Provenance for Visualizations: Reproducibility and Beyond

By Claudio T. Silva, Juliana Freire, and Steven P. Callahan

The demand for the construction of complex visualizations is growing in many disciplines of science, as users are faced with ever increasing volumes of data to analyze. The authors present VisTrails, an open-source provenance management system that provides infrastructure for data exploration and visualization.

Computing has been an enormous accelerator for science, leading to an information explosion in many different fields. Future scientific advances depend on our ability to comprehend the vast amounts of data currently being produced and acquired. To analyze and understand this data, though, we must assemble complex computational processes and generate insightful visualizations, which often require combining loosely coupled resources, specialized libraries, and grid and Web services. Such processes could generate yet more data, adding to the information overload scientists currently deal with.

Today, the scientific community uses ad hoc approaches to data exploration, but such approaches have serious limitations. In particular, scientists and engineers must expend substantial effort managing data (such as scripts that encode computational tasks, raw data, data products, images, and notes) and recording provenance information (that is, all the information necessary for reproducing a certain piece of data) so that they can answer basic questions: Who created a data product and when? When was it modified, and who modified it? What process was used to create the data product? Were two data products derived from the same raw data? Not only is this process time-consuming, it's also error-prone.

Without provenance, it's difficult (and sometimes impossible) to reproduce and share results, solve problems collaboratively, validate results with different input data, and understand the process used to solve a particular problem. In addition, data products' longevity becomes limited—without precise and sufficient information about how the data product was generated, its value diminishes significantly.

The lack of adequate provenance support in visualization systems motivated us to build VisTrails, an open source provenance-management system that provides infrastructure for data exploration and visualization through workflows. VisTrails transparently records detailed provenance of exploratory computational tasks and leverages this information beyond just the ability to reproduce and share results. In particular, it uses this information to simplify the process of exploring data through visualization.

Visualization Systems

Visualization systems such as MayaVi (http://mayavi.sourceforge.net) and ParaView (www.paraview.org)—which are built on top of Kitware’s Visualization Toolkit (VTK)—as well as SCIRun (http://software.sci.utah.edu/scirun.html) enable users to interactively create and manipulate complex visualizations. Such systems are based on the notion of data flows, and they provide visual interfaces for producing visualizations by assembling pipelines out of modules (or functions) connected in a network. SCIRun supports an interface that lets users directly edit data flows. MayaVi and ParaView have a different interaction paradigm that implicitly builds data flows as the user makes “task-oriented” choices (such as selecting an isosurface value).

Although these systems let users create complex visualizations, they lack the ability to support data exploration at a large scale. Notably, they don’t adequately support collaborative creation and exploration of multiple visualizations. Because these systems don’t distinguish between the definition of a data flow and its instances, to execute a given data flow with different parameters (for example, different input files), users must manually set these parameters through a GUI. Clearly, this process doesn’t scale to more than a few visualizations at a time. Additionally, modifications to parameters or to a data flow’s definition are destructive—the systems don’t maintain any change history. This requires the user to first construct the visualization and then remember the input data sets, parameter values, and the exact dataflow configuration that led to a particular image.

Finally, before constructing a visualization, users must often acquire,
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This first column discusses the benefits of provenance and makes a case that better provenance mechanisms are needed for visualization. In upcoming columns of the Visualization Corner, we will attempt to inform the scientific community at large about the benefits and technologies related to provenance. In particular, we want to promote the idea of reproducible visualizations. We encourage authors of articles published in the department to provide metadata for visualizations in their articles that let readers reproduce images as well as generate related ones (for example, using different data). Ultimately, our hope is that this trend will spread to the point that published articles will contain not only textual descriptions of the techniques, but links to data, code, and the complete overall process used to generate the scientific results.

As a mechanism to capture and share provenance metadata, authors can use VisTrails to produce specifications of the figures and plots presented in their articles. We’ll archive this information at www.vistrails.org/index.php/GiSE. The data and processes associated with this column are already available on the Web site, so you can reproduce them, right now, from your desktop!

Reproducibility and Sharing Data and Processes for the Visualization Corner

By Claudio Silva and Joel E. Tohline

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VisTrails: Provenance for Visualization

The VisTrails system (www.vistrails.org) we developed at the University of Utah is a new visualization system that provides a comprehensive provenance-management infrastructure and can be easily combined with existing visualization libraries. Unlike previous systems, VisTrails uses an action-based provenance model that uniformly captures changes to both parameter values and pipeline definitions by unobtrusively tracking all changes that users make to pipelines in an exploration task. We refer to this detailed provenance of the pipeline evolution as a visualization trail, or vistrail.

The stored provenance ensures that users will be able to reproduce the visualizations and lets them easily navigate through the space of pipelines created for a given exploration task. The VisTrails interface lets users query, interact with, and understand the visualization process’s history. In particular, they can return to previous versions of a pipeline and change the specification or parameters to generate a new visualization without losing previous changes.

Another important feature of the action-based provenance model is that it enables a series of operations that greatly simplify the exploration process and could reduce the time to insight. In particular, it allows the flexible reuse of pipelines and provides a scalable mechanism for creating and comparing numerous visualizations as well as their corresponding pipelines. Although we originally built VisTrails to support exploratory visualization tasks, its extensible infrastructure lets users integrate a wide range of libraries. This makes the system suitable for other exploratory tasks, including data mining and integration.

Creating an Interactive Visualization with VisTrails

To illustrate the issues involved in creating visualizations and how provenance can aid in this process, we present the following scenario, common in medical data visualization.

Starting from a volumetric computed tomography (CT) data set, we generate different visualizations by exploring the data through volume rendering, isosurfacing (extracting a contour), and slicing. Note that with proper modifications, this example also works for visualizing other types of data (for example, tetrahedral meshes).

Dataflow Processing Networks and Visual Programming

A useful paradigm for building visualization applications is the dataflow model. A data flow is a directed graph in which nodes represent computations,
and edges represent data streams: each node or module corresponds to a procedure that’s applied on the input data and generates some output data as a result. The flow of data in the graph determines the order in which a dataflow system executes the processing nodes. In visualization, we commonly refer to a dataflow network as a visualization pipeline. (For this article, we use the terms workflow, data flow, and pipeline interchangeably.) Figure 1b shows an example of the data flow used to derive the images shown in Figure 1c. The green rectangles represent modules, and the black lines represent connections. Most of the modules Figure 1 shows are from VTK, and labels on each module indicate the corresponding VTK class. In this figure, we naturally think of data flowing from top to bottom, eventually being rendered and presented for display.

We can use different mechanisms for creating visualization pipelines—for example, “scripting” in a modern dynamic language, such as Python. Consider Figure 1a, which defines the workflow via a script written in Python that uses VTK to read a volume data set from a file, extract an isosurface, map the isosurface to renderable geometry, and then finally render it in an interactive window.

Visual programming interfaces for designing data flows have become popular and several systems, such as SCIRun, have adopted them. These interfaces give users a more intuitive view of the pipeline. They also dynamically perform type checking and guide the connection between modules’ input and output ports—once the user selects a module’s output, connections are allowed only to the target module’s appropriate input. VisTrails automatically pulls edges toward the correct input port. As we discuss later, another benefit of having a high-level, structured workflow description is that we can use expressive languages for querying and updating workflows.

Comparing and Exploring Multiple Visualizations

Regardless of the specific mechanism we use to define a pipeline, the visualization process’s end goal is to gain insight from the data. To obtain such insight, users must often generate and compare multiple visualizations. Going back to our scenario, several alternatives exist for rendering our CT data. Isosurfacing is a commonly used technique. Given a function \( f: \mathbb{R}^n \rightarrow \mathbb{R} \) and a value \( a \), an isosurface consists of the set of points in a domain that map to \( a \)—that is, \( S_a = \{ x \in \mathbb{R}^n : f(x) = a \} \).

The range of \( a \) values determines all possible isosurfaces that the user can generate. To identify “good” \( a \) values that represent a data set’s important features, we can look at the range of values taken by \( a \), and their frequency, in the form of a histogram.

Figure 1. Dataflow programming for visualization. (a) We commonly use a script to describe a pipeline from existing libraries such as the Visualization Toolkit (VTK). (b) Visual programming interfaces, such as the one VisTrails provides, facilitate the creation and maintenance of these dataflow pipelines. The green rectangles represent modules, and the black lines represent connections. (c) The end result of the script or the VisTrails pipeline is a set of interactive visualizations.
Using VisTrails, we can straightforwardly extend the isosurface pipeline to also display a histogram of the data. VisTrails provides a very simple plugin functionality that you can use to add packages and libraries, including your own. For our example, we used matplotlib’s 2D plotting functionality (http://matplotlib.sourceforge.net) to generate the histogram at the top of Figure 1c. This histogram helps in data exploration by suggesting regions of interest in the volume. The plot shows that the highest frequency features lie between the ranges [0,25] and [58,68]. To identify the features that correspond to these ranges, we must explore these regions directly through visualization.

**Scalable exploration of parameter spaces.** VisTrails provides an interface for parameter exploration that lets users specify a set of parameters to explore, as well as how to explore, group, and display them. As a simple 1D example, Figure 2 shows an exploration of the isosurface value as four steps between 50 and 70, displayed horizontally in the VisTrails spreadsheet.

The VisTrails spreadsheet lets us compare visualizations in different dimensions (row, column, sheet, and time), and we can link the spreadsheet’s cells to synchronize the interactions between visualizations. Note that VisTrails leverages the dataflow specifications to identify and avoid redundant operations. By using the same cache for different cells in the spreadsheet, VisTrails lets users efficiently explore numerous related visualizations.

**Comparing different visualization techniques.** Volume rendering is a powerful computer graphics technique for visualizing 3D data. While many visualization algorithms focus on creating a rendering of surfaces—although they might be surfaces of 3D objects—volume rendering lets us see “inside” the volume. This technique models the volume as cloud-like cells of semitransparent material. Although a surface rendering of the human body might show only the skin, for example, a complete volume rendering might also show the bones and internal organs.

Volume rendering and isosurfacing are complementary techniques, and they can generate very similar imagery depending on parameters. In fact, distinguishing between them can be difficult. The VisTrails system lets us compare workflows using a visual difference interface. To demonstrate this capability, we compute the difference between the original isosurface generation pipeline and the new volume rendering pipeline. Figure 3 shows the visual difference of the workflows that we can inspect, along with their resulting visualizations. In Figure 3a, we use volume rendering to create the image, in which we can see the skin on top of the bone structure; Figure 3b shows only the bone structure rendered with our standard isosurface technique. This ability to (efficiently) compare workflows and visualizations is one of the benefits of the VisTrails action-based provenance model and becomes increasingly important as a workflow becomes more complex and is shared among collaborators.

With other workflow systems, these comparisons are challenging because they require module-by-module (visual programming) or line-by-line
Visualizing comparisons. Although the former can be computationally intractable (the related decision problem of subgraph isomorphism is NP-complete), the latter could lead to results that are hard to interpret.

**Interacting with visualizations.** The images we generated so far correspond to simple, static workflows. To perform a more dynamic comparison between volume rendering and isosurfing, we used VisTrails, a tool that allows users to interact with visualizations. VisTrails provides a fully browseable history of the exploration process that led to this final set of visualizations.

Figure 3. A visual difference between different pipelines in VisTrails. We show the difference between pipelines that generated (a) volume rendering and (b) isosurface visualizations. (c) The interface distinguishes shared modules in dark gray, the modules unique to isosurfing in blue, those unique to direct volume rendering in orange, and those with parameter changes in light gray.

Figure 4. Multiple rendering techniques. (a) VisTrails renders the visualizations by combining volume rendering and isosurfacing and updates them with user interactions. (b) The corresponding pipeline represents the data flow for creating interactive visualizations. (c) VisTrails provides a fully browseable history of the exploration process that led to this final set of visualizations.
and isosurfacing, we add a feedback loop into the workflow to let users adjust the visualization interactively. We build a new workflow that uses the isosurfacing and volume rendering algorithms simultaneously. We add a clipping plane into the volume visualization to assign the volume region that we display in distinct spreadsheet cells. The pipeline interactively updates these slices along with the plane during user interaction. Figure 4 shows the resulting visualizations along with the complex dynamic workflow required to produce them.

Provenance and Exploratory Visualization
The combination of multiple visualization algorithms, different libraries, and the interactions between them considerably complicates the workflow specification. In addition, creating a set of visualizations from data is not always a linear process and often involves several iterations as a user formulates and tests hypotheses. Whereas for simple experiments, manual approaches to provenance management might be feasible, complex computational tasks involving large volumes of data or multiple researchers require automated approaches. As these tasks’ complexity and scale increases, data organization becomes a major component of the process.

VisTrails manages the data manipulated and metadata created in the course of an exploratory task. As a user (or group of users) generates a series of visualizations, VisTrails transparently tracks all the steps this exploration followed—that is, the modules and connections added and deleted, parameter value changes, and so on. Figure 4c shows a history tree of the different pipelines created in the course of our running example. The nodes in this tree correspond to pipelines, and an edge between two pipelines corresponds to changes performed on the parent pipeline to obtain its child. For readability, by default, only the nodes
in the tree that the user tags as important are displayed.

By tracking all the changes made to a workflow ensemble, VisTrails properly captures each step, leaving a complete trail of the work. Having access to the different pipelines’ specifications lets others reproduce and share the results of each step in the exploratory process.

To demonstrate this, we made the vis-trail associated with this example available for download with the VisTrails system (see the “VisTrails System” sidebar). You can recreate each figure shown in this article by executing the different nodes in the history tree.

Note that by using the action-based provenance model, we obtain a very concise representation of the history, which uses substantially less space than the alternative of explicitly storing multiple versions of a pipeline.\(^3\)

The exploration trail VisTrails captures also supports various activities that are crucial for performing reflective reasoning and obtaining insights, such as following chains of reasoning backward and forward and comparing different results.\(^4\) The tree-based view lets users

- seamlessly navigate over the history tree and return to previous pipeline versions after reaching a dead end;
- undo bad changes;
- reuse pipelines and pipeline fragments from previous versions;
- compare different pipelines and their results; and
- be reminded, in an intuitive way, of the actions that led to a particular result.

Thus, users can efficiently explore several related visualizations.

The issue of reproducibility for visualization has been considered before,\(^5\) we should note that whereas some visualization and workflow systems provide support for provenance tracking, their focus has been on data provenance—that is, information about how the system derived a given data product, including the parameter values used\(^6\)—and on interaction provenance (such as capturing a visualization’s viewing manipulations).\(^7\) VisTrails is the first system to capture information about how workflows evolve over time.

For instance, to generate the composite visualization in our final example, we extended our pipeline labeled “Volume Rendering” to include modules from the pipeline labeled “Isosurfacings.” Having two pipelines lets us further explore the visualization—by trying different isosurface values, for example (see Figure 2). In addition, we can compare the pipelines by dragging one node on top of the other (see Figure 3). These computed differences

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**Table 1. Query examples.**

<table>
<thead>
<tr>
<th>Query</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>volume</td>
<td>Highlights all nodes in the history tree where the string “volume” appears (for example, in a module name, parameter name, annotation)</td>
</tr>
<tr>
<td>user:juliana</td>
<td>Highlights all nodes in the history tree created by the user “juliana”</td>
</tr>
<tr>
<td>before: March 30, 2007</td>
<td>Highlights all nodes in the history tree created before “March 30, 2007”</td>
</tr>
</tbody>
</table>

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Figure 5. The VisTrails query by example interface. (a) Users can define a set of modules and parameters in the visual programming interface to create a query template. (b) The query results are shown in the history tree, which users can browse for specific instances of the match (inset).
are useful for understanding the visualization process, and the user can also reuse them. In this case, we applied the modules unique to “Isosurfacing” to “Volume Rendering” to create a new pipeline called “Combined Rendering” that uses a cutting plane to define regions for the rendering methods. VisTrails can automatically apply pipeline differences (like a patch) to derive new pipelines in a process we call visualization creation by analogy.9

Another benefit to having a high-level specification of the visualization process is that users can query the pipelines and their execution instances. Scientists can query a vistrail to find anomalies in previously generated visualizations and locate data products and visualizations based on operations applied in the visualization process. VisTrails supports simple, keyword-based queries as well as structured queries. In addition to providing information about the results (for example, workflow identifiers and attributes), VisTrails can visually display query results by highlighting the workflows and modules that satisfy the query. Table 1 shows an example.

Users might also define queries by example.8 As Figure 5 illustrates, users can construct (or copy and paste) a pipeline fragment into the VisTrails query tab to identify in the history tree all nodes that contain that fragment. They can then browse through the highlighted nodes and click on one to display the workflow and highlight the modules that match the query. Users can then click on the individual modules to view execution log records associated with them.

The VisTrails project has focused on creating an infrastructure to address the need to manage the provenance data of exploratory tasks. With this infrastructure in place, our research focus is now on what we can do with all the provenance that is accumulated. By mining this information, we hope to learn useful patterns that can help guide users in assembling and refining complex computational tasks.

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References

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