BuildUGrid.vt
- **vtkIcicleView:** infovis.vt
- **vtkIdList:** BuildUGrid.vt, marching.vt
- **vtkImageActor:** Medical3.vt
- **vtkImageDataGeometryFilter:** BandContourTerrain.vt, imageWarp.vt
- **vtkImageLuminance:** imageWarp.vt
- **vtkImageMapToColors:** brain_vistrail.vt, Medical3.vt
- **vtkImageReslice:** terminator.vt
- **vtkImageShiftScale:** lung.vt - raycasted
- **vtkImageShrink3D:** BandContourTerrain.vt
- **vtkImplicitBoolean:** iceCream.vt, ExtractGeometry.vt
- **vtkImplicitModeller:** hello.vt
- **vtkImplicitPlaneWidget:** terminator.vt, vtk.vt, ImplicitPlaneWidget.vt
- **vtkImplicitSum:** PerlinTerrain.vt
- **vtkIntArray:** Arrays.vt
- **vtkInteractionHandler:** ProbingWithPlaneWidget.vt, StreamlinesWithLineWidget.vt, terminator.vt, vtk.vt - Implicit Plane Clipper, TransformWithBoxWidget.vt, Cone.vt - 6 , ImplicitPlaneWidget.vt, ProbeWithPointWidget.vt, VolumeRenderWithBoxWidget.vt
- **vtkInteractorStyleImage:** terminator.vt
- **vtkInteractorStyleTrackballCamera:** Cone.vt - 5
- **vtkLight:** cubeAxes.vt, faultLines.vt
- **vtkLine:** BuildUGrid.vt
- **vtkLineSource:** streamSurface.vt, xyPlot.vt
- **vtkLineWidget:** StreamlinesWithLineWidget.vt
- **vtkLODActor:** TestText.vt, stl.vt, CADPart.vt, vtk.vt - Implicit Plane Clipper, TransformWithBoxWidget.vt, BandContourTerrain.vt, cubeAxes.vt, ImplicitPlaneWidget.vt, FilterCADPart.vt, ColorIsosurface.vt
- **vtkLookupTable:** brain_vistrail.vt, vtk_book_3rd_p193.vt, pointToCellData.vt, BandContourTerrain.vt, ExtractUGrid.vt, Medical3.vt, rainbow.vt, PseudoVolumeRendering.vt

- **vtkMaskPoints:** vtk_book_3rd_p193.vt, spikeF.vt
- **vtkMassProperties:** triangle_area.vt - CalculateArea
- **vtkMergeFilter:** imageWarp.vt
- **vtkOpenGLVolumeTextureMapper3D:** lung.vt - TextureWithShading
- **vtkOutlineFilter:** VisQuad.vt, probeComb.vt, ExtractGeometry.vt, vtk_book_3rd_p189.vt, cubeAxes.vt, VolumeRenderWithBoxWidget.vt, Contours2D.vt, Medical1.vt, Medical2.vt, Medical3.vt
- **vtkPDBReader:** protein_visualization.vt, structure_or_id_webservice.vt
- **vtkPerlinNoise:** PerlinTerrain.vt
- **vtkPiecewiseFunction:** lung.vt, SimpleRayCast.vt, mummy.xml - volume rendering, SimpleTextureMap2D.vt, VolumeRenderWithBoxWidget.vt
- **vtkPixel:** BuildUGrid.vt
- **vtkPlane:** lung.vt - TS and plane, CutCombustor.vt, terminator.vt, vtk.vt - Implicit Plane Clipper, ImplicitPlaneWidget.vt, iceCream.vt, PerlinTerrain.vt, ClipCow.vt
- **vtkPlanes:** VolumeRenderWithBoxWidget.vt
- **vtkPlaneSource:** Tplane.vt, terminator.vt, probeComb.vt
- **vtkPlaneWidget:** ProbingWithPlaneWidget.vt
- **vtkPLOT3DReader:** ProbingWithPlaneWidget.vt, StreamlinesWithLineWidget.vt, CutCombustor.vt, SubsampleGrid.vt, TextureThreshold.vt, xyPlot.vt, probeComb.vt, ProbeWithPointWidget.vt, rainbow.vt, ColorIsosurface.vt, streamSurface.vt, warpComb.vt, PseudoVolumeRendering.vt
- **vtkPointData:** marching.vt, Arrays.vt, BuildUGrid.vt
- **vtkPointDataToCellData:** pointToCellData.vt
- **vtkPoints:** CreateStrip.vt, marching.vt, constrainedDelaunay.vt, Arrays.vt, BuildUGrid.vt
- **vtkPointSource:** GenerateTextureCoords.vt, officeTube.vt
- **vtkPointWidget:** ProbeWithPointWidget.vt
- **vtkPolyData:** CreateStrip.vt, ProbingWithPlaneWidget.vt, constrainedDelaunay.vt, StreamlinesWithLineWidget.vt, Arrays.vt, ProbeWithPointWidget.vt, ClipCow.vt
- **vtkPolyDataInspector:** ClipCow.vt
- **vtkPolyDataNormals:** brain_vistrail.vt, pointToCellData.vt, Medical1.vt, faultLines.vt, ExtractUGrid.vt, smoothFran.vt, cubeAxes.vt, Medical2.vt, Medical3.vt, ClipCow.vt, ColorIsosurface.vt, warpComb.vt, PerlinTerrain.vt, spikeF.vt, PseudoVolumeRendering.vt, BandContourTerrain.vt
- **vtkPolyDataReader:** hello.vt, faultLines.vt, smoothFran.vt, spikeF.vt
- **vtkPolygon:** BuildUGrid.vt
- **vtkPolyLine:** BuildUGrid.vt
- **vtkPolyVertex:** BuildUGrid.vt
- **vtkProbeFilter:** brain_vistrail.vt, ProbingWithPlaneWidget.vt, xyPlot.vt, probeComb.vt, ProbeWithPointWidget.vt
- **vtkProperty2D:** xyPlot.vt
- **vtkPyramid:** BuildUGrid.vt
- **vtkQuad:** BuildUGrid.vt

- **vtkQuadraticDecimation:** spx.vt - Decimate
- **vtkQuadric:** VisQuad.vt, ExtractGeometry.vt, vtk_book_3rd_p189.vt, Contours2D.vt
- **vtkRandomGraphSource:** infovis.vt - hello_world
- **VTKRenderOffscreen:** offscreen.vt
- **vtkRibbonFilter:** StreamlinesWithLineWidget.vt
- **vtkRuledSurfaceFilter:** streamSurface.vt
- **vtkRungeKutta4:** StreamlinesWithLineWidget.vt, officeTube.vt, streamSurface.vt
- **vtkSampleFunction:** VisQuad.vt, ExtractGeometry.vt, vtk_book_3rd_p189.vt, iceCream.vt, Contours2D.vt, PerlinTerrain.vt
- **vtkScaledTransferFunction:** head.vt - volume rendering, terminator.vt
- **vtkShrinkFilter:** ExtractGeometry.vt
- **vtkShrinkPolyData:** marching.vt, filterCADPart.vt
- **vtkSmoothPolyDataFilter:** xyPlot.vt
- **vtkSphere:** iceCream.vt, ExtractGeometry.vt
- **vtkSphereSource:** TestText.vt, marching.vt, assembly.vt, vtk.vt - Implicit Plane Clipper, TransformWithBoxWidget.vt, ImplicitPlaneWidget.vt
- **vtkSTLReader:** stl.vt, CADPart.vt, FilterCADPart.vt
- **vtkStreamLine:** StreamlinesWithLineWidget.vt, officeTube.vt, streamSurface.vt
- **vtkStripper:** brain_vistrail.vt, Medical2.vt, Medical3.vt, ClipCow.vt
- **vtkStructuredGridGeometryFilter:** CutCombuster.vt, officeTube.vt, TextureThreshold.vt, rainbow.vt, warpComb.vt
- **vtkStructuredGridOutlineFilter:** StreamlinesWithLineWidget.vt, officeTube.vt, SubsampleGrid.vt, TextureThreshold.vt, xyPlot.vt, probeComb.vt, ProbeWithPointWidget.vt, rainbow.vt, ColorIsosurface.vt, streamSurface.vt, warpComb.vt, PseudoVolumeRendering.vt, ProbingWithPlaneWidget.vt, CutCombustor.vt
- **vtkStructuredGridReader:** officeTube.vt
- **vtkStructuredPointsReader:** lung.vt, vtk_book_3rd_p193.vt, SimpleRayCast.vt, TextureThreshold.vt, head.vt - volume rendering, mummy.xml - volume rendering, head.vt - alias, mummy.xml - Isosurface, terminator.vt, SimpleTextureMap2D.vt
- **vtkTetra:** BuildUGrid.vt
- **vtkTextActor:** TestText.vt
- **vtkTextProperty:** TestText.vt, xyPlot.vt, cubeAxes.vt
- **vtkTexture:** Tplane.vt, TextureThreshold.vt, terminator.vt, GenerateTextureCoords.vt
- **vtkTextureMapToCylinder:** GenerateTextureCoords.vt
- **vtkThreshold:** pointToCellData.vt
- **vtkThresholdPoints:** vtk_book_3rd_p193.vt, marching.vt
- **vtkThresholdTextureCoords:** TextureThreshold.vt
- **vtkTransform:** marching.vt, terminator.vt, xyPlot.vt, TransformWithBoxWidget.vt, Cone.vt - 6, probeComb.vt, ExtractGeometry.vt, spikeF.vt

- **vtkTransformPolyDataFilter:** marching.vt, xyPlot.vt, probeComb.vt, spikeF.vt
- **vtkTransformTextureCoords:** GenerateTextureCoords.vt
- **vtkTreeMapView:** infovis.vt
- **vtkTreeRingView:** infovis.vt
- **vtkTriangle:** BuildUGrid.vt
- **vtkTriangleFilter:** triangle_area.vt - CalculateArea, ClipCow.vt
- **vtkTriangleStrip:** BuildUGrid.vt
- **vtkTubeFilter:** marching.vt, constrainedDelaunay.vt, officeTube.vt, officeTubes.vt, xyPlot.vt, faultLines.vt, PseudoVolumeRendering.vt
- **vtkUnstructuredGrid:** BuildUGrid.vt, marching.vt
- **vtkUnstructuredGridReader:** offscreen.vt, spx.vt, pointToCellData.vt
- **vtkVectorText:** textOrigin.vt, marching.vt
- **vtkVertex:** BuildUGrid.vt
- **VTKViewCell:** infovis.vt
- **vtkViewTheme:** infovis.vt - cone_layout
- **vtkVolume:** lung.vt, SimpleRayCast.vt, head.vt - volume rendering, mummy.xml - volume rendering, terminator.vt, SimpleTextureMap2D.vt, VolumeRenderWithBoxWidget.vt
- **vtkVolume16Reader:** VolumeRenderWithBoxWidget.vt, Medical1.vt, Medical2.vt, Medical3.vt
- **vtkVolumeProperty:** lung.vt, SimpleRayCast.vt, head.vt - volume rendering, mummy.xml - volume rendering, terminator.vt, SimpleTextureMap2D.vt, VolumeRenderWithBoxWidget.vt
- **vtkVolumeRayCastCompositeFunction:** lung.vt - raycasted, SimpleRayCast.vt, mummy.xml - volume rendering, terminator.vt - SW, VolumeRenderWithBoxWidget.vt
- **vtkVolumeRayCastMapper:** lung.vt - raycasted, SimpleRayCast.vt, mummy.xml - volume rendering, terminator.vt - SW, VolumeRenderWithBoxWidget.vt
- **vtkVolumeTextureMapper2D:** SimpleTextureMap2D.vt
- **vtkVolumeTextureMapper3D:** head.vt - volume rendering, terminator.vt - HW
- **vtkVoxel:** BuildUGrid.vt
- **vtkWarpScalar:** imageWarp.vt, BandContourTerrain.vt, warpComb.vt
- **vtkWarpVector:** pointToCellData.vt, ExtractUGrid.vt
- **vtkWedge:** BuildUGrid.vt
- **vtkWindowLevelLookupTable:** terminator.vt
- **vtkXMLTreeReader:** infovis.vt
- **vtkXYPlotActor:** xyPlot.vt

INTERMEDIATE CONCEPTS AND VISTRAILS PACKAGES

4.1 Parameter Widgets

4.1.1 Introduction to Parameter Widgets

Parameter widgets are editable parameters inside modules in the pipeline view. They can be used to give an overview of the parameters in a workflow, or to quickly edit parameters without the usual clicking on a module and selecting the parameter in the ‘Module Info’ panel. *Figure 1* shows a complete workflow using parameter widgets. (open in [vistrails](#))

Enabling Parameter Widgets

Parameter widgets are hidden by default, but can be enabled by toggling the pencil icon in the ‘Module Info’ panel (See *Figure 2*). This will show all existing parameter widgets as well as the pencil icons in ‘Module Info’ for adding new ones.

Adding a parameter widget to a module

A parameter widget can be enabled or disabled in the ‘Module Info’ panel by toggling the pencil icon (See *Figure 3*). Only parameters of constant type that have widgets for editing can be added.

Constant modules such as String and Integer show a parameter widget for ‘value’ by default, but it can be removed using the ‘Module Info’ panel if needed.

Limitations

On some platforms (Such as Mac) some parameter widgets may look unsharp or pixelated. This is because no widget for that type has been created for use in the pipeline view, and the default one from the ‘Module Info’ pane has been used instead.

Only one parameter widget per port can be visible right now. In the ‘Module Info’ pane it is possible to specify several function parameters for each port.

Zooming out will hide all the edit widgets for performance reasons, it would also be difficult to edit anything in that size.

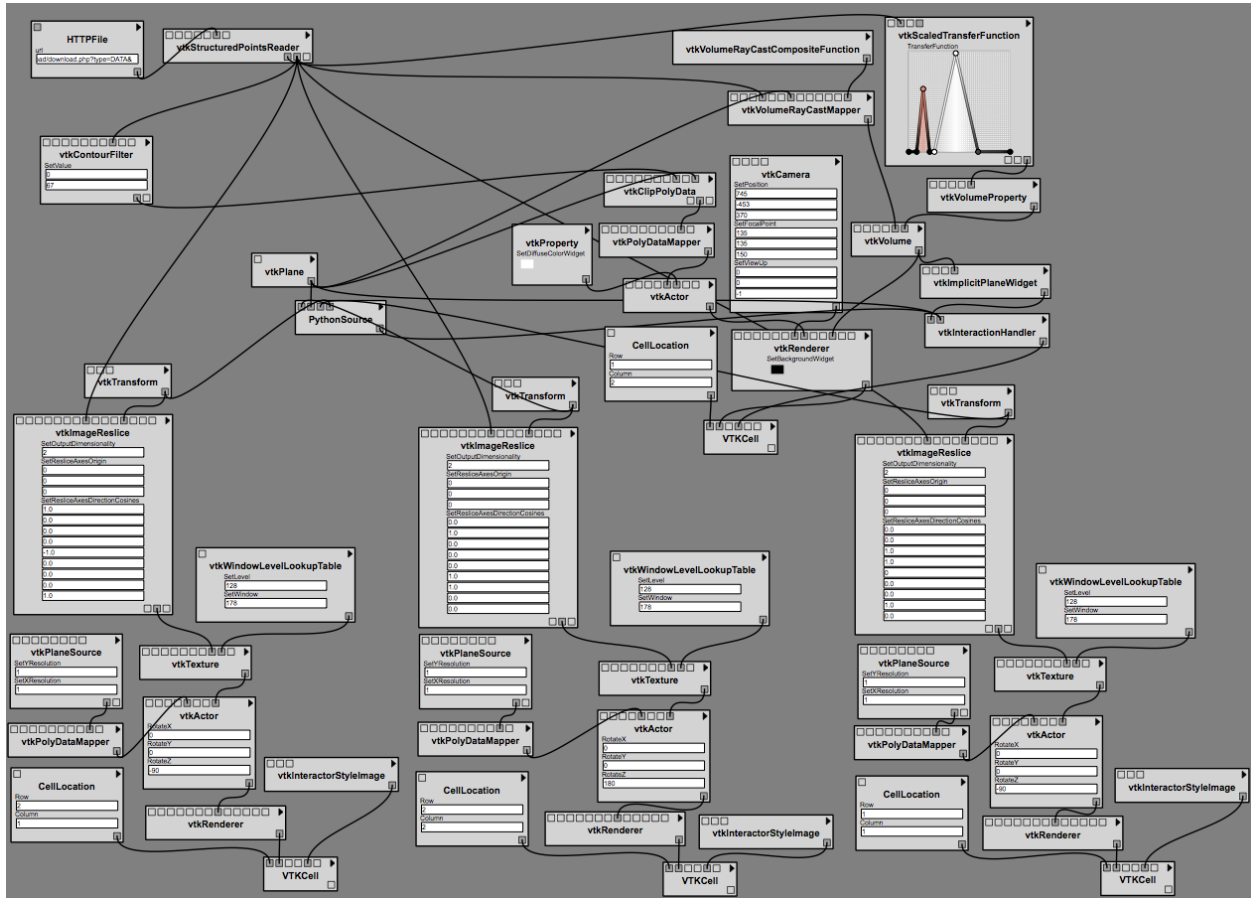


Fig. 4.1: Figure 1 - Complex Workflow with Parameter Widgets.

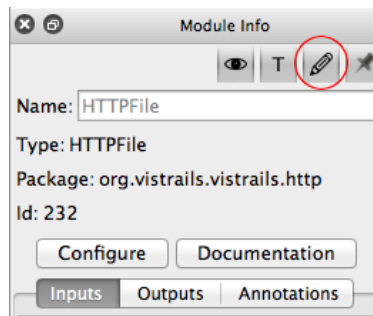


Fig. 4.2: Figure 2 - How to enable/disable the Parameter Widgets mode.

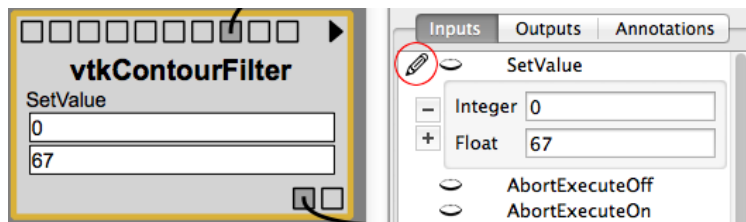


Fig. 4.3: Figure 3 - How to add/remove Parameter Widgets from modules.

4.2 Control Flow in VisTrails

Scientific workflows usually follow a dataflow model, but, in some cases, control structures, including loops and conditionals, are necessary to accomplish certain tasks. VisTrails provides the `Control Flow` package to support these and other structures. To create your own `Control Flow` modules, please refer to the Developer's Guide (*Creating a Control Flow Loop Module*). Or, if you would like to use the Control Flow Assistant, to simplify the process described in this chapter, please refer to *The Control Flow Assistant*.

This package also provides some related modules that operate on lists.

4.2.1 The Map operator

In functional programming, `map` is a high-order function that applies a given function to a list (each element of the list is processed using this function) and returns a sequence of results. The `Map` module provides this functionality for workflows in VisTrails. Note that this module provides simple looping as it can be used to iterate through a list of inputs.

The `Map` module has four input ports:

- “FunctionPort”: this port receives the module (via the “self” output port) that represents the function to be applied for each element of the input list; if the function uses more than one module, you must use a `Group` (see Chapter *Groups and Subworkflows*) or a `SubWorkflow` and connect that composite module to this port;
- “InputPort”: this port receives a list of the names of the input ports that represent the individual arguments of the function;
- “OutputPort”: this port receives the name of the output port that represents the individual result of the function;
- “InputList”: this port receives the input list for the loop; it must be a list of tuples if more than one function input port was chosen.

The output port “Result” produces a list of results, one for each element in the input list.

Try it Now!

To better show how to use the `Map` module, let's use a workflow as an example. Inside the “examples” directory of the VisTrails distribution, open the “triangle_area.vt” vistrail. Now, select the “Surface Area” version. This version basically calculates the area of a given isosurface. We are going to modify this version, in order to calculate the areas of the isosurface given by contour values in a list. Then, we will create a 2D plot to show all the areas.

Begin by deleting the `StandardOutput` modules, and the connection between the `vtkDataSetReader` and the `vtkContourFilter` modules. Then, drag the following modules to the canvas:

- `Map`
- `CartesianProduct`
- `List` (under “Basic Modules”)
- `MplSource` (under “matplotlib”)
- `MplFigure` (under “matplotlib”)
- `MplFigureCell` (under “matplotlib”)
- `InputPort` (under “Basic Modules”) - you will need two of them
- `OutputPort` (under “Basic Modules”)
- `PythonSource` (under “Basic Modules”)

Notice that when you drag `Map` to the pipeline canvas it will be drawn in a different shape from the other modules. This is a visual cue to help distinguish control modules from other modules. All control modules have the same shape.

Next Step!

Select the `vtkContourFilter` module and delete its method “SetValue” in the `Module Information` tab. Then, make this port visible by clicking on the first column left of its name in the “inputs” tab to toggle the eye icon..

Connect the modules as shown in Figure *Connecting a subset of the modules to be grouped as a SubWorkflow*.

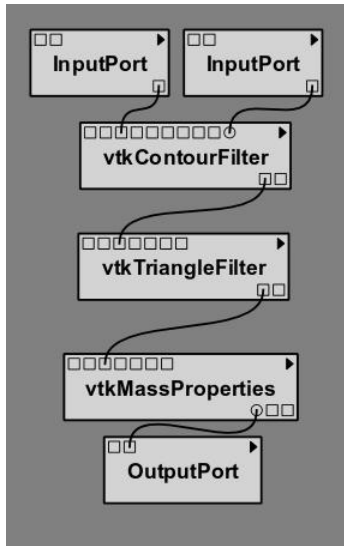


Fig. 4.4: Connecting a subset of the modules to be grouped as a SubWorkflow

These modules represent the function we wish to map: each element of the input list will be processed using them. Because we have more than one module, we need to create a `Group` or a `SubWorkflow` to identify the entire function. The `InputPort` and the `OutputPort` modules are necessary to expose these ports in the `Group/SubWorkflow` structure.

Next Step!

In this example, we will use a `SubWorkflow` structure. Select all the modules shown in Figure *Connecting a subset of the modules to be grouped as a SubWorkflow*, go to the `Workflow` menu, and then click on `Create SubWorkflow`. You can name it `CalculateArea`. Enable the self output port in the ‘outputs’ panel: you will need it to connect to the “Map” module

Note

When using `Map`, the module (or subworkflow) used as function port in the map module **MUST** be a function, i.e., it can only define 1 output port.

Next Step!

Now, select the `MplSource` module and open its configuration dialog. Inside it, add two input ports of type `List`: “`InputList`” and “`X_Values`”. Also, copy the code listed below, in order to create the necessary information for the 2D plot, into the source text area and save your changes.

```

subplot (212)

dashes = [1, 3]
xaxis = []

for i in xrange(len(InputList)):
    xaxis.append(X_Values[i][1])

l, = plot(xaxis, InputList, marker="o", markerfacecolor="red",
          markersize=7, label="IsoSurface Areas", linewidth=1.5)

l.set_dashes(dashes)

```

Next Step!

Next, edit the `PythonSource` module by adding an output port “result” of type `List`, copying the following code to the source text area, and saving these changes. The code will create a range of contour values that we will use as our input list.

```

result = []

for i in xrange(4, 256, 4):
    result.append(i)

```

Next Step!

It may be helpful to identify this `PythonSource` module by labeling it as `RangeList`. Connect all the modules as shown in Figure *All the modules connected in the canvas*.

Next Step!

You will set some parameters now:

- `DownloadFile`: set the parameter “url” to <http://www.sci.utah.edu/~cscheid/stuff/head.120.vtk>
- `List`: set the parameter “value” to `[0]`
- `Map`: set the parameter “InputPort” to `["SetValue"]` and the parameter “OutputPort” to `GetSurfaceArea`

The workflow is now ready to be executed. When you execute the workflow, you will see the `SubWorkflow CalculateArea` executing several times (one time for each value of the input list). It’s important to notice that, although only the module connected to `Map` (in this example, the `SubWorkflow Calculate Area`) will be in the loop, the modules above it will be also used in each loop iteration; the difference is that they are going to be executed only for the first iteration; in all other iterations, the results will be taken from the cache.

When the workflow finishes its execution, the VisTrails Spreadsheet will contain a 2D plot (Figure *The result in the VisTrails Spreadsheet*).

This example can be found in the version “Surface Area with Map”, inside the `triangle_area.vt` vistrail.

4.2.2 Filtering results

When computing large lists of results, it can be useful to selectively reduce the list during execution to avoid unnecessary computation.

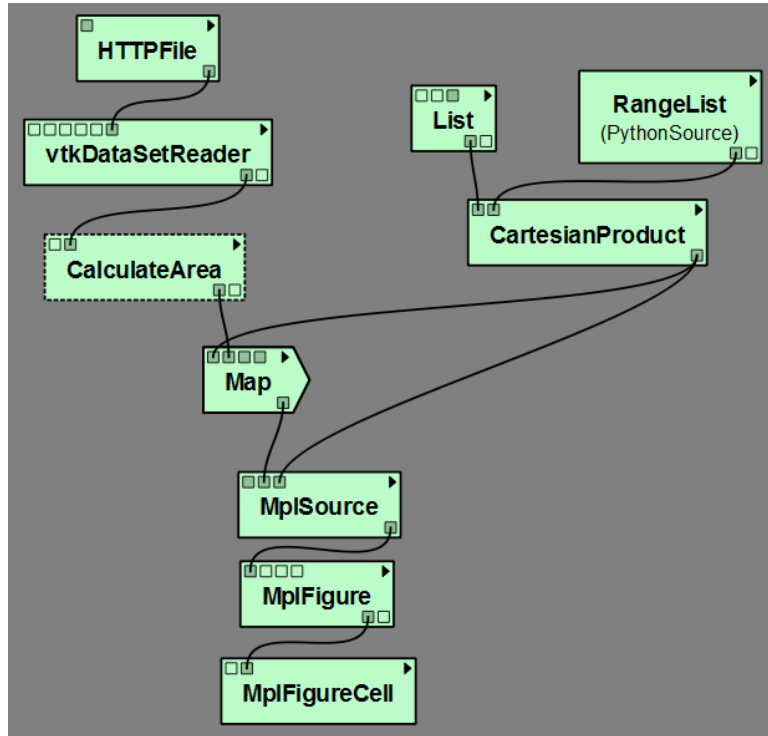


Fig. 4.5: All the modules connected in the canvas

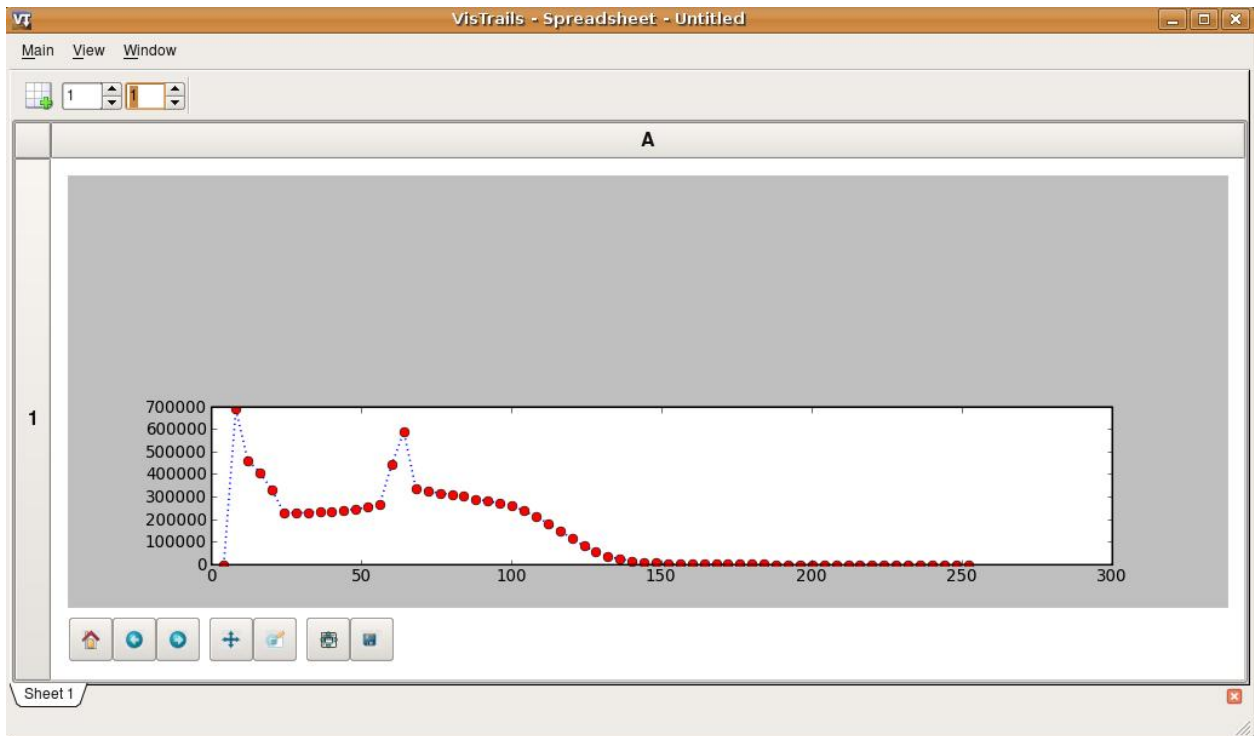


Fig. 4.6: The result in the VisTrails Spreadsheet

The `Filter` module was developed to address this issue. It receives an input list and, based on a specified boolean condition, returns only elements of the list that satisfy the condition. Its ports are the same as those in the `Map` module. The difference between these modules is related to the function module: in `Filter`, the output of that module is not the value to keep, but a boolean indicating whether to keep (`True`) or discard (`False`) the value from the original list.

Try it Now!

To better understand how `Filter` works, let's modify our earlier example to filter out areas less than 200,000. With the previous vistrail open (you can use the "Surface Area with Map" version), add the following modules to the canvas:

- `Filter`
- `PythonSource` (under "Basic Modules")

Edit the configuration of `PythonSource` by adding an input port of type `Float` named "Area", and an output port of type `Boolean` named "Condition", and writing the following code inside the source text area:

```
if Area > 200000.00:
    Condition = True
else:
    Condition = False
```

Next Step!

Press the OK button. You can label this `PythonSource` as `FilterCondition`. Now, reorganize the modules in the canvas as shown in Figure *The new organization of the modules in the canvas*.

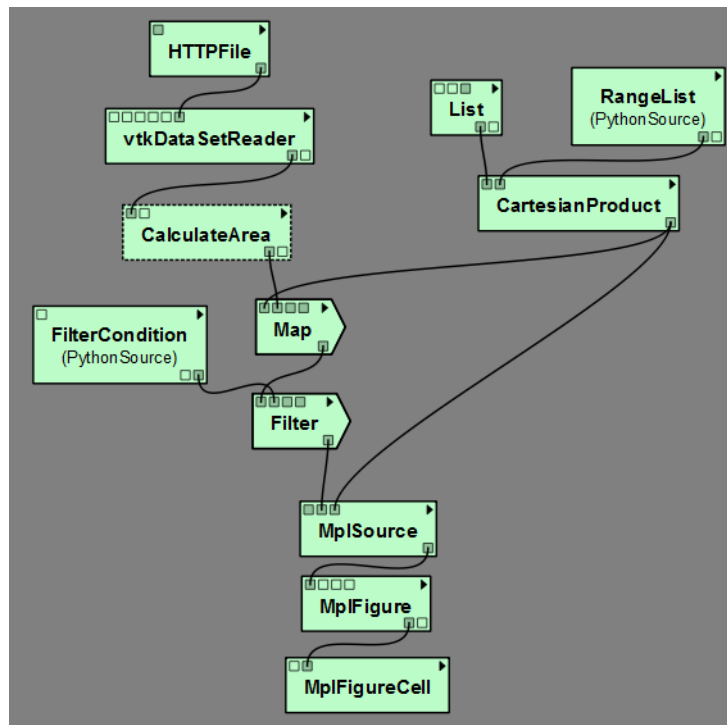


Fig. 4.7: The new organization of the modules in the canvas

Next Step!

Select the `Filter` module and set the values of its parameters to the following:

- “InputPort”: [`Area`]
- “OutputPort”: `Condition`

When you execute this workflow, it will generate another plot that is similar to the one from the `Map` example, but only areas above 200,000 are considered (Figure *The result in the VisTrails spreadsheet*).

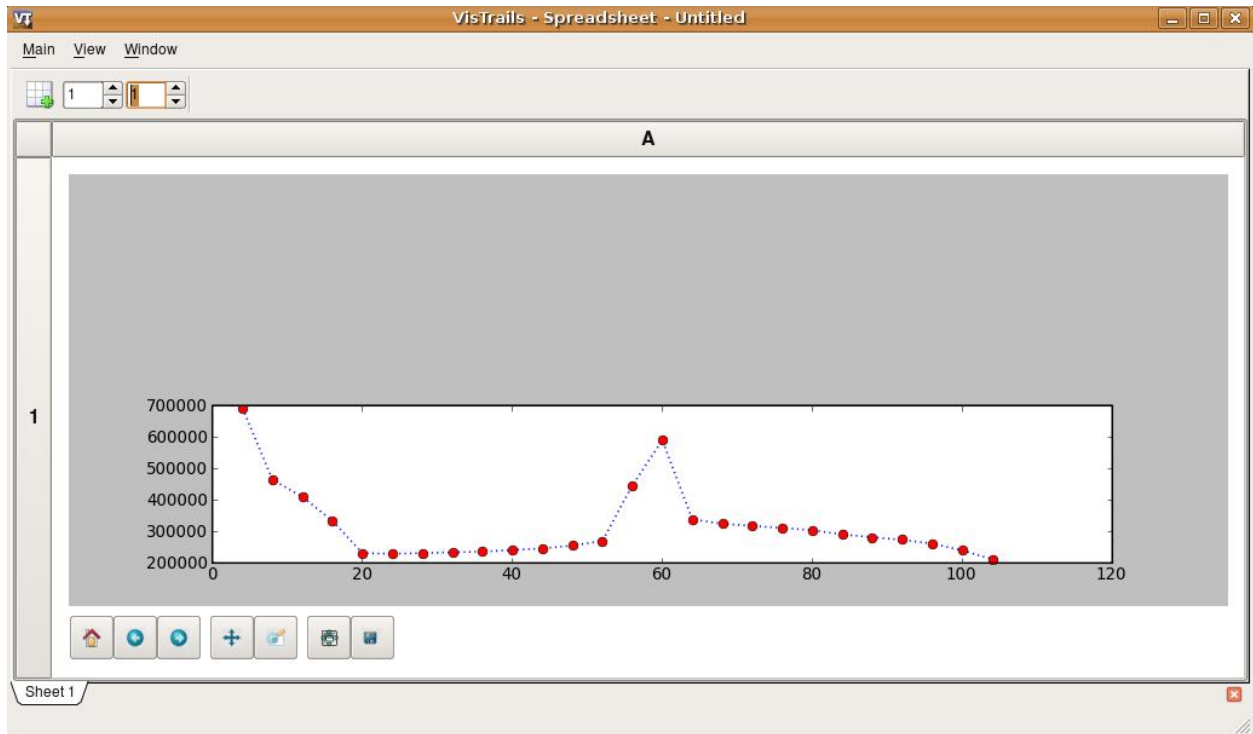


Fig. 4.8: The result in the VisTrails spreadsheet

This example is already inside the `triangle_area.vt` vistrail, in the “Surface Area with Map and Filter” version.

Later in this chapter, you will see how to combine `Map` and `Filter` in one single module, by creating your own control structure.

4.2.3 Conditional module

Conditional statements are a very important control flow structure frequently used in programming languages, and the `if` structure is probably the most common of these structures. In scientific workflows, for example, an `if` structure can be used to select the part of the pipeline to be executed based on a boolean condition.

For this reason, the `Control Flow` package also includes an `If` module. Its input ports are:

- “Condition”: this port receives a boolean value that will specify the direction of computation;
- “TruePort”: this port receives the part of the workflow that will be executed if the condition value is `True`; you don’t need to group or make a `SubWorkflow` in this case: just connect the output port “self” of the last module in this port;

- “FalsePort”: this port receives the part of the workflow that will be executed if the condition value is `False`; as with the
- “TruePort” port, you don’t need to group or make a `SubWorkflow`;
- “TrueOutputPorts”: this port receives a list that contains the names of the output ports of the module connected to “TruePort” that you want the result of; this port is optional;
- “FalseOutputPorts”: this port receives a list that contains the names of the output ports of the module connected to “FalsePort” that you want the result of; this port is optional.

The `If` module has an output port named “Result” that returns a list with the results of the specified output ports of “TrueOutputPorts” or “FalseOutputPorts”, depending on the condition value. If only one output port is chosen, the result of this port will not be returned in a list. If “TrueOutputPorts” or “FalseOutputPorts” are not enabled, “Result” returns `None`.

Let’s do a simple example to show how this module works.

Try it Now!

Our example will contain 2 different text strings. The string that is used by the workflow will depend on the condition of the `If` module. The final text will be rendered in a spreadsheet cell. You can change the final text by changing the condition on the `If` module. Create a new workflow and add the following modules:

- `Boolean` (under “Basic Modules”)
- `String` (under “Basic Modules”) - you will need two of them
- `If` (under “Control Flow”)
- `WriteFile` (under “Basic Modules”)
- `RichTextCell` (under “VisTrails Spreadsheet”)

Name the `Boolean` module “Condition”, the first `String` module “True Branch”, and the second `String` module “False Branch”. Connect the modules as shown in Figure *Simple If example*. The `Condition` should be connected to the “Condition” port on the `If` module and will determine which of the branches that will be executed. `True Branch` should be connected to the “TruePort” on the `If` module and will be executed when the `If` module evaluates to `True`. `False Branch` should be connected to the “FalsePort” on the `If` module and will be executed when the `If` module evaluates to `False`. On the `If` module, set parameters “TrueOutputPorts” and “FalseOutputPorts” to “[value]”. This will tell the `If` module to output the “value” port on the `String` modules. Finally, set the “value” port on the `Condition` module to either `True` or `False`. Execute the workflow and see that the branch specified by the `If` condition has been executed.

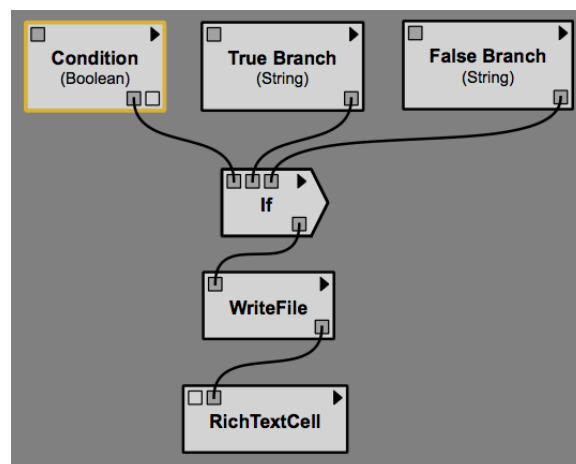


Fig. 4.9: Simple If example

Lets do a more advanced example from the bioinformatics domain. This workflow will take a string as the input. If this string is a structure identifier, a web service from the European Bioinformatics Institute - EBI (<http://www.ebi.ac.uk/>) is used to put the structure into PDB format (a standard representation for macromolecular structure) and the VTK package is used to show the protein in the VisTrails Spreadsheet. Otherwise, the input is assumed to be invalid and a message is generated in the Spreadsheet.

Try it Now!

First, the EBI's web service must be enabled. For this, you need to add the following url to the `wSDLList` configuration:

`http://www.ebi.ac.uk/Tools/webservices/wSDL/WSDbfetch.wSDL`

Don't forget to ensure that the `SudsWebServices` package is enabled in the Preferences dialog. For more information about web services in VisTrails, see Chapter *Example: Web Services*.

Now, you're going to drag the following modules to the canvas:

- If
- `fetchData` (under "Methods" for the current web service)
- `WriteFile` (under "Basic Modules")
- `vtkPDBReader` (under "VTK")
- `vtkDataSetMapper` (under "VTK")
- `vtkActor` (under "VTK")
- `vtkRenderer` (under "VTK")
- `VTKCell` (under "VTK")
- `PythonSource` (under "Basic Modules") - you will need two of them
- `String` (under "Basic Modules")
- `RichTextCell` (under "VisTrails Spreadsheet")

Set some parameters of `fetchData`:

- "format": `pdb`
- "style": `raw`

Next, connect some modules as shown in Figure *Some modules of the workflow connected*.

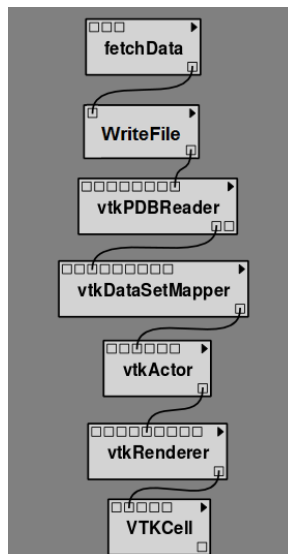


Fig. 4.10: Some modules of the workflow connected

The aim of this group of modules is to get the PDB format of the structure ID, through the web service, and then make the visualization with the VTK package. This is the part of the workflow that will be executed if the input is a structure identifier.

Next Step!

Next, select one of the `PythonSource` modules and open its configuration dialog. One input port named “Structure”, of type `String`, and one output port named “Is_ID”, of type `Boolean`, must be added, as well as the code below:

```

1  if "\n" in Structure:
2      lineLen = Structure.index("\n")
3  else:
4      lineLen = -1
5  if lineLen < 1:
6      lineLen = len(Structure)
7
8  if ":" in Structure:
9      index = Structure.index(":")
10 else:
11     index = -1
12
13 if Structure[0] != "ID " and index > 0 and index < lineLen:
14     Is_ID = True
15 else:
16     Is_ID = False

```

Next Step!

Name this module as `Is_ID`. This module will be the condition for the `If` structure. Now, select the last `PythonSource` module, and, inside its configuration, add one input port of type `String`, named “Input”, and one output port of type `File`, named “html”. Then, copy the code below:

```

1  output = self.interpreter.filePool.create_file()
2  f = open(str(output.name), 'w')
3  text = '<HTML><TITLE>Protein Visualization</TITLE><BODY BGCOLOR="#FFFFFF">'
4  f.write(text)
5  text = '<H2>Protein Visualization Workflow</H2>'
6  f.write(text)
7  text = '<H3>The following input is not an ID from a protein:</H3>'
8  text += '<H4>' + Input + '</H4>'
9  text += '<H3>The visualization cannot be done.</H3>'
10 f.write(text)
11
12 text = '</BODY></HTML>'
13 f.write(text)
14
15 self.set_output('html', f)
16
17 f.close()

```

Next Step!

Name this `PythonSource` as `Not_ID`. This module will print a message in the VisTrails Spreadsheet when the input is not a structure identifier.

Finally, the `String` module can be named as `Workflow_Input`, to make it clear that it takes the input of the workflow. Also, open the configuration dialog of `RichTextCell` to enable the output port “self”, so it can be connected to the `If` module. Then, connect all the modules as shown in Figure *All the modules connected*.

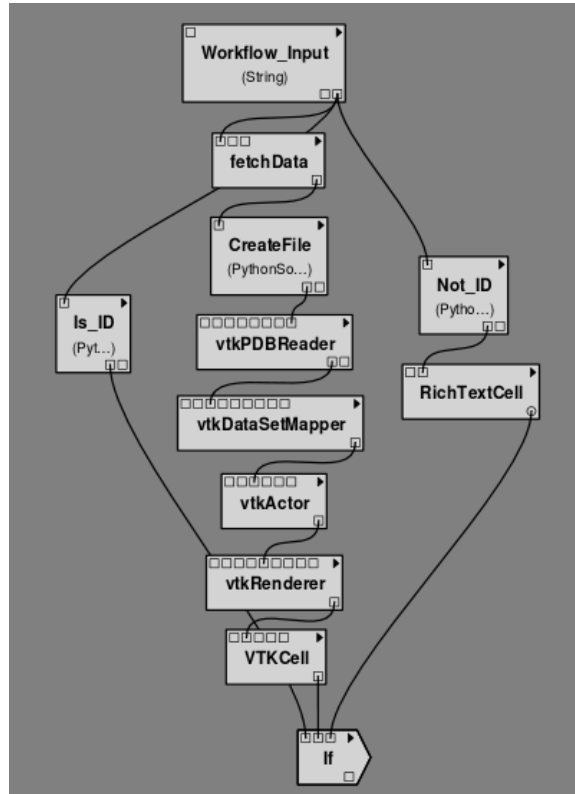


Fig. 4.11: All the modules connected

Next Step!

In order to better organize the disposal of the modules, group all the modules shown in Figure *Some modules of the workflow connected* by selecting them, going to the Edit menu and clicking on Group. Name it as `Generate_Visualization`. Your workflow must correspond to the one shown in Figure *The final workflow, using the Group structure*.

Note that this implementation follows exactly the initial specification of the workflow. If the input is a structure identifier (`Is_ID` returns `True`), `Generate_Visualization` will be executed; otherwise (`Is_ID` returns `False`), `Not_ID` and `RichTextCell` will create an error message in the VisTrails Spreadsheet.

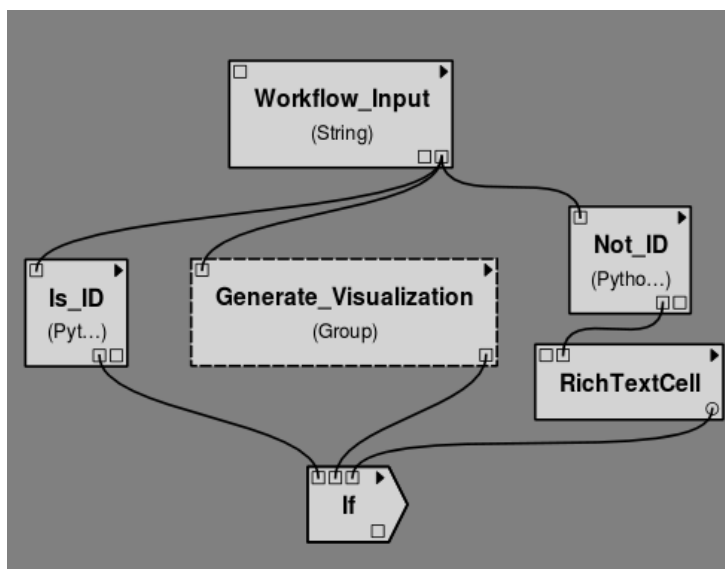


Fig. 4.12: The final workflow, using the Group structure

Next Step!

For the workflow execution, set the parameter “value” of the `Workflow_Input` module to `PDB:3BG0`. This entry is an ID from a protein; so, the condition will be `True`, and the `Generate_Visualization` group will be executed, generating the visualization shown in Figure *The visualization of the protein in the VisTrails Spreadsheet*.

If you change the value from the input port “value” to `protein`, for example, the condition will be `False`, and the message shown in Figure *The message in the Spreadsheet, generated when the input is not a structure ID* will be generated in the Spreadsheet.

This example can be found inside the “examples” directory, in the `protein_visualization.vt` vistrail. It was partially based on the workflow “Structure_or_ID”, which can be found at <http://www.myexperiment.org/workflows/225>.

4.2.4 While loop

The while loop is a common construct of programming languages, allowing the repetition of an operation until some condition becomes true.

It runs a single module (possibly a Group or Subworkflow) whose `self` output port is connected to the `FunctionPort` input of the `While` module (just like the `Map` module). It gets the value of the ports whose name are set on the `ConditionPort`, `OutputPort` and `StateOutputPorts`. As long as the port designated by `ConditionPort` does not return true, the module is run again, with on its `StateInputPorts` the values that were output on the `StateOutputPorts` in the previous run.

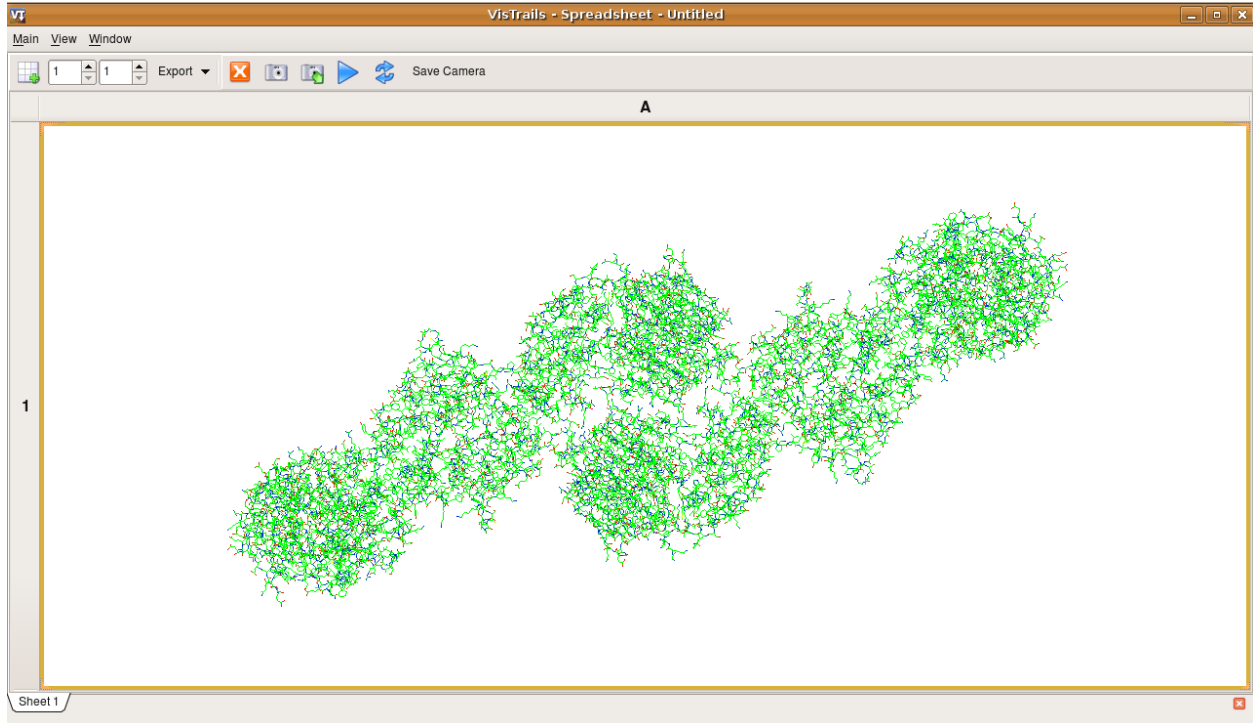


Fig. 4.13: The visualization of the protein in the VisTrails Spreadsheet

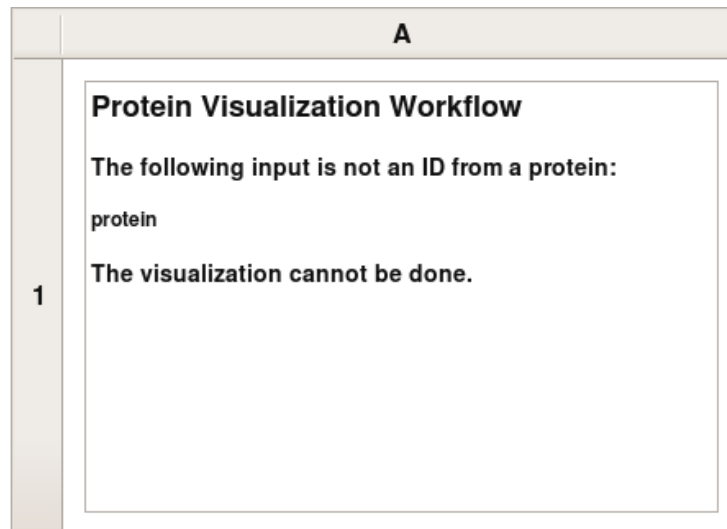


Fig. 4.14: The message in the Spreadsheet, generated when the input is not a structure ID

Try it Now!

In this example, we are going to compute the GCD of two integers using Euclid's algorithm. Keep in mind that VisTrails is meant for data-oriented workflows and that we are twisting its execution model a little, but this will demonstrate the functionality should you actually need it.

Note that you can find the completed example here: [gcd.vt](#).

The modules we are going to need are:

- And
- InputPort (under "Basic Modules")
- List (under "Basic Modules")
- PythonSource (under "Basic Modules")
- 3 OutputPort (under "Basic Modules")
- 2 Tuple and one Untuple (under "Basic Modules")
- 2 PythonCalc (under "PythonCalc")
- 2 If

The structure is a little complicated and comports 4 parts (see Figure *The grouped pipeline for Euclid's algorithm*):

- (I) compares a and b, and outputs the biggest one as 'result'
- (II) makes the (a, b-a) Tuple (if a < b)
- (III) is like (II) but makes (a-b, b) (if a >= b)
- (IV) sets the 'continue' port, if both a and b are not null.

The Integer modules marked 'a' and 'b' are only here to make the workflow clearer, they simply repeat the values from Untuple.

Next Step!

The PythonCalc are substractions (operation '-').

The PythonSource has two Integer inputs a and b, and a Boolean o output; the code should be `o = a < b`

The Tuple and Untuple modules have two Integer ports each.

You will need to use the List module's configuration widget to add one additional port, so you can connect a and b to the head and item0 ports.

The If modules each have ['value'] for both FalseOutputPorts and TrueOutputPorts.

Next Step!

Set names on the InputPort and OutputPort modules. For example, you can use nbs for the InputPort and (from left to right) state, result and continue for the OutputPort.

Once this is done, you can simply select everything and Workflow/Group. Then, add a While module, fill in the port names, and set the nbs port of the Group to 15 and 6 (or any couple of integers). Also add a StandardOutput module to display the result.

4.2.5 For loop

The For module is very similar to Map, except that it uses input values from a range. It can be used to make a module or group run several times with successive integer input, or just to repeatedly execute a task (optionally waiting between each iteration).

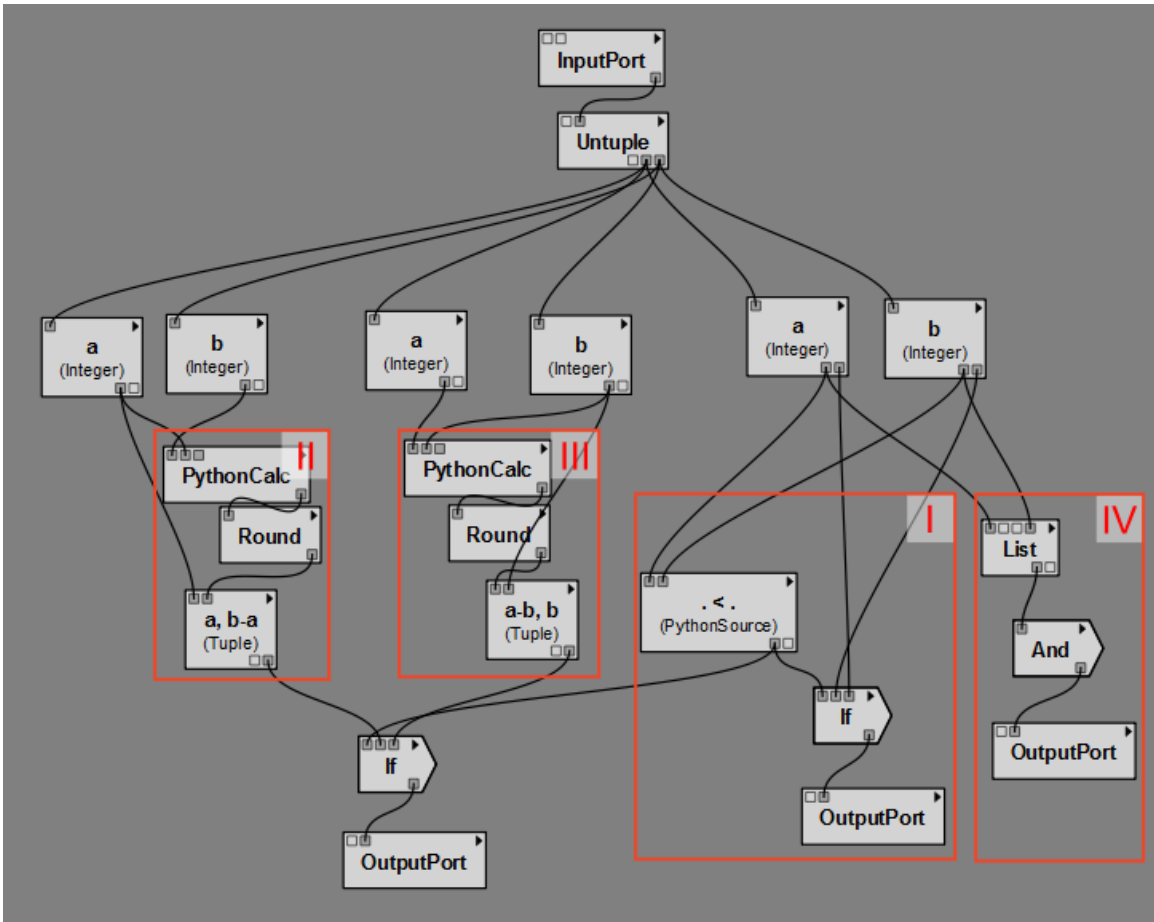


Fig. 4.15: The grouped pipeline for Euclid's algorithm

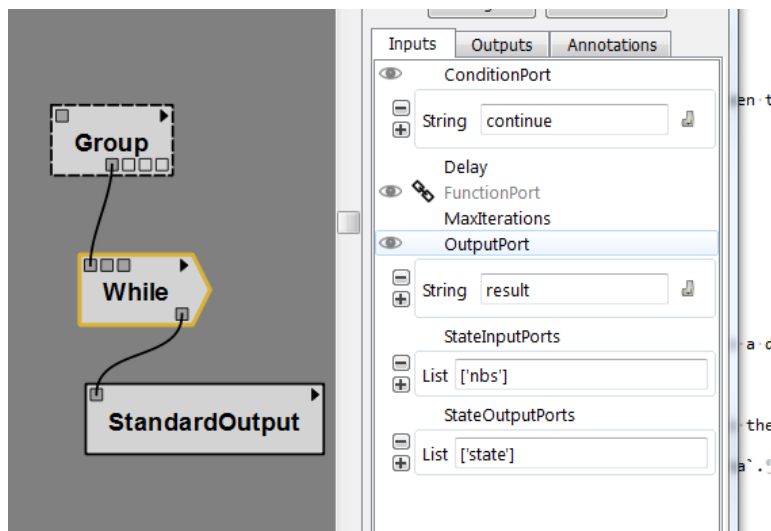


Fig. 4.16: The final pipeline

4.2.6 Boolean operations

The `And` and `Or` modules are simple boolean operations. They take a list of booleans and output a single boolean. They are useful when building workflows with structures that need booleans, such as the `Filter`, `While` and `If` modules.

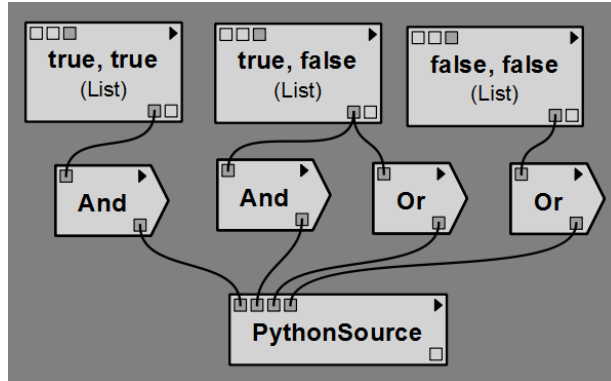


Fig. 4.17: Example usage of And and Or modules; outputs (True, False, True, False)

4.2.7 Vector operations

This packages also provides some general modules for lists, or vectors of numbers.

The `Sum` module computes the sum of the elements in a list of numbers. Example: `Sum([1, 2, 3]) = 6`

The `Cross` module takes two 3-element lists and computes the cross product of these vectors. It returns a 3-element list as well. Example: `Cross([1, 2, -1], [0, 2, 5]) = [12, -5, 2]`

The `Dot` module performs the dot product of two lists, i.e. returns the sum of the pairwise products of the two lists' elements. It is the same thing as connecting an `ElementwiseProduct` to a `Sum` module. Example: `Dot([2, 0, -1], [4, 2, 3]) = 5`

If `NumericalProduct` is `true` (the default), the `ElementwiseProduct` module outputs a list where each element is the product of the elements of both input lists. Example: `ElementwiseProduct([1, 2, 3], [2, 0, -1]) = [2, 0, -3]`

Else, the elements are concatenated instead of multiplied. Example: `ElementwiseProduct([1, 2, 3], [2, 0, -1]) = [(1, 2), (2, 0), (3, -1)]`

4.3 The Control Flow Assistant

4.3.1 Using the Control Flow Assistant (CFA)

In order to simplify the process of creating a control flow loop that uses the `Map` module, VisTrails has a Control Flow Assistant (CFA). To use the CFA, you must:

1. Enable all ports (in the Module Information panel) that you wish to use as inputs or outputs.
2. Select the modules in the workflow that will form the basis of your mapped input-output loop.
3. Go to 'Edit->Control Flow Assistant' to launch the CFA using the selected modules.
4. Select the input ports that you wish to loop over using List modules as input.

5. Select the output port that you wish to use for the values in the output List.
6. Click OK, and the CFA will generate the control flow structure as a Group module.
7. Connect a List input to each of the inputs on the control flow Group.
8. Connect the Group's output List (output port 'Result') to a suitable module/port, or create a PythonSource module to handle the List output.

Note: All existing connections to input and output ports selected in steps 4 and 5 will be removed.

List Input

By default, the List inputs will be used sequentially, one from each List, which requires that all List inputs be the same length. As another option, the Group created by the CFA has a boolean 'UseCartesianProduct' parameter. If this parameter is set to 'true' then the cartesian product of all of the input Lists will be used as the input for the Map. Use caution when using this parameter, as the number of inputs can grow very rapidly with just a few List inputs.

List Output

There are several ways to handle the output List. One option would be to send the output List to a StandardOutput module to display its contents. Another option is to simply ignore the output List, in the case where you just want part of the workflow to execute multiple times using different inputs. For example, if the mapped portion of the workflow contains a VTKCell, and you just want to generate a new VTKCell for each input, you should select the 'self' port of the VTKCell module when choosing the output port in the CFA, and then ignore the output List. For more specialized handling of the output List, you may wish to create a PythonSource module.

Custom List

For advanced users, the default behavior, or cartesian product behavior may not be sufficient for your needs. If this is the case, the 'UserDefinedInputList' parameter allows you to manually specify the input list. If this parameter is defined, it will override any input lists already defined or connected. The format for this user-provided input list must be a list of lists of tuples. Each inner list represents a single loop execution, and contains tuples (or single values for functions taking only one argument) representing the arguments for each input function to be used in that loop execution. The order of the argument tuples in the inner lists should match the order in which the functions appear on the module generated by the CFA.

For example, if the loop has two input functions defined, in order, as SetXY(x, y) and SetZ(z), and we want two executions of the loop, the input list would be: `[[x1, y1], z1], [(x2, y2), z2]]`

Parameter Exploration

One useful purpose for the CFA is to provide a version-based approach to parameter exploration. To create a parameter exploration for a workflow, you could simply select all modules in the workflow, making sure the ports for the desired parameters are enabled, then launch the CFA and select the ports of the parameters you wish to explore. By providing a list for each parameter, you can create a parameter exploration that directly uses the version tree.

Try it Now!

Processing a List of values with PythonCalc:

1. Go to 'Edit->Preferences', select the 'Module Packages' tab, and enable the 'pythonCalc' package if it is not already enabled.
2. Click on File->New to start a new VisTrail.
3. Add the following modules from the module registry to the VisTrail: a) One 'PythonCalc' module from the 'pythonCalc' package b) One 'List' module from the 'Basic Modules' package c) One 'StandardOutput' module from the 'Basic Modules' package
4. Set the List 'value' parameter to: [1.0, 2.0, 3.0, 4.0, 5.0]
5. Set the PythonCalc 'op' parameter to: '*'
6. Set the PythonCalc 'value2' parameter to: 2.0
7. With the PythonCalc module selected, go to 'Edit->Control Flow Assistant' (see Figure [Example 1.1](#)):
 - (a) Click on the input port 'value1' and ensure it is highlighted
 - (b) Click on the output port 'value' and ensure it is highlighted
 - (c) Click 'OK' to close the window and build the loop structure as a Group module (see Figure [Example 1.2](#))
8. Connect the 'List' module's output port 'value' to the 'Group' module's input port 'value1'.
9. Connect the 'Group' module's output port 'Result' to the 'StandardOutput' module's input port 'value' (see Figure [Example 1.3](#))
10. Execute the current workflow.
11. In your Standard Output console, you should see a List containing the computation for each element in the input list: [2.0, 4.0, 6.0, 8.0, 10.0] ([Open result](#))

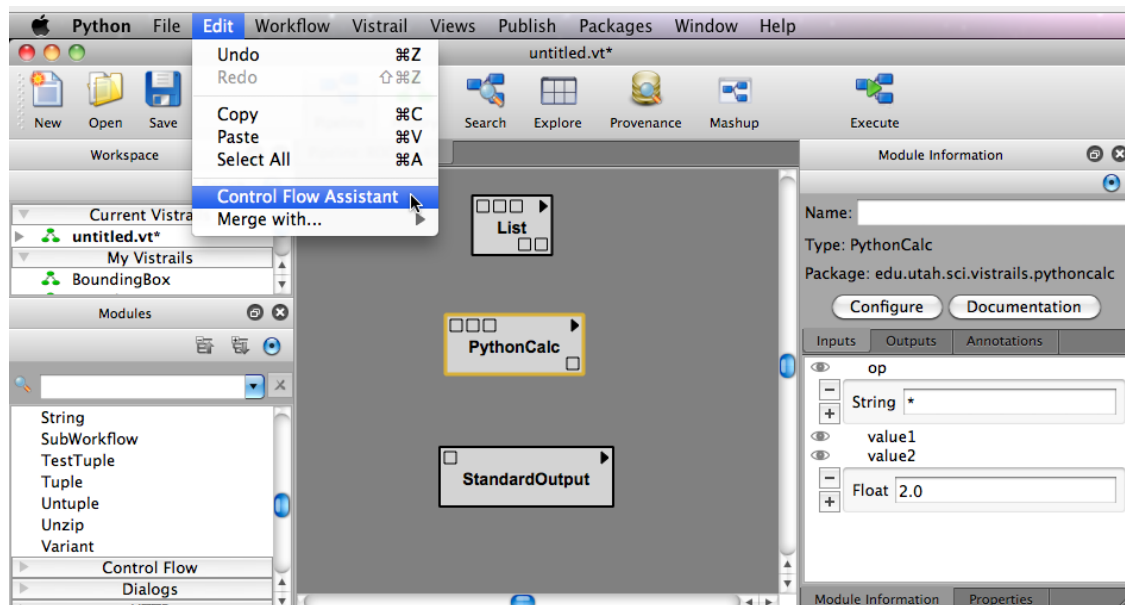


Fig. 4.18: Example 1.1 - Running the Control Flow Assistant

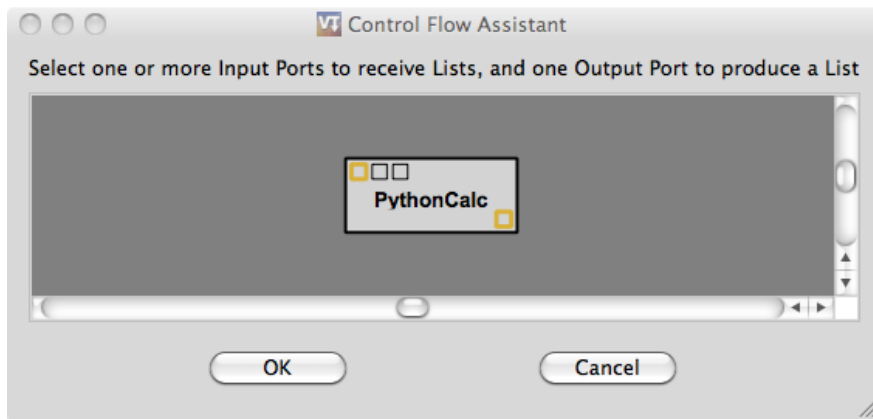


Fig. 4.19: Example 1.2 - Selecting relevant ports.

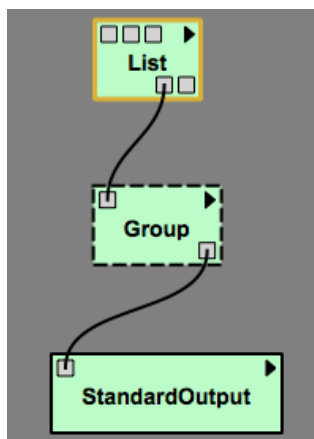


Fig. 4.20: Example 1.3 - The connected pipeline.

Try it Now!

Performing a Parameter Exploration:

1. Go to 'File->Open', explore to the VisTrails examples folder, and open `spx.vt`.
2. Open the History view and select the version tagged as 'decimate'.
3. Open the Pipeline view.
4. Select the 'vtkContourFilter' module and enable the 'SetValue' input port by clicking to the left of 'Set-Value' in the Module Information panel (see Figure [Example 2.1](#)).
5. Click on 'Edit->Select All'.
6. With all modules selected, go to 'Edit->Control Flow Assistant':
 - (a) Click on the 'vtkContourFilter' module's input port 'SetValue' and ensure it is highlighted
 - (b) Click on the 'VTKCell' module's output port 'self' and ensure it is highlighted (see Figure [Example 2.2](#))
 - (c) Click 'OK' to close the window and build the loop structure as a Group module
7. Select the newly created 'Group' module, and set the 'SetValue' parameter to: [(0, 0.5), (0, 0.75), (0, 1.0)]
8. Execute the current workflow.
9. In your VisTrails Spreadsheet, you should see three visualizations, one for each set of input parameters to the 'SetValue' port of 'vtkContourFilter' (see Figure [Example 2.3](#)). (Open result)

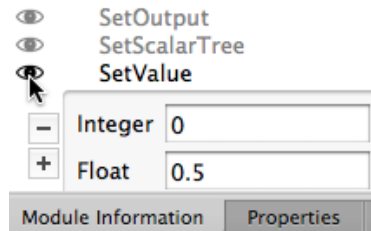


Fig. 4.21: Example 2.1 - Enabling a port for use with the control flow assistant.

4.4 List Handling in VisTrails

In VisTrails you can pass typed and *untyped* lists between modules. Ports on modules have a depth parameter specifying the list depth it supports. 0 means no list, 1 is a list, 2 is a list of lists etc. Port depth can be specified either by module developers or by using a `PythonSource` or similar module.

It is important to know how connections of mismatching list depths are handled:

- **List wrapping** - If the destination port has a larger list depth, the source will be wrapped in lists until the list depth is matched.
- **Iterating over lists** - If the source port has a larger list depth, the destination module will be executed once for each element in the list.

4.4.1 The List type

The `List` type represents an untyped list and can contain a list of any type. The `visitrails Variant` type matches any type and a `List` is equal to a `Variant` of list depth 1. List depth specified on `List` types does not include the `List` itself: A `List` type with list depth 1 are considered a `Variant` with list depth 2.

There is one important exception: `Variant` connects directly to `List`. This is because `Variant` ports are allowed to contain lists.

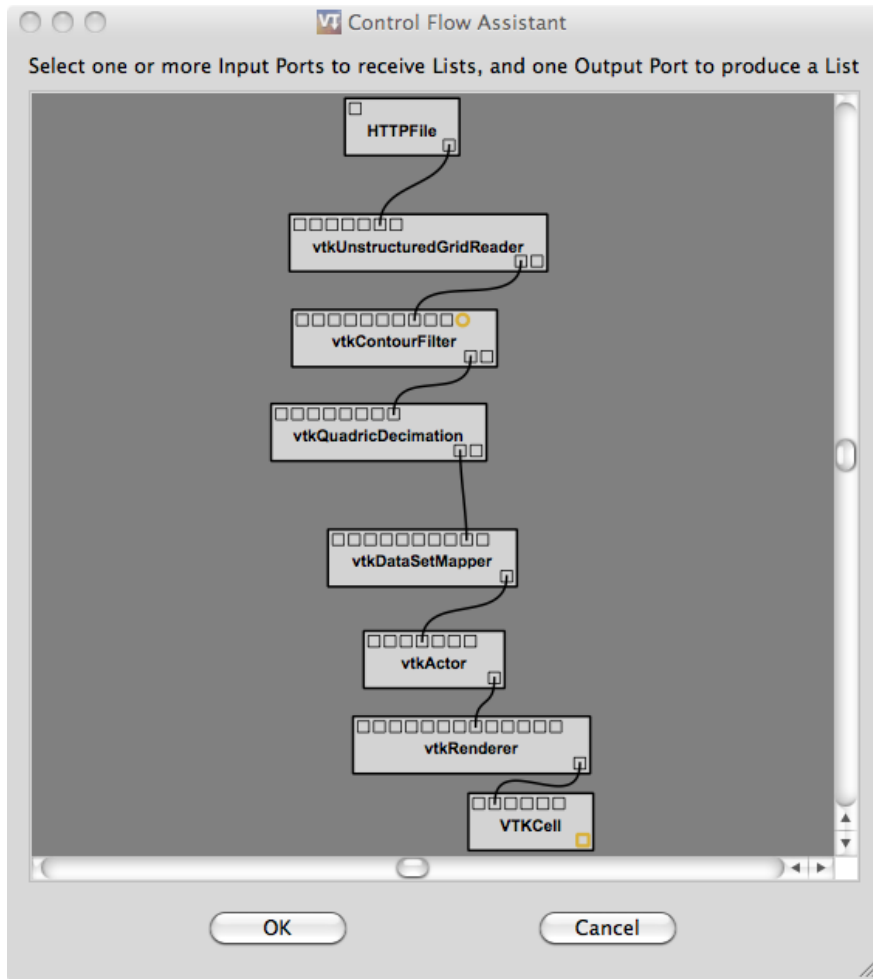


Fig. 4.22: Example 2.2 - Selecting relevant ports.



Fig. 4.23: Example 2.3 - The spreadsheet results using the list: [(0, 0.5), (0, 0.75), (0, 1.0)] as input to the contour filter via the control flow assistant.

4.4.2 Iterating over lists

Passing a list to a module that does not support lists will cause that module to be executed once for each element in the list. When passing lists on multiple input ports, the inputs will be combined. The default combination is cartesian product, where each element in a list is combined with each element in another list. This combination can be changed by selecting “Looping Options” in the module menu. The options are `Cartesian`, `Pairwise` (where the elements are combined pairwise), and `Custom`. `Custom` gives you complete control over how inputs are combined and allows you to use both pairwise/cartesian combiners as well as reordering them. The output of an iterated module will be an ordered list with the individual results of the module execution. This will cause modules downstream to also be iterated over, unless they accept a list as input. Iterated modules will have duplicated connections to show that they are being iterated over. A list of lists will have the connection triplicated etc.

Try it Now!

Lets create a simple example showing how to combine strings. First we will create a module that generates lists of strings. Create a new workflow and add a `PythonSource` module. Give it three output ports named `s1`, `s2`, `s3` of type `String` and set their list depth to 1. Enter this code:

```
s1 = ['A', 'B', 'C']
s2 = ['+', '-', '*']
s3 = ['1', '2', '3']
```

Next Step!

Add a `ConcatenateString` module, connect `s1->str1`, `s2->str2`, `s3->str3`. Notice how the connections going into `ConcatenateString` are duplicated. This indicates that `ConcatenateString` will iterate over the list inputs. Add a `StandardOutput` module and connect `ConcatenateString.value` to `StandardOutput.value`. This connection will be duplicated in both ends, indicating they will both be iterated over. Your workflow should now look like Figure *The complete workflow*.

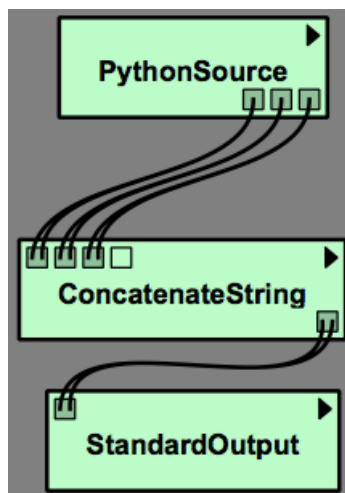


Fig. 4.24: The complete workflow

Next Step!

By default `ConcatenateString` will combine the inputs using cartesian product `["A+1", "A+2", "A+3", "A-1", ...]`. Lets change this. Go to `Module Menu->Looping Options` and click `custom`. Right click in the port list and add a pairwise product. Rearrange the ports so that it looks like Figure *A custom list combiner*.

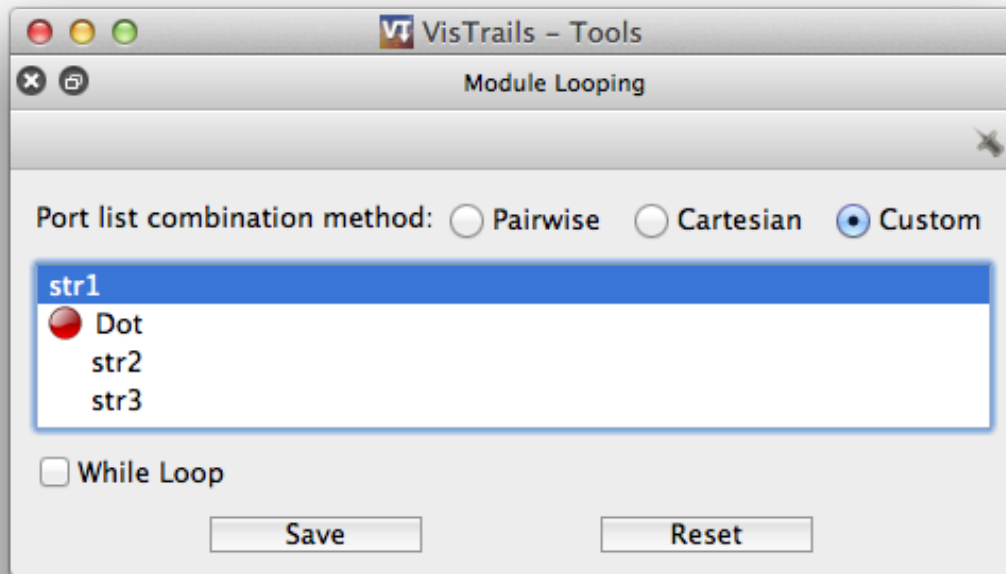


Fig. 4.25: A custom list combiner

Finally:

`str2` and `str3` will now be combined pairwise and then combined with `str1` using cartesian product. Open the `visitrails` console and execute the workflow. You should see this output: ([Open result](#))

```
A+1
A-2
A*3
B+1
B-2
B*3
C+1
C-2
C*3
```

4.5 Streaming in VisTrails

Streaming data may be useful for a number of reasons, such as to incrementally update a visualization, or to process more data than would fit into memory. VisTrails supports streaming data through the workflow. By implementing modules that supports streaming, data items will be passed through the whole workflow one at a time.

4.5.1 Using Streaming

Streaming is similar to list handling (see Chapter *List Handling in VisTrails*). Modules that create streams should output a port with list depth 1. Downstream modules that do not accept lists will be executed once for each item in the stream. Modules with multiple input streams will combine them pairwise. For this reason the input streams should contain the same number of items (or be unlimited).

Modules accepting a type with list depth 1, but not supporting streaming, will see their input collected into a list, and will execute after the streaming has ended.

Try it Now!

Let's use PythonSources to create a simple example that incrementally sums up a sequence of numbers. First we will create a module that streams the natural numbers up to some value. Create a new workflow and add a PythonSource module. Give it an input port named `inputs` of type `Integer`, which will specify the maximum number to stream, and an output port named `out` of type `Integer` with list depth 1, which will be the output stream. An output stream can be created by using `self.set_streaming_output`, which takes the port name, an iterator object, and an optional length of the input items. To create an integer iterator we can use `xrange`. Add this to the PythonSource:

```
self.set_streaming_output('out',
                          iter(xrange(inputs)),
                          inputs)
```

Next Step!

Now let's create a module that processes each item in the sequence. Add a second PythonSource module below the first one. Give it an input port named `integerStream` of type `Integer` and list depth 1 that will be our input stream. An input stream can be captured by adding the magic string `# pragma: streaming` to the PythonSource code and calling `self.set_streaming` with a generator method as argument. The generator method should take the module as an input. It should first initialize its value, in our case set `intsum=0`. Then it should receive the inputs in a loop ending with `yield`. In each iteration the module will be updated to contain a new input in the stream. Similar to a normal module, the loop should:

1. get inputs
2. compute outputs
3. set outputs
4. call `yield`

Below is the complete example. Add it to the PythonSource.

```
# pragma: streaming - This tag is magic, do not change

def generator(module):
    intsum = 0
    while 1:
        i = module.get_input('integerStream')
        intsum += i
```

```
        print "Sum so far:", intsum
        yield

self.set_streaming(generator)
```

Finally:

Connect the two PythonSources, set `inputs` to 100 in the first PythonSource, open the VisTrails console and execute. See how the output is printed to the console while the stream runs and how the progress of the modules increase. The output should look like this: ([open in vistrails](#))

```
Sum so far: 0
Sum so far: 1
Sum so far: 3
...
Sum so far: 4851
Sum so far: 4950
```

4.6 Parallel Flow in VisTrails

When dealing with large datasets, the ability to leverage multiple cores or machines allows to speed up workflow execution time. VisTrails provides support for parallelization of tasks using [IPython](#).

4.6.1 Setting up an IPython cluster

This package uses the standard `IPython.parallel` machinery to execute jobs. You will need to create and configure the IPython profile that you want VisTrails to use.

VisTrails is capable of running the `ipcontroller` and `ipengine` commands for you to start a controller or a set of engines locally, but for more complex setups, you can run `ipcluster` yourself from a terminal with the necessary options.

4.6.2 Interacting with the cluster

In the `Packages/Parallel Flow` menu, you will find the following options:

Start new engine processes Use `ipengine` to start multiple new workers on the machine, using the current IPython profile. These processes will be shutdown on exit, unless detached using `Cleanup`

Show information on the cluster Indicates whether we are connected to an IPython controller, the number of engines in the cluster, and which processes were started locally. Lists some basic information on each engine.

Change profile Selects a different IPython profile. Performs cleanup first if a cluster was connected.

Cleanup started processes Disconnects from the cluster and “forgets” the processes that were started from VisTrails. It is either possible to terminate them, or to leave them running in the background (for example, to be reuse by the next VisTrails session).

Request cluster shutdown Sends the shutdown signal to the controller, regardless of whether it was started locally or not. If accepted, the controller will ask every connected engine to terminate and exit.

Note that when VisTrails is exited, it will shutdown the engines that it started. If it started the controller, it will also be shutdown, along with every engine that might have connected to it from other machines. To prevent that, use the

‘cleanup’ button and choose not to stop them; they will detach from VisTrails and won’t be killed automatically. You will still be able to use the ‘cluster shutdown’ button explicitly.

4.6.3 The Map module

Map allows you to execute a single module or a Group in parallel using input values taken from a list. It works in exactly the same way as the regular Map module from the *Control Flow* package.

Contrary to the standard Map module, the elements of the list will be submitted to the IPython controller which will execute them in a load-balanced manner on the engines currently connected.

4.7 Connecting to a Database

As an environment for collaborative scientific exploration, VisTrails supports both stand-alone, file-based storage and relational storage of vistrails. With a relational database supporting VisTrails, multiple users can easily collaborate on projects without copying files back and forth. At the same time, if you choose to work without being connected to a database, you can save your work locally to files. Finally, VisTrails can import and export to both types of storage so you can import a vistrail from the database, save it locally as a file on your computer, make and save changes, and export those changes back to the database. Remember that because the complete workflow evolution is always saved, other users will not overwrite your changes, and vice versa. This prevents users from “stepping on each other’s feet.”

By default, VisTrails works with local files stored in the “.vt” format (essentially compressed XML). You can save a vistrail as uncompressed XML by saving the file with a “.xml” extension. When saving a vistrail, the system displays a standard save dialog. These files have a version associated with them so when the schema for these files may change, VisTrails will be able to import older versions. The current version of the XML schema can be found in the distribution at:

```
vistrails/db/versions/v1_0_2/schemas/xml/vistrail.xsd
```

where `v1_0_2` is the current version.

4.7.1 Setup

As described earlier, VisTrails supports relational database storage as well as file-based storage. Currently, VisTrails has been tested with MySQL, but in the future, we plan to support most standard relational database systems.

Setting up the database

Before using VisTrails with a relational database, you must have a database installed and have access to create, access, and modify that database. If you are planning to deploy for institution-wide access, you should consult your system administrator to determine the correct configuration. The database schema for VisTrails can be found in the distribution at:

```
vistrails/db/versions/v1_0_2/schemas/sql/vistrails.sql
```

where `v1_0_2` is the current version. This schema contains a sequence of SQL commands that define the tables needed for storing vistrails.

After you or someone else has created the database for the vistrails, you will need the following information:

1. *hostname*: the name or IP address of the machine that stores the database (`localhost` if it is your own machine)
2. *port*: the port number that you connect to the database on

3. *user*: the username that should be used to access and modify the vistrails database
4. *password*: the password for the account corresponding to the given user
5. *database name*: the name of the database where the vistrails are to be stored.

Setting up VisTrails

If you are planning to use the database for most of your work, you can configure VisTrails to open vistrails from the database by default. To do so, select the `Preferences` option from the `Edit` menu. (On Mac OS X, the `Preferences` option is found under the `VisTrails` menu.) When the `Preferences` window opens, select the appropriate option from the “Read/Write to database by default” box in the `General Configuration` tab.

4.7.2 Opening from a database

To open a vistrail from a relational database, choose the `Import` option from the `File` menu. You should see a dialog like the one pictured in Figure *Opening a vistrail from the database*. (Alternatively, if you have set VisTrails to use a relational database by default (see Section *Setting up VisTrails*), then you should select `File` → `Open` from the menu or the `Open` button on the toolbar.)

If you have previously connected to databases using VisTrails, you should see a list of these databases in the left column of the dialog. If not, you will need to add one. To do so, click the `+` icon in the lower-left corner. This will bring up a dialog like that shown in Figure *Creating a new database connection*. To set up a connection, you will need the database connection information outlined in Section *Setting up the database*. After filling in that information, you can test the connection by clicking the `Test` button. If the test succeeds, click the `Create` button to add the database to the available sources for vistrails.

The database you wish to use should now be listed in the left column. Clicking on that row will query the database for a list of vistrails available from the database and display them in the right column. To open a vistrail, select the desired vistrail and click the `Open` button or simply double-click the vistrail. When the vistrail has loaded, you will be able to interact with it in exactly the same way as a vistrail loaded from a file.

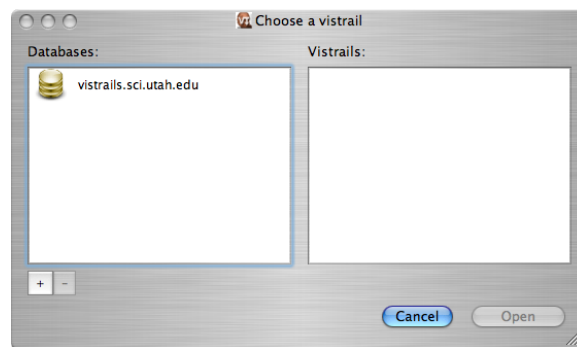


Fig. 4.26: Opening a vistrail from the database

4.7.3 Saving to a database

If you opened a vistrail from the database, the default save action will be to save that vistrail back to the database. There will be no dialogs displayed—the database the vistrail was loaded from will be automatically updated.

If you opened the vistrail from a file, you will need to select either `Save As` or `Export` from the `File` menu, depending on whether VisTrails uses the database by default (see Section *Setting up VisTrails*). You will be shown a

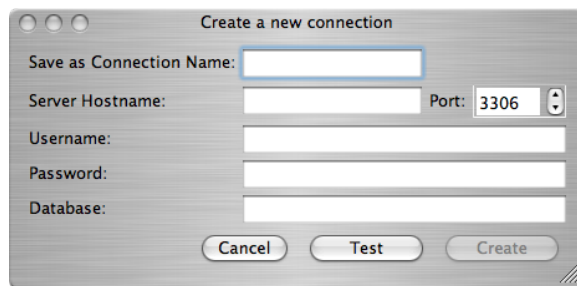


Fig. 4.27: Creating a new database connection

dialog similar to the one in Figure *Saving a vistrail to the database*. As discussed in Section *Opening from a database*, you can create a new connection to the database or use an existing one. Note that the name of the vistrail must differ from those already stored on the database, and clicking the *Save* button will persist the changes to the database.

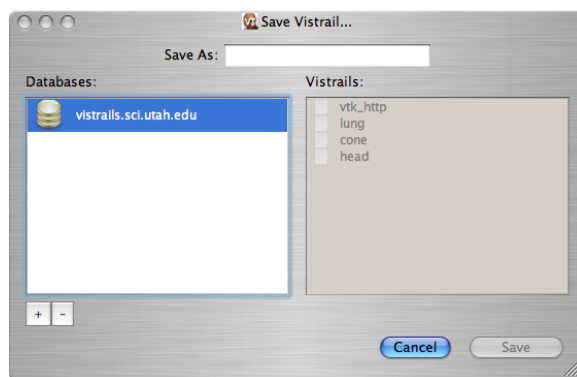


Fig. 4.28: Saving a vistrail to the database

4.7.4 Known Issues

Currently, saving a vistrail to the database will *overwrite* the vistrail currently stored on the database. However, we plan to add synchronization soon so that all explorations are captured. Thus, be aware that if two users have the same vistrail loaded from the database at the same time, and both users save their changes, only the second user's changes will be captured.

4.8 Example: Web Services

A *web service* grants you programmatic access to an online data source via a straightforward API. In this chapter, you will learn how to invoke web services from within VisTrails workflows. We will build a simple workflow that invokes a web service and generates an HTML table with the results. Our current example is intentionally simple; for more in-depth examples, please refer to the VisTrails website.

Where we're going in this chapter: The European Bioinformatics Institute maintains ChEBI,¹ a database of over 15,000 chemical compounds. Each entity is referenced by a unique ID number, called its *chebiID*. To see an example of the kind of queries we will build in this example, go to <http://www.ebi.ac.uk/chebi/webServices.do> and scroll down until you find the web form labeled "getCompleteEntity." (Figure (a) *Web browser interface for the ChEBI database*).

¹ ChEBI is an acronym for Chemical Entities of Biological Interest.

If you type 15357 into the text field, it will return a long string of data in XML format about this chemical. We learn, among other things, that this chemical’s name is *acetylenedicarboxylate(-2)*.

To try another query, scroll down to the area labeled “getOntologyChildren” and type 15357 into the text field. This returns an XML representation of this chemical’s ontology children. In this case, the result is a single chemical, *acetylenedicarboxylate(-1)*, whose chebiID is 30782 (Figure (b) *Results from a “getOntologyChildren” query*).

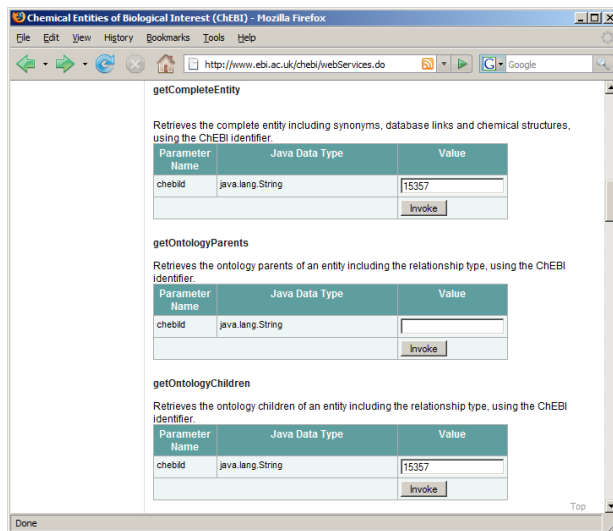


Fig. 4.29: (a) Web browser interface for the ChEBI database

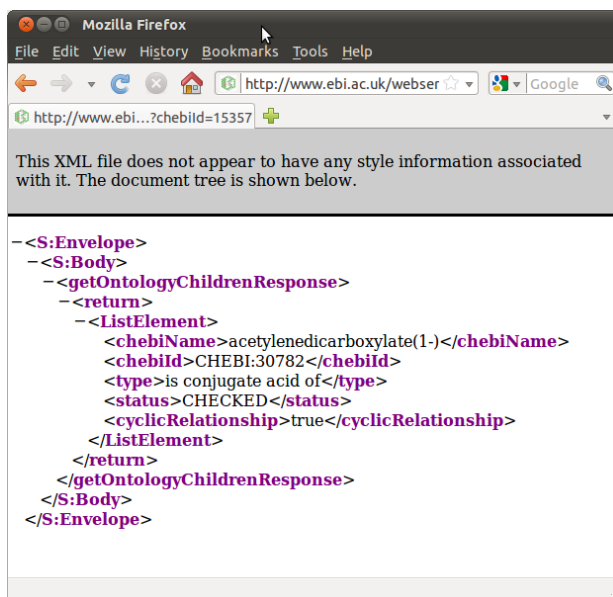


Fig. 4.30: (b) Results from a “getOntologyChildren” query

In this example, we will build a workflow that accesses a web service to perform the second of these two queries. Because we’re using a web service, we don’t need a browser — we will perform this query programmatically within VisTrails.

4.8.1 Enabling the SUDSWebServices Package

In order to use web services in VisTrails, you need to ensure that the `SUDSWebServices` package is enabled in the `Preferences` dialog. (Please refer to Chapter *Writing VisTrails Packages* for more information on enabling packages.)

4.8.2 Adding Web Service Packages

Within the `Module Packages` tab of the `Preferences` dialog, click the `Configure` button to open the configuration dialog for this package (`SUDSWebServices`). Select the `wsdlList` and click on the `Value` field. This is where you will enter the URL(s) of the web service(s) you wish to access. If there is more than one URL, place a semicolon (;) between each URL, but *not* after the final URL. In other words, the URLs must be semicolon-delimited, but not semicolon-terminated.

For our example, we need the following URL:

```
http://www.ebi.ac.uk/webservices/chebi/2.0/webservice?wsdl
```

After closing the dialog, you need to reload the `SUDSWebServices` package in order to load the changes. Then, close the `Preferences` dialog. A new package will be created for each URL provided.

Alternatively, you may add a web service package by clicking the secondary mouse button on the “SUDS Web Services” package in the module palette and entering the corresponding URL. You may remove a web service by clicking the secondary mouse button on the corresponding package in the module palette and selecting `Remove this Web Service`.

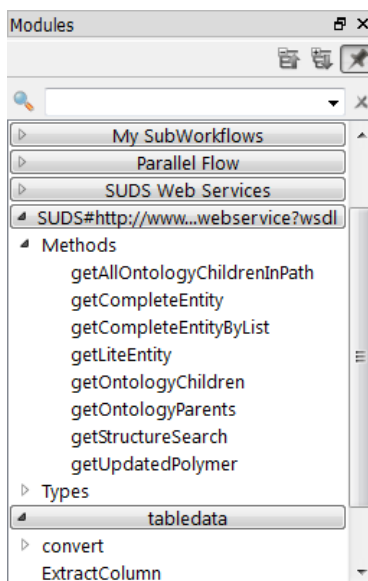


Fig. 4.31: The available modules in the `webServices` module are shown in the `Modules` panel.

4.8.3 Creating a new vistrail

After configuring the `SUDSWebServices` package properly, there will be a `SUDSWebServices` entry in your `Modules` panel. The `SUDSWebServices` package will generate a module for each published method in a web service.

Start with a new empty workflow in the `Pipeline` view, and drag the following modules to the canvas.

- String (under “Basic Modules”)
- getOntologyChildren (under “Methods” for the current web service)
- getOntologyChildrenResponse (under “Types” for the current web service)
- OntologyDataItemList (under “Types” for the current web service)
- PythonSource (under “Basic Modules”)
- RichTextCell (under “Spreadsheet”)

As discussed in Chapter *Creating and Modifying Workflows*, PythonSource has no input and output ports by default; we need to create some. Open the configuration dialog for PythonSource by selecting this module in the pipeline canvas and typing ‘Ctrl-E’. Add a new input port named “ontologyDataItemList” of type List, and a new output port named “outfile” of type File. (Please refer to Chapter *Creating and Modifying Workflows* for more information about configuring and using the PythonSource module.)

We will now add some Python code to this module. This code generates a simple HTML table based on the information retrieved from the web service query. Type or paste the following source code into the PythonSource configuration dialog:

```
dataitemlist = self.get_input("ontologyDataItemList")
output1 = self.interpreter.filePool.create_file()
f1 = open(str(output1.name), "w")
text = "<HTML><TITLE>Chebi WebService</TITLE><BODY BGCOLOR=#FFFFFF>"
f1.write(text)
text = "<H2>getOntologyChildren Query</H2><BR>"
f1.write(text)
text = "<CENTER><table border = 1><tr><TH>ChebiId</TH> <TH>ChebiName</TH>"
text += "<TH>Comments</TH> <TH>Type</TH> <TH>Status</TH>"
text += "<TH>CyclicRelationship</TH></tr>"
f1.write(text)
for element in dataitemlist:
    if not hasattr(element, 'Comments') or str(element.Comments) == '[]':
        comment = ""
    else:
        comment = str(element.Comments)
    line = "<tr><td>" + str(element.chebiId) + "</td><td>" + str(element.chebiName)
    line += "</td><td>" + comment + "</td><td>" + str(element.type) + "</td><td>"
    line += str(element.status) + "</td><td>" + str(element.cyclicRelationship)
    line += "</td></tr>"
    f1.write(line)
text = "</table></CENTER></BODY></HTML>"
f1.write(text)
self.set_output("outfile", output1)
f1.close()
```

Close the dialog. One of the ports we need to use is an optional port. Select the OntologyDataItemList module and select the Outputs tab from the Module Information panel. Click in the left column next to ListElement so the eye icon appears. Now connect the modules together as shown in Figure *Our example pipeline*.

Our workflow is now complete except for one crucial element: the starting point. We need to pass a chebiID string to the workflow in order to look up information about a chemical. We do this by assigning a chebiID string to the String module at the top of the pipeline. Highlight the String module in the canvas, then in the Module Information panel on the right, make sure the Inputs tab is selected and click on value and type CHEBI:15357 into the String input box that comes up.

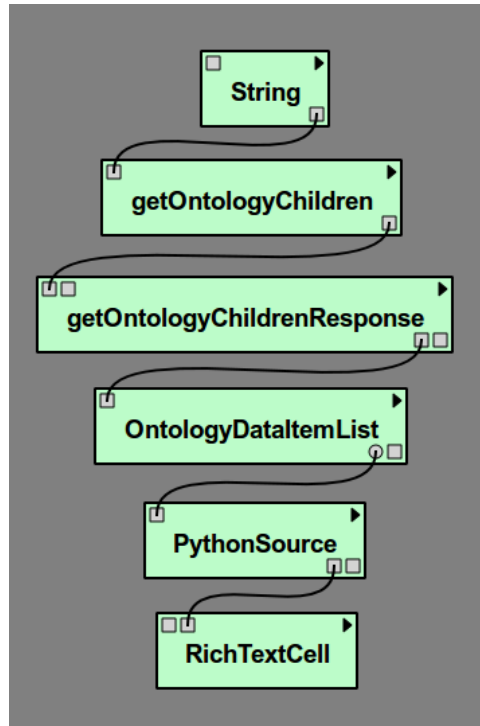


Fig. 4.32: Our example pipeline

4.8.4 Executing the workflow

The workflow is now ready to be visualized. Click the `Execute` button to send the current pipeline with the current parameters to a `RichTextCell` within the VisTrails Spreadsheet. Your result should resemble Figure *The HTML table generated by our workflow*. As you can see, the “ontology children” query returns the same information as before, but without the use of a web browser. In addition, we used a small Python program (via the `PythonSource` module) to transform the raw XML into a readable HTML table.

4.9 Example: ITK

4.9.1 Introduction to ITK

The *Insight Toolkit*,² or ITK, is an open-source software system initially designed to support the Visible Human Project [C1]. ITK is under continual development, being updated to employ cutting-edge segmentation and registration algorithms for multiple dimensions. For more information about ITK, please refer to [C2] and [C3].

In order to facilitate the implementation of processing mechanisms specific to the medical imaging community, ITK provides a robust set of general purpose image processing tools. These image processing tools are available to users through the standard ITK Filter interface. Although ITK is implemented in C++, through the use of CMake³ and CableSwig⁴, the functionality of ITK is made available to languages such as TCL, Java, and Python. In addition, much of the functionality of ITK is also available in a VisTrails package. The ITK package is not currently included in the binary distribution of VisTrails, but it may be downloaded separately from the VisTrails website.

² The Insight Toolkit is sometimes referred to by the longer name *Insight Segmentation and Registration Toolkit*.

³ CMake cross-platform make system. <http://www.cmake.org>

⁴ CableSwig Interface generator. <http://www.itk.org/HTML/CableSwig.html>

ChebiId	ChebiName	Comments	Type	Status	CyclicRelationship
CHEBI:30782	acetylenedicarboxylate(1-)		is conjugate acid of	CHECKED	True

Fig. 4.33: The HTML table generated by our workflow

Note: The WrapITK library, upon which the VisTrails ITK package depends, is well-tested on Linux and Mac OS X platforms. It is, however, known to have issues under Windows.

4.9.2 Preparing ITK

At the time of this writing, the latest stable release of ITK is 3.6.0. In order to incorporate the functionality of ITK into the VisTrails system, it first must be built and installed. In the following sections, we will describe in detail the process of downloading, building, and installing ITK and all the required components needed to use it.

Downloading ITK

ITK can be downloaded in either source tarballs or via public CVS access to the ITK source repository. The following instructions take advantage of the CVS source repository; however, source tarballs can be downloaded from: <http://www.itk.org/>

These instructions can be found, in part, at the ITK website. To use CVS, you must have a CVS client installed on your system. To download the ITK library, issue the following commands:

```
cvs -d :pserver:anonymous@www.itk.org:/cvsroot/Insight login
password: insight
```

```
cvs -d :pserver:anonymous@www.itk.org:/cvsroot/Insight co Insight
```

Change directory into the newly created Insight/Utilities directory and issue the following command:

```
cvs -d :pserver:anonymous@public.kitware.com:/cvsroot/CableSwig co CableSwig
```

This checkout includes CableSwig in the ITK system, allowing it to be built automatically during compilation of ITK itself.

Building the ITK Libraries

ITK requires CMake to be installed and available on your system. As of ITK version 3.2.0, CMake version 2.4.6 or greater must be used to prevent compilation errors. In order to simplify updating ITK to later versions of the software,

we perform an out-of-source build. To do this, we first create a directory outside the **Insight** directory created for us during the CVS checkout process.

```
mkdir itk
cd itk
```

We now run CMake, or the GUI-based version `ccmake`, in this directory. If you're using Windows, you may wish to run the Windows-specific `cmake-gui.exe` instead.

```
ccmake ../Insight
```

Note: The above command assumes that the **Insight** directory exists at the same level as the **itk** directory that we just created.

The following advanced CMake variables must be set to the appropriate values:

CMake Variable	Value
BUILD_SHARED_LIBS	ON
INSTALL_WRAP_ITK_COMPATIBILITY	ON
ITK_CSWIG_PYTHON	OFF
ITK_USE_REVIEW	ON
USE_WRAP_ITK	ON
WRAP_ITK_PYTHON	ON
WRAP_ITK_JAVA	OFF

Note: Some CMake variables are only available based on the state of others. If a variable is missing from the list, set what is visible and re-configure, this will often allow you to see and set additional parameters.

After generating the appropriate files and exiting `ccmake`, the standard build process can be completed. To compile (on Linux or Mac OS X), run:

```
make
sudo make install
```

On Windows, the build process is governed by the type of project or Makefile generated by CMake.

Note:

It is possible to use ITK without installing it. To do this, the environment variables `LD_LIBRARY_PATH` and `PYTHONPATH` must be set to the appropriate build directories:

```
LD_LIBRARY_PATH=/Path_To_itk/bin
PYTHONPATH=/Path_To_itk/Wrapping/WrapITK/Python
```

At this point, ITK is build and installed. To validate this, open a Python shell and issue the following commands:

```
>>> import itk
>>> itk.Image[itk.US, 2]
```

The above commands should both complete without error, and should produce the output:

```
<class 'itkImage.itkImageUS2'>
```

The `WrapITK` implementation used to wrap ITK for use in Python lazily instantiates required classes. This means that even if the import succeeds, the instantiation of the above `itk.Image` class may fail. This is particularly common if the environment variable `LD_LIBRARY_PATH` is incorrectly set.

4.9.3 ITK and VisTrails

When built and installed with the appropriate Python bindings included, ITK can be used from VisTrails through the ITK package. As mentioned previously, ITK is a third-party package and is not included in the general VisTrails distribution. However, like many third-party packages, it is available from the VisTrails website.⁵

The VisTrails ITK package is under continual development with the latest versions being announced on the VisTrails website. After downloading the package and extracting it into the `.vistrails/userpackages` directory, you can enable it through the `Module Packages` tab in the Preferences dialog. Please refer to Chapter [Writing VisTrails Packages](#) for instructions on how to do this.

Upon starting VisTrails, the ITK package modules will be made available to the Builder Window.

ITK Package Organization

The ITK VisTrails package loosely mimics the ITK functionality hierarchy. The package's top level consists of base classes, containers, and file readers as shown in Figure (a) *The VisTrails ITK Package Structure Overview*. Also available at the top level is the `PixelType` module and the specific types used to create and execute ITK-based pipelines.

Currently, the ITK Image Filters are organized into functional groups. The five filter types, as show in Figure (c) *The ITK Package Filter Structure*, are:

- Feature Extraction Filters
- Image Intensity Filters
- Segmentation Filters
- Image Selection Filters
- Image Smoothing Filters

All filter types currently have at least one representative ITK filter wrapped and usable from within the VisTrails environment.

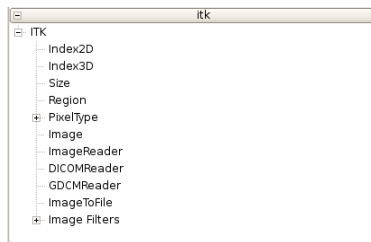


Fig. 4.34: (a) The VisTrails ITK Package Structure Overview

Reading DICOM Volumes

DICOM is a standard format for exchanging medical images. ITK includes DICOM support through the GDCM libraries.⁶ It is worthwhile to note that at this time these libraries are currently not a complete implementation of the DICOM standard.

⁵ Please Note: At the time of this writing, the VisTrails ITK package is not a complete wrapping of all ITK functionality. If you would like to contact the author regarding the wrapped functionality, please do so through the e-mail address on the VisTrails website.

⁶ Grass roots DiCoM Project. <http://www.creatis.insa-lyon.fr/Public/Gdcm/>

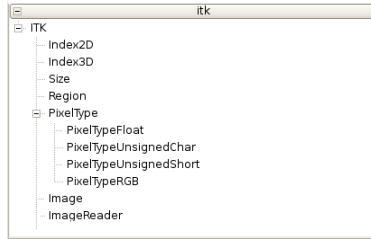


Fig. 4.35: (b) The ITK Package Supported PixelTypes

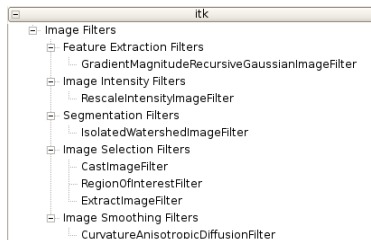


Fig. 4.36: (c) The ITK Package Filter Structure

DICOM volumes can be integrated into VisTrails through the use of either the `GDCMReader` or `DICOMReader` modules in the ITK package. For the rest of this example, we will use the `GDCMReader` module as its performance is slightly higher than the `DICOMReader` implementation.

Figure *VisTrails workflow utilizing ITK to extract a single slice...* shows the use of the `GDCMReader` module. In order to properly read a DICOM volume, the `GDCMReader` must be supplied with the dimension of the volume to be read and the directory containing the series to read. By default, `WrapITK` supports two- and three-dimensional volumes. In order to include support for higher dimensions, the appropriate `WrapITK` variable must be set within `CMake`, *before* compiling ITK.

Volume Processing With ITK and VisTrails

Typically, DICOM volumes are written with no 16-bit unsigned shorts. Unfortunately, most systems allow the display of only 8-bit values. Because of the higher precision inherent in DICOM data, it is often preferable to perform any computation, segmentation, or processing on the data prior to rescaling in order to utilize as much information as possible.

Volume Processing With ITK and VisTrails

ITK image filters are typically templated based on the dimensionality of the data being processed, as well as the data type being processed. In VisTrails, these parameters are handled through the use of `PixelType` modules. Although any ITK Filter wrapped in `vistrails` can accept any of these `PixelTypes`, the underlying implementation may not be compatible with the input `PixelType`. Using `PixelTypes` incompatible with the underlying filter implementations is the most frequent cause of error when executing otherwise functional pipelines in VisTrails.

When processing volumes, it is often necessary to extract a single slice from the volume at different stages of the processing pipeline. This is possible in VisTrails through the use of the `ExtractImageFilter`. Given a volume, a `Region`, and `Dimensionality` information, the `ExtractImageFilter` can extract a single slice from the data volume that can be used in further processing, previewing the results, or writing to disk. An example workflow that extracts a slice from a DICOM volume can be seen in Figure *VisTrails workflow utilizing ITK to extract a single slice...*

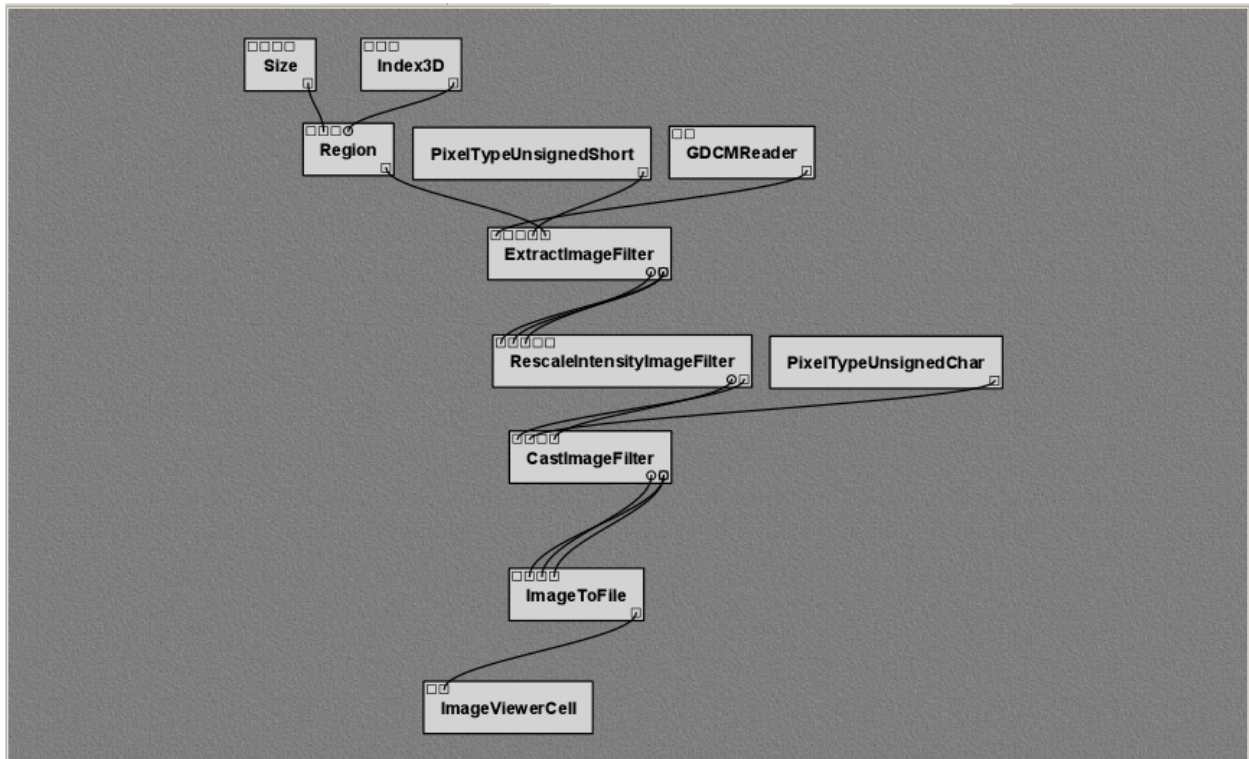


Fig. 4.37: VisTrails workflow utilizing ITK to extract a single slice from a DICOM volume. The slice is chosen by first forming a Region to extract. The result is viewed through the use of standard VisTrails Spreadsheet modules.

Visualizing the results

Although ITK's processing filters and the DICOM standard both support 16-bit processing and storage, many image viewers are capable of displaying in only 8-bit resolution using the unsigned char `PixelType`. Since the output of an ITK processing workflow is an image, it makes sense to view it as such. This means that we are required to both remap the data values in the image to 8 bits as well as perform a casting operation to change the data type from unsigned shorts to unsigned chars. These operations are performed through the use of the `RescaleIntensityImageFilter` and the `CastImageFilter`. Figure *VisTrails workflow utilizing ITK to extract a single slice...* demonstrates the use of the `RescaleIntensityImageFilter` and the `CastImageFilter` in conjunction with the `ImageToFile` and `ImageViewerCell` modules to view the resulting slice in the VisTrails Spreadsheet.

Citations

4.10 Persistence in VisTrails

The `Persistent Archive` package in VisTrails provides a persistent file store with searchable metadata. It makes it easy for users to store files permanently with meaningful information so that they can be retrieved and exploited later, without having to manually organize and reference them.

At the simplest level, you can use it to cache files to disk, so that your pipelines can retrieve them later and avoid lengthy recomputations by inserting a `CachedFile` module.

4.10.1 Getting Started With Persistence

This package builds upon the `file_archive` tool. Should you need to insert or extract files from the store from outside VisTrails, you will find the store in `~/vistrails/file_archive`.

Files are stored uncompressed in the store, along with metadata in the form of key-value pairs. VisTrails stores the generating module location and signature in their, but you can add all the meaningful metadata you might need for later identification.

VisTrails provides 4 types of modules:

PersistedInputDir and PersistedInputFile

This allows you to persist an input file inside the store. It will use the matching file from the store, unless a new file is provided and differs from the store.

Use it for example to record the result of a computation, or to keep track of your experiment's input for later reference even though you might change or delete the original.

PersistedDir and PersistedFile

These modules insert data into the store, along with metadata. Additionally, if an entry can be found for the signature of the upstream subpipeline, the module will simply use that file, skipping the execution of these upstream modules.

Use it for example to persistent an important result that is part of your pipeline.

CachedDir and CachedFile

These are variants of `PersistedDir` and `PersistedFile` that don't accept additional metadata. Files will be marked as cache files and won't be shown by default in the viewer. You can use this for unimportant pieces of data that you only persist to speed up your pipeline.

QueriedInputDir and QueriedInputFile

These simply get a previous result, or any entry from the store, from conditions on the metadata. It accepts more general queries than `PersistedInputFile` which only compares for equality of the metadata.

Use it for example to analyse previous results.

4.10.2 Managing the store

All the files currently stored in the archive can be listed by clicking on the *Packages* menu > *Persistent Archive* > *Show archive content*.

4.10.3 Examples

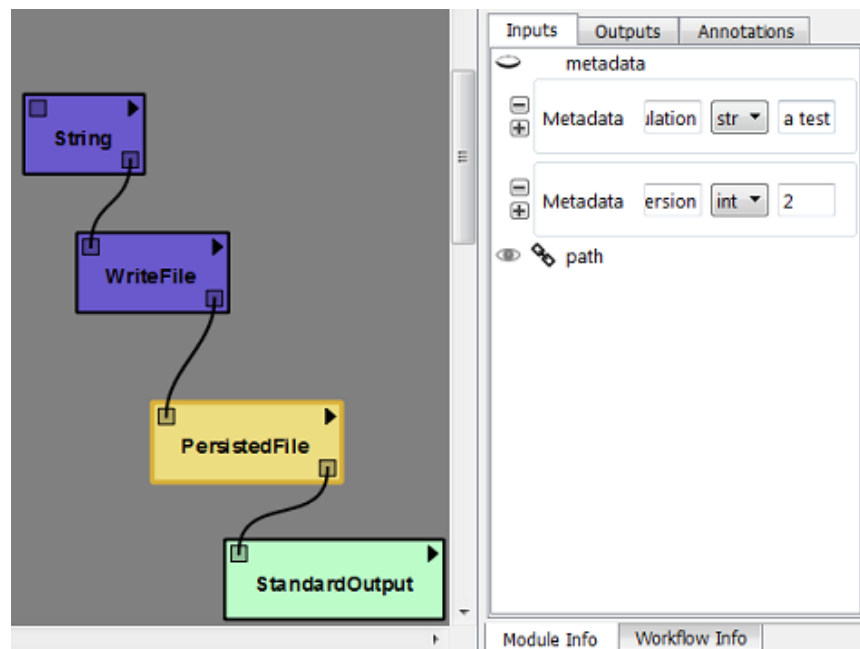


Fig. 4.38: Example: Using `PersistedFile` in a workflow with metadata. Upstream is not re-executed.

4.11 Running commands on a remote server

The `tej` tool provides a way to start job on any remote server through SSH, associate it with an identifier, and monitor its status. When the job is complete, it can download the resulting files through SCP.

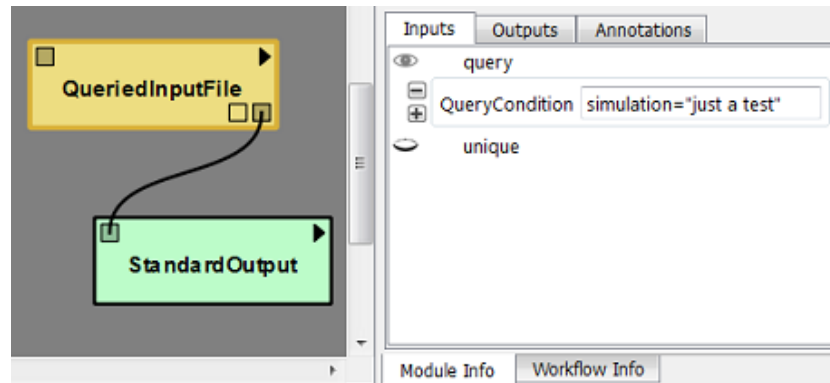


Fig. 4.39: Example: Querying a file from the archive with text conditions.

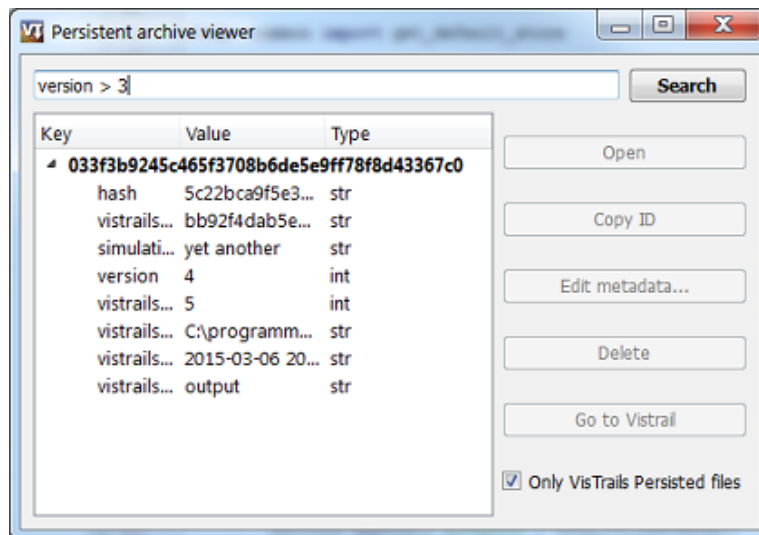


Fig. 4.40: Example: Searching for archive entries with the *Show archive content* dialog.

In VisTrails, the subpipeline’s signature is used as the job identifier. This means that once you have run your pipeline one and the job has been submitted, running it again will match it to the existing job, and will either wait for the job to complete or download the existing results without running it again.

4.11.1 Referencing a queue

The first thing you need to do is setup a `Queue` module that indicates which server to connect to (and optionally, where on the filesystem should the jobs be stored).

No setup is required on the server (though VisTrails/tej needs to be able to connect to it via SSH, so you might want to setup public key authentication), the directory will be created on the server with the necessary structure and helpers.

4.11.2 Submitting a job

The `SubmitJob` module upload a job to a server if it doesn’t exist there already (checking for the same subpipeline) and returns a `Job` object suitable for downloading its results. Regardless of whether the job is created or it already existed, VisTrails will wait for it to complete before carrying on executing your workflow; if you click “cancel” however, it will add the job to the job monitor and keep tabs on the server, alerting you when the job is done so you can resume executing the workflow.

The job is simply a directory that will be uploaded to the server, with a `start.sh` script that will be executed there (or whatever name is set on the `script` input port). Remember to use relative paths in there so that different jobs don’t overwrite their files.

A different module, `SubmitShellJob`, makes it easy to submit a job consisting of a single shell script that you can enter directory in the module configuration window. Its output (`stdout`, `stderr`) is downloaded and returned as files on the corresponding output ports.

4.11.3 Downloading output files

You can connect `SubmitJob`’s output to `DownloadFile` modules to retrieve generated files from the server and use them in the following steps of your pipeline. The module only needs a `filename` parameter, which is relative to the job’s directory. The `DownloadDirectory` module works in the same way but downloads a whole subdirectory recursively.

4.11.4 Example

In this example, we’ll submit a simple Python script to a server via SSH. That script searches for the largest prime factor of a given number and prints it to the console.

Try it Now!

First, create the Python script. You can use the `String` module, entering the script in the configuration widgets; connect it to a `WriteFile` module to get a file suitable for uploading.

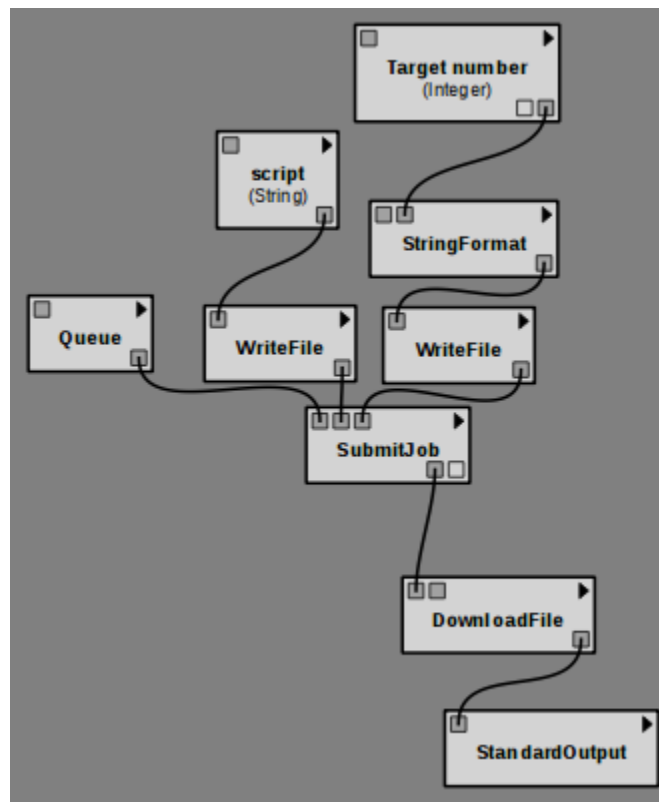
```
#!/usr/bin/env python
with open('input') as fp:
    number = int(fp.read().strip())

largest = None
n = 2
while n <= number:
    while number % n == 0:
        number /= n
    if number == 1:
        largest = n
        break
    n += 1

with open('output', 'w') as fp:
    if largest is not None:
        fp.write("%d" % largest)
```

As you can see, this script reads the target number from a file, `input`, and writes the result to another file, `output`. You can create the `input` file from an `Integer` using the `StringFormat` module (setting the *format* to `{target}` for example).

Add a `DownloadFile` module to download `output` and print the file with `StandardOutput` for example. The end result should look like this (or open it from here):



Running it will start the job on the server. The job monitor window will pop up to indicate that it knows about the remote job, and that it is currently running. Clicking the “check” button or re-running the workflow will update the status, and eventually run the rest of the pipeline when the job is done, displaying the result.

Because the job identifier is computed from the signature of the subpipeline consisting of `SubmitJob` and its upstream modules, anyone running the same job on the same server will hit the same job, and will reuse your results without triggering a recomputation. But if you change the script, or choose a different target number to factorize, a new job will be submitted, that will not affect the result seen by other users and other workflows.

4.11.5 Setting up ssh keys

tej requires the servers ssh key to be registered in `known_hosts` in a format supported by Paramiko.

If the key is missing, or in the wrong format, you will see something like:

```
paramiko.SSHEXception: Unknown server 127.0.0.1
```

The easiest way to add the key is to connect with `ssh` and accept the prompt (“Are you sure you want to continue connecting?”); `ssh` will add the server to the known hosts automatically and you can disconnect.

If this does not work, the key used by SSH is probably in a format not supported by Paramiko (like ECDSA). To force using the RSA key (from [here](#)):

```
ssh -o HostKeyAlgorithms=ssh-rsa -o FingerprintHash=md5 user@yourserver.com
```

4.12 VisTrails Server Setup

- lets assume that everything is going to be put in the `/server` dir:

```
$ cd /server
$ mkdir vistrails
```

- put VisTrails Source in `vistrails/` folder:

```
$ cd vistrails
$ git clone git://vistrails.org:vistrails.git git # or just download the latest release or night
```

- make a logs dir for the server:

```
$ mkdir logs
```

- if you are running the server without `crowdLabs` or as a remote server, you need to create a media directory with the following structure:

```
/path/to/media_dir/
    wf_execution/
    graphs/
        workflows/
        vistrails/
    medleys/
    images/
```

You can run `python scripts/create_server_media_dir_structure.py /path/to/media_dir` to create the directory structure automatically.

- Determine how you will start the vistrails server. You have a choice of using `Xvfb` or not. If you use it, `/server/vistrails/git/scripts/start_vistrails_xvfb.sh` is what you will use, otherwise, use `start_vistrails.sh`

Using Xvfb is slower and not recommended if your workflows will make use of volume rendering or other graphics-card intensive techniques.

4.12.1 Using Xvfb

- edit `/server/vistrails/git/scripts/start_vistrails_xvfb.sh` file and make sure it is consistent with your system setup:

```
LOG_DIR=/server/vistrails/logs
Xvfb_CMD=/usr/bin/Xvfb
VIRTUAL_DISPLAY=":6"
VISTRAILS_DIR=/server/vistrails/git/vistrails
ADDRESS="<your_server.com>"
PORT="8081" #the port where the server will listen for requests
CONF_FILE="server.cfg"
NUMBER_OF_OTHER_VISTRAILS_INSTANCES="1"
MULTI_OPTION="-M" #execute the main instance multithreaded
```

- The setup above will execute 2 instances of the server. You can add more instances by changing the variable `NUMBER_OF_OTHER_VISTRAILS_INSTANCES`. When using multiple instances, the ports and virtual displays will be used incrementally, so if the main instance is using port 8081 and virtual display `:6`, the next instance will use port 8082 and virtual display `:7`, and so on.

4.12.2 Connecting to X server directly

- If you decide no to use Xvfb, edit `/server/vistrails/git/scripts/start_vistrails.sh` file and make sure it is consistent with your system setup:

```
LOG_DIR=/server/vistrails/logs
VISTRAILS_DIR=/server/vistrails/git/vistrails
ADDRESS="<your_server.com>"
PORT="8081" #the port where the server will listen for requests
CONF_FILE="server.cfg"
NUMBER_OF_OTHER_VISTRAILS_INSTANCES="2"
MULTI_OPTION="-M" #execute the main instance multithreaded
```

- The setup above will execute 3 instances of the server. You can add or remove more instances by changing the variable `NUMBER_OF_OTHER_VISTRAILS_INSTANCES`. When using multiple instances, the ports will be used incrementally, so if the main instance is using port 8081, the next instance will use port 8082, and so on.

4.12.3 Basic Configuration

- If the vistrails server will receive requests from the outside world and if you are using a firewall, make sure the ports used by the vistrails server are open and accessible.
- create a file called `server.cfg` in `/server/vistrails/git/vistrails/` as follows:

```
[access]
permitted_addresses = localhost, 127.0.0.1, <crowdlabs-server-address>

[media]
media_dir=/server/crowdlabs/site_media/media

[database]
host = <vistrail database address>
read_user = <read user>
```

```
read_password = <read password>
write_user = <write user>
write_password = <write user password>

[script]
script_file=/server/vistrails/git/scripts/start_vistrails.sh
virtual_display=<virtual display number>
```

- change `permitted_addresses` variable in to include the address of the machine running of the crowdLabs server (or other machines you want to be able to connect to the server):

```
[access]
permitted_addresses = localhost, 127.0.0.1, <crowdlabs-server-address>
```

- Add the password for the full permission mysql user:

```
write_user = <write user>
write_password = <write user password>
```

- Configure the full path to the script file and if you are using Xvfb, also specify the virtual display of the main instance:

```
[script]
script_file=/server/vistrails/git/scripts/start_vistrails.sh
virtual_display=0 #not using any display
```

- run vistrails in server mode:

```
$ cd /server/vistrails/git/scripts
# If you are running Xvfb:
$ ./start_vistrails_xvfb.sh
# Or if you are connecting to X server directly:
$ ./start_vistrails.sh
```

4.13 Embedding VisTrails Files Via Latex

The VisTrails Latex extension allows you to embed the result from a VisTrails file into a Latex document. Images to be included in the Latex document will be generated through VisTrails and can be linked to the VisTrails file and version from which it was generated. In other words, Latex calls VisTrails to generate an image for a resulting PDF document. The resulting image can be set up so, when clicked, the generated VisTrails file will be opened in VisTrails.

4.13.1 Latex Setup and Commands

This section contains instructions for setting up Latex files to use VisTrails. For a complete example of this setup, you may also refer to `example.tex` in VisTrails' `extensions/latex` directory.

To use the Latex extension, copy `vistrails.sty` and `includevistrail.py` from the `extensions/latex` directory to the same directory as your `.tex` files. Then, add the following line to the beginning of the latex file:

```
\usepackage{vistrails}
```

By default, VisTrails will be executed at `www.vistrails.org` and the images downloaded to your hard drive. This allows any user that downloads your paper to execute the workflows on the server.

Local Setup

If you want to run a local copy of VisTrails instead, add the following path to your python file or executable:

```
\renewcommand{\vistrailspath}{/path/to/vistrails/run.py}
```

Depending on how you are running VisTrails and on which OS you are running, the vistrailspath should be configured appropriately. Please check head.tex in VisTrails' extensions/latex directory for detailed instructions on the configuration for the different platforms.

By default, images are set up to link to their corresponding vistrail. This means that on a local setup, clicking on an image will open the local .vt file or will try to connect to the database if you loaded the vistrail from a database. This may not work when other users click on the images on different machines. However, if you are using your own web server, additional setup is required (see *Setup For Use With Files on MediaWiki or a Web Server*). Otherwise, to setup the images without links (not clickable), add:

```
\renewcommand{\vistrailsdownload}{}
```

Finally, if you are running VisTrails from source and don't have python on your path, use this to set the python interpreter:

```
\renewcommand{\vistrailspythonpath}{/path/to/python/executable}
```

Note: If you set the vistrailspythonpath to an invalid path VisTrails will use cached files if they exist.

Setup For Use With Files on MediaWiki or a Web Server

Many VisTrails files and/or data are stored in a database that readers of a pdf document might not have access to. If the files are also accessible through the web, the following instructions explain setup that will allow readers to download the VisTrail or workflow through MediaWiki or a web server.

MediaWiki

To setup your MediaWiki for use with VisTrails:

- In your wiki/extensions folder, create a config.php file based on the config.php.sample file located in VisTrails' extensions/http folder.
- Copy download.php, functions.php, and vistrailsExtension.php from the extensions/mediawiki folder to your wiki/extensions folder and update these files according to your needs.
- Configure your .tex files with:

```
\renewcommand{\vistrailsdownload}{http://yourwebserver.somethingelse/download.php}
```

Web Server

To configure VisTrails to run on your web server:

- Create a config.php file based on the config.php.sample file located in VisTrails' extensions/http folder.
- Copy functions.php and downloads.php from the extensions/mediawiki folder and update them according to your needs.
- **Depending on the functionality you want to make available, copy any or all of the following files:**
 - run_vistrails.php - will execute workflows and return images and pdf files
 - get_db_vistrail_list.php - will return a list of VisTrails available in the database
 - get_vt_xml.php - will return a VisTrail in xml format
 - get_wf_pdf.php - will return a workflow graph in pdf format
 - get_wf_xml.php - will return a workflow in xml format

- Configure your .tex files with:

```
\renewcommand{\vistrailspath}{http://yourwebserver.somethingelse/run_vistrails.php}
\renewcommand{\vistrailsdownload}{http://yourwebserver.somethingelse/download.php}
```

4.13.2 Including VisTrails Results in Latex

There are two ways of including VisTrails' objects in a Latex file. Usually you start with a workflow in a vistrail (the vistrail can be loaded from a file or from a database):

- In History view, select the version node representing the workflow.
- In Pipeline view, ensure that the workflow is being displayed.

Now you can select Publish → To Paper... to launch a dialog with embedding options (see Figure *Embedding Options*).

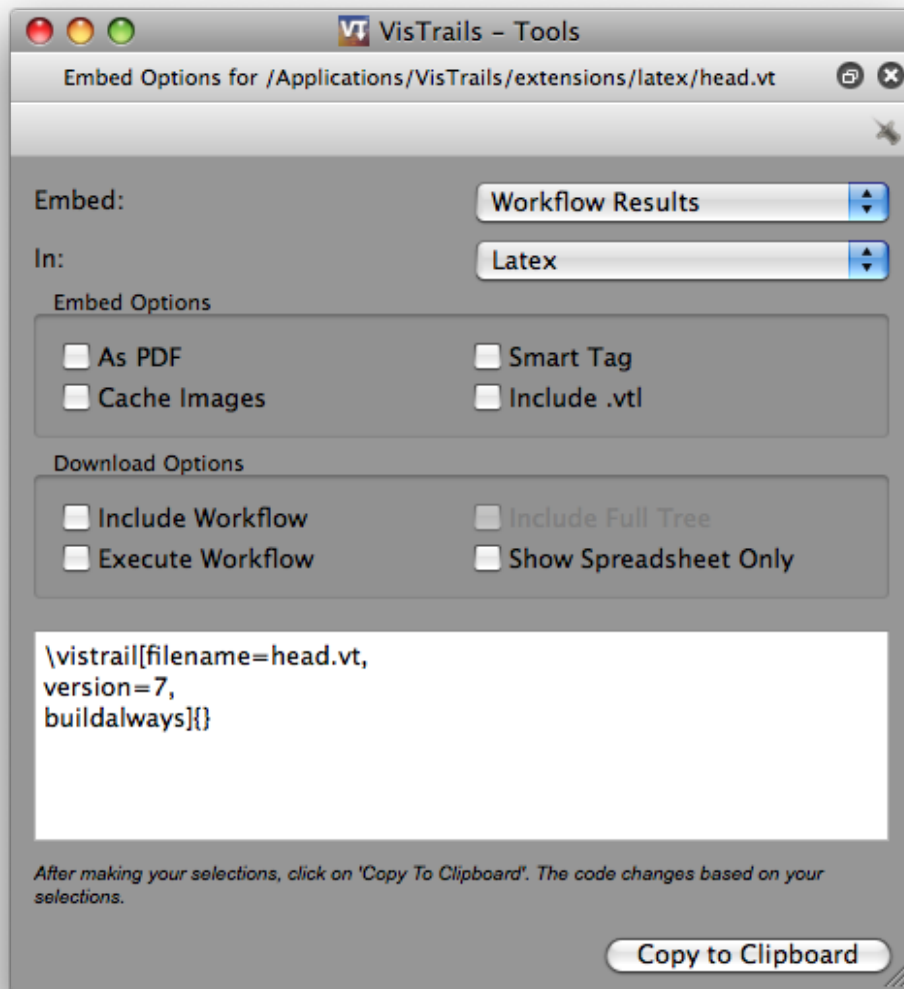


Fig. 4.41: Embedding Options

Then perform the following steps:

- Select the type of object that you would like to display. The choices are: Workflow Results, Workflow Graph, and History Tree Graph.
- Make sure that `Latex` is displayed in the `In:` combobox.
- You should then choose from a number of “Embed” and “Download” options which will be explained in the tables below.
- Press the “Copy to Clipboard” button
- Paste clipboard contents into you Latex document
- Run `pdflatex` with the `-shell-escape` option: `pdflatex -shell-escape example.tex`.

Note on using local VisTrails files: Relative or absolute filenames can be used in the `.tex` file, but absolute filenames are used in the pdf. Thus, if the absolute location of the file has changed, the pdf will need to be regenerated even if the relative location of the file has not changed. Also, the `VisTrails Embed` function assumes the `.vt` file is in the same directory as the `.tex` file. You will need to change this to an absolute filename if it is not.

Table 4.1: Configuration Options

Option	Latex Flag	Description
Workflow Results	<code>version=<...></code>	Show the results of the specified version.
Workflow Graph	<code>version=<...></code> <code>showworkflow</code>	Show the workflow instead of the results.
History Tree Graph	<code>showtree</code>	Show the version tree instead of the results.

Table 4.2: Embed Options

Option	Latex Flag	Description
As PDF	<code>pdf</code>	Download images as pdf files. If this is not checked, a png image is used.
Smart Tag	<code>tag=<...></code>	Allows you to include a version’s tag. If a tag is provided, version can be omitted and <code>buildalways</code> is implicit.
Cache Images	<code>buildalways</code> (do not include for caching)	When caching desired, the <code>buildalways</code> flag should not be included. If it is included, VisTrails will be called regardless of whether or not it has been called for the same host, db, version, port and <code>vt_id</code> .
Include <code>.vtl</code>	<code>getvtl</code>	Causes the <code>.vtl</code> file to be downloaded when compiling the pdf file. This is useful when you want to package the workflows together with your paper for archiving.

Table 4.3: Download Options

Option	Latex Flag	Description
Include Workflow	embedworkflow	When clicking on the image in the pdf, download the workflow only.
Execute Workflow	execute	Will cause the workflow to be executed when it is opened.
Include Full Tree	includefulltree	When clicking on the image, download the complete VisTrail.
Show Spreadsheet Only	showspreadsheetonly	When opening the workflow it will initially only show the spreadsheet. The execute option is implicit.

Example

The following is an example command for including the execution results the workflow `aliases` from `examples/head.vt` in a pdf and caching the images. When clicking on the images, the user will start VisTrails showing only the spreadsheet:

```
\vistrail[filename=head.vt,
version=15,
pdf,
execute,
showspreadsheetonly,
]{width=0.45\linewidth} %Options you would give to the \includegraphics{}
command.
```

See `head.tex` in the `extensions/latex` directory for a complete example of usage.

Additional Notes

After running at least once, VisTrails will cache the images and latex instructions. The latex code will be in the “cached” folder and the images in `vistrails_images`.

VisTrails will create in the current directory a directory called `vistrails_images/filename_version_options` with the `png/pdf` files generated by the spreadsheet.

4.13.3 Including crowdlabs.org workflow results in Latex

It is also possible to embed results of workflows that are in `www.crowdlabs.org`.

To use the `crowdLabs` extension, copy `crowdlabs.sty` and `includecrowdlabs.py` from the `extensions/latex` directory to the same directory as your `.tex` files. Then, add the following line to the beginning of the latex file:

```
\usepackage{crowdlabs}
```

The `vistrial` you would like to use must be already in `crowdLabs`. Visit the page of the workflow, for example, go to:

<http://www.crowdlabs.org/vistrails/workflows/details/1046/>

And click on the `Embed this Workflow` tab located below the image. Copy the snippet in the `In LaTeX` box:

```
\vistrail[wfid=1046,  
buildalways=false]{width=4cm}
```

And paste it in the latex file.

Currently crowdLabs supports only embedding workflow results in the png format. Do not use this extension together with the `vistrails` extension above.

4.14 Example: scikit-learn

4.14.1 Introduction to scikit-Learn

`scikit-learn` is a python based open-source machine learning library. It provides implementations of popular machine learning algorithms together with evaluation and preprocessing utilities. For more information, refer to the [extensive documentation](#).

4.14.2 Installing scikit-learn

VisTrails should be able to automatically install `scikit-learn` via `pip`. If this fails, try to install it manually:

```
pip install --user scikit-learn
```

If this also fails, consult the [installation instructions](#).

4.14.3 Using scikit-learn via VisTrails

Datasets

For testing purposes and the examples, there are two multi-class classification datasets made available as VisTrails modules, the Digits and the Iris datasets. These have as output ports training data and classification targets, to quickly test a pipeline. Both datasets are very simple toy datasets and should not be used as benchmarks.

The Digits dataset consists of 1797 handwritten digits as represented as 8x8 grey scale images, resulting in 64 features. The digits belong to the classes 0 to 9. The `Iris` dataset consists of 150 data points with four features, belonging to one of three classes.

Splitting data into training and test set

As machine learning is inherently about generalization from training to test data, it is essential to separate a data set into training and test parts. The `TrainTestSplit` module is a convenient way to do this:

Basic usage

The VisTrails `sklearn` package contains most algorithms provided in `scikit-learn`. In machine learning, applying an algorithm to a dataset usually means training it on one part of the data, the training set, and then applying it to another part, the test set.

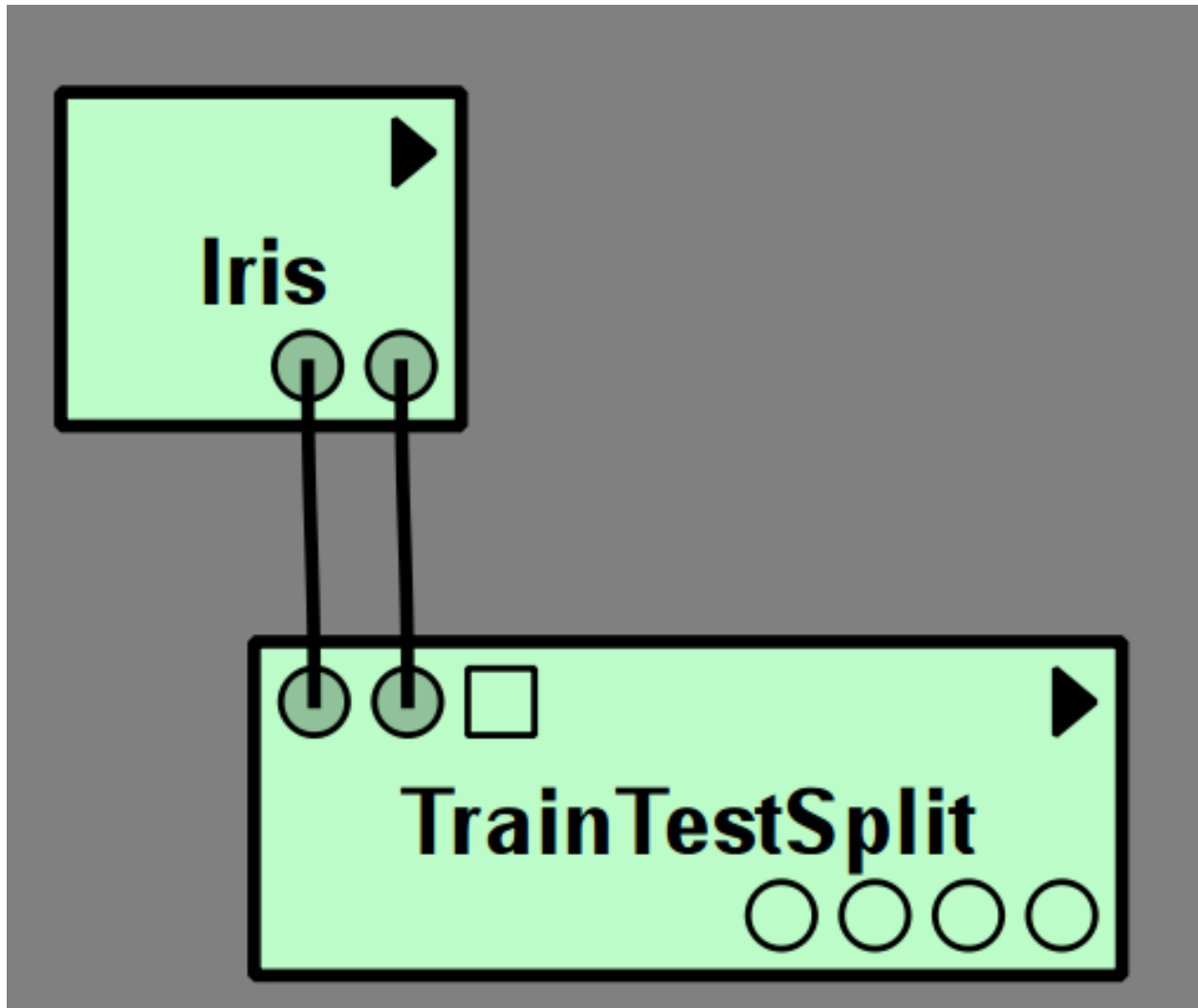
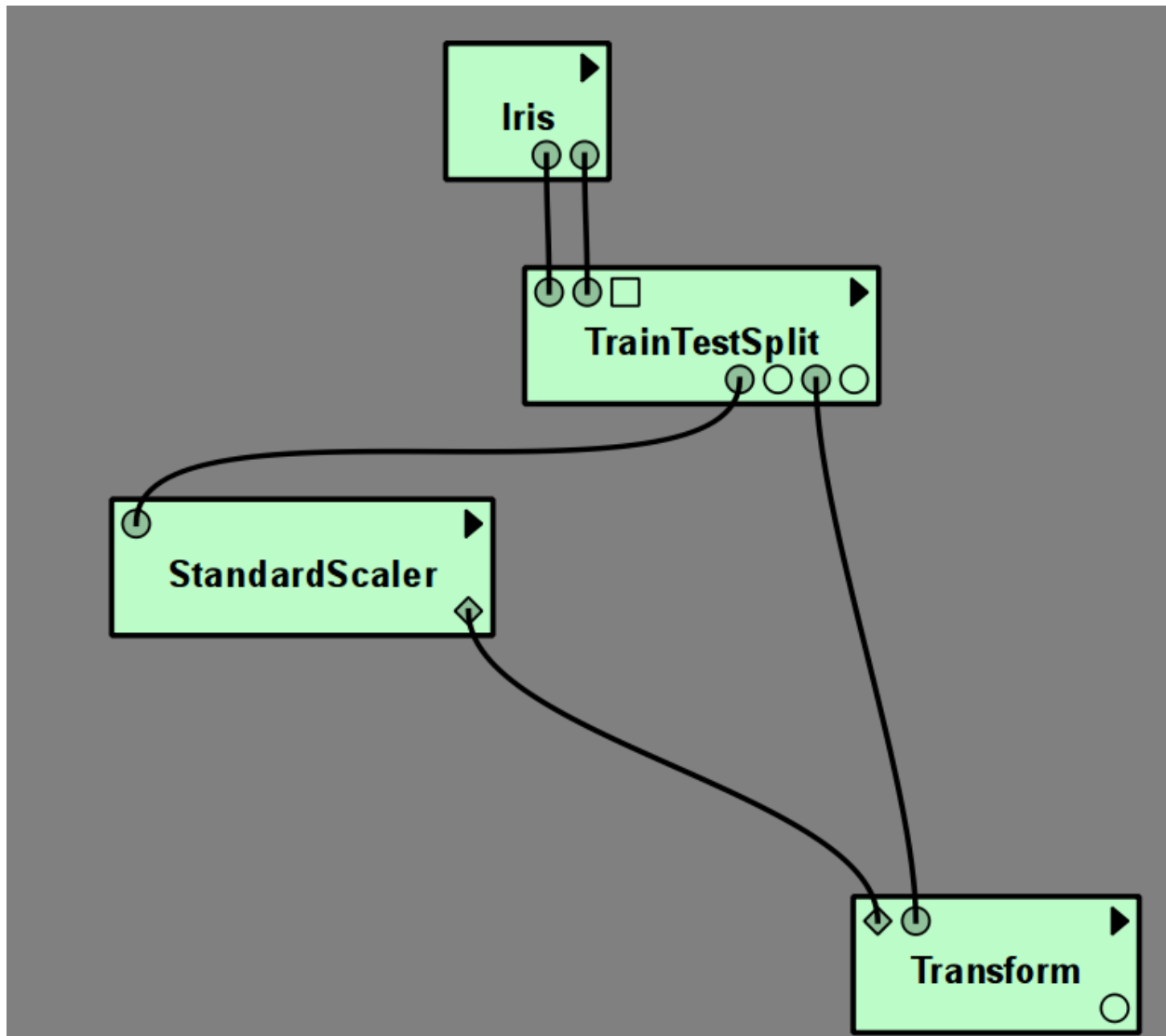


Fig. 4.42: The round output ports of the Iris dataset correspond to training data and training targets, which are fed into `TrainTestSplit`. The outputs of `TrainTestSplit` are data and labels for two subsets of the data, corresponding to the four round output ports. First are training data and training labels, then test data and test labels. The split is done randomly with 25% test data by default.

Each algorithm in scikit-learn has a corresponding VisTrails module, which has input ports for training data, and outputs the model that was learned (with the exception of the *Manifold learning* module). To apply the model to new data, connect it to a `Predict` module (for classification and regression) or to a `Transform` module (for data transformations like feature selection and dimensionality reduction).



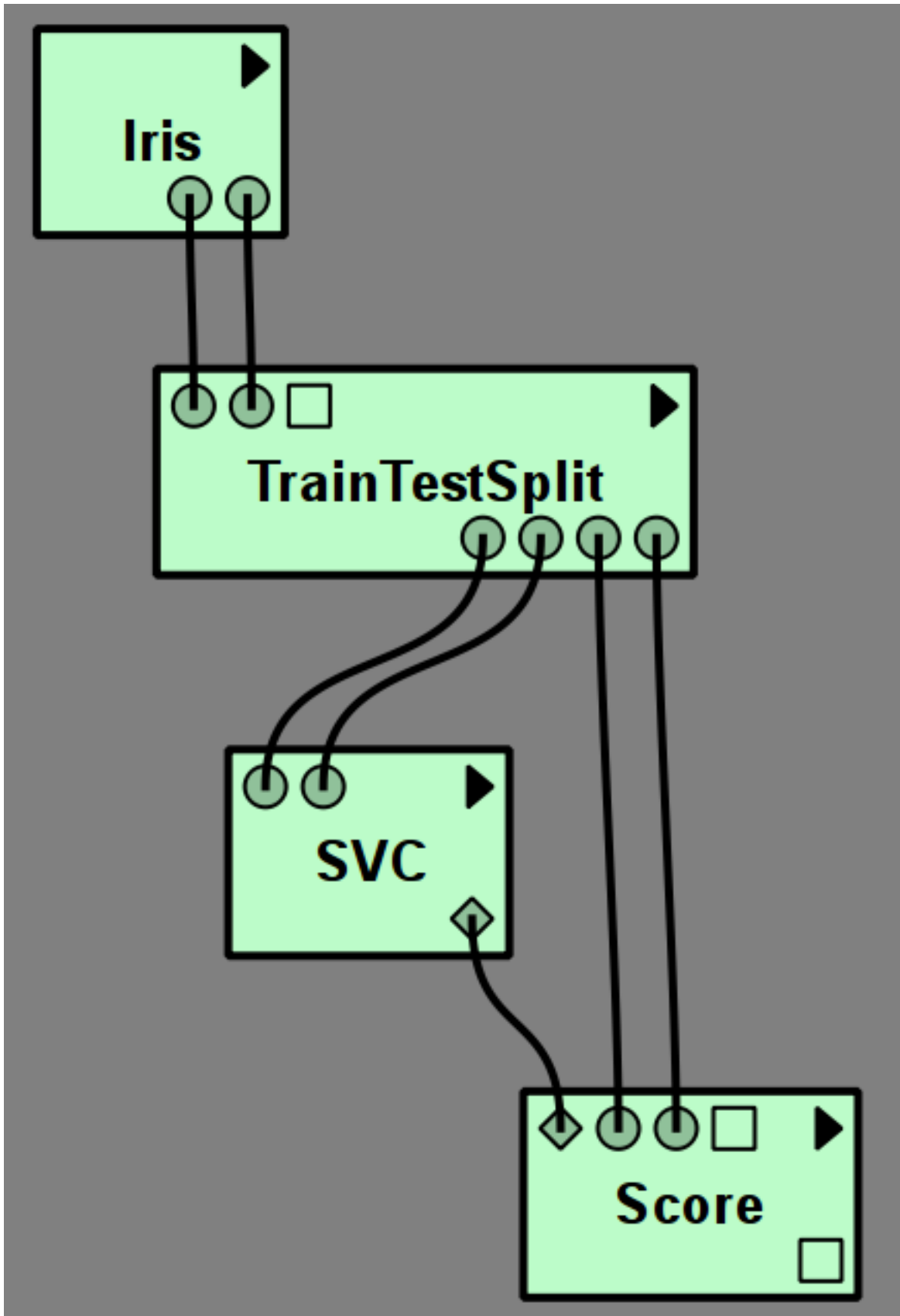
It is also possible to directly compute performance metrics like the accuracy or mean squared error using the `Score` module.

The resulting Scores can be output with a `GenericOutput`, or more advanced string formatting.

To make connecting the ports easier, ports that represent models are diamond shaped, while ports that represent data or label arrays are round. The remaining square ports are either parameters of the models or additional information provided as output.

Manifold learning

Manifold learning algorithms are algorithms that embed high-dimensional data into a lower-dimensional space, often for visualization purposes. Most manifold learning algorithms in scikit-learn embed data, but cannot transform new



data using a previously learned model. Therefore, manifold learning modules will directly output the transformed data.

Cross Validation and Grid Search

To perform a cross validation or grid search with a model, simply create a module for the model, without providing any training data. The output will be an unfitted model that can be used as input for grid search or cross validation:

`GridSearch` needs as additional input a dictionary of parameter values, that is best specified using a `PythonSource` module:

`GridSearch` itself has a model output port, so that the grid search can be used, for example, in `CrossValScore` to perform a nested cross-validation.

Pipelines of scikit-learn models

To perform cross validation or grid search over a chain of estimators, such as preprocessing followed by classification, scikit-learn provides a `Pipeline` module. Each step of a pipeline is defined by an input port specifying a model. All but the last model in the pipeline must be transformers, the last can be arbitrary. Currently the VisTrails scikit-learn package only supports up to four steps in a pipeline.

As any other model, a pipeline can either be fit on data and then evaluated using `Predict`, `Transform` or `Score` modules, or can serve as the input model to `CrossValScore` or `GridSearchCV`.

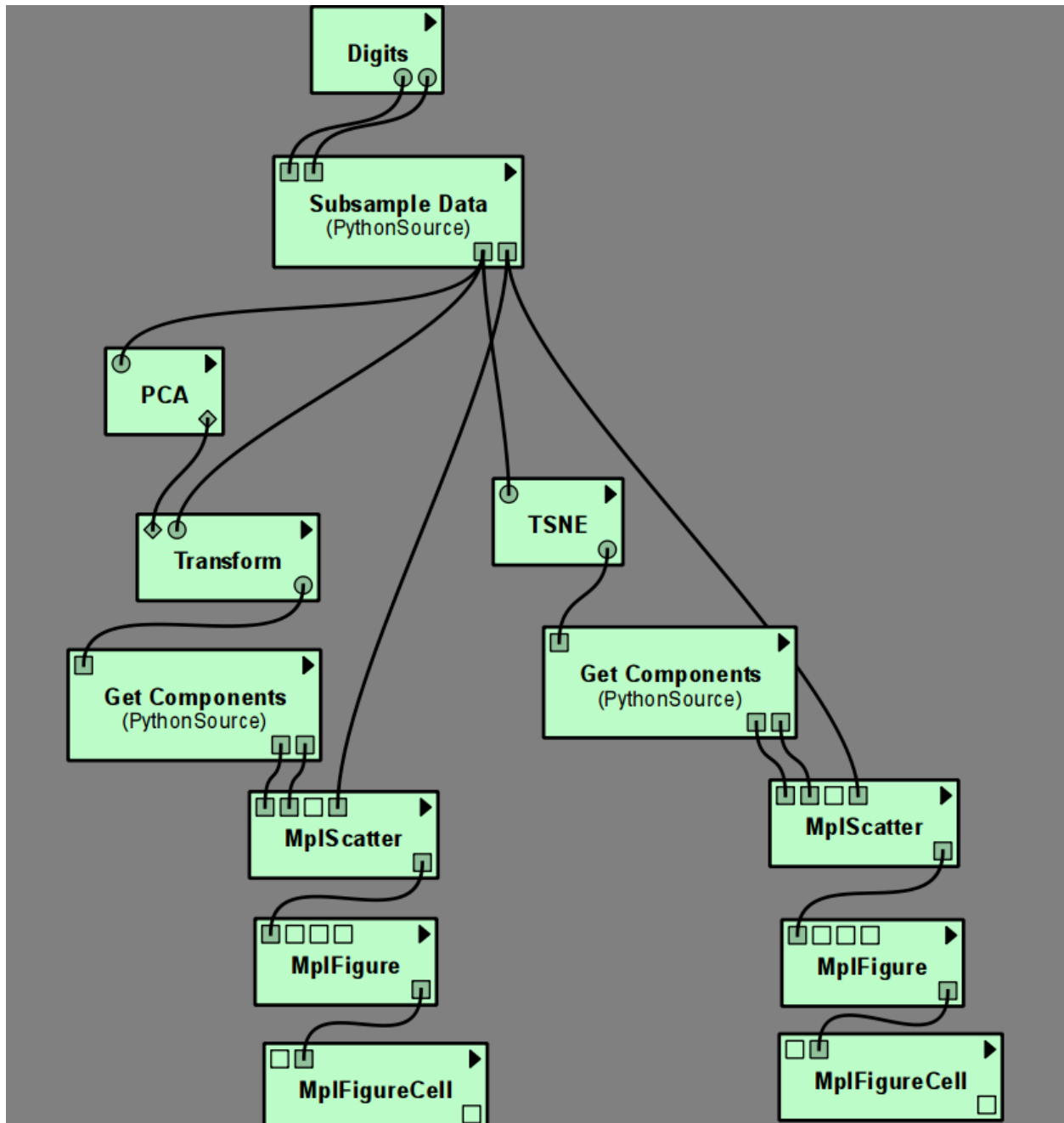
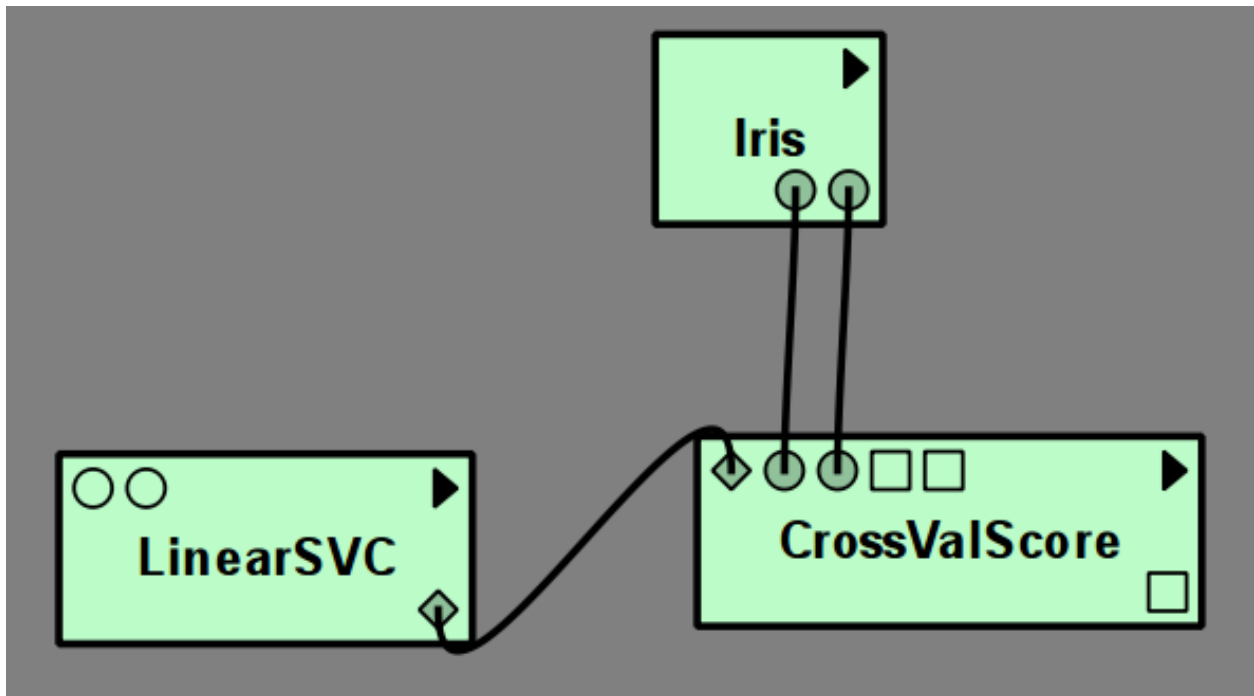


Fig. 4.43: The left hand side of the pipeline uses PCA, which can use Transform to be applied to new data. The right hand side uses the manifold learning method TSNE, which cannot be applied to new data, and therefore directly produces the transformed input data (in contrast to PCA, which produces a model).



A diagram illustrating a workflow with four modules: SVC, Grid Parameters (PythonSource), Iris, and GridSearchCV. The Grid Parameters module is highlighted with a yellow border. The GridSearchCV module has four input ports (diamonds) and two output ports (squares). Lines connect the output port of SVC to the first input port of GridSearchCV. Lines connect the output ports of Grid Parameters to the second and third input ports of GridSearchCV. Lines connect the output ports of Iris to the fourth and fifth input ports of GridSearchCV.

Module Configuration

	Input Port Name	Type	List Depth
1			
	Output Port Name	Type	List Depth
1	parameters	Dictionary (org.vistrails....	0
2			

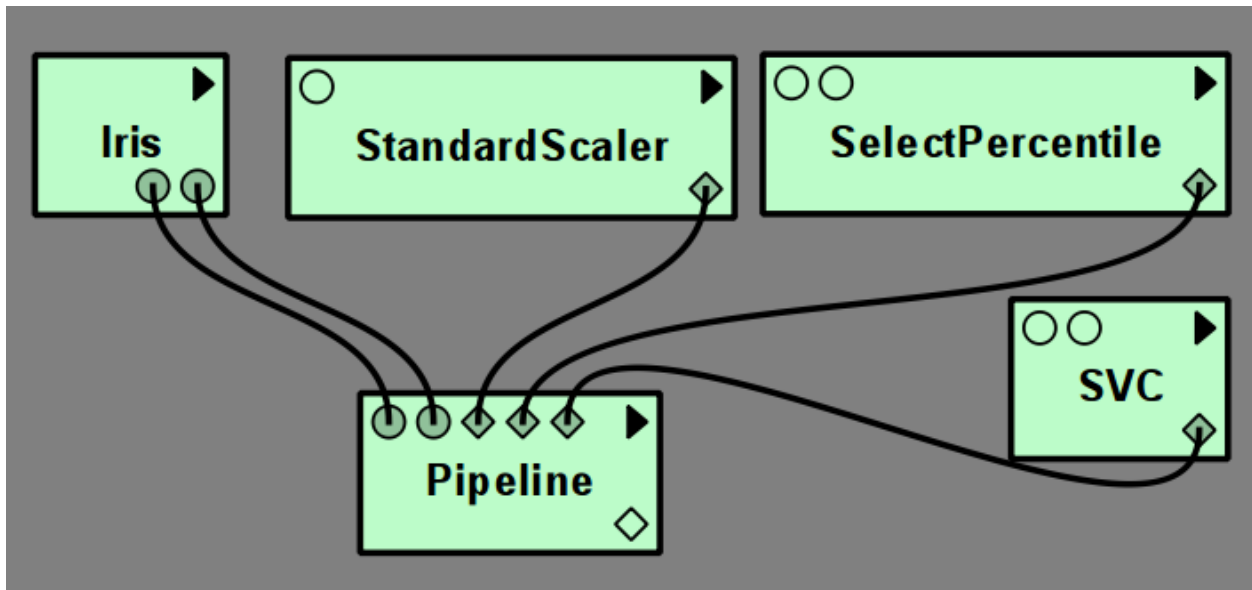
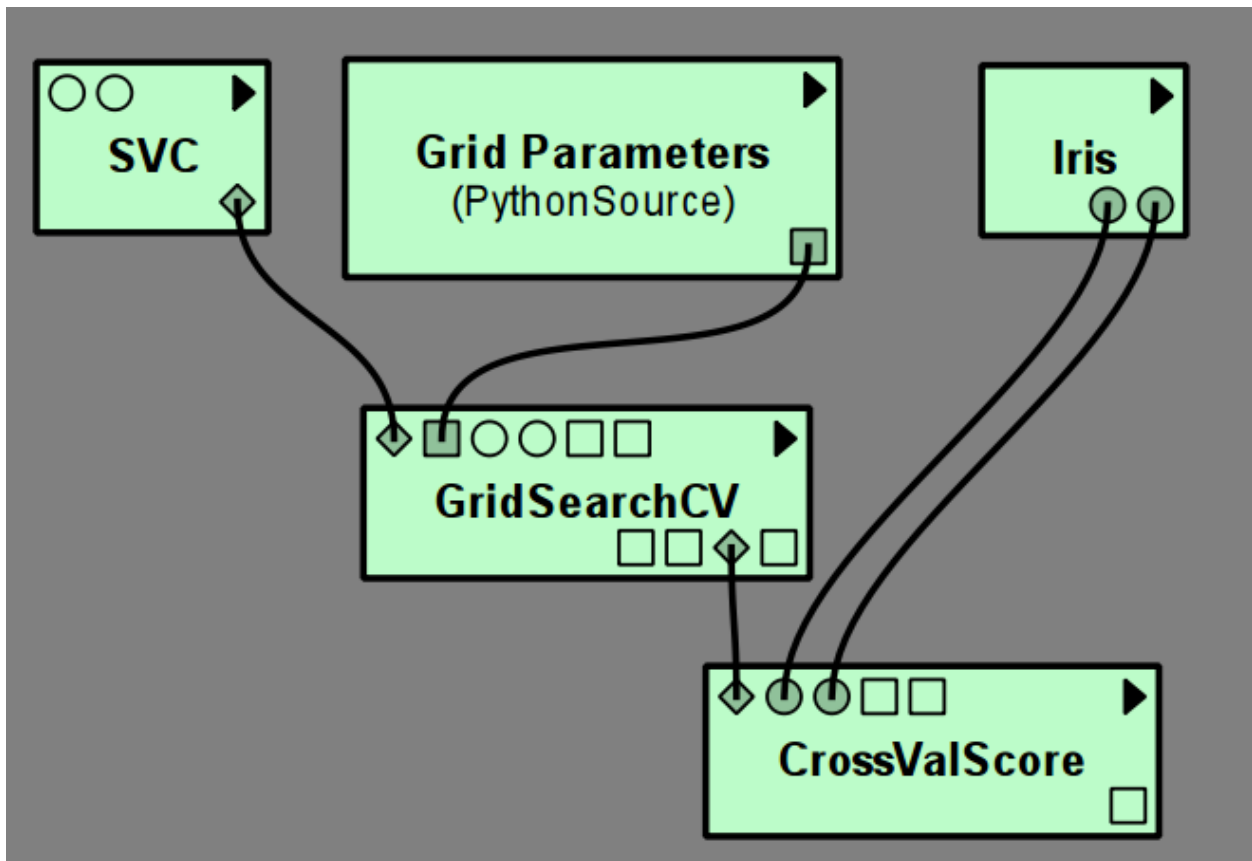
```

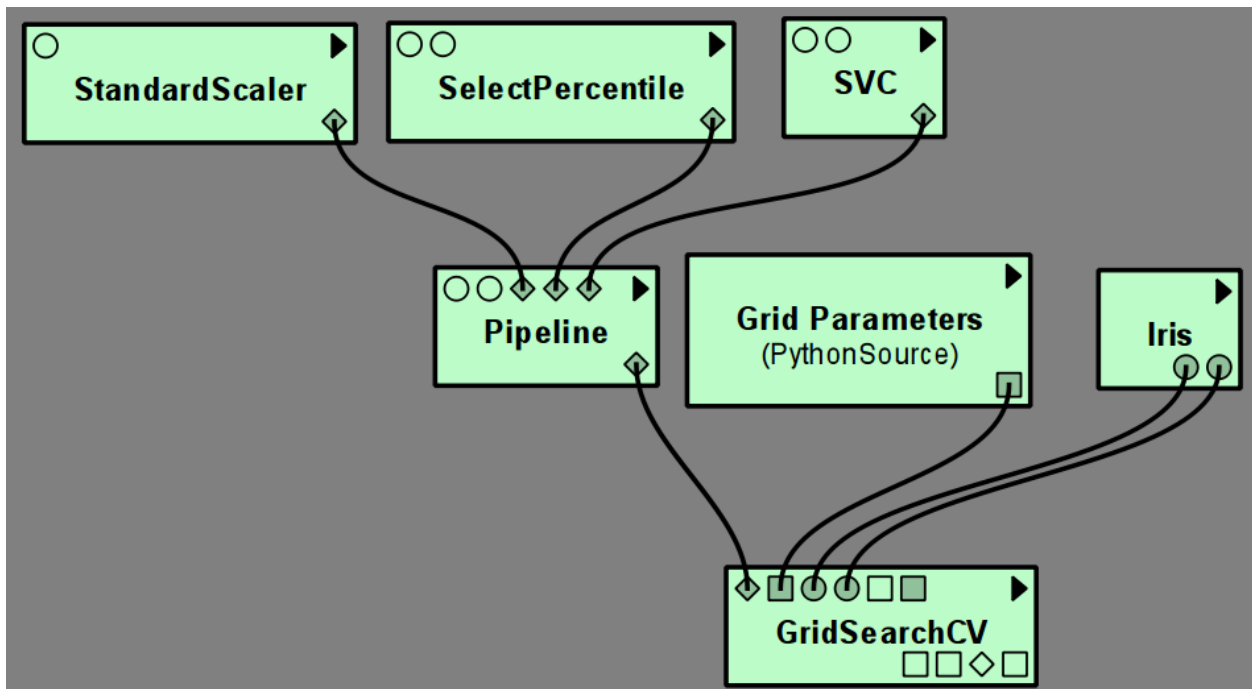
1 import numpy as np
2 parameters = {'C': 10. ** np.arange(-3, 3),
3 'gamma': 10. ** np.arange(-3, 3)}

```

Line: 1 / Col: 1

Show read-only window Save Reset





Part II

Developer's Guide

WRITING VISTRAILS PACKAGES

5.1 Introduction

VisTrails provides a plugin infrastructure to integrate user-defined functions and libraries. Specifically, users can incorporate their own visualization and simulation code into pipelines by defining custom modules (or wrappers). These modules are bundled in what we call *packages*. A VisTrails package is simply a collection of Python classes stored in one or more files, respecting some conventions that will be described shortly. Each of these classes will represent a new module. In this chapter, we will build progressively more complicated modules. Note that even though each section introduces a specific large feature of the VisTrails package mechanism, new small features are highlighted and explained as we go along. Because of this, we recommend at least skimming through the entire chapter at least once.

5.2 Who Should Read This Chapter?

This chapter is written for developers who wish to extend VisTrails with customized modules, tailored for their specific needs. It is assumed that you have experience writing code in the Python programming language. Teaching the syntax of Python is beyond the scope of this manual; for experienced programmers who would like a compact introduction to Python, we recommend the book *Python in a Nutshell* by Alex Martelli (published by O'Reilly).

However, if you do not yet know Python but are familiar with another object-oriented language such as Java or C#, you should be able to get the gist of these examples from looking at the code and by reading our line-by-line commentaries.

5.3 An Example Module

Here is the definition of a very simple module:

```
1 class Divide(Module):
2     _input_ports = [IPort(name='arg1',\
3                          signature='basic:Float',\
4                          label="dividend"),
5                    IPort(name='arg2',\
6                          signature='basic:Float',\
7                          label='divisor')]
8     _output_ports = [OPort(name='result',\
9                            signature='basic:Float',\
10                           label='quotient')]
11
12     def compute(self):
13         arg1 = self.get_input("arg1")
```

```

14     arg2 = self.get_input("arg2")
15     if arg2 == 0.0:
16         raise ModuleError(self, "Division by zero")
17     self.set_output("result", arg1 / arg2)

```

New VisTrails modules must subclass from *Module*, the base class that defines basic functionality. The only required override is the *compute()* method, which performs the actual module computation. Input and output is specified through ports, which must be explicitly registered with VisTrails using the *_input_ports* and *_output_ports* lists. Simple ports are specified using *InputPort* (*IPort*) and *OutputPort* (*OPort*) objects.

5.4 An Example Package

The previous section only shows the definition of a single module. To create a full package that loads and runs in VisTrails, a few more items are required. In this example, we define a basic calculator package named *PythonCalc*. Note that this package includes *two* files, *__init__.py* and *init.py* that live in a directory named *pythonCalc*; each file is an important piece of a VisTrails package.

__init__.py

```

1  """This package implements a very simple VisTrails module called
2  PythonCalc. This is intended as a simple example that can be referred
3  to by users to create their own packages and modules later.
4
5  If you're interested in developing new modules for VisTrails, you
6  should also consult the documentation in the User's Guide and in
7  core/modules/vistrails_module.py.
8  """
9
10 identifier = 'org.vistrails.vistrails.pythoncalc'
11 name = 'PythonCalc'
12 version = '0.9.2'

```

init.py

```

1  #####
2  # PythonCalc
3  #
4  # A VisTrails package is simply a Python class that subclasses from
5  # Module. For this class to be executable, it must define a method
6  # compute(self) that will perform the appropriate computations and set
7  # the results.
8  #
9  # Extra helper methods can be defined, as usual. In this case, we're
10 # using a helper method op(self, v1, v2) that performs the right
11 # operations.
12
13 from vistrails.core.modules.vistrails_module import Module, ModuleError
14 from vistrails.core.modules.config import IPort, OPort
15
16 class PythonCalc(Module):
17     """PythonCalc is a module that performs simple arithmetic operations
18     on its inputs."""
19
20     # You need to report the ports the module wants to make
21     # available. This is done by creating _input_ports and
22     # _output_ports lists composed of InputPort (IPort) and OutputPort
23     # (OPort) objects. These are simple ports that take only one

```

```

24 # value. We'll see in later tutorials how to create compound ports
25 # which can take a tuple of values. Each port must specify its
26 # name and signature. The signature specifies the package
27 # (e.g. "basic" which is shorthand for
28 # "org.vistrails.vistrails.basic") and module (e.g. "Float").
29 # Note that the third input port (op) has two other arguments.
30 # The "enum" entry_type specifies that there are a set of options
31 # the user should choose from, and the values then specifies those
32 # options.
33 _input_ports = [IPort(name="value1", signature="basic:Float"),
34                 IPort(name="value2", signature="basic:Float"),
35                 IPort(name="op", signature="basic:String",
36                       entry_type="enum", values=["+", "-", "*", "/])]
37 _output_ports = [OPort(name="value", signature="basic:Float")]
38
39 # This constructor is strictly unnecessary. However, some modules
40 # might want to initialize per-object data. When implementing your
41 # own constructor, remember that it must not take any extra
42 # parameters.
43 def __init__(self):
44     Module.__init__(self)
45
46 # This is the method you should implement in every module that
47 # will be executed directly. VisTrails does not use the return
48 # value of this method.
49 def compute(self):
50     # get_input is a method defined in Module that returns
51     # the value stored at an input port. If there's no value
52     # stored on the port, the method will return None.
53     v1 = self.get_input("value1")
54     v2 = self.get_input("value2")
55
56     # You should call set_output to store the appropriate results
57     # on the ports. In this case, we are only storing a
58     # floating-point result, so we can use the number types
59     # directly. For more complicated data, you should
60     # return an instance of a VisTrails Module. This will be made
61     # clear in further examples that use these more complicated data.
62     self.set_output("value", self.op(v1, v2))
63
64 def op(self, v1, v2):
65     op = self.get_input("op")
66     if op == '+':
67         return v1 + v2
68     elif op == '-':
69         return v1 - v2
70     elif op == '*':
71         return v1 * v2
72     elif op == '/':
73         return v1 / v2
74     # If a module wants to report an error to VisTrails, it should raise
75     # ModuleError with a descriptive error. This allows the interpreter
76     # to capture the error and report it to the caller of the evaluation
77     # function.
78     raise ModuleError(self, "unrecognized operation: '%s'" % op)
79
80 # VisTrails will only load the modules specified in the _modules list.
81 # This list contains all of the modules a package defines.

```

```
82 _modules = [PythonCalc,]
```

To create and install this package in VisTrails, first create a new directory named `pythonCalc` in the `.vistrails/userpackages` subdirectory of your home directory. Then, save the two code blocks above to the corresponding `__init__.py` and `init.py` files in the newly created `pythonCalc` directory. Now, click on the Edit menu (or the VisTrails menu on Mac OS X), select the Preferences option and select the Module Packages tab. A dialog similar to what is shown in Figure *All available packages...* should appear. Select the `pythonCalc` package, then click on Enable. This should move the package to the Enabled packages list. Close the dialog. The package and module should now be visible in the VisTrails builder.

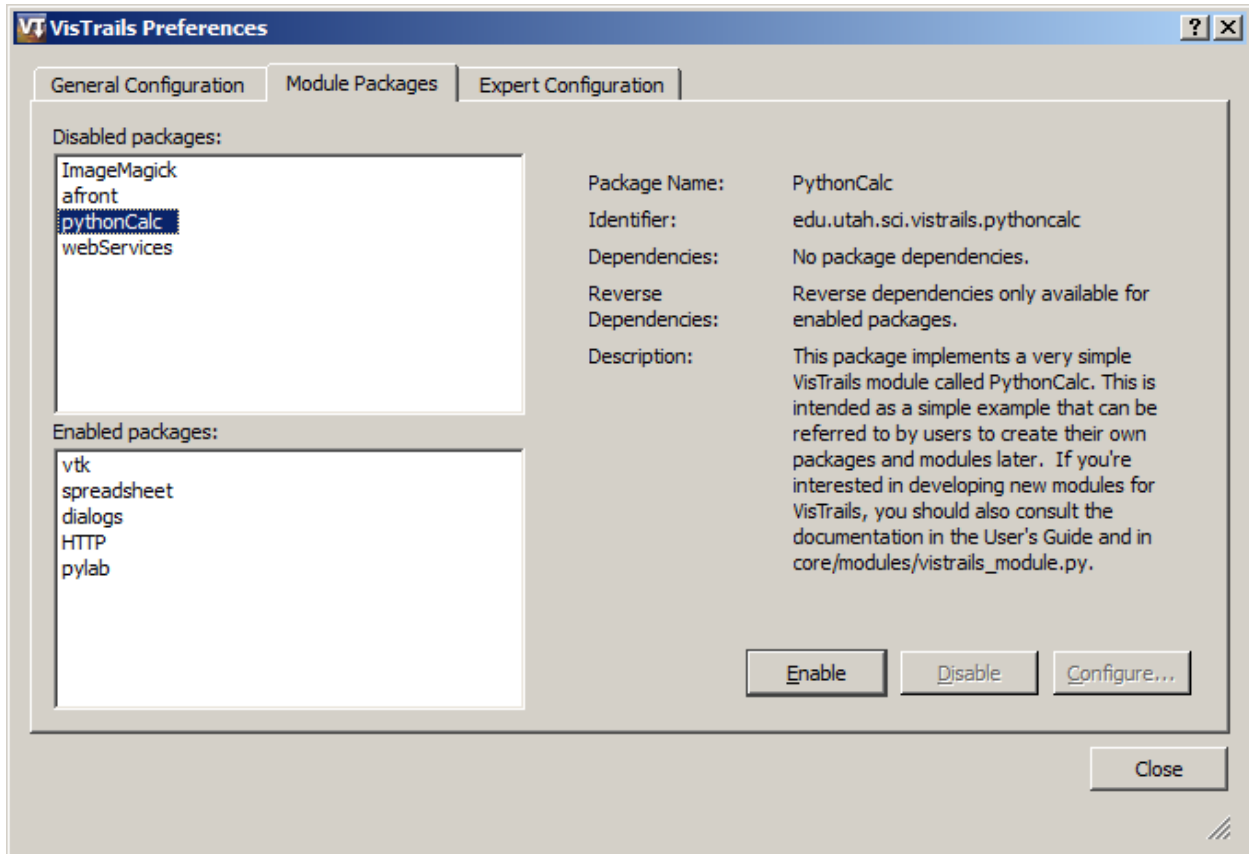


Fig. 5.1: All available packages can be enabled and disabled with the VisTrails preferences dialog.

Now create a workflow similar to what is shown in Figure *A simple workflow that uses PythonCalc...* When executed, this workflow will print the following on your terminal:

```
7.0
```

Let's now examine how this works. The `__init__.py` file provides metadata about the package. `Version` is simply information about the package version. This might be tied to the underlying library or not. The only recommended guideline is that compatibility is not broken across minor releases, but this is not enforced in any way. `Name` is a human-readable name for the package.

The most important piece of metadata, however, is the package *identifier*, stored in the variable called `identifier`. This is a string that must be globally unique across all packages, not only in your system, but in any possible system. We recommend using an identifier similar to Java's package identifiers. These look essentially like regular DNS names, but the word order is reversed. This makes sorting on the strings a lot more meaningful. You should generally go for

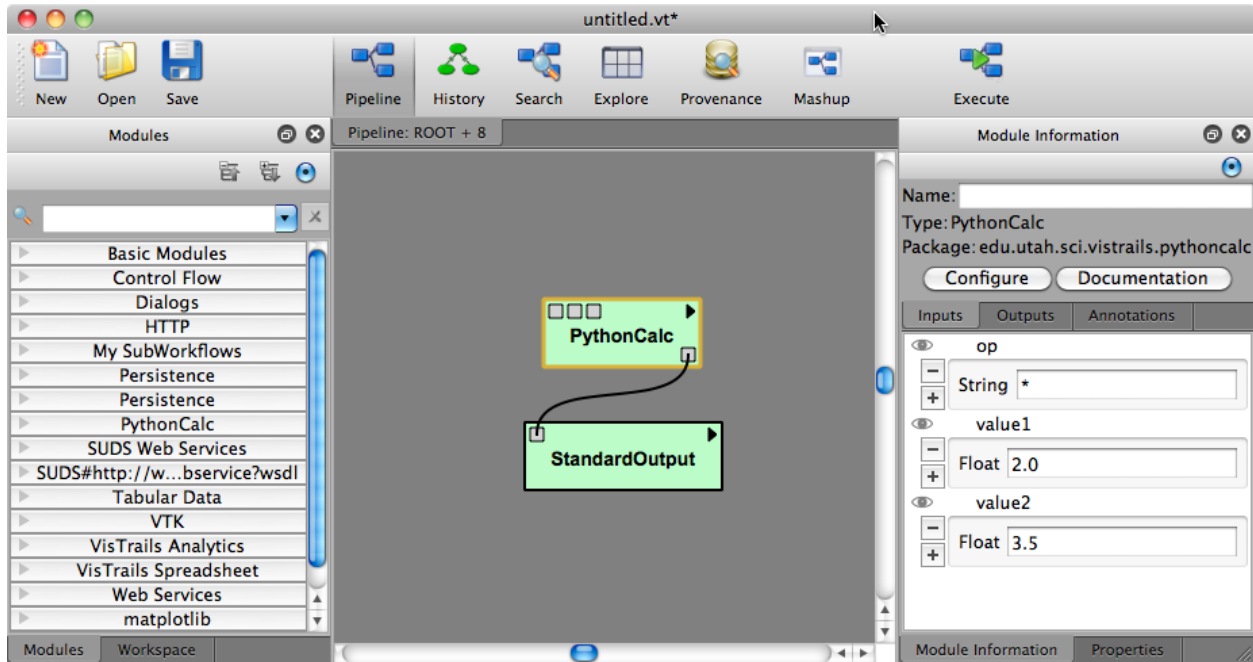


Fig. 5.2: A simple workflow that uses `PythonCalc`, a user-defined module.

`institution.project.packagename` for a package related to a certain project from some institution, and `institution.creatorname` for a personally developed package. If you are wrapping third-party functionality, *do not* use their institution's DNS, use your own. The rationale for this is that the third party itself might decide to create their own VisTrails package, and you do not want to introduce conflicts.

The `init.py` file contains the actual definitions of the modules. Every VisTrails module corresponds to a Python class that ultimately derives from the `Module` class, which is defined in `vistrails.core.modules.vistrails_module`. Each module must define input ports and output ports as well as implement a `compute()` method that takes no extra parameters.

We need to tell VisTrails about the input and output ports we want to expose in a module. Input ports are set in the `_input_ports` list and output ports in the `_output_ports` list. Each object in these lists is defined from a type from `vistrails.core.modules.config`. The most basic port types are `InputPort` (aka `IPort`) and `OutputPort` (aka `OPort`). Each requires two arguments, the *name* of the port and the *signature* of the port. A name may be any string, but must be unique across all inputs or outputs. The same name may be used both for an input and an output. The signature defines the type of the port; VisTrails allows any module to also be a type. A signature is a string composed of the module's package identifier followed by a colon and the module's name. Many basic module types including `String`, `Float`, and `Integer` are defined by VisTrails in the Basic Modules package. Thus, the `Float` module's signature is `org.vistrails.vistrails.basic:Float`. Any core package that is distributed with VisTrails has an identifier that begins `org.vistrails.vistrails` and thus you may omit that prefix for brevity; `basic:Float` defines the same signature. There are a number of other options for ports, but we will cover these later.

The `compute` method on Line 49 defines the actual computation that happens in a module. This computation typically involves getting the necessary input and generating the output. Lines 53-54 shows how to extract input from a port. Specifically, we're getting the values passed to input ports `value1` and `value2`. We then perform some operation with these values, and need to report the output on an output port, so that it is available for downstream modules. This is done on Line 62, where the result is set to port `value`.

Let us now look more carefully at the remainder of the class definition. Notice that developers are allowed to define

extra helper methods, for example the `op` method on Line 64. These helper methods can naturally use the ports API. The other important feature of the `op` method is *error checking*. `PythonCalc` requires a string that represents the operation to be performed with the two numbers. If the string is invalid, it signals an error by simply raising a Python exception, `ModuleError`, that is provided in `vistrails.core.modules.vistrails_module`. This exception expects two parameters: the module that generated the exception (typically `self`) and a string describing the error. In the Pipeline view, this error message is displayed in the tooltip that appears when the user moves the cursor over the `PythonCalc` module icon.

The final step is to specify the list of modules your package defines. This is done via the `_modules` list which is simply a list of all the modules the package wishes to define. Leaving a class out of that list will mean it will *not appear* as an available module for use in VisTrails. That is it — you have successfully created a new package and module. From now on, we will look at more complicated examples, and more advanced features of the package mechanism.

Note

Older versions of VisTrails used explicit calls to the `ModuleRegistry` in an `initialize()` method. These calls like `ModuleRegistry.add_module()`, `ModuleRegistry.add_input_port()`, and `ModuleRegistry.add_output_port()` are still supported though their use is discouraged as the new syntax places all attributes and configuration options in the module definition, making code more readable and localized. The arguments available in the registry functions are mirrored in the new configuration objects used for `_settings`, `_input_ports`, and `_output_ports`.

5.5 Package Specification

5.5.1 Structure

A package should contain the following files inside a directory named for the package:

- `__init__.py` – identifiers and configuration
- `init.py` – modules, other imports

Optionally, it might also contain:

- `identifiers.py` – the identifiers might be specified here and imported in `__init__.py`
- `widgets.py` – any GUI widgets the package’s modules use
- any other files and/or python submodules that the package depends on in

The reason for the separation between `__init__.py` and `init.py` is that VisTrails inspects packages for identification, configurations, and information to populate the list of available packages, and for large packages with dependent libraries, including everything (including the subpackage imports) in `__init__.py` would take significant time. Thus, we encourage package developers to define modules and include sub-imports only from `init.py` to speed up loading times. The optional `identifiers.py` allows developers to import configuration information, like the identifier and version, into both `__init__.py` and `init.py`. Then, `__init__.py` may consist of the line `from identifiers import *`. `widgets.py` is a suggested separation between GUI configuration widgets and the module definitions because VisTrails can run in batch mode or as a python package without Qt/PyQt, and if the widgets are imported into or defined from `init.py`, VisTrails will unnecessarily try to import the Qt/PyQt libraries. Instead, modules can define their configuration widgets as *path strings* (see [Configuration Widgets](#)), and the widgets will only be imported when the GUI is running.

Most third-party packages should be installed into a user’s `~/vistrails/userpackages` directory. The package’s `codepath` is the name of the directory in that `userpackages` directory. A few third-party packages install

into the `packages` directory of the VisTrails codebase due to specific dependencies or to install for all users of the application. If you are interested in such installation features, please contact us.

The `identifier`, `name`, `version`, `configuration`, and `package_dependencies` fields/methods should be specified or imported into `__init__.py`. An example of `__init__.py` from VisTrails' `matplotlib` package follows.

```

1 identifier = 'org.vistrails.vistrails.matplotlib'
2 name = 'matplotlib'
3 version = '1.0.1'
4 old_identifiers = ['edu.utah.sci.vistrails.matplotlib']
5
6 def package_dependencies():
7     import vistrails.core.packagemanager
8     manager = vistrails.core.packagemanager.get_package_manager()
9     if manager.has_package('org.vistrails.vistrails.spreadsheet'):
10        return ['org.vistrails.vistrails.spreadsheet']
11    else:
12        return []
13
14 def package_requirements():
15    import vistrails.core.requirements
16    if not vistrails.core.requirements.python_module_exists('matplotlib'):
17        raise vistrails.core.requirements.MissingRequirement('matplotlib')
18    if not vistrails.core.requirements.python_module_exists('pylab'):
19        raise vistrails.core.requirements.MissingRequirement('pylab')

```

The `old_identifiers` field is used to identify packages whose identifiers have changed. This allows VisTrails to migrate old vistrails to the new packages. Other imports (excluding `vistrails.core.configuration`), other class definitions, and the `initialize` method should be in the `init.py` file.

5.5.2 Configuration

In addition to “pure-python” packages, VisTrails packages can also be designed to wrap existing libraries and command-line tools (see *Wrapping Command-line tools* for more information). For command-line tools, there are often some configuration options that may change from machine to machine. In addition, there may also be flags (e.g. for debugging) that a user may wish to toggle on or off depending on the situation. VisTrails provides the configuration package attribute for such situations; the `ConfigurationObject` stored here is accessible both during module computations and from the GUI in the `Preferences` dialog.

In the following example, we have some code from a package designed to control runs of `afrofront`, a command-line program for generating 3D triangle meshes.¹ It uses a general `run()` method to run each command, and we use the configuration object to determine where the executable lives and whether we should print debugging information.

```

1 import os
2
3 from vistrails.core.configuration import ConfigurationObject
4 from vistrails.core.modules.vistrails_module import Module, ModuleError
5 from vistrails.core.system import list2cmdline
6
7 configuration = ConfigurationObject(path=(None, str),
8                                   debug=False)
9
10 class AfrofrontRun(object):
11
12     def run(self, args):

```

¹ This package is not included in binary distributions of VisTrails, but is available in the source code distribution. The stand-alone `Afront` utility is available at <http://afrofront.sourceforge.net>.

```

13     if configuration.check('path'): # there's a set directory
14         afront_cmd = os.path.join(configuration.path, 'afront')
15     else: # Assume afront is on path
16         afront_cmd = 'afront'
17     cmd = [afront_cmd, '-nogui'] + args
18     cmdline = list2cmdline(cmd)
19     if configuration.debug:
20         print cmdline
21     ...
22 ...

```

Let us first look at how to specify configuration options. Named arguments passed to the `ConfigurationObject` constructor (Lines 6 and 7) become attributes in the object. If the attribute has a default value, simply pass it to the constructor. If the attribute should be unset by default, pass the constructor a pair whose first element is `None` and second element is the *type* of the expected parameter. Currently, the valid types are `bool`, `int`, `float` and `str`.

To use the configuration object in your code, you can simply access the attributes (as on line 18). This is fine when there is a default value set for the attribute. In the case of `path`, however, the absence of a value is encoded by a tuple (`None`, `str`), so using it directly is inconvenient. That is where the `check()` method comes in (line 12). It returns `False` if there is no set value, and returns the value otherwise.

Perhaps the biggest advantage of using a configuration object is that the values can be changed through a GUI, and they are persistent across VisTrails sessions. To configure a package, open the Preferences menu (VisTrails → Preferences on Mac OS X, or Edit → Preferences on other platforms). Then, select the package you want to configure by clicking on it (a package must be enabled to be configurable). If the Configure button is disabled, it means the package does not have a configuration object. When you do click Configure, a dialog like the one in Figure *Configuration window for a package...* will appear.

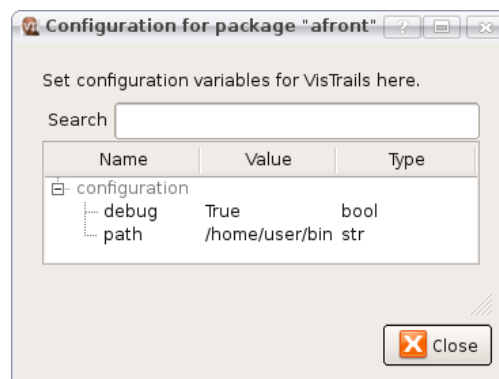


Fig. 5.3: Configuration window for a package that provides a configuration object.

To edit the value for a particular field, double-click on it, and change the value. The values set in this dialog are persistent across VisTrails sessions, being saved on a per-user basis.

5.5.3 Menu Items

As we saw in Section *Configuration*, using the `ConfigurationObject` class is one way to “hook” your custom package into the VisTrails GUI. However, this is not the only way to integrate your package with the user interface. VisTrails also supports a mechanism whereby your package can add new options underneath the Packages menu (Figure *Packages can integrate their own commands...*).

This is done by adding a function named `menu_items` to your main package file. This function takes no parameters, and should return a tuple of pairs for each new menu item to be added. The first element of each pair is the label of

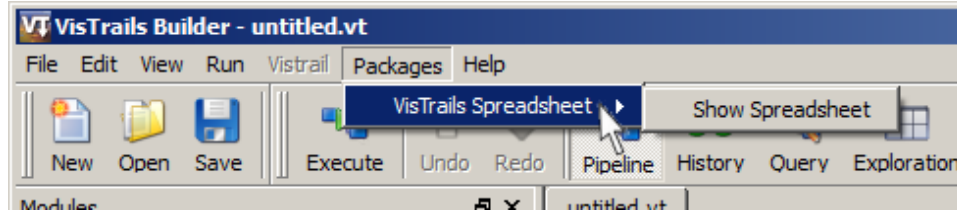


Fig. 5.4: Packages can integrate their own commands into the main VisTrails menu.

the menu item as it should appear in the GUI. The second element of the pair is the name of the callback function to be invoked when the user selects that menu item.

As an example, we include below the implementation of `menu_items` from the VisTrails Spreadsheet package:

```

1 def menu_items():
2     """menu_items() -> tuple of (str,function)
3     It returns a list of pairs containing text for the menu and a
4     callback function that will be executed when that menu item is selected.
5     """
6
7     def show_spreadsheet():
8         spreadsheetWindow.show()
9         lst = []
10        lst.append(("Show Spreadsheet", show_spreadsheet))
11        return tuple(lst)

```

Writing your own `menu_items` function is straightforward; simply use the provided example as a basis, and substitute labels and callback functions as appropriate for your specific module. Although the Spreadsheet package currently only implements one new menu option, you are free to add as many as you see fit; just append additional pairs to the list (see Line 10 of the example code) before the function returns.

The Packages menu is organized hierarchically, as illustrated in Figure *Packages can integrate their own commands...* Each package that contributes a `menu_items` function will receive an entry in the Packages menu. The actual menu items for each package will appear in a submenu.

5.5.4 Dependencies

When creating more sophisticated VisTrails packages, you might want to create a new module that requires a module *from another package*. For example, using modules from different packages as input ports, or even subclassing modules from other packages, require management of interpackage dependencies. VisTrails needs to know about these so that packages can be initialized in the correct order. To specify these dependencies, you should add a function named `package_dependencies` to your package. This function should return a list containing the identifier strings of the required packages.

As an example of this function's usage, let's take a look at a (simplified) code segment from the VTK package, which is included in the standard VisTrails distribution:

```

1 def package_dependencies():
2     return ['org.vistrails.vistrails.spreadsheet']

```

As you can see, the `package_dependencies` function is quite straightforward; it simply returns a list of the identifiers for the packages required by the VTK package. In this case, the list contains just a single string, as the VisTrails Spreadsheet is the only package dependency for the VTK package.

The simple approach taken by the above code works well for the majority of cases, but in practice you may want to add some error-checking to your `package_dependencies` function. This allows VisTrails to recover gracefully

in the unlikely event that the Spreadsheet package is missing. Below is the complete `package_dependencies` function for the VTK package:

```
1 def package_dependencies():
2     import vistrails.core.packagemanager
3     manager = vistrails.core.packagemanager.get_package_manager()
4     if manager.has_package('org.vistrails.vistrails.spreadsheet'):
5         return ['org.vistrails.vistrails.spreadsheet']
6     else:
7         return []
```

The above code segment also demonstrates the VisTrails API function `has_package` which simply verifies that a given package exists in the system.

5.5.5 Requirements

In Section *Dependencies*, we saw how packages can depend on other packages. However, some packages may also depend on the presence of external libraries (in the form of Python modules) or executable files in order to run correctly.

Python Modules

To check for the presence of a required Python module, you should add a function named `package_requirements` to your package. This function need not return any value; however it may raise exceptions or output error messages as necessary. Here is an example of the syntax of the `package_requirements` function, taken from the VisTrails VTK package:

```
1 def package_requirements():
2     import vistrails.core.requirements
3     if not vistrails.core.requirements.python_module_exists('vtk'):
4         raise vistrails.core.requirements.MissingRequirement('vtk')
5     if not vistrails.core.requirements.python_module_exists('PyQt4'):
6         print 'PyQt4 is not available. There will be no interaction',
7         print 'between VTK and the spreadsheet.'
8     import vtk
```

A key element of `package_requirements` is the use of the function `python_module_exists` (see Lines 3 and 5), which checks whether a given module has been installed in your local Python system.

Automatically Installation

A more advanced method is to attempt to install a python module automatically using a system package manager. This method currently works for apt- and rpm-based systems. By using `core.bundles.py_import`, you can attempt to automatically install a system dependency, all you need to specify is the python module name and the name of the package that contains it. The following example can be put in your `init.py` file, with the desired module and package names changed:

```
1 from vistrails.core.bundles import py_import
2 from vistrails.core import debug
3 try:
4     pkg_dict = {'linux-ubuntu': 'your-apt-package',
5               'linux-fedora': 'your-deb-package'}
6     your-py-module = py_import('your-py-module', pkg_dict)
7 except Exception, e:
8     debug.critical("Exception: %s" % e)
```

Note that, if you use this method, you should not specify it in the `package_requirements`, because that would block the install attempt.

Executables

As explained in Section *Wrapping Command-line tools*, a common motivation for writing new VisTrails modules is to wrap existing command-line tools. To this end, the VisTrails API provides a function called `executable_file_exists` which checks for the presence of specific executables on the path.

Here is an example of its usage, taken from the `initialize` function of the `ImageMagick` package. This package is included in the standard VisTrails distribution. The following code snippet checks to see if `convert`, a command-line program associated with the *ImageMagick* suite of graphics utilities, is on the path.

```

1 import vistrails.core.requirements
2
3 ...
4
5     if (not vistrails.core.requirements.executable_file_exists('convert')):
6         raise vistrails.core.requirements.MissingRequirement("ImageMagick suite")

```

Note that this function is not strictly required in order to wrap third party executables into a module. Using a `Configuration` object (see Section *Configuration*) that lets the user specify the path to an executable may be a cleaner solution.

For additional information or examples of any of the functions described above, please refer to the VisTrails source code or contact the VisTrails development team.

5.5.6 Upgrades

When revising a package, it is important that workflows containing old modules can be translated to their corresponding new versions. If no upgrade is explicitly specified, VisTrails attempts to automatically upgrade the old module to the new version. However, if a module's interface has changed (e.g. a port was added or removed or the name was changed), the automated upgrade will fail. For such cases, VisTrails provides hooks for developers to specify the upgrade paths. The recommended method is to use the `_upgrades` attribute in the package to specify a dictionary where each key is a module name and the corresponding value is a list of potential upgrade paths for those modules. The upgrade path is specified by an `UpgradeModuleRemap` instance which specifies the versions for which the upgrade is valid, the output version, the new module, and a set of remaps for module entities. For example,

```

1 _upgrades = {"TestUpgradeA":
2     [UpgradeModuleRemap('0.8', '0.9', '0.9', None,
3         function_remap={'a': 'aa'},
4         src_port_remap={'z': 'zz'}),
5     UpgradeModuleRemap('0.9', '1.0', '1.0', None,
6         function_remap={'aa': 'aaa'},
7         src_port_remap={'zz': 'zzz'})]}

```

Here, we have two upgrade paths for the module `TestUpgradeA`. The first works for version 0.8 through—but not including—0.9, and the second for 0.9 to 1.0. The output versions are 0.9 and 1.0, respectively, and both specify `None` as the new module type which means that the new module has the same name as the old one. The new module type could also be a string representing a different module name. There are four remap types: `function_remap`, `src_port_remap`, `dst_port_remap`, and `annotation_remap`. Each one is a dictionary where the name of affected function, port, or annotation is the key and the value specifies either the output name (if this is just a name change) or a function to be used to perform the remap. For example, one might write a method that transforms the value of a temperature parameter from Fahrenheit to Celsius. Such a method should return a list of actions that accomplish this change. Note that because the `dst_port_remap` and `function_remap` both affect input ports, any remaps for `dst_port_remap` are also used for functions unless explicitly overridden.

If you require more control over the upgrade process, you may also define a `handle_module_upgrade_request` method in the VisTrails package. It will be passed the controller, id of the module needing an upgrade, and the current pipeline as inputs, and should return a set of actions that will upgrade that single module to the latest version.

5.6 Module Specification

In this section, we will explore different options for specifying modules and associated attributes, including those which affect their appearance and organization in the GUI. Details about all of the options available for modules can be found in the *VisTrails API Documentation*. VisTrails provides the `ModuleSettings` class to offer a number of configuration options for modules. A module should define the `_settings` attribute in the class to use these settings.

5.6.1 Caching

VisTrails provides a caching mechanism, in which portions of pipelines that are common across different executions are automatically shared. However, some modules should not be shared. Caching control is therefore up to the package developer. By default, caching is enabled. So a developer that doesn't want caching to apply must make small changes to the module. For example, look at the `StandardOutput` module:

```
from vistrails.core.modules.vistrails_module import Module, newModule, NotCacheable, ModuleError
from vistrails.core.modules.config import IPort

...

class StandardOutput(NotCacheable, Module):
    """StandardOutput is a VisTrails Module that simply prints the
    value connected on its port to standard output. It is intended
    mostly as a debugging device."""

    _input_ports = [IPort(name="value", signature="basic:Module")]

    def compute(self):
        v = self.get_input("value")
        print v
```

By subclassing from `NotCacheable` and `Module` (or one of its subclasses), we are telling VisTrails not to cache this module, or anything downstream from it.

VisTrails also allows a more sophisticated decision on whether or not to use caching. To do that, a user simply overrides the method `is_cacheable` to return the appropriate value (the default implementation returns `True`). For example, in the *teem* <<http://teem.sourceforge.net/>> package, there's a module that generates a scalar field with random numbers. This is non-deterministic, so shouldn't be cached. However, this module only generates non-deterministic values in special occasions, depending on its input port values. To keep efficiency when caching is possible, while still maintaining correctness, that module implements the following override:

```
class Unu1op(Unu):
    (...)
    def is_cacheable(self):
        return not self.get_input('op') in ['rand', 'nrand']
    (...)
```

Notice that the module explicitly uses inputs to decide whether it should be cached. This allows reasonably fine-grained control over the process.

5.6.2 Namespaces

`ModuleSettings.namespace` can be used to define a hierarchy for modules in a package that is used to organize the module palette. Hierarchies can be nested through the use of the ‘|’ character. For example,

```

1 class MyModule1(Module):
2     _settings = ModuleSettings(namespace="MyNamespace")
3     ...
4
5 class MyModule2(Module):
6     _settings = ModuleSettings(namespace="ParentNamespace|\
7                                 ChildNamespace")
8     ...

```

5.6.3 Documentation

The docstring you set on your `Module` subclass will be displayed to the user when he clicks on the ‘Documentation’ button in the ‘Module Information’ panel. Be sure to put a readable description and your usage information there.

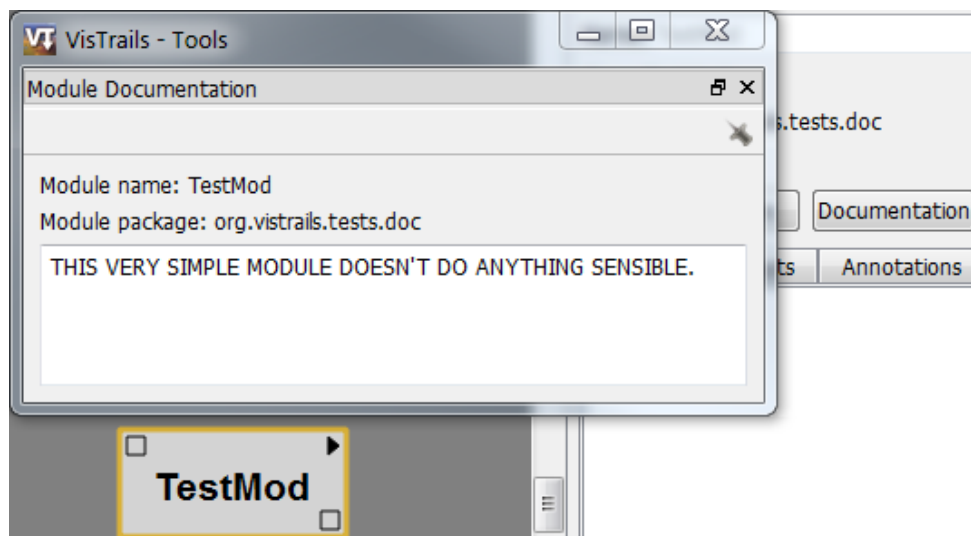
If you want to customize that documentation, you can provide a staticmethod or classmethod ‘`get_documentation`’ on your `Module`. The string it returns will be used as the documentation.

```

1 class TestMod(Module):
2     """This very simple module doesn't do anything sensible.
3     """
4
5     @classmethod
6     def get_documentation(cls, docstring, module=None):
7         return docstring.upper()

```

The function receives two arguments: the string that was about to be used (the module’s docstring or an empty string), and the module object from the pipeline if the documentation was requested for a specific instance of that module (else, `None` is passed).



5.6.4 Visibility

`ModuleSettings.abstract` and `ModuleSettings.hide_descriptor` can be used to prevent modules from appearing in the module palette. `abstract` is for use with modules that should never be instantiated in the workflow and will not add the item to the module palette. On the other hand, `hide_descriptor` will add the item to the palette, but hides it. This will prevent users from adding the module to a pipeline, but allow code to add it programmatically. To use either of these options, `abstract` or `hide_descriptor`, set it to `True`:

```

1 class AbstractModule(Module):
2     _settings = ModuleSettings(abstract=True)
3     ...
4
5 class InvisibleModule(Module):
6     _settings = ModuleSettings(hide_descriptor=True)
7     ...

```

5.6.5 Shape and Color

VisTrails allows users to assign custom colors and shapes to modules by using the `ModuleSettings.color` and `ModuleSettings.fringe` options. For example,

```

class FancyModule(Module):
    _settings = ModuleSettings(color=(1.0, 0.0, 0.0),
                               fringe=[(0.0, 0.0),
                                       (0.2, 0.0),
                                       (0.2, 0.4),
                                       (0.0, 0.4),
                                       (0.0, 1.0)])

```

produces



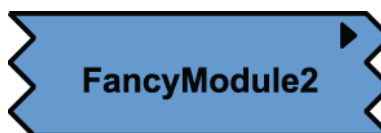
and

```

class FancyModule2(Module):
    _settings = ModuleSettings(color=(0.4, 0.6, 0.8),
                               fringe=[(0.0, 0.0),
                                       (0.2, 0.0),
                                       (0.0, 0.2),
                                       (0.2, 0.4),
                                       (0.0, 0.6),
                                       (0.2, 0.8),
                                       (0.0, 1.0)])

```

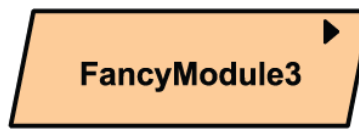
produces



The `ModuleSettings.color` parameter must be a tuple of three floats between 0 and 1 that specify RGB colors for the module background, while `ModuleSettings.fringe` is a list of pairs of floats that specify points as they go around a side of the module (the same one is used to go from the top-right corner to bottom-right corner, and from the bottom-left corner to the top-left one. If this is not enough, let the developers know!)

Alternatively, you may use different fringes for the left and right borders:

```
class FancyModule3(Module):
    _settings = ModuleSettings(color=(1.0,0.8,0.6),
                               left_fringe=[(0.0, 0.0),
                                             (-0.2, 0.0),
                                             (0.0, 1.0)],
                               right_fringe=[(0.0, 0.0),
                                              (0.2, 1.0),
                                              (0.0, 1.0)])
```



5.6.6 Configuration Widgets

There are two types of widgets that are associated with modules. The first, the *module configuration widget*, is available to all modules regardless of inheritance. This type of widget allows users to configure modules in ways other than with the ports list in the Module Information panel. For example, the PythonSource module uses a special widget that allows users to add ports as well as write code in a editor with line numbers and highlighting features. Developers wishing to create similar widgets should subclass from `vistrails.gui.modules.module_configure.StandardModuleConfigurationWidget` and implement the `saveTriggered` and `resetTriggered` methods. Note that both the *module* and *controller* are passed into the constructor and are available as `self.module` and `self.controller`.

The second type of widget is the *constant configuration widget* which can only be defined for constant modules, that is those which subclass from `vistrails.core.modules.basic_modules.Constant`. When such a module is used as the type of an input port, the user is allowed to edit the value in the ports list of the Module Information panel. The constant configuration widget is used to display and allow the user to edit the value of a parameter. The default widget is a simple line edit widget, but certain basic types in VisTrails like `Color` and `File` have specialized widgets that make specification easier.

Creation

Developers may build new constant configuration widgets using the `vistrails.gui.modules.constant_configuration.ConstantWidgetBase` or `vistrails.gui.modules.constant_configuration.ConstantEnumWidgetBase` base classes. **Note** that these base classes should be the *second* base class listed; the first should be a `QWidget` subclass. `ConstantWidgetBase` is intended for use with “normal” while `ConstantEnumWidgetBase` is intended for use with ports where the possible values are enumerated. For `ConstantWidgetBase` subclasses, developers should implement the `setContents` and `contents` methods and optionally the `setDefault` method. For `ConstantEnumWidgetBase` subclasses, developers should implement the `setValues` method and optionally the `setFree` and `setNonEmpty` methods.

As an example, consider the following widget:

```
1 from PyQt4 import QtCore, QtGui
2 from vistrails.gui.modules.constant_configuration import ConstantEnumWidgetBase
```

```

3
4 class NumericSliderWidget (QtGui.QSlider, ConstantEnumWidgetBase):
5     def __init__(self, param, parent=None):
6         QtGui.QSlider.__init__(self, parent)
7         self.setOrientation(QtCore.Qt.Horizontal)
8         self.setTracking(False)
9         self.setTickPosition(QtGui.QSlider.TicksBelow)
10        ConstantEnumWidgetBase.__init__(self, param)
11        self.connect(self, QtCore.SIGNAL("valueChanged(int)"),
12                    self.update_parent)
13
14        def setValues(self, values):
15            self.setMinimum(int(values[0]))
16            self.setMaximum(int(values[1]))
17
18        def contents(self):
19            return unicode(self.value())
20
21        def setContentts(self, contents, silent=True):
22            if contents:
23                self.setValue(int(contents))
24                if not silent:
25                    self.update_parent()

```

Registration

To make VisTrails aware of these new widgets, developers should specify them in the *ModuleSettings* options. For example,

```

1 class TestWidgets (Constant):
2     _settings = ModuleSettings (configure_widget="widgets:MyWidget",
3                               constant_widget="widgets:ConstWgt")

```

Note that the `PathString` is best specified relative to the base path of the package. **Important:** If `MyWidget` is defined in the `widgets` module of the `test_widgets` package in `userpackages`, its full path might be `userpackages.test_widgets.widgets:MyWidget`, but we only include the inner path (`widgets:MyWidget`). (The full path is used for internal packages, but this should be avoided for third-party packages.)

For constant widgets, VisTrails allows users to associate different widgets with different *uses*. A widget used for query may differ from the default display & edit widget, and developers may specify different widgets for these uses. Current uses include “query” and “paramexp” (parameter exploration). In addition, individual ports may specify different constant widgets using the *InputPort.entry_type* setting. These specifications are tied to the widget’s *type*. To specify these associations, developers should use the *ConstantWidgetConfig* settings. Also, *QueryWidgetConfig* and *ParamExpWidgetConfig* provide shortcuts for configurations for query and parameter exploration uses, respectively. Multiple widgets can be specified via the `ModuleSettings.constant_widgets` setting. For example,

```

1 class TestWidgets (Constant):
2     _settings = ModuleSettings (constant_widgets=[
3         ConstantWidgetConfig (widget="widgets:MyEnumWidget",
4                               widget_type="enum"),
5         QueryWidgetConfig (widget="widgets:MyQueryWidget")])

```

Note that if a query or parameter exploration widget is not specified, VisTrails will generically adapt the default widget for those uses so you do not need to create a widget for each use.

5.7 Port Specification

5.7.1 Defaults and Labels

In versions 2.0 and greater, package developers can add labels and default values for parameters. To add this functionality, you need to use the `default(s)` and `label(s)` keyword arguments. For example,

```

1 class TestDefaults (Module) :
2     _input_ports = [IPort ('word', 'basic:String',
3                           default="Hello",
4                           label="greeting"),
5                     CIPort ('center', 'basic:Float, basic:Float',
6                             defaults=[10.0, 10.0], labels=["x", "y"])]

```

Note that simple ports use the singular `InputPort.default` and `InputPort.label` kwargs while compound input ports use *plural* forms, `CompoundInputPort.defaults` and `CompoundInputPort.labels`.

5.7.2 Optional Ports

An optional port is one that will not be visible by default in the module shape. For modules with many ports, developers might less-used ports optional to reduce clutter. To make a port optional, set the `optional` flag to true:

```

1 class ModuleWithManyPorts (Module) :
2     _input_ports = [IPort ('Port14', 'basic:String',
3                           optional=True)]

```

5.7.3 Cardinality

By default, ports will accept any number of connections or parameters. However, the `Module.get_input()` method will only access *one* of the inputs, and which one is not well-defined. To access *all* of the inputs, developers should use the `Module.get_input_list()` method. The spreadsheet package uses this feature, so look there for usage examples ([vistrails/packages/spreadsheet/basic_widgets.py](#))

In addition, VisTrails 2.1 introduced new port configuration arguments `min_conns` and `max_conns` that allow developers to enforce specific cardinalities on their ports. For example, a port that required at least two inputs could set `min_conns=2`, and a port that does not accept more than a single input could set `max_conns=1`. Currently, the values for `min_conns` and `max_conns` default to 0 and -1, respectively, which means that no connections are required and any number of connections are allowed. These will eventually be enforced by the GUI to help users building workflows.

5.7.4 Shape

As with modules, port shape can also be customized. There are three basic types besides the default square, “triangle”, “circle”, and “diamond”. Such types are specified as string values to the `shape` setting. In addition, the triangle may be rotated by appending the degree of rotation (90, 180, or 270 only!) in the string. Finally, custom shapes are supported in a similar fashion to the module fringe. The shape should be defined in the [0,1] x [0,1] domain with 0 representing the top/left) and 1 being the bottom/right.

```

1 class FancyPorts (Module) :
2     _input_ports = [IPort ("normal", "basic:Float"),
3                     IPort ("triangle", "basic:Float",
4                             shape="triangle"),
5                     IPort ("triangle90", "basic:Float",

```

```

6         shape="triangle90"),
7         IPort("circle", "basic:Float",
8             shape="circle"),
9         IPort("diamond", "basic:Float",
10            shape="diamond"),
11        IPort("pentagon", "basic:Float",
12            shape=[(0.0, 0.0), (0.0, 0.66),
13                  (0.5, 1.0), (1.0, 0.66),
14                  (1.0, 0.0)])]

```

This produces a module with ports that look like the following figure:



5.7.5 Signatures

We recommend using strings to define ports, but we still allow the actual classes to be used instead for backward compatibility. For example,

```

1 from vistrails.core.modules.basic_modules import String
2
3 class MyModule(Module):
4     _input_ports = [IPort("a", String)]

```

This is **not recommended** for non-basic types due to the required import of the dependent package modules. If a package developer wants to use a module from another package, they must determine where in that package the module is defined, import that specific module, and then hope that future versions of that package do not change the location of that module. String-based signatures do not face the same issues as code reorganization is independent of the package definition. The grammar for a simple port signature is

```

1 <module_string> := <package_identifier>[:<namespace>|]<module_name>
2 <port_signature> := "<module_string>"

```

and for a compound port:

```

1 <compound_string> := ,<module_string>
2 <port_signature> := "<module_string><compound_string>*"

```

For example,

```

class MyModule(Module):
    _input_ports = ("myInputPort", "org.suborg.pkg_name:Namespace|ModuleB")

```

5.7.6 Variable Output

There may be cases where a port may output values of different types. There are a few ways to tackle this—each has its own benefits and pitfalls. Because VisTrails modules obey inheritance principles, a port of a given type may produce/accept subclasses of itself. For example, an output port of type `Constant` may output `String`, `Float`, or `Integer` values since all are subclasses of `Constant`. For input ports, `Module` (the base class for all modules) is the most general input type and will accept any input. For example, the `StandardOutput` module's input port

value is of type `Module` and it prints the string representation of the input value to `stdout`. However, for output ports, note that having an output of type `Module` is less useful because there may be cases where a user wishes to use a general output as an input to a port that accepts a specific type. For example, consider a `GetItem` module that takes a `List` module and a `Integer` parameter and outputs the element at the specified index. Its output port must be the most general type (e.g. `Module`), but that means that a user who knows the list only contains floats cannot pass the output to a calculator that only takes floats as inputs. To address this issue, VisTrails provides the `Variant` type which allows connections to any input port. VisTrails attempts to do run-time type-checking to ensure that the type passed in to the module is as advertised but allows general computations to remain general. For example, the `GetItem` module might be constructed as:

```

1 class GetItem(Module):
2     _input_ports = [IPort("list", "basic:List"),
3                     IPort("index", "basic:Integer")]
4     _output_ports = [OPort("value", "basic:Variant")]

```

5.7.7 Connectivity

In some cases, it may be desirable to know which outputs are used before running a computation. The `outputPorts` dictionary of the module stores connection information. Thus, you should be able to check

```
("myPortName" in self.outputPorts)
```

on the parent module to check if there are any downstream connections from the port “myPortName”. **Note**, however, that the caching algorithm assumes that all outputs are computed so adding a new connection to a previously unconnected output port will not work as desired if that module is cached. For this reason, we would currently recommend making such a module not cacheable. Another possibility is overriding the `update()` method to check the output ports and set the `upToDate` flag if they are not equal. Here is an example:

```

1 class TestModule(Module):
2     _output_ports = [('a1', 'basic:String'),
3                     ('a2', 'basic:String')]
4     def __init__(self):
5         Module.__init__(self)
6         self._cached_output_ports = set()
7
8     def update(self):
9         if len(set(self.outputPorts) - self._cached_output_ports) > 0:
10             self.upToDate = False
11             Module.update(self)
12
13     def compute(self):
14         if "a1" in self.outputPorts:
15             self.set_output("a1", "test")
16         if "a2" in self.outputPorts:
17             self.set_output("a2", "test2")
18         self._cached_output_ports = set(self.outputPorts)

```

5.8 Generating Modules Dynamically

When wrapping existing libraries or trying to generate modules in a more procedural manner, it is useful to dynamically generate modules. In our work, we have created some shortcuts to make this easier. In addition, the list of modules can also be based on the package configuration. Here is some example code:

```
__init__.py
```

```

1 from vistrails.core.configuration import ConfigurationObject
2
3 identifier = "org.vistrails.examples.auto_example"
4 version = "0.0.1"
5 name = "AutoExample"
6
7 configuration = ConfigurationObject(use_b=True)

```

init.py

The `expand_ports` and `build_modules` methods are functions to help the construction of the modules easier. The key parts are the `new_module` call and setting the `_modules` variable.

```

1 from vistrails.core.modules.vistrails_module import new_module, Module
2
3 identifier = "org.vistrails.examples.auto_example"
4
5 def expand_ports(port_list):
6     new_port_list = []
7     for port in port_list:
8         port_spec = port[1]
9         if type(port_spec) == str: # or unicode...
10            if port_spec.startswith('('):
11                port_spec = port_spec[1:]
12            if port_spec.endswith(')'):
13                port_spec = port_spec[:-1]
14            new_spec_list = []
15            for spec in port_spec.split(','):
16                spec = spec.strip()
17                parts = spec.split(':', 1)
18                print 'parts:', parts
19                namespace = None
20                if len(parts) > 1:
21                    mod_parts = parts[1].rsplit('|', 1)
22                    if len(mod_parts) > 1:
23                        namespace, module_name = mod_parts
24                    else:
25                        module_name = parts[1]
26                    if len(parts[0].split('.')) == 1:
27                        id_str = 'org.vistrails.vistrails.' + parts[0]
28                    else:
29                        id_str = parts[0]
30                else:
31                    mod_parts = spec.rsplit('|', 1)
32                    if len(mod_parts) > 1:
33                        namespace, module_name = mod_parts
34                    else:
35                        module_name = spec
36                    id_str = identifier
37                if namespace:
38                    new_spec_list.append(id_str + ':' + module_name + \
39                                        ':' + namespace)
40                else:
41                    new_spec_list.append(id_str + ':' + module_name)
42                port_spec = '(' + ','.join(new_spec_list) + ')'
43            new_port_list.append((port[0], port_spec) + port[2:])
44    print new_port_list
45    return new_port_list
46

```



```

47 def build_modules(module_descs):
48     new_classes = {}
49     for m_name, m_dict in module_descs:
50         m_doc = m_dict.get("_doc", None)
51         m_inputs = m_dict.get("_inputs", [])
52         m_outputs = m_dict.get("_outputs", [])
53         if "_inputs" in m_dict:
54             del m_dict["_inputs"]
55         if "_outputs" in m_dict:
56             del m_dict["_outputs"]
57         if "_doc" in m_dict:
58             del m_dict["_doc"]
59         klass_dict = {}
60         if "_compute" in m_dict:
61             klass_dict["compute"] = m_dict["_compute"]
62             del m_dict["_compute"]
63         m_class = new_module(Module, m_name, klass_dict, m_doc)
64         m_class._input_ports = expand_ports(m_inputs)
65         m_class._output_ports = expand_ports(m_outputs)
66         new_classes[m_name] = (m_class, m_dict)
67     return new_classes.values()
68
69 def initialize():
70     global _modules
71     def a_compute(self):
72         a = self.get_input("a")
73         i = 0
74         if self.has_input("i"):
75             i = self.get_input("i")
76         if a == "abc":
77             i += 100
78         self.set_output("b", i)
79
80     module_descs = [("ModuleA", {"_inputs": [("a", "basic:String")],
81                                     "_outputs": [("b", "basic:Integer")],
82                                     "_doc": "ModuleA documentation",
83                                     "_compute": a_compute,
84                                     "namespace": "Test"}),
85                    ("ModuleB", {"_inputs": [("a", "Test|ModuleA")],
86                                     "_outputs": [("b", "Test|ModuleA")],
87                                     "_doc": "ModuleB documentation"})]
88
89
90     if configuration.use_b:
91         _modules = build_modules(module_descs)
92     else:
93         _modules = build_modules(module_descs[:1])
94
95     _modules = []

```

5.9 Wrapping Command-line tools

Many existing programs are readily available through a command-line interface. Also, many existing workflows are first implemented through scripts, which work primarily with command-line tools. This section describes how to wrap command-line applications so they can be used with VisTrails. We will use as a running example the `afrofront` package, which wraps `afrofront`, a command-line program for generating 3D triangle meshes. We will wrap the basic

functionality in three different modules: `Afront`, `AfrontIso`, and `MeshQualityHistogram`.

Each of these modules will be implemented by a Python class, and they will all invoke the `afront` binary. `Afront` is the base execution module, and `AfrontIso` requires extra parameters on top of the original ones. Because of this, we will implement `AfrontIso` as a subclass of `Afront`. `MeshQualityHistogram`, however, requires entirely different parameters, and so will not be a subclass of `Afront`. A first attempt at writing this package might look something like this:

`__init__.py`

```
1 name = "Afront"
2 version = "0.1.0"
3 identifier = "edu.utah.sci.vistrails.afront"
```

`init.py`

```
1 from vistrails.core.modules.vistrails_module import Module
2 ... # other import statements
3
4 class Afront(Module):
5     def compute(self):
6         ... # invokes afront
7
8 class AfrontIso(Afront):
9     def compute(self):
10        ... # invokes afront with additional parameters
11
12 class MeshQualityHistogram(Module):
13     def compute(self):
14        ... # invokes afront with completely different parameters
15
16 _modules = [Afront, AfrontIso, MeshQualityHistogram, ...]
```

5.9.1 Class Mixins

While this approach is a good start, it does require significant duplication of effort. Each module must contain code to invoke the `afront` binary and pass it some parameters. Since this functionality is required by all three modules, we would like to put this code in a separate class called, say, `AfrontRun`, and let each of our modules inherit from it. `AfrontRun` itself is not a module, and thus does not extend the `Module` class. So our three modules will inherit from *both* `AfrontRun` and `Module`. Helper classes such as this are often referred to as *mixin classes*.² *hi* hello

```
1 from vistrails.core.modules.vistrails_module import Module, ModuleError
2 from vistrails.core.system import list2cmdline
3 import os
4
5 class AfrontRun(object):
6     _debug = False
7     def run(self, args):
8         cmd = ['afront', '-nogui'] + args
9         cmdline = list2cmdline(cmd)
10        if self._debug:
11            print cmdline
12        result = os.system(cmdline)
13        if result != 0:
```

² Programmers who are more comfortable with single-inheritance languages like Java and C# may be unfamiliar with mixins. A mixin class is similar to an *interface* in Java or C#, except that a mixin provides an implementation as well. Python's support for multiple inheritance allows subclasses to "import" functionality as needed from a mixin class, without artificially cluttering the base class's interface.

```

14         raise ModuleError(self, "Execution failed")
15
16 class Afront(Module, AfrontRun):
17     ...
18
19 class MeshQualityHistogram(Module, AfrontRun):
20     ...

```

Now every module in the `afront` package has access to `run()`. The other new feature in this snippet is `list2cmdline`, which turns a list of strings into a command line. It does this in a careful way (protecting arguments with spaces, for example). Notice that we use a call to a shell (`os.system()`) to invoke `afront`. This is frequently the easiest way to get third-party functionality into VisTrails.

5.9.2 Temporary File Management

Command-line programs typically generate files as outputs. On complicated pipelines, many files get created and passed to other modules. To facilitate the use of files as communication objects, VisTrails provides basic infrastructure for temporary file management. This way, package developers do not have to worry about file ownership and lifetimes.

To use this infrastructure, it must be possible to tell the program being called which filename to use as output. VisTrails can accommodate some filename requirements (in particular, specific filename extensions might be important in Windows environments, and these can be set), but it must be possible to direct the output to a certain filename.

We will use `Afront`'s `compute()` method to illustrate the feature.

```

1  ...
2  class Afront(Module, AfrontRun):
3
4      def compute(self):
5          o = self.interpreter.filePool.create_file(suffix='.m')
6          args = []
7          if not self.has_input("file"):
8              raise ModuleError(self, "Needs input file")
9          args.append(self.get_input("file").name)
10         if self.has_input("rho"):
11             args.append("-rho")
12             args.append(str(self.get_input("rho")))
13         if self.has_input("eta"):
14             args.append("-reduction")
15             args.append(str(self.get_input("eta")))
16         args.append("-outname")
17         args.append(o.name)
18         args.append("-tri")
19         self.run(args)
20         self.set_output("output", o)
21     ...

```

Line 5 shows how to create a temporary file during the execution of a pipeline. There are a few new things happening, so let us look at them one at a time. Every module holds a reference to the current *interpreter*, the object responsible for orchestrating the execution of a pipeline. This object has a `filePool`, which is what we will use to create a pipeline, through the `create_file` method. This method takes optionally a named parameter `suffix`, which forces the temporary file that will be created to have the right extension.

The file pool returns an instance of `basic_modules.File`, a module that is provided by the basic VisTrails packages. There are two important things you should know about `File`. First, it has a `name` attribute that stores the name of the file it represents. In this case, it is the name of the recently-created temporary file. This allows you to safely use this file when calling a shell, as seen on Line 17. The other important feature is that it can be passed directly to an output port, so that this file can be used by subsequent modules. This is shown on Line 20.

The above code also introduces the boolean function `has_input` (see Lines 7, 10, and 13). This is a simple error-checking function that verifies that the port has incoming data before the program attempts to read from it. It is considered good practice to call this function before invoking `get_input` for any input port.

Accommodating badly-designed programs Even though it is considered bad design for a command-line program not to allow the specification of an output filename, there do exist programs that lack this functionality. In this case, a possible workaround is to execute the command-line tool, and move the generated file to the name given by VisTrails.

5.10 For System Administrators

Most users will want to put their custom packages in their

```
~/vistrails/userpackages
```

directory, as described in Section *An Example Package*. This makes the package available to the current user only. However, if you are a power user or a system administrator, you may wish to make certain packages available to all users of a VisTrails installation. To do this, copy the appropriate package files and/or directories to the

```
vistrails/packages
```

directory of the VisTrails distribution. The packages will be made visible to users the next time they launch VisTrails.

COMMAND-LINE ARGUMENTS

6.1 Starting VisTrails via the Command Line

VisTrails supports a number of command-line arguments that let you modify certain attributes and behaviors of the program. When invoking VisTrails from the command line, the arguments are placed after the “run.py” filename. For example,

```
python vistrails/run.py -b
```

starts VisTrails in batch mode. Table table-batch-cli contains a complete list of the command line switches supported by vistrails. Each command line switch has both a short form and a long form. The two forms are logically equivalent, and which one you use is a matter of personal preference. The short form consists of a single minus sign “-” followed by a single letter. The longer form uses two minus signs “--” followed by a descriptive word. For example, the above command for batch mode could have been written as:

```
python vistrails/run.py --batch
```

In addition to the explicit switches listed in Table table-batch-cli, the VisTrails command line also lets you indicate the filename of the vistrail you wish to open. For example, assuming your “examples” directory is one level above your current working directory, this is how you would tell VisTrails to load the “lung.vt” example at startup:

```
python vistrails/run.py examples/lung.vt
```

Moreover, if you want VisTrails to start on a *specific version* of the pipeline within the vistrail, you can indicate that version’s tag name on the command line. The filename and version tag should be separated by a colon. For example, to start VisTrails with the `colormap` version of the “lung.vt” vistrail, use:

```
python vistrails/run.py examples/lung.vt:colormap
```

In the event that the version you want to open contains a space in its tag name, simply surround the entire “filename:tag” pair in double quotes. For example:

```
python vistrails/run.py "examples/lung.vt:Axial View"
```

You can also open up multiple vistrails at once by listing more than one vistrail file on the command line. This causes the vistrails to be opened in separate tabs, just as if you had opened them via the GUI. For example:

```
python vistrails/run.py examples/lung.vt examples/head.vt
```

You can specify version tags in conjunction with multiple filenames. Here is an example of an elaborate command-line invocation that opens two vistrails and sets each one to a specific version:

```
python vistrails/run.py "examples/lung.vt:Axial View"  
examples/head.vt:bone
```

```
usage: run.py [-h] [--version] [-S DIR] [--subworkflows-dir DIR]  
             [--data-dir DIR] [--package-dir DIR] [--user-package-dir DIR]  
             [--file-dir DIR] [--log-dir DIR] [--temporary-dir DIR]
```

```

[--thumbs-auto-save | --no-thumbs-auto-save]
[--thumbs-mouse-hover | --no-thumbs-mouse-hover]
[--thumbs-tags-only | --no-thumbs-tags-only]
[--thumbs-cache-dir DIR] [--thumbs-cache-size THUMBS.CACHESIZE]
[--host URL] [--port PORT] [--db DB] [--user USER]
[--rpc-server RPCSERVER] [--rpc-port RPCPORT]
[--rpc-log-file DIR] [--rpc-instances RPCINSTANCES]
[--multithread] [--rpc-config DIR] [--web-repository-url URL]
[--web-repository-user WEBREPOSITORYUSER]
[--job-check-interval JOBCHECKINTERVAL]
[--job-autorun JOBAUTORUN] [--job-list] [--job-info] [-E] [-b]
[-o DIR] [-p OUTPUTSETTINGS] [--parameters PARAMETERS]
[--parameter-exploration] [--show-window]
[--output-version-tree] [--output-pipeline-graph]
[--graphs-as-pdf] [--enable-usage] [--disable-usage]
[--maximize-windows | --no-maximize-windows]
[--multi-heads | --no-multi-heads]
[--show-splash | --hide-splash] [--auto-save | --no-auto-save]
[--db-default | --no-db-default] [--cache | --no-cache]
[--stop-on-error | --no-stop-on-error]
[--execution-log | --no-execution-log]
[--error-log | --no-error-log]
[--default-file-type DEFAULTFILETYPE] [-v DEBUGLEVEL]
[--show-vistrails-news | --hide-vistrails-news]
[--upgrades | --no-upgrades]
[--migrate-tags | --no-migrate-tags]
[--hide-upgrades | --no-hide-upgrades]
[--upgrade-delay | --no-upgrade-delay]
[--upgrade-module-fail-prompt | --no-upgrade-module-fail-prompt]
[--auto-connect | --no-auto-connect]
[--detach-history-view | --no-detach-history-view]
[--show-connection-errors | --hide-connection-errors]
[--show-variant-errors | --hide-variant-errors]
[--show-debug-popups | --hide-debug-popups]
[--show-scrollbar | --hide-scrollbar]
[--show-inline-parameter-widgets | --hide-inline-parameter-widgets]
[--shell-font-face SHELL.FONTFACE]
[--shell-font-size SHELL.FONTSIZE]
[--max-recent-vistrails MAXRECENTVISTRAILS]
[--view-on-load VIEWONLOAD]
[--custom-version-colors | --no-custom-version-colors]
[--fixed-custom-version-color-saturation | --no-fixed-custom-version-color-saturation]
[--enable-packages-silently | --no-enable-packages-silently]
[--load-packages | --no-load-packages]
[--install-bundles | --no-install-bundles]
[--install-bundles-with-pip | --no-install-bundles-with-pip]
[--repository-local-path DIR] [--repository-httpurl URL]
[--single-instance | --no-single-instance]
[--static-registry DIR]
[vistrail [vistrail ...]]

```

Positional arguments:

vistrails Vistrail to open

Options:

--version	show program's version and exit
-S, --dot-vistrails	The location to look for VisTrails user configurations and storage. Defaults to ~/.vistrails.
--subworkflows-dir	The location where a user's local subworkflows are stored.
--data-dir	The location that VisTrails uses as a default directory for data.
--package-dir	The directory to look for VisTrails core packages (use userPackageDir for user-defined packages).
--user-package-dir	The location for user-installed packages (defaults to ~/.vistrails/userpackages).
--file-dir	The location that VisTrails uses as a default directory for specifying files.
--log-dir	The path that indicates where log files should be stored.
--temporary-dir	The directory to use for temporary files generated by VisTrails.
--thumbs-auto-save	Whether to save thumbnails of results when executing VisTrails.
--no-thumbs-auto-save	Inverse of --thumbs-auto-save
--thumbs-mouse-hover	Whether to show thumbnails when hovering over a version in the version tree.
--no-thumbs-mouse-hover	Inverse of --thumbs-mouse-hover
--thumbs-tags-only	If True, only stores thumbnails for tagged versions. Otherwise, stores thumbnails for all versions.
--no-thumbs-tags-only	Inverse of --thumbs-tags-only
--thumbs-cache-dir	The directory to be used to cache thumbnails.
--thumbs-cache-size	The size (in MB) of the thumbnail cache.
--host	The hostname for the database to load the vistrail from.
--port	The port for the database to load the vistrail from.
--db	The name for the database to load the vistrail from.
--user	The username for the database to load the vistrail from.
--rpc-server	Hostname or ip address where this xml rpc server will work.
--rpc-port	Port where this xml rpc server will work.
--rpc-log-file	Log file for XML RPC server.
--rpc-instances	Number of other instances that vistrails should start.
--multithread	Server will start a thread for each request.
--rpc-config	Config file for server connection options.
--web-repository-url	The URL of the web repository that should be attached to VisTrails (e.g. www.crowdlabs.org).
--web-repository-user	The default username for logging into a VisTrails web repository like crowdLabs.
--job-check-interval	How often to check for jobs (in seconds, default=600).

--job-autorun	Run jobs automatically when they finish.
--job-list	List running workflows.
--job-info	List jobs in running workflow.
-E, --no-execute	Do not execute specified workflows.
-b, --batch	Run vistrails in batch mode instead of interactive mode.
-o, --output-directory	Directory in which to place output files
-p, --output-settings	One or more comma-separated key=value parameters.
--parameters	List of parameters to use when running workflow.
--parameter-exploration	Open and execute parameter exploration specified by the version argument after the .vt file.
--show-window	Show the main VisTrails window.
--output-version-tree	Output the version tree as an image.
--output-pipeline-graph	Output the workflow graph as an image.
--graphs-as-pdf	Generate graphs in PDF format instead of images
--enable-usage	Enable sending anonymous usage statistics
--disable-usage	Disable sending anonymous usage statistics
--maximize-windows	Whether the VisTrails windows should take up the entire screen space.
--no-maximize-windows	Inverse of --maximize-windows
--multi-heads	Whether or not to use multiple screens for VisTrails windows.
--no-multi-heads	Inverse of --multi-heads
--show-splash	Whether the VisTrails splash screen should be shown on startup.
--hide-splash	Inverse of --show-splash
--auto-save	Automatically save vistrails to allow recovery from crashes, etc.
--no-auto-save	Inverse of --auto-save
--db-default	Use a database as the default storage location for vistrails entities.
--no-db-default	Inverse of --db-default
--cache	Cache previous results so they may be used in future computations.
--no-cache	Inverse of --cache
--stop-on-error	Whether or not VisTrails stops executing the rest of the workflow if it encounters an error in one module.
--no-stop-on-error	Inverse of --stop-on-error
--execution-log	Track execution provenance when running workflows.
--no-execution-log	Inverse of --execution-log
--error-log	Write errors to a log file.
--no-error-log	Inverse of --error-log
--default-file-type	Defaults to .vt but could be .xml.

- v, --debug-level** How much information VisTrails should alert the user about (0: Critical errors only, 1: Critical errors and warnings, 2: Critical errors, warnings, and log messages).
- show-vistrails-news** Show news from VisTrails on startup. Each message will only be displayed once.
- hide-vistrails-news** Inverse of `--show-vistrails-news`
- upgrades** Whether to upgrade old workflows so they work with newer packages.
- no-upgrades** Inverse of `--upgrades`
- migrate-tags** Whether or not the tag on a workflow that was upgraded should be moved to point to the upgraded version.
- no-migrate-tags** Inverse of `--migrate-tags`
- hide-upgrades** Don't show the "upgrade" nodes in the version tree.
- no-hide-upgrades** Inverse of `--hide-upgrades`
- upgrade-delay** Persist upgrade only after other changes.
- no-upgrade-delay** Inverse of `--upgrade-delay`
- upgrade-module-fail-prompt** Whether to alert the user when an upgrade may fail when upgrading a subworkflow.
- no-upgrade-module-fail-prompt** Inverse of `--upgrade-module-fail-prompt`
- auto-connect** Try to automatically connect a newly dragged in module to the rest of the workflow.
- no-auto-connect** Inverse of `--auto-connect`
- detach-history-view** Show the version tree in a separate window.
- no-detach-history-view** Inverse of `--detach-history-view`
- show-connection-errors** Alert the user if the value along a connection doesn't match connection types.
- hide-connection-errors** Inverse of `--show-connection-errors`
- show-variant-errors** Alert the user if the value along a connection coming from a Variant output doesn't match the input port.
- hide-variant-errors** Inverse of `--show-variant-errors`
- show-debug-popups** Always show the debug popups or only if there is a modal widget.
- hide-debug-popups** Inverse of `--show-debug-popups`
- show-scrollbar** Whether VisTrails should show scrollbars on the version tree and workflow canvases.
- hide-scrollbar** Inverse of `--show-scrollbar`
- show-inline-parameter-widgets** Show editable parameters inside modules.
- hide-inline-parameter-widgets** Inverse of `--show-inline-parameter-widgets`
- shell-font-face** The font to be used for the VisTrails console.
- shell-font-size** The font size used for the VisTrails console.

- max-recent-vistrails** How many recently opened vistrails should be stored for “Open Recent” access.
- view-on-load** Whether to show pipeline or history view when opening vistrail. Can be either appropriate/pipeline/history.
- custom-version-colors** Allow setting custom colors for versions, and display these colors in the version tree.
- no-custom-version-colors** Inverse of `--custom-version-colors`
- fixed-custom-version-color-saturation** Don’t change the saturation according to the age of the version if it has a custom color.
- no-fixed-custom-version-color-saturation** Inverse of `--fixed-custom-version-color-saturation`
- enable-packages-silently** Do not prompt the user to enable packages, just do so automatically.
- no-enable-packages-silently** Inverse of `--enable-packages-silently`
- load-packages** Whether to load the packages enabled in the configuration file.
- no-load-packages** Inverse of `--load-packages`
- install-bundles** Automatically try to install missing Python dependencies.
- no-install-bundles** Inverse of `--install-bundles`
- install-bundles-with-pip** Whether to try to use pip to install Python dependencies or use distribution support.
- no-install-bundles-with-pip** Inverse of `--install-bundles-with-pip`
- repository-local-path** Path used to locate packages available to be installed.
- repository-httppurl** URL used to locate packages available to be installed.
- single-instance** Whether or not VisTrails should only allow one instance to be running.
- no-single-instance** Inverse of `--single-instance`
- static-registry** If specified, VisTrails uses an XML file defining the VisTrails module registry to load modules instead of from the packages directly.

6.2 Specifying a User Configuration Directory

In addition to the default `.vistrails` directory, VisTrails allows you to create and use additional configuration directories. First, you will need to create a new directory. This is done by running: `python vistrails/run.py -S /path_to_new_directory/new_directory_name`.

This will both create a new directory containing default configuration files and directories, and launch VisTrails, which will use the newly created files for configuration. The user is then free to add desired configurations to the new directory. Once a configuration directory exists, subsequent calls using the directory name (`python vistrails/run.py -S /path_to_directory/existing_directory`) will launch VisTrails using the ‘existing_directory’ for configuration and a new directory will not be created.

Note: If you would like to copy configuration directories, you must change the references in `copy_of_directory/startup.xml` to point to the new directory instead of the original.

6.3 Passing Database Parameters on the Command Line

As discussed in Chapter *Connecting to a Database*, VisTrails can read and write vistrails stored in a relational database as well as in a filesystem. VisTrails allows you to specify the name of the database server, the database name, the port number, and the username on the command line. This potentially saves you the trouble of filling out the same information on the database connection dialog. Note that, for security reasons, VisTrails does not allow you to include a database password on the command line; you must still type your password into the database connection dialog when VisTrails opens.

The last four rows of Table `table-batch-cli` show the command-line switches that pertain to database connectivity. Be advised that these switches were designed primarily for use by VTL files (see Section *Using “Vistrail Link” Files*) and as such, are not necessarily user-friendly. In particular, these switches are ignored unless you also specify the vistrail ID and version name on the command line. For example, to open the `contour` version of the the “spx” vistrail (whose ID is 5) from the database “vistrails” residing on the host “vistrails.sci.utah.edu” with a username of “vistrails”:

```
python vistrails/run.py --host=vistrails.sci.utah.edu --db=vistrails
--user=vistrails 5:contour
```

Once VisTrails opens, you will be prompted to enter the password. Upon successful authentication, the vistrail is loaded from the database and opened to the pipeline corresponding to the specified version.

6.3.1 Using “Vistrail Link” Files

As discussed in Chapter *Connecting to a Database*, one of the advantages of storing your vistrails on a database is that you can collaborate with others without having to pass around a `.vt` file or force all users to use a shared filesystem. A disadvantage is that you need to remember the parameters with which to connect to the database. Using a “Vistrail Link” (VTL) file reduces this inconvenience, and also eliminates the need to include the associated command-line switches to connect to the database.

A VTL is a very small text (XML) file that contains the parameters required to load a vistrail from a database. VTL files are intended for use with a VisTrails-enabled wiki. You can open a VTL either by saving the file and passing its filename to the command line, or by configuring your web browser to do this for you. Here is the syntax for using a VTL file on the command line:

```
python vistrails/run.py sample.vtl
```

Internally, VisTrails parses the VTL file and loads the vistrail from the database exactly as if you had included its full parameter list on the command line.

Note:

VTL is a relatively new feature of VisTrails, and as such is neither fully developed nor completely documented. Please contact the VisTrails development team with any bug reports and/or suggestions.

6.4 Running VisTrails in Batch Mode

Although VisTrails is primarily intended to be run as an interactive, graphical client application, it also supports non-interactive use. VisTrails can thus be invoked programmatically, eg as part of a shell script. You can tell VisTrails to start in non-interactive mode by using the “-b” or “-batch” command line switch when launching vistrails.¹

Running VisTrails in non-interactive mode has little effect, however, without an additional command line argument indicating which vistrail to load. Since we are running VisTrails as part of a batch process, it only makes sense to

¹ The parameter “-b” stands for “batch.” In this chapter, we use the terms “batch mode” and “non-interactive mode” synonymously.

execute vistrails whose output is something tangible, such as a file. A vistrail whose only output is an interactive rendering in a `VTKCell`, for instance, would not be well-suited for running in batch mode.

Consider the following example. The “`offscreen.vt`” vistrail (included in the “`examples`” directory) has a variety of output options, depending on which version you select in the `History` view (Figure *The different versions of the `offscreen.vt` vistrail...*). The version tagged `only vtk` displays its output as an interactive VTK rendering. The version tagged `html` creates a simple web page in the Spreadsheet. The `offscreen` version, however, outputs an image file named “`image.png`”. Since its output (a file) can be easily accessed outside of VisTrails, this version is an ideal candidate for running in batch mode. To try it, invoke VisTrails as shown, specifying both the name of the vistrail file and the desired version:

```
python vistrails/run.py -b examples/offscreen.vt:offscreen
```

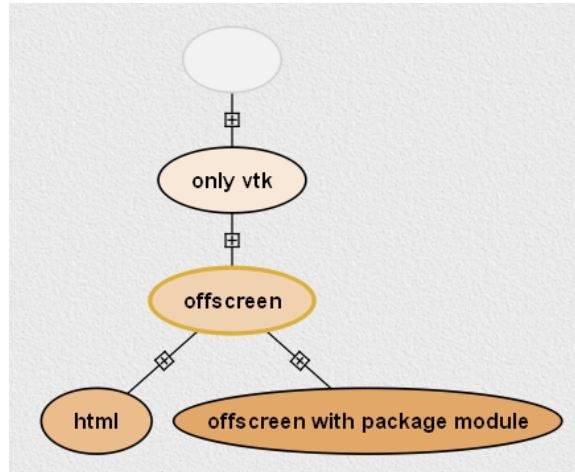


Fig. 6.1: The different versions of the “`offscreen.vt`” vistrail offer various forms of output.

As you would expect, this command runs to completion without opening any windows. Instead, it silently loads the requested pipeline, executes it, and closes. Assuming it ran correctly, this pipeline should have created a file named “`image.png`” in the current directory. When you view this file, it should resemble the picture in Figure *Running the `offscreen` version of `offscreen.vt` in batch mode...*

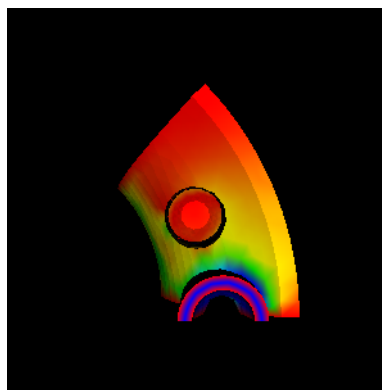


Fig. 6.2: Running the `offscreen` version of “`offscreen.vt`” in batch mode produces an image named “`image.png`”.

6.4.1 Running a Specific Workflow in Batch Mode

To run a specific workflow in batch mode, call VisTrails with the following options:

```
python vistrails/run.py -b path_to_vistrails_file:pipeline
```

where pipeline can be a version **tag name** or version **id**.

Note

If you downloaded the MacOS X bundle, you can run VisTrails from the command line via the following commands in the terminal. Change the current directory to wherever VisTrails was installed (often /Applications), and then type: `Vistrails.app/Contents/MacOS/vistrails` [`<cmd_line_options>`]

6.4.2 Running a Workflow with Specific Parameters

An alias is a name assigned to a parameter that allows you to reference that parameter in batch mode. An alias is created by clicking on the type of an existing parameter in VisTrails, then entering a name for it.



Fig. 6.3: Example of creating an alias

Users can change workflow parameters that have an alias through the command line.

For example, offscreen pipeline in `offscreen.vt` always creates the file called `image.png`. If you want generate it with a different filename:

```
python vistrails/run.py -b examples/offscreen.vt:offscreen
--parameters="filename=other.png"
```

`filename` in the example above is the alias name assigned to the parameter in the value method inside the String module. When running a pipeline from the command line, VisTrails will try to start the spreadsheet automatically if the pipeline requires it. For example, this other execution will also start the spreadsheet (note that `$` characters need to be escaped when running on bash; if running on windows, you should remove the backslashes):

```
python vistrails/run.py -b examples/head.vt:aliases --parameters="isovalue=30\$\&\$diffuse_
0.4, 0.2"
```

You can also execute more than one pipeline on the command line:

```
python vistrails/run.py -b examples/head.vt:aliases ../examples/spx.vt:spx \
--parameters="isovalue=30"
```

Use `--parameters` only once regardless the number of pipelines.

6.4.3 Accessing a Database in Batch Mode

As discussed in Section *Passing Database Parameters on the Command Line*, you can specify most of the parameters of your database connection on the command line, but the password must be entered through the GUI. This poses a problem for running VisTrails in non-interactive mode, since no database connection dialog will be opened. If your batch process needs to access vistrails stored on a database, the current workaround is to create a special account on the database (probably one with read-only access) that does *not* require a password, and use this account for connecting to the database in batch mode.

6.4.4 Using VisTrails as a Server

Using the VisTrails server mode, it is possible to execute workflows and control VisTrails through another application. For example, the CrowdLabs Web portal (<http://www.crowdlabs.org>) accesses a VisTrails sever to execute workflows, retrieve and display vistrail trees and workflows.

The way you access the server is by doing XML-RPC calls. In the current VisTrails release, we include a set of PHP scripts that can talk to a VisTrails server instance. They are in “extensions/http” folder. The files are reasonably well documented. Also, it should be not difficult to create python scripts to access the server (just use xmlrpclib module).

Note that the VisTrails server requires the provenance and workflows to be in a database. More detailed instructions on how to setup the server and the database are available in *VisTrails Server Setup* and in *Setting up the database*.

If what you want is just to execute a series of workflows in batch mode, a simpler solution would be to use the VisTrails client in batch mode (see Section *Running VisTrails in Batch Mode*).

6.5 Executing Workflows in Parallel

The VisTrails server can only execute pipelines in parallel if there’s more than one instance of VisTrails running. The command

```
self.rpcserver=ThreadedXMLRPCServer((self.temp_xml_rpc_options.server,
self.temp_xml_rpc_options.port))
```

starts a multithreaded version of the XML-RPC server, so it will create a thread for each request received by the server. The problem is that Qt/PyQT doesn’t allow these multiple threads to create GUI objects. Only the main thread can. To overcome this limitation, the multithreaded version can instantiate other single threaded versions of VisTrails and put them in a queue, so workflow executions and other GUI-related requests, such as generating workflow graphs and history trees can be forwarded to this queue, and each instance takes turns in answering the request. If the results are in the cache, the multithreaded version answers the requests directly.

Note that this infrastructure works on Linux only. To make this work on Windows, you have to create a script similar to `start_vistrails_xvfb.sh` (located in the scripts folder) where you can send the number of other instances via command-line options to VisTrails. The command line options are:

```
python vistrails_server.py --host=<ADDRESS> --port=<PORT>
-O<NUMBER_OF_OTHER_VISTRAILS_INSTANCES> [-M] &
```

If you want the main vistrails instance to be multithreaded, use the `-M` at the end.

After creating this script, update function `start_other_instances` in `vistrails/gui/application_server.py` lines 1007-1023 and set the script variable to point to your script. You may also have to change the arguments sent to your script (line 1016: for example, you don’t need to set a virtual display). You will need to change the path to the `stop_vistrails_server.py` script (on line 1026) according to your installation path.

6.6 Executing Parameter Explorations from the Command Line

Named parameter explorations can be executed from the command line in different ways using the `-P` flag. The parameter after the vistrail will then indicate the parameter exploration name in place of the workflow version. To open vistrails and execute a parameter exploration named “final” in `terminator.vt` run:

```
python vistrails/run.py -P terminator.vt:final
```

To only show the spreadsheet run:

```
python vistrails/run.py -P -i terminator.vt:final
```

To execute the spreadsheet in batch mode, and to output the spreadsheet as images to a directory, use the `-b` flag and specify a directory with the `-e` flag:

```
python vistrails/run.py -P -b -e ./final_images terminator.vt:final
```

This will create an image for each cell and also create a composite image for each sheet in the spreadsheet.

6.7 Finding Methods Via the Command Line

We have tried to make some methods more accessible in the console via an api. You can import the api via `import api` in the console and see the available methods with `dir(api)`. To open a vistrail:

```
import api
api.open_vistrail_from_file('/Applications/VisTrails/examples/terminator.vt')
```

To execute a version of a workflow, you currently have to go through the controller:

```
api.select_version('Histogram')
api.get_current_controller().execute_current_workflow()
```

Currently, only a subset of VisTrails functionality is directly available from the api. However, since VisTrails is written in python, you can dig down starting with the `VistrailsApplication` or `controller` object to expose most of our internal methods. If you have suggestions for calls to be added to the api, please let us know.

One other feature that we're working on, but is still in progress is the ability to construct workflows via the console. For example:

```
vtk = load_package('org.vistrails.vistrails.vtk')
vtk.vtkDataSetReader() # adds a vtkDataSetReader module to the pipeline
# click on the new module
a = selected_modules()[0] # get the one currently selected module
a.SetFile('/vistrails/examples/data/head120.vtk') # sets the SetFile\
parameter for the data set reader
b = vtk.vtkContourFilter() # adds a vtkContourFilter module to the\
pipeline and saves to var b
b.SetInputConnection0(a.GetOutputPort0()) # connects a's GetOutputPort0\
port to b's SetInputConnection0
```


JOB SUBMISSION

VisTrails provides a mechanism for running external jobs. This is used for long-running executions and jobs that are run in parallel. These jobs are executed asynchronously in the background while the workflow execution suspends on the client side. The state of running jobs are persisted in the vistrail file, so that workflows with running jobs can be resumed even after restarting VisTrails.

To use the Job mechanism, it needs to be implemented by Modules. VisTrails will then detect the jobs and handle it accordingly. Jobs are implemented either using *JobMixin* (recommended) or *raising ModuleSuspended directly*.

Note: To run the examples, first install the example package by copying it from *vistrails/tests/resources/myjob.py* to *~/vistrails/userpackages* (Or run a workflow that does this automatically)

7.1 Monitoring Jobs

Jobs are tracked by the Job Monitor when started from the VisTrails GUI. It keeps track of all jobs and enables you to:

- Check jobs - Checks if the job has completed through the handle mechanism, either the selected workflow/module or all.
- Pause jobs - A paused workflow will not be checked by the timer or *Check All* button.
- View standard output/error for running jobs - If implemented by the handle.
- Delete running workflows/modules.
- Set time interval for automatic job checking.
- Set flag for waiting for job to finish (Automatic job execution).

7.2 Job Handles

A handle is used by the the Job Monitor to poll the job. This is a class instance with a *finished()* method that knows how to check the job. Below is an example with a simple time condition.

```
class TimedJobMonitor(object):
    """ Example that will complete when the specified time have passed

    """
    def __init__(self, start_time, how_long=10):
        self.start_time = start_time
        self.how_long = how_long
```

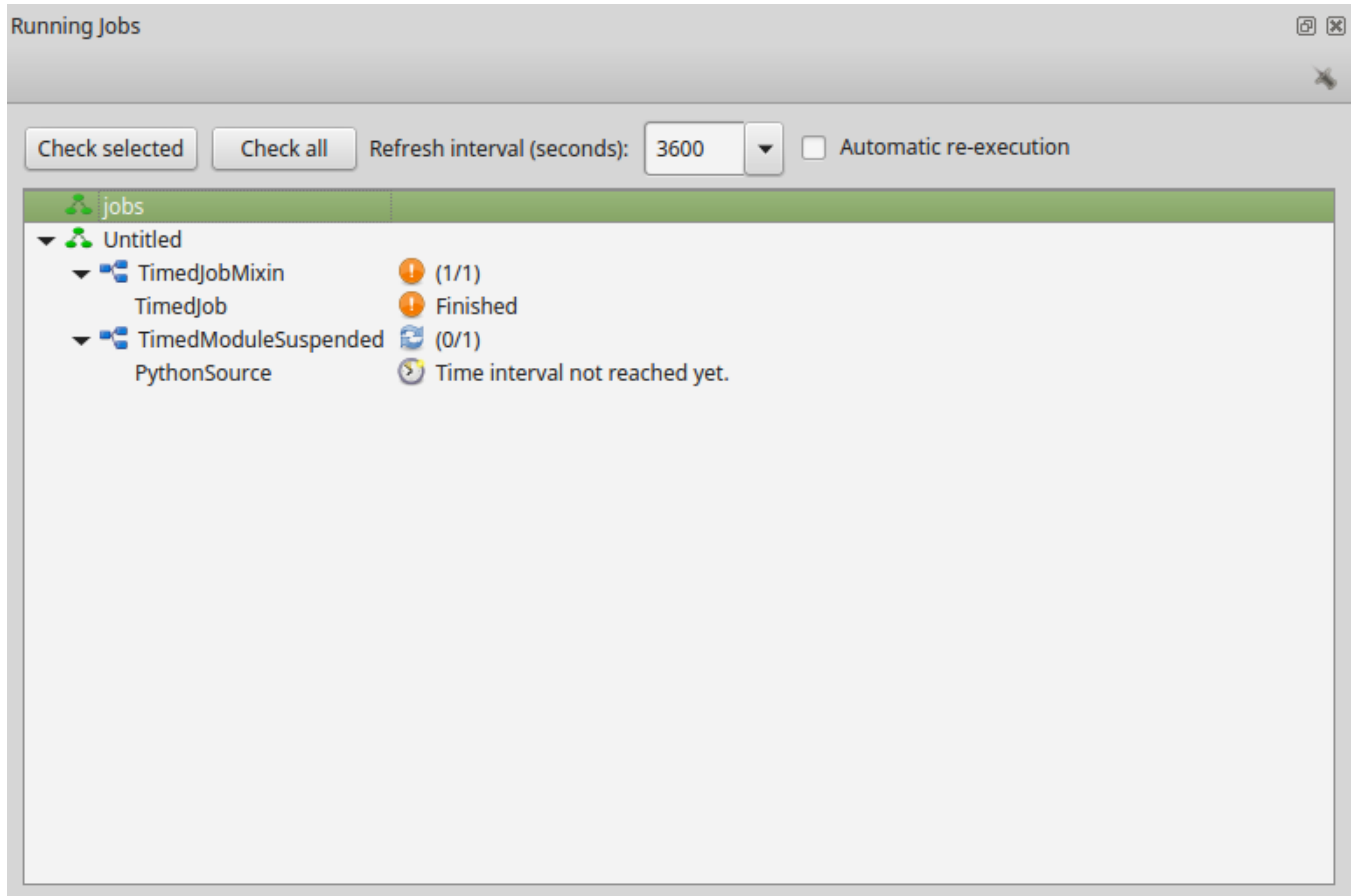


Fig. 7.1: The Job Monitor with one running and one finished workflow.

```
def finished(self):
    return (time.time()-self.start_time) > self.how_long
```

7.3 Using ModuleSuspended

ModuleSuspended (found in *vistrails.core.modules.vistrails_module*) is a low-level method to use the job mechanism. It is mainly used as a simple method to suspend *PythonSource*'s. (The preferred way is to use *JobMixin*). Raising *ModuleSuspended* will detach the job execution and suspend that branch of the workflow.

A Module that implements a job needs to:

- Check if the job is already running and if not, start it.
- Check if the job has completed, and raise *ModuleSuspended* if it has not.

Raising *ModuleSuspended* will suspend the module execution (unless a flag is set to wait for each job to finish). Other workflow branches will continue to be executed until all branches are either suspended or completed, until finally the workflow stops execution and enter a suspended state.

ModuleSuspended takes a *handle* that is used to check the job. Below is an example using the *TimedJobMonitor* above. (Open in vistrails)

```
handle = TimedJobMonitor(start_time)
if not handle.finished():
    raise ModuleSuspended(self, 'Time interval not reached yet.', handle)
```

Warning: The drawback with this method is that the upstream of the suspended modules will be executed each time the workflow is resumed. So make sure the upstream can be executed multiple times without creating a new job each time.

7.4 Using JobMixin

JobMixin (in *vistrails.core.vistrails.job*) is the preferred method to create job modules. It exposes a set of methods to implement that is needed to handle the job. One advantage of *JobMixin* is that it will resume jobs without re-executing the upstream of the module, as opposed to *ModuleSuspended*. This means the upstream will only be executed once for each job. Below is an example from the package *MyJobs* (*vistrails.packages.myjob*). (Open in vistrails)

```
class TimedJob(JobMixin, Module):
    """ A module that suspends until 'how_long' seconds have passed

    """
    _input_ports = [IPort("how_long", "basic:Integer", default=10)]
    _output_ports = [OPort("finished", "basic:Boolean")]

    def job_read_inputs(self):
        """ Implemented by modules to read job parameters from input ports.

        Returns the `params` dictionary used by subsequent methods.
        """
        return {'how_long': self.force_get_input('how_long') or 10}

    def job_start(self, params):
        """ Implemented by modules to submit the job.
```

```
Gets the `params` dictionary and returns a new dictionary, for example
with additional info necessary to check the status later.
"""

# this example gets the current time and stores it
# this time represents the information necessary to check the status of the job

params['start_time'] = time.time()
return params

def job_finish(self, params):
    """ Implemented by modules to get info from the finished job.

    This is called once the job is finished to get the results. These can
    be added to the `params` dictionary that this method returns.

    This is the right place to clean up the job from the server if they are
    not supposed to persist.
    """
    return params

def job_set_results(self, params):
    """ Implemented by modules to set the output ports.

    This is called after job_finished() or after getting the cached results
    to set the output ports on this module, from the `params` dictionary.
    """
    self.set_output('finished', True)

def job_get_handle(self, params):
    """ Implemented by modules to return the JobHandle object.

    This returns an object following the JobHandle interface. The
    JobMonitor will use it to check the status of the job and call back
    this module once the job is done.

    JobHandle needs the following method:
    * finished(): returns True if the job is finished
    """
    return TimedJobMonitor(params['start_time'], params['how_long'])
```

ACCESSING THE EXECUTION LOG

The code responsible for storing execution information is located in the “core/log” directories, and the code that generates much of that information is in “core/interpreter/cached.py”. Modules can add execution-specific annotations to provenance via `annotate()` calls during execution, but much of the data (like timing and errors) is captured by the `LogController` and `CachedInterpreter` (the execution engine) objects. To analyze the log from a `vistrail (.vt)` file, you might have something like the following:

```
import core.log.log
import db.services.io
```

```
def run(fname):
    # open the .vt bundle specified by the filename "fname"
    bundle = db.services.io.open_vistrail_bundle_from_zip_xml(fname) [0]
    # get the log filename
    log_fname = bundle.vistrail.db_log_filename
    if log_fname is not None:
        # open the log
        log = db.services.io.open_log_from_xml(log_fname, True)
        # convert the log from a db object
        core.log.log.Log.convert(log)
        for workflow_exec in log.workflow_execs:
            print 'workflow version:', workflow_exec.parent_version
            print 'time started:', workflow_exec.ts_start
            print 'time ended:', workflow_exec.ts_end
            print 'modules executed:', [i.module_id
                                       for i in workflow_exec.item_execs]
    if __name__ == '__main__':
        run("some_vistrail.vt")
```

You should be able to see what information is available by looking at the “core/log” classes.

CREATING A CONTROL FLOW LOOP MODULE

This chapter explains how to extend the `Control Flow` package by creating additional loop modules. For more information on `Control Flow` or the `Control Flow Assistant`, please refer to *Control Flow in VisTrails* or *The Control Flow Assistant* in the User's Guide.

9.1 Building your own loop structure

In functional programming, `fold` is a high-order function used to encapsulate a pattern of recursion for processing lists. A simple example of a `fold` is summing the elements inside a list. If you `fold` the list `[1, 2, 3, 4]` with the sum operator, the result will be $((1+2)+3)+4 = 10$. It's common to start with an initial value too. In the sum example, the initial value would be 0, and the result would be $((0+1)+2)+3)+4 = 10$.

With this function, a programmer can do any type of recursion. In fact, the `map` and `filter` functions, shown previously, can be implemented with `fold`. The `Control Flow` package provides a `Fold` module to enable this functionality, and the `Map` and the `Filter` modules inherit from the `Fold` class.

In fact, any control module that has this kind of recursion uses the `Fold` class. To use this functionality for your own control modules, instead of defining the `compute()` method, you need to define two other methods:

- `setInitialValue()`: in this method, you will set the initial value of the fold operator through the `self.initialValue` attribute;
- `operation()`: in this method, you must implement the function to be applied recursively to the elements of the input list (e.g., the sum function). More specifically, you need to define the relationship between the previous iteration's result (`self.partialResult` attribute) and the current element of the list (`self.element` attribute); this method must be defined after the `setInitialValue()` one.

It's important to notice that all modules inheriting from `Fold` will have the same ports, as `Map` and `Filter`, but you can add any other ports that will be necessary for your control structure. Also, you do not need to use the input ports "FunctionPort", "InputPort" and "OutputPort". You will only use them when you create an operator like `Map` and `Filter`, which need a function to be applied for each element of the input list.

As an example, we will create a simple `Sum` module to better understand the idea. Create a new package, and the code inside it would be as follows:

```
1 from controlflow import Fold, registerControl
2
3 version = "0.1"
4 name = "My Control Modules"
5 identifier = "org.vistrails.my_control_modules"
6
7 def package_dependencies():
8     return ["org.vistrails.vistrails.control_flow"]
9
```

```

10 class Sum(Fold):
11     def setInitialValue(self):
12         self.initialValue = 0
13
14     def operation(self):
15         self.partialResult += self.element
16
17 def initialize(*args, **keywords):
18     registerControl(Sum)

```

We begin by importing the `Fold` class and the `registerControl` function from the `Control Flow` package (Line 1). The `registerControl` function is used to register the control modules, so the shape of them can be set automatically.

Also, define the variables `version`, `name` and `identifier`, as it's done for all packages. The interpackage dependency (include reference of the package chapter) is used too, as `My Control Modules` requires a module and a function from `Control Flow` (Lines 7 and 8); in this way, `VisTrails` can initialize the packages in the correct order. Then, create the class `Sum`, which inherits from `Fold`. Inside it, set the initial value to 0 inside the `setInitialValue()` method (Lines 11 and 12), and define the sum operator inside `operation()`, as shown clearly by the relation between `self.partialResult` and `self.element` (Lines 14 and 15).

The last thing we must do is define the `initialize()` method, so the package can be loaded in `VisTrails`. However, instead of calling the registry, if you do not need any other ports, you just have to call the `registerControl()` function (Line 18).

Save this package and enable it inside `VisTrails`. Create a similar workflow as shown in Figure *A workflow using the Sum module*.

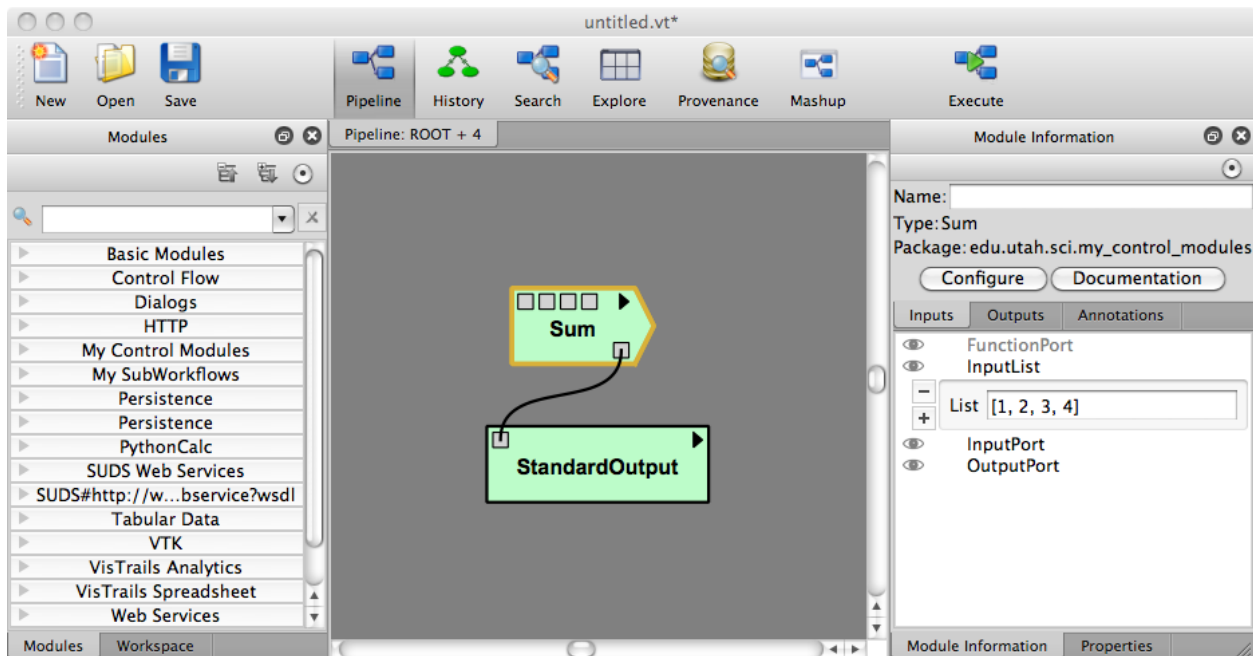


Fig. 9.1: A workflow using the `Sum` module

Upon executing this workflow, the sum $((((0+1)+2)+3)+4)$, should be printed on your terminal as follows:

```
10
```


Note that the input ports “FunctionPort”, “InputPort” and “OutputPort” were not necessary for this module. Now, let’s see another example that does use them. Open the workflow we used to calculate the area of isosurfaces (in “triangle_area.vt”, “Surface Area with Map and Filter” version), and delete the Map, the Filter, and the FilterCondition (PythonSource) modules.

Now, create a single module that maps the list and filters the results, named as AreaFilter. Inside your package, add the following class:

```

1 class AreaFilter(Fold):
2     def setInitialValue(self):
3         self.initialValue = []
4
5     def operation(self):
6         area = self.elementResult
7
8         if area>200000:
9             self.partialResult.append(area)

```

The initial value is an empty list, so the result of each element can be appended to it (Line 3). In the operation() method, the self.elementResult attribute is used (Line 6); it represents the result of the port chosen in “OutputPort”; so, it means that “FunctionPort”, “InputPort” and “OutputPort” will have connections. In this workflow, self.elementResult is the area for each contour value inside the input list, and, if the area is above 200,000, it will be appended to the final result (Lines 8 and 9). We can easily see that this module does exactly the same as Map and Filter combined.

Don’t forget to register this module in the initialize() function. After doing this, save the package and load it again inside VisTrails. Then, just connect AreaFilter as in Figure *The same workflow, but now with AreaFilter*.

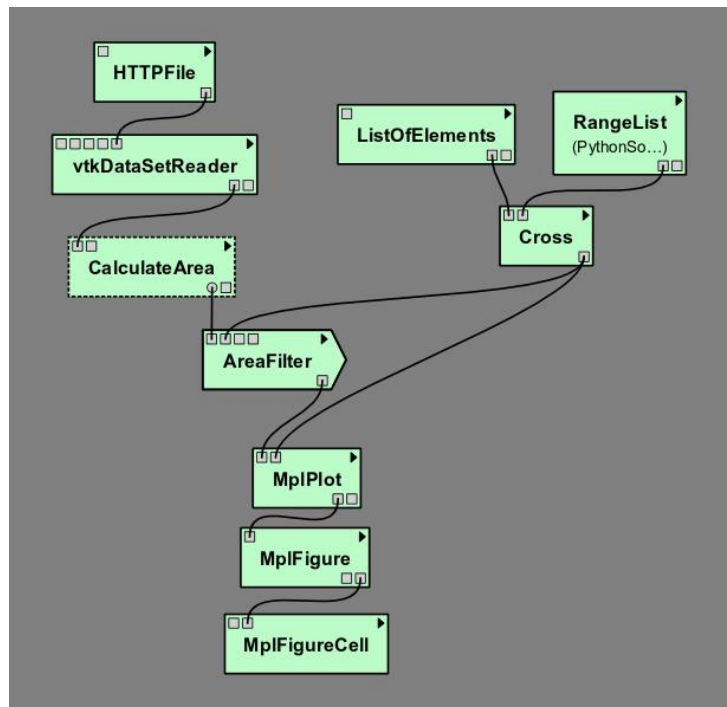


Fig. 9.2: The same workflow, but now with AreaFilter

Now, you must set some values in the following parameters of AreaFilter:

- “InputPort”: [”SetValue”]

- “OutputPort”: *GetSurfaceArea*

When you execute this workflow, the result in the VisTrails Spreadsheet will be the same as shown previously (Figure *The result in the VisTrails spreadsheet*). It shows the flexibility of doing a recursion function by inheriting from `Fold`.

USING PARALLELIZATION IN VISTRAILS MODULES

This chapters presents different techniques for using parallelization inside the code of your VisTrails modules.

10.1 Threading

VisTrails is single-threaded: the modules are executed one after the other, and while you are free to use threads in your module's `compute()` method, you should not interact with VisTrails from other threads.

Note that because of the restrictions of the CPython interpreter, you might not improve performance by using this type of parallelization: the interpreter has a lock, preventing two threads from executing Python code at the same time. If you are not already, consider using packages such as [NumPy](#) which provides efficient numerical functions implemented in C (and parallelizable).

10.2 Multiprocessing

Use of the `multiprocessing` package introduced with Python 2.6 is possible in VisTrails. This is generally the preferred way of performing multiple computational tasks in parallel in Python, and will effectively leverage multiple cores; please refer to the [official documentation](#) for more details.

10.3 IPython

You can access IPython clusters through the *Parallel Flow* package, via the provided API. Simply declare it in your package's dependencies, and import `vistrails.packages.parallelflow.api`. This module provides the following:

`get_client(ask=True)` -> `IPython.parallel.Client` or `None` Low-level function giving you a Client connected to the cluster, or `None`. If not connected to a cluster or if no engines are available, the `ask` parameter controllers whether to offer the user to take automatic action.

`direct_view(ask=True)` -> `IPython.parallel.DirectView` or `None` Gives you a view on the engines of the cluster, which you can use to submit tasks. This is currently equivalent to calling `get_client()[:]`.

You should probably use `load_balanced_view()` instead.

`load_balanced_view(ask=True)` -> `IPython.parallel.LoadBalancedView` or `None` Gives you a load-balanced view on the engines of the cluster, which you can * use to submit tasks. It is the preferred way of submitting tasks. This is currently equivalent to calling `get_client().load_balanced_view()`.

WRAPPING COMMAND LINE TOOLS USING PACKAGE CLTOOLS

11.1 Package CLTools

The package CLTools provide a way to wrap command line tools so that they can be used as modules in VisTrails. It includes a wizard that simplifies the creation of wrappers. To use the package, enable CLTools in the package configuration window. The package will be empty until you add a wrapper for a command line tool. When you have added a wrapper you need to reload the wrappers by either pressing the reload button in the wizard, reloading the CLTools package, or selecting Packages->CLTools->Reload All Scripts on the menu.

11.1.1 Using the CLTools Wizard

You can run the Wizard from within VisTrails. First, make sure the CLTools package is enabled. Then, on the menu, select Packages->CLTools->Open Wizard.

Or, to launch the wizard from the command line run: `python vistrails/package/CLTools/wizard.py`

The wizard allows you to create and edit wrappers for command line tools. Input/output ports can be created as arguments to the command or using pipes (stdin, stdout, or stderr). *Figure 1.1* shows the main interface. Command line arguments can be added, removed and rearranged. Pipes can be added and configured. There is a preview line where you can see how your command will look when executed. You can also push the preview button to see which ports will be available for the vistrails module, as shown in the bottom right. This example shows some of the most common ways to specify arguments. In order: The standard output is used as a string output port, an integer attribute using the `-i` flag, a boolean flag `-A` that can be turned on or off, an input file using a prefix, an output file using the `-o` flag, and finally a simple string input. Note the way arguments correspond to ports in the bottom right.

Arguments can represent either input ports, output ports, both, or constant strings. Ports can handle different types such as boolean flags, strings, integers, floats, or files. Lists of strings and files are also possible. Each argument can have a flag before it such as `-f` or a prefix such as `--file=`.

A file ending can be specified for files that are used as outputs using **file suffix**.

You can view and import flags from man and help pages (See *Figure 1.2*).

Files should be saved as `{modulename}.clt` in the directory `.vistrails/CLTools/`

Supported flags:

```
-c Import a command with arguments automatically
For example, to create a wrapper for ls with two flags -l and -A run:
python wizard.py -c ls -l -A
```

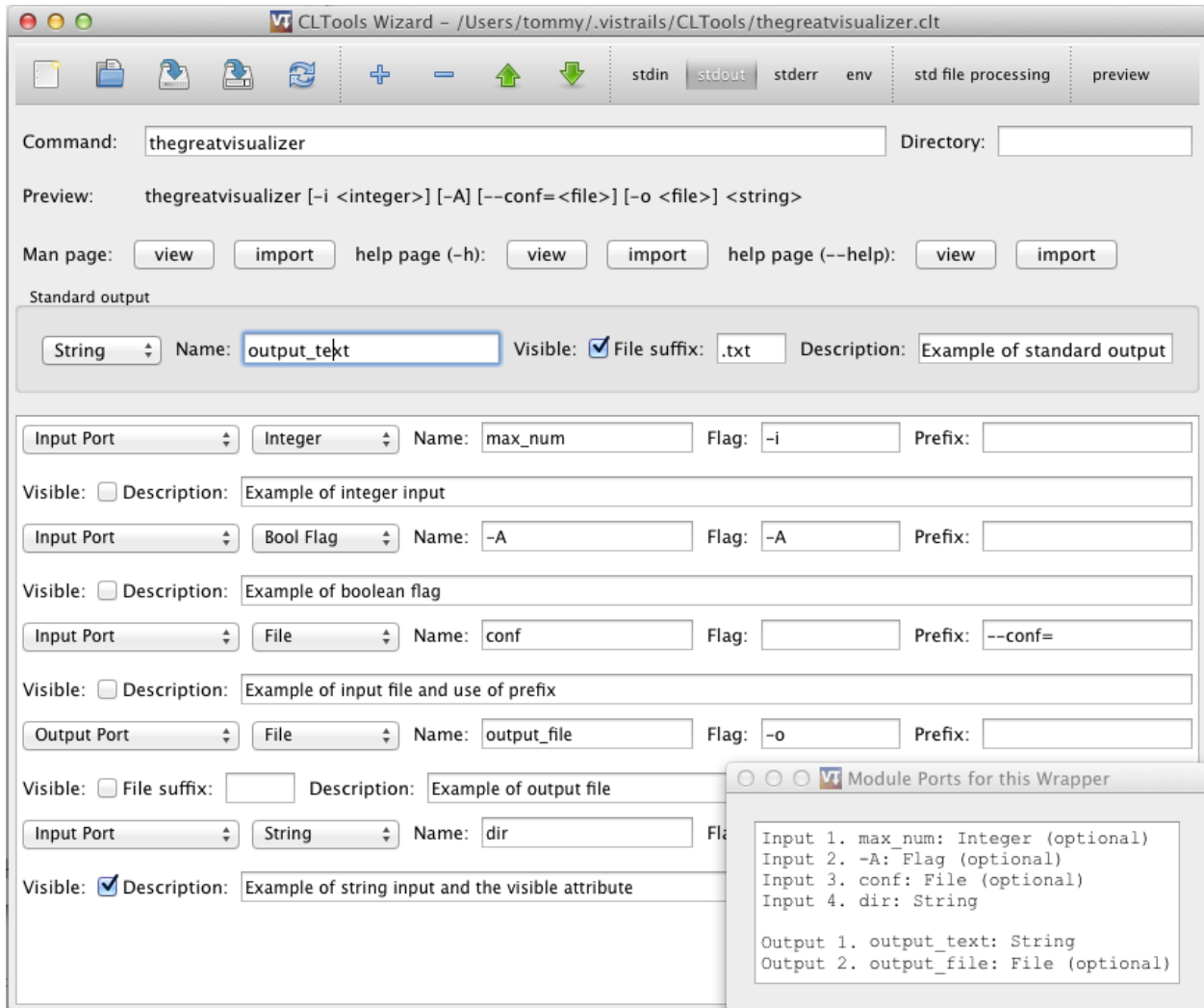


Fig. 11.1: Figure 1.1 - CLTools Wizard main window

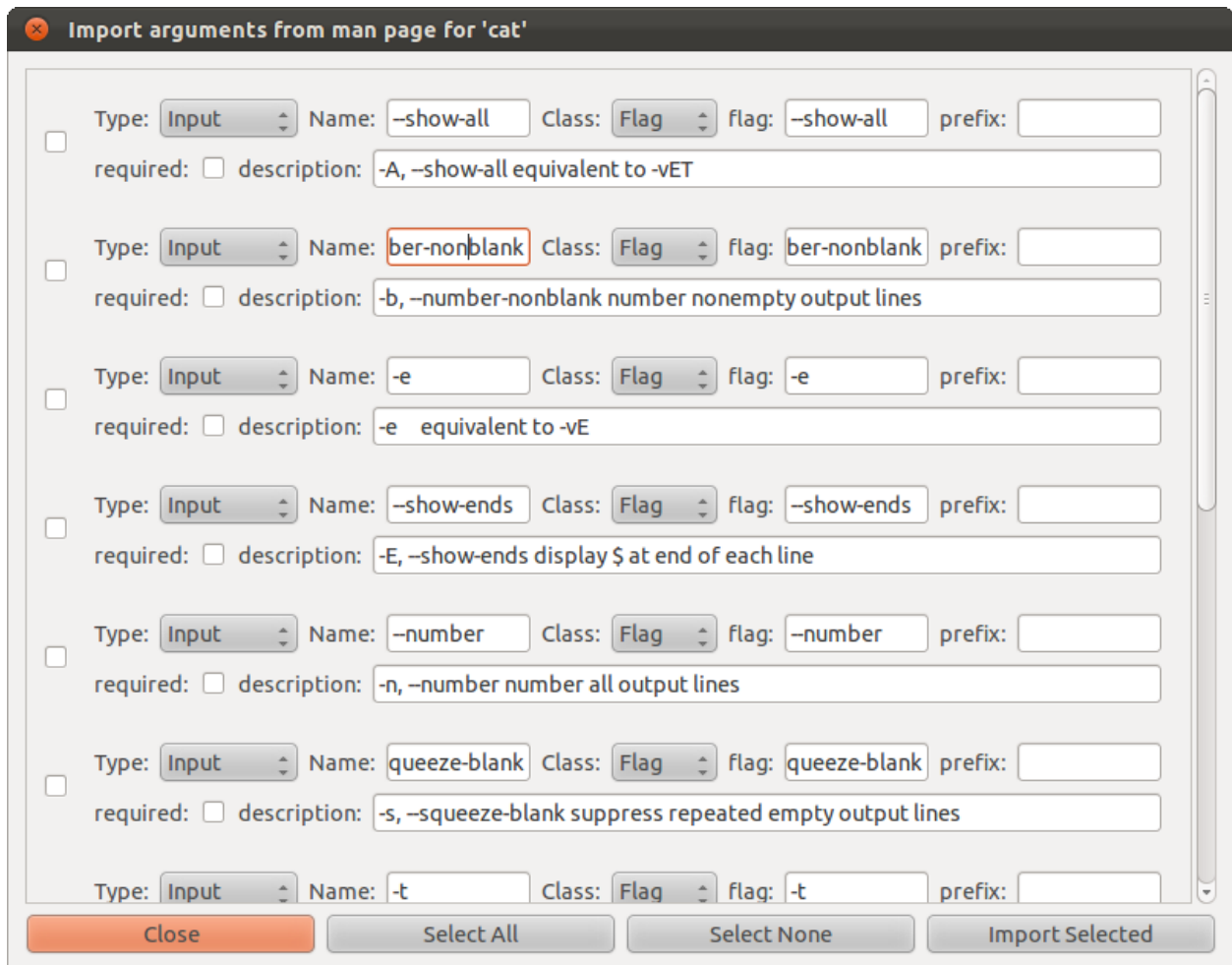


Fig. 11.2: Figure 1.2 - Import Arguments Window

Try it Now!

Create a wrapper that takes a file as input and generate a file as output using `-o`. The ports should always be visible. The command looks like:

```
filter infile -o outfile
```

Your wrapper should look like in figure [Figure 1.3](#). Note that the order of the arguments is always preserved:

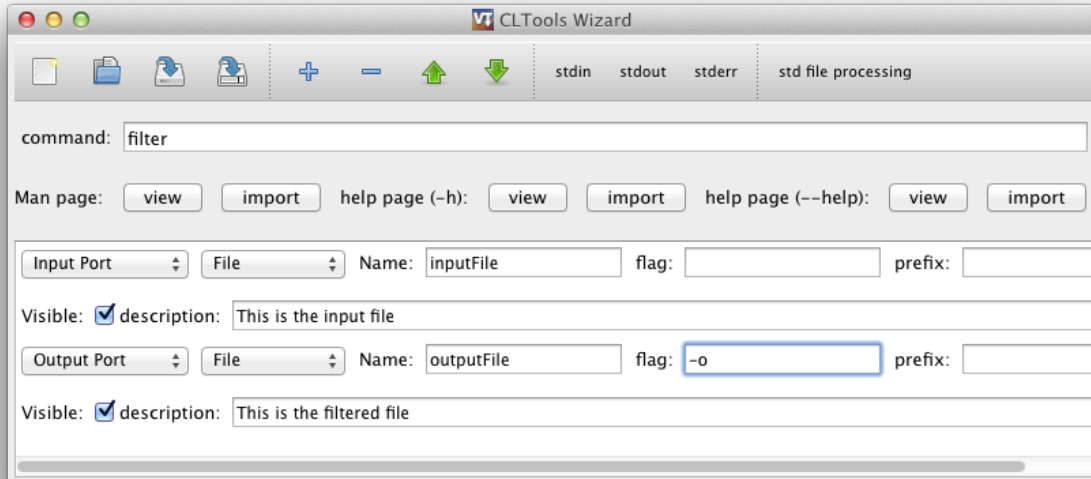


Fig. 11.3: Figure 1.3 - An infile outfile wrapper

11.1.2 Port visibility

[Figure 1.4](#) shows how the **visible** setting affects ports in VisTrails. Visible ports are meant to be connected to other modules, and are shown as square input or output ports on the module, while non-visible ports are meant to be optional, or added as parameters on the input port list to the right. Non-visible ports can be made visible on the module by clicking on the left side of the ports pane, so that an eye icon is displayed. The example below has 2 visible input ports and one visible output port. The input list to the right shows available inputs, both visible and non-visible. The first input in the input list to the right is visible by default, which is shown by a greyed-out eye. The second port is non-visible by default but has been made visible as shown by the eye icon. The second input is non-visible but can be made visible on the module by clicking so that the eye icon becomes visible.

11.1.3 Environment Variables

There are three ways to set environment variables in CLTools. If your environment variables is platform-dependent, you should set the **env** configuration variable for the CLTools package. In VisTrails, go to the Preferences->Module Packages dialog, select **CLTools**, make sure it is enabled, and select **Configure...**. Set the **env** variable to the preferred environment. Separate name and value using `=` and variables using `;`, like this:

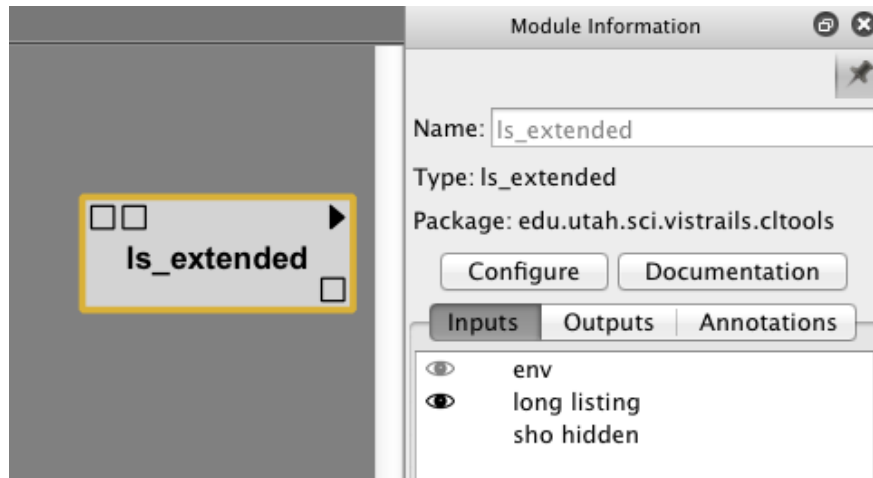


Fig. 11.4: Figure 1.4 - Port visibility in VisTrails

```
PATH=/my/custom/path;DEBUG=;MYVAR=32
```

If you want to specify the variables in your workflow, you can enable the **env** input port on your module by checking the **env** option in the top toolbar in the CLTools wizard. Then you can specify environment variables either as parameters to your module or by connecting the **env** input port to other modules. Multiple parameters can be specified as a single string or by adding multiple **env** parameters. These variables overrides variables specified using the other two methods.

For modules that always need the same environment variables, they can be added to the module by editing the `.clt` file directly and adding an **env** entry in the options section as shown below. These variables overrides the ones specified in the CLTools configuration:

```
{
  "command": "ls",
  "options": {
    "env": "MYVAR=/my/custom/path;MYVAR2=64"
  }
}
```

Note that if you replace e.g. the **PATH** variable, you should include the existing path, which can be found by running e.g. `echo $PATH` on the command line.

11.1.4 Setting working directory

The **Directory** field to the right of the command field can be used to specify the working directory where the command will be executed. It does **not** specify the directory where the command is found. Use the `PATH` environment variable for that.

11.1.5 InputOutput files

The **InputOutput** port should be used for commands that modifies a file in-place, so that it is used both as an input and an output. An example of using the InputOutput module is shown in *Figure 1.5*. When executed, the input file will be copied to a temporary file before it is passed to the command and used as an output. This is because you should not (if you can avoid it) modify the inputs to your modules, because they may be used by other modules, or re-executed by the same module. It may be useful to set the file suffix attribute to make sure the copied file is of the same type as

the original. There is currently no way of passing the original file to the command, since it is discouraged. But if this is necessary in a particular case, CLTools can be easily modified to do this.

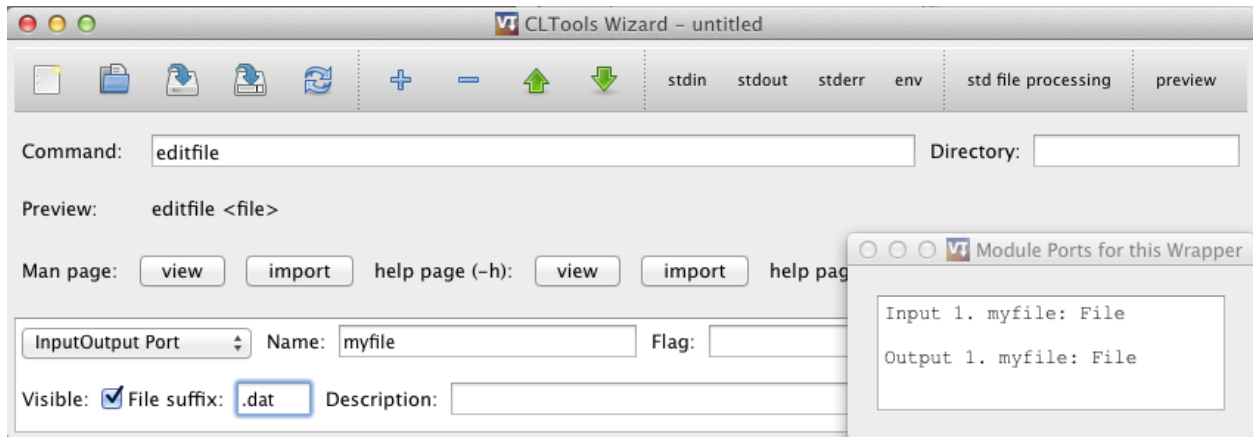


Fig. 11.5: Figure 1.5 - Example of an InputOutput port

11.1.6 Creating a standalone package

When you have a working set of wrappers and want to distribute them, you should put them in a separate module package. This allows you to name and version your package, and makes sure there are no conflicts with modules using the same name as yours. One warning: workflows using the old modules will need to be recreated to use the modules in this new package instead, so it is better to start building workflows after a separate package has been created. Below are the steps to follow in order to set up a new package.

1. Create a new directory in `$HOME/.vistrails/userpackages/`
2. Copy `__init__.py` and `init.py` from `vistrails/packages/CLTools` to this new directory
3. Update **name**, **identifier**, and **version** in `__init__.py` to the desired values
4. Move all desired tools (`*.clt` files) to this new directory
5. Enable and test your new package!

11.1.7 File Format

The wrapper is stored as a `JSON` file and can be edited using a text editor if needed. It uses the following schema:

`ROOT` is a dict with the following possible keys:

- **command** (required) - value is the command to execute like “`cat`” or “`/home/tommy/cat`”
- **stdin** - handle stdin - value is a 3-list [”port name”, `CLASS`, `OPTIONDICT`]
- **stdout** - handle stdout - value is a 3-list [”port name”, `CLASS`, `OPTIONDICT`]
- **stderr** - handle stdout - value is a 3-list [”port name”, `CLASS`, `OPTIONDICT`]
- **args** - list of ordered arguments that can either be constants, inputs, or outputs. See `ARG`.
- **dir** - value is the working directory to execute the command from
- **options** - a dict of module options - see `OPTIONDICT`

OPTIONDICT is a dict with module specific options, recognized options are:

- **std_using_files** - connect files to pipes so that they need not be stored in memory. This is useful for large files but may be unsafe since it does not use subprocess.communicate
- **env** - A list of environment variables to set when executing the command, with entries separated by ; and key/value pairs separated by =. This overrides all other environment variables set, except for the env_port, and should only be used when they are not expected to change. It can only be set by editing the .clt files directly with a text editor.
- **env_port** - Set to add an input port **env** for specifying the environment variables to use, this overrides all other environment variables set

ARG is a 4-list containing [TYPE, "name", KCLASS, ARGOPTIONDICT] TYPE is one of:

- **input** - create input port for this arg
- **output** - create output port for this arg
- **inputoutput** - create both input and output port for this arg. The type must be **File** and a copy of the original file will be processed and used as output.
- **constant** - use "port name" directly as a constant string

CLASS indicates the port type and can be one of the following. **String** is used by default.

- **File** - A vistrails **File** type. The filename will be used as the argument
- **String** - A vistrails **String** type. The string will be used as the argument
- **Integer** - A vistrails **Integer** type. Its string value will be used as the argument
- **Float** - A vistrails **Float** type. Its string value will be used as the argument
- **Flag** - A vistrails **Bool** type. A boolean flag that when set to true will add the value of the argument to the command.
- **List** - A list of values of the type specified by the **type** option. All values in the list will be added as arguments.

ARGOPTIONDICT is a dict containing argument options. recognized options are:

- **type: CLASS** - used by List-types to specify subtype.
- **flag: name** - Append name as a short-style flag before the specified argument. If type is **List** it is appended before each item
- **prefix: name** - Append name as a long-style prefix to the final argument. If it is also a list it is appended to each item.
- **required: None** - Makes the port always visible in VisTrails.
- **suffix: name** - Specifies the file ending for created files

Try it Now!

Wrap the command “cat” that takes 2 files as input named “first” and “second”. Also take a list of files as input named “rest”. Catch stdout as file, name it “combined”. Catch stderr as string, name it “stderr”. Show “first” and “combined” by default.

Your wrapper should now look like this:

```
{ "command": "cat",
  "args": [ ["input", "first", "File", {"required":""}],
            ["input", "second", "File", {}],
            ["input", "rest", "List", {"type":"File"}] ],
  "stdout": ["combined", "File", {"required":""}],
  "stderr": ["stderr", "String", {}]
}
```

Save as {yourhomedirectory}/.vistrails/CLTools/cat.clt Reload CLTools package in VisTrails. Test the new module.

VISTRAILS API DOCUMENTATION

12.1 Module Definition

12.1.1 Module

class `vistrails.core.modules.vistrails_module.Module`

Module is the base module from which all module functionality is derived from in VisTrails. It defines a set of basic interfaces to deal with data input/output (through ports, as will be explained later), as well as a basic mechanism for dataflow based updates.

Execution Model

VisTrails assumes fundamentally that a pipeline is a dataflow. This means that pipeline cycles are disallowed, and that modules are supposed to be free of side-effects. This is obviously not possible in general, particularly for modules whose sole purpose is to interact with operating system resources. In these cases, designing a module is harder – the side effects should ideally not be exposed to the module interface. VisTrails provides some support for making this easier, as will be discussed later.

VisTrails caches intermediate results to increase efficiency in exploration. It does so by reusing pieces of pipelines in later executions.

Terminology

Module Interface: The module interface is the set of input and output ports a module exposes.

Designing New Modules

Designing new modules is essentially a matter of subclassing this module class and overriding the `compute()` method. There is a fully-documented example of this on the default package ‘pythonCalc’, available on the ‘packages/pythonCalc’ directory.

Caching

Caching affects the design of a new module. Most importantly, users have to account for `compute()` being called more than once. Even though `compute()` is only called once per individual execution, new connections might mean that previously uncomputed output must be made available.

Also, operating system side-effects must be carefully accounted for. Some operations are fundamentally side-effectful (creating OS output like uploading a file on the WWW or writing a file to a local hard drive). These modules should probably not be cached at all. VisTrails provides an easy way for modules to report that they should not be cached: simply subclass from the `NotCacheable` mixin provided in this python module. (NB: In order for the mixin to work appropriately, `NotCacheable` must appear *BEFORE* any other subclass in the class hierarchy declarations). These modules (and anything that depends on their results) will then never be reused.

Intermediate Files

Many modules communicate through intermediate files. VisTrails provides automatic filename and handle management to alleviate the burden of determining tricky things (e.g. longevity) of these files. Modules can request temporary file names through the file pool, currently accessible through `self.interpreter.filePool`.

The FilePool class is available in `core/modules/module_utils.py` - consult its documentation for usage. Notably, using the file pool will make temporary files work correctly with caching, and will make sure the temporaries are correctly removed.

`__input_ports`

Class attribute that stores the list of input ports for the module. May include instances of `InputPort` and `CompoundInputPort`.

`__output_ports`

Class attribute that defines the list of output ports for the module. May include instances of `OutputPort` and `CompoundOutputPort`.

`__settings`

Class attribute that stores a `ModuleSettings` object that controls appearance, configuration widgets, and other module settings.

`compute()`

This method should be overridden in order to perform the module's computation.

`get_input(port_name, allow_default=True)`

Returns the value coming in on the input port named **port_name**.

Parameters

- **port_name** (*str*) – the name of the input port being queried
- **allow_default** (*bool*) – whether to return the default value if it exists

Returns the value being passed in on the input port

Raises `ModuleError` if there is no value on the port (and no default value if `allow_default` is `True`)

`get_input_list(port_name)`

Returns the value(s) coming in on the input port named **port_name**. When a port can accept more than one input, this method obtains all the values being passed in.

Parameters **port_name** (*str*) – the name of the input port being queried

Returns a list of all the values being passed in on the input port

Raises `ModuleError` if there is no value on the port

`set_output(port_name, value)`

This method is used to set a value on an output port.

Parameters

- **port_name** (*str*) – the name of the output port to be set
- **value** – the value to be assigned to the port

`check_input(port_name) → None`

Raises an exception if the input port named `port_name` is not set.

Parameters **port_name** (*str*) – the name of the input port being checked

Raises `ModuleError` if there is no value on the port

`has_input(port_name)`

Returns a boolean indicating whether there is a value coming in on the input port named **port_name**.

Parameters `port_name` (*str*) – the name of the input port being queried

Return type `bool`

force_get_input (*port_name*, *default_value=None*)

Like `get_input()` except that if no value exists, it returns a user-specified `default_value` or `None`.

Parameters

- `port_name` (*str*) – the name of the input port being queried
- `default_value` – the default value to be used if there is no value on the input port

Returns the value being passed in on the input port or the default

force_get_input_list (*port_name*)

Like `get_input_list()` except that if no values exist, it returns an empty list

Parameters `port_name` (*str*) – the name of the input port being queried

Returns a list of all the values being passed in on the input port

annotate (*d*)

Manually add provenance information to the module's execution trace. For example, a module that generates random numbers might add the seed that was used to initialize the generator.

Parameters `d` (*dict*) – a dictionary where both the keys and values are strings

12.1.2 ModuleError

```
class vistrails.core.modules.vistrails_module.ModuleError (module,          errmsg,
                                                         abort=False,      error-
                                                         Trace=None)
```

`ModuleError` should be passed the module instance that signaled the error and the error message as a string.

12.1.3 ModuleSettings

```
class vistrails.core.modules.config.ModuleSettings (name=None,           config-
                                                         ure_widget=None,   con-
                                                         stant_widget=None,  con-
                                                         stant_widgets=None,
                                                         signature=None,     con-
                                                         stant_signature=None, color=None,
                                                         fringe=None,        left_fringe=None,
                                                         right_fringe=None,  ab-
                                                         stract=False,       package=None,
                                                         namespace=None,     version=None,
                                                         package_version=None,
                                                         hide_namespace=False,
                                                         hide_descriptor=False,
                                                         is_root=False,      ghost_package=None,
                                                         ghost_package_version=None,
                                                         ghost_namespace=None)
```

name (*String*)

An optional string that will identify the module (defaults to the module class's `__name__`).

configure_widget (*QWidget* | *PathString*)

An optional module configuration widget that is provided so that users can configure the module (e.g. PythonSource uses a widget to display a code editor more suited for writing code).

constant_widget (*ConstantWidgetConfig* | *QWidget* | *PathString*)

If not None, the registry will use the specified widget(s) or import path string(s) of the form “<module>:<class>” to import the widget. A tuple allows a user to specify the widget_type (e.g. “default”, “enum”, etc.) as the second item and the widget_use (e.g. “default”, “query”, “paramexp”). If the plural form is used, we expect a list, the singular form is used for a single item.

constant_widgets (*List(constant_widget)*)

See *ModuleSettings.constant_widget*

signature (*Callable*)

If not None, then the cache uses this callable as the function to generate the signature for the module in the cache. The function should take three parameters: the pipeline (of type *vistrails.core.vistrail.Pipeline*), the module (of type *vistrails.core.vistrail.Module*), and a dict that stores parameter hashers. This dict is supposed to be passed to *vistrails/core/cache/haser.py:Hasher*, in case that needs to be called.

constant_signature (*Callable*)

If not None, the cache uses this callable as the function used to generate the signature for parameters of the associated module’s type. This function should take a single argument (of type *vistrails.core.vistrail.module_param.ModuleParam*) and returns a SHA hash.

color (*(Float, Float, Float)*)

In the GUI, the module will be colored according to the specified RGB tuple where each value is a float in [0,1.0].

fringe (*List((Float, Float))*)

If not None, generates custom lateral fringes for the module boxes. *module_fringe* must be a list of pairs of floats. The first point must be (0.0, 0.0), and the last must be (0.0, 1.0). This will be used to generate custom lateral fringes for module boxes. All x values must be positive, and all y values must be between 0.0 and 1.0. Alternatively, the user can set *ModuleSettings.left_fringe* and *ModuleSettings.right_fringe* to set two different fringes.

left_fringe (*List((Float, Float))*)

See *ModuleSettings.fringe*.

right_fringe (*List((Float, Float))*)

See *ModuleSettings.fringe*.

abstract (*Boolean*)

If True, means the module only serves as a base class for other modules. It will not appear in the module palette but may be used as an input or output port type.

package (*String*)

If not None, then we use this package instead of the current one. This is only intended to be used with local per-module module registries (in other words: if you don’t know what a local per-module registry is, you can ignore this option).

namespace (*String*)

If not None, then we associate a namespace with the module. A namespace is essentially appended to the package identifier so that multiple modules inside the same package can share the same name. Namespaces may be nested using the “|” separator. For example, “Tools|Mathematical” specified the Mathematical namespace inside of the Tools namespace.

version (*String*)

The module version. This is usually used with subworkflows where the underlying module may have different versions. Not recommended for general use at this time.

package_version (*String*)

The current package version for the module. As with `ModuleSettings.package`, you should not use this unless you know what you are doing as VisTrails will automatically fill in this information for any normal package.

hide_namespace (*Boolean*)

If True, the module palette will not display the namespace for the module. Used for subworkflows, otherwise it may be confusing for users.

hide_descriptor (*Boolean*)

If True, the module palette will not display that module in its list (similar to abstract, but can be used when the module is not truly abstract).

is_root (*Boolean*)

Internal use only. This is used to designate the base Module class and should not be used by any other module.

ghost_package (*String*)

If not None, then the 'ghost_identifier' is set on the descriptor, which will cause the module to be displayed under that package in the module palette, rather than the package specified by the package argument (or current package).

ghost_package_version (*String*)

If not None, then the attribute 'ghost_package_version' is set on the descriptor. Currently this value is unused, but eventually if multiple packages with the same identifier but different package versions are loaded simultaneously, this will allow overriding the package_version to clean up the module palette.

ghost_namespace (*String*)

If not None, the descriptor will be displayed under the specified namespace instead of the 'namespace' attribute of the descriptor.

12.2 Port Specification

12.2.1 InputPort (IPort)

```
class vistrails.core.modules.config.InputPort (name=None, signature=None, optional=False, sort_key=-1, docstring=None, shape=None, min_conns=0, max_conns=-1, depth=0, label=None, default=None, values=None, entry_type=None)
```

name (*String*)

The name of the of the port

signature (*String*)

The signature of the of the port (e.g. "basic:Float")

optional (*Boolean*)

Whether the port should be visible by default (defaults to True)

sort_key (*Integer*)

An integer value that indicates where, relative to other ports, this port should appear visually

docstring (*String*)

Documentation for the port

shape (“triangle” | “diamond” | “circle” | [(Float,Float)])

The shape of the port. If triangle, appending an angle (in degrees) rotates the triangle. If a list of (x,y) tuples, specifies points of a polygon in the [0,1] x [0,1] region

min_conns (*Integer*)

The minimum number of values required for the port

max_conns (*Integer*)

The maximum number of values allowed for the port

depth (*Integer*)

The list depth of the port. Default is 0 (no list)

label (*String*)

A label to be shown with a port

default

The default value for a constant-typed port

values (*List*)

A list of enumerated values that a *ConstantWidgetConfig* uses to configure the widget. For example, the “enum” widget uses the entries to present an exclusive list of choices.

entry_type (*String*)

The type of the configuration widget that should be used with this port. Developers may use custom widgets on a port-by-port basis by adding widgets with different *ConstantWidgetConfig.widget_type* values and defining the port’s *entry_type* to match.

class `vistrails.core.modules.config.IPort`

Synonym for *InputPort*

12.2.2 OutputPort (OPort)

class `vistrails.core.modules.config.OutputPort` (*name=None, signature=None, optional=False, sort_key=-1, docstring=None, shape=None, min_conns=0, max_conns=-1, depth=0*)

name (*String*)

The name of the of the port

signature (*String*)

The signature of the of the port (e.g. “basic:Float”)

optional (*Boolean*)

Whether the port should be visible by default (defaults to True)

sort_key (*Integer*)

An integer value that indicates where, relative to other ports, this port should appear visually

docstring (*String*)

Documentation for the port

shape (“triangle” | “diamond” | “circle” | [(Float,Float)])

The shape of the port. If triangle, appending an angle (in degrees) rotates the triangle. If a list of (x,y) tuples, specifies points of a polygon in the [0,1] x [0,1] region

min_conns (*Integer*)

The minimum number of values required for the port

max_conns (*Integer*)

The maximum number of values allowed for the port

depth (*Integer*)

The list depth of the port. Default is 0 (no list)

class `vistrails.core.modules.config.OPort`

Synonym for `OutputPort`

12.2.3 CompoundInputPort (CIPort)

class `vistrails.core.modules.config.CompoundInputPort` (*name=None, signature=None, optional=False, sort_key=-1, docstring=None, shape=None, min_conns=0, max_conns=-1, depth=0, items=None, labels=None, defaults=None, values=None, entry_types=None*)

name (*String*)

The name of the of the port

signature (*String*)

The signature of the port (e.g. “basic:Integer, basic:Float”). Note that for compound ports, this may be instead included on a per-component basis in `InputPortItem.signature`.

optional (*Boolean*)

Whether the port should be visible by default (defaults to True)

sort_key (*Integer*)

An integer value that indicates where, relative to other ports, this port should appear visually

docstring (*String*)

Documentation for the port

shape (“triangle” | “diamond” | “circle” | [(Float,Float)])

The shape of the port. If triangle, appending an angle (in degrees) rotates the triangle. If a list of (x,y) tuples, specifies points of a polygon in the [0,1] x [0,1] region

min_conns (*Integer*)

The minimum number of values required for the port

max_conns (*Integer*)

The maximum number of values allowed for the port

depth (*Integer*)

The list depth of the port. Default is 0 (no list)

items (*List(InputPortItem)*)

Either use this field and break individual labels/defaults/values/entry_types into `InputPortItem` components or use the other four fields.

labels (*List(String)*)

A list of `InputPort.label`

defaults (*List*)

A list of `InputPort.default`

values (*List(List)*)

A list of `InputPort.values`

entry_types (*List(String)*)
A list of *InputPort.entry_type*

class `vistrails.core.modules.config.CIPort`
Synonym for *CompoundInputPort*

12.2.4 CompoundOutputPort (COPort)

class `vistrails.core.modules.config.CompoundOutputPort` (*name=None, signature=None, optional=False, sort_key=-1, docstring=None, shape=None, min_conns=0, max_conns=-1, depth=0, items=None*)

name (*String*)
The name of the of the port

signature (*String*)
The signature of the port (e.g. “basic:Integer, basic:Float”). Note that for compound ports, this may be instead included on a per-component basis in *OutputPortItem.signature*.

optional (*Boolean*)
Whether the port should be visible by default (defaults to True)

sort_key (*Integer*)
An integer value that indicates where, relative to other ports, this port should appear visually

docstring (*String*)
Documentation for the port

shape (*“triangle” | “diamond” | “circle” | [(Float,Float)]*)
The shape of the port. If triangle, appending an angle (in degrees) rotates the triangle. If a list of (x,y) tuples, specifies points of a polygon in the [0,1] x [0,1] region

min_conns (*Integer*)
The minimum number of values required for the port

max_conns (*Integer*)
The maximum number of values allowed for the port

depth (*Integer*)
The list depth of the port. Default is 0 (no list)

items (*List(OutputPortItem)*)
Either use this field and break individual signatures into *OutputPortItem* components or use the signature field.

class `vistrails.core.modules.config.COPort`
Synonym for *CompoundOutputPort*

12.2.5 InputPortItem (IPItem)

class `vistrails.core.modules.config.InputPortItem` (*signature=None, label=None, default=None, values=None, entry_type=None*)

signature (*String*)
See *InputPort.signature*

label (*String*)

See *InputPort.label*

default

See *InputPort.default*

values (*List*)

See *InputPort.values*

entry_type (*String*)

See *InputPort.entry_type*

class `vistrails.core.modules.config.IPItem`

Synonym for *InputPortItem*

12.2.6 OutputPortItem (OPItem)

class `vistrails.core.modules.config.OutputPortItem` (*signature=None*)

signature (*String*)

See *InputPort.signature*

class `vistrails.core.modules.config.OPItem`

Synonym for *OutputPortItem*

12.3 Parameter Widget Configuration

12.3.1 ConstantWidgetConfig

class `vistrails.core.modules.config.ConstantWidgetConfig` (*widget*, *widget_type=None*,
widget_use=None)

widget (*QWidget* | *String*)

The widget to be used either as the class itself or a string of the form `<py_module>:<class>` (e.g. “`vistrails.gui.modules.constant_configuration:BooleanWidget`”)

widget_type (*String*)

A developer-available type that links a widget to a port *entry_type*

widget_use (*String*)

Intended to differentiate widgets for different purposes in VisTrails. Currently uses the values `None`, “`query`”, and “`paramexp`” to define widget uses in parameter, query, and parameter exploration configurations, respectively.

12.3.2 QueryWidgetConfig

class `vistrails.core.modules.config.QueryWidgetConfig` (*widget=None*, *wid-*
get_type=None, *wid-*
get_use='query')

widget (*QWidget* | *String*)

The widget to be used either as the class itself or a string of the form `<py_module>:<class>` (e.g. “`vistrails.gui.modules.constant_configuration:BooleanWidget`”)

widget_type (*String*)

A developer-available type that links a widget to a port entry_type

widget_use (*String*)

Like *ConstantWidgetConfig.widget_use*, just defaulted to “query”

12.3.3 ParamExpWidgetConfig

```
class vistrails.core.modules.config.ParamExpWidgetConfig (widget=None,          wid-
                                                         get_type=None,          wid-
                                                         get_use='paramexp')
```

widget (*QWidget | String*)

The widget to be used either as the class itself or a string of the form <py_module>:<class> (e.g. “vistrails.gui.modules.constant_configuration:BooleanWidget”)

widget_type (*String*)

A developer-available type that links a widget to a port entry_type

widget_use (*String*)

Like *ConstantWidgetConfig.widget_use*, just defaulted to “paramexp”

Part III

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