VisTrails: Workflow Management System on NEX

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Outline

1. Goals
2. Workflows Background
3. VisTrails Overview
4. Demo
5. VisTrails and NASA Earth Exchange (NEX)

Goals

- Provide background on workflows with emphasis on the VisTrails workflow management system.
- Demonstrate some of VisTrails features

(Not an in-depth tutorial, but rather an introduction to a software package that provide capabilities for provenance, transparency, reproducibility, and collaboration)

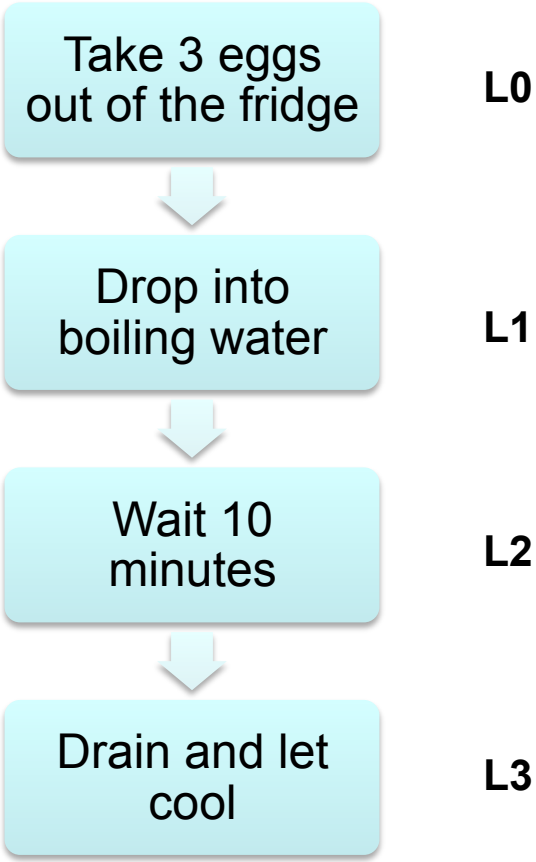
Some Terminology

- Workflow
  - Basically sequence of (connected) steps
  - Originated in manufacturing – think assembly line
- Workflow Management System
  - Manages the execution of a workflow (flow of data and information)
  - Enables users to define and execute new workflows.
- Workflow Engine
  - Implement the coordination (orchestration) of the steps in a workflow
  - Dozens of workflow engines (Business, manufacturing, science, …) – can be hard to navigate

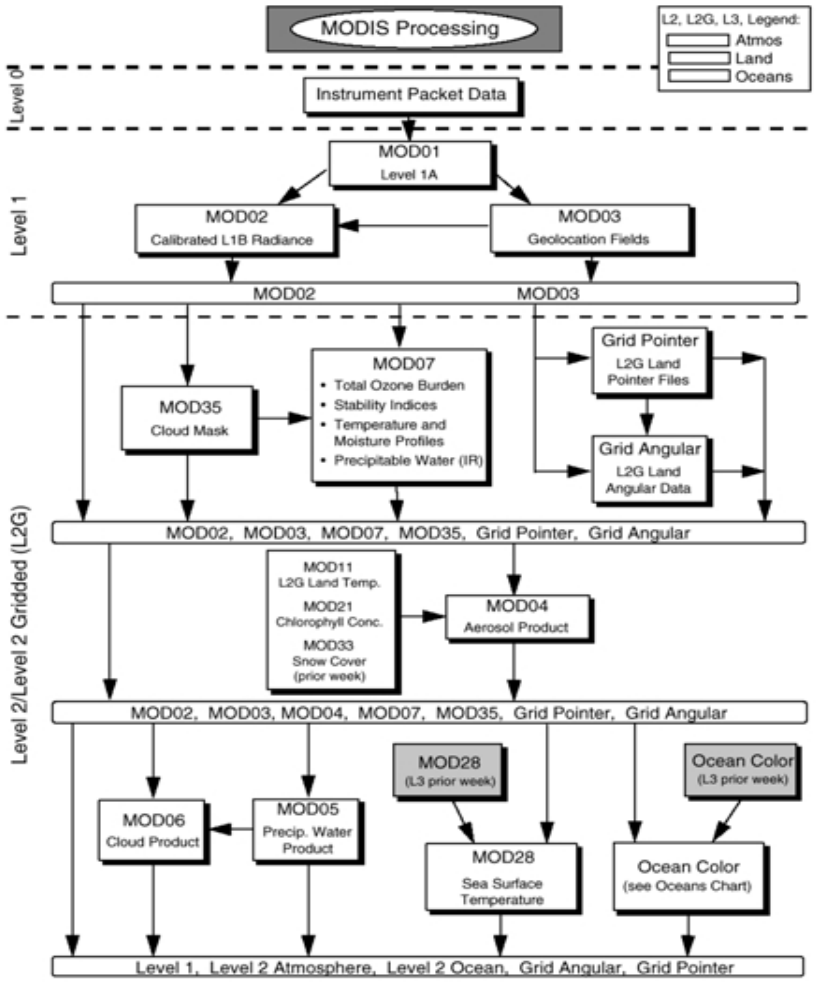
Some Examples

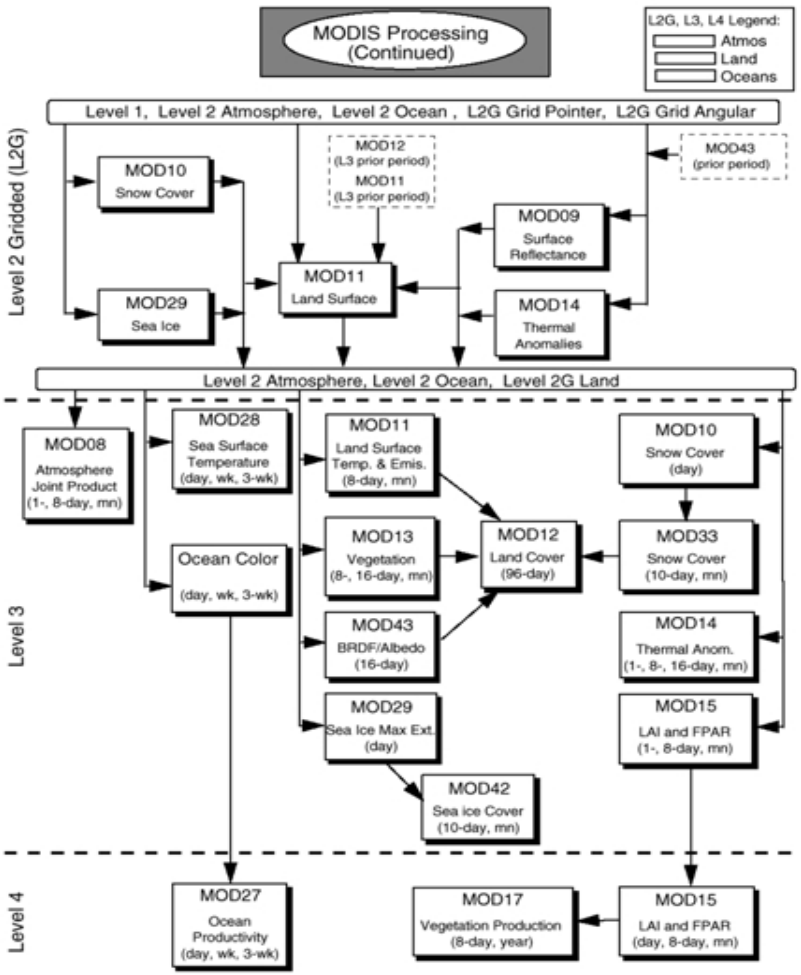
- Apache ODE
  - For execution of business processes written in WS-BPEL standard
- Taverna Workbench
  - Graphical interface for building and execution of workflows
  - myExperiment collaboration site
- SciFlo (JPL)
  - Web services orchestration of scientific workflows
  - Can move operations to data – this may still be problematic if your data is distributed in many places.

Workflows can be simple …



… or complicated

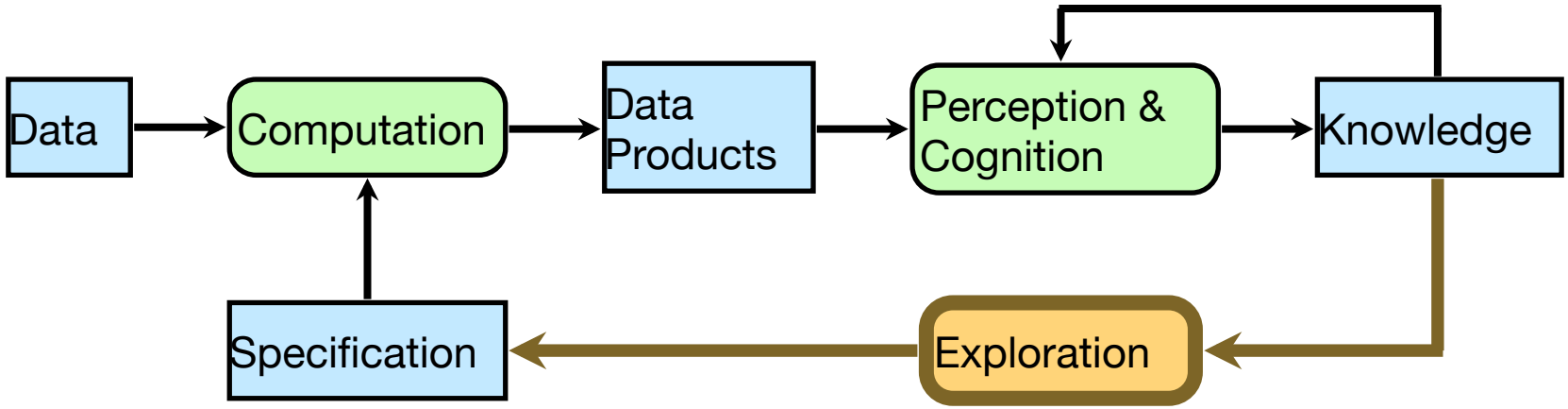




Why VisTrails

- Provides built-in provenance capabilities
- Python based
  - Just as a majority of the NEX platform development
- Excellent graphics capabilities
  - Important to convey the message
- **Easy integration of legacy software**

Data Analysis and Visualization



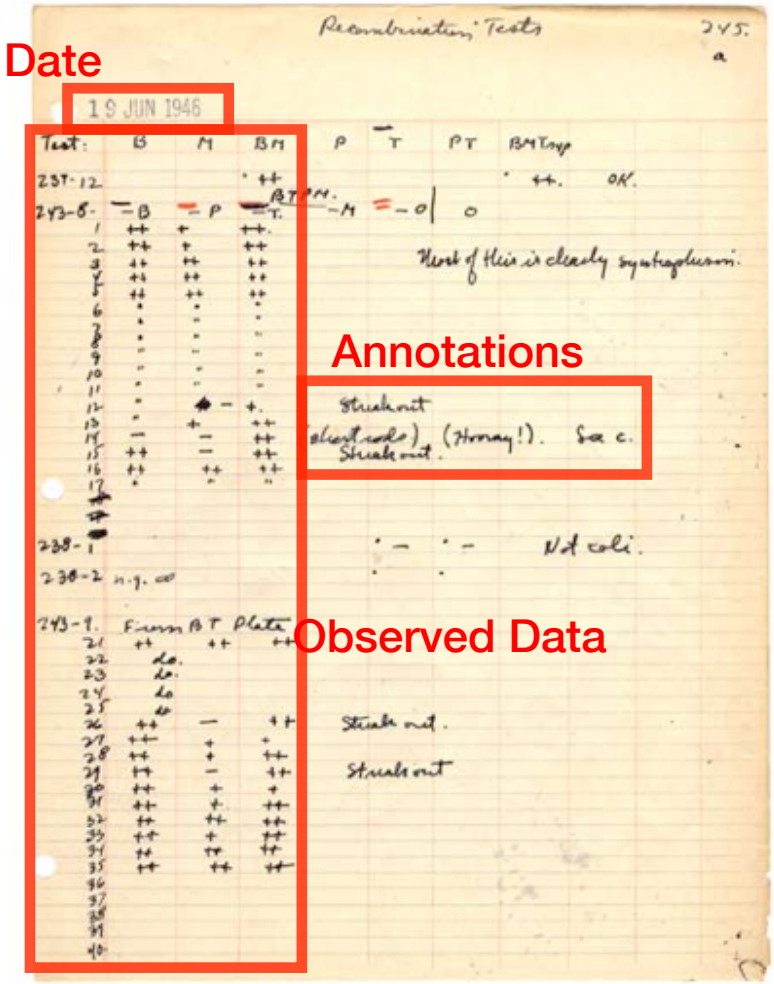
[Modified from Van Wijk, Vis 2005]

"Reflective thought requires the ability to store temporary results, to make inferences from stored knowledge, and to follow chains of reasoning backward and forward, sometimes backtracking when a promising line of thought proves to be unfruitful. The process takes time." – Donald A. Norman

[Courtesy of D. Koop, VisTrails]

Provenance in Science

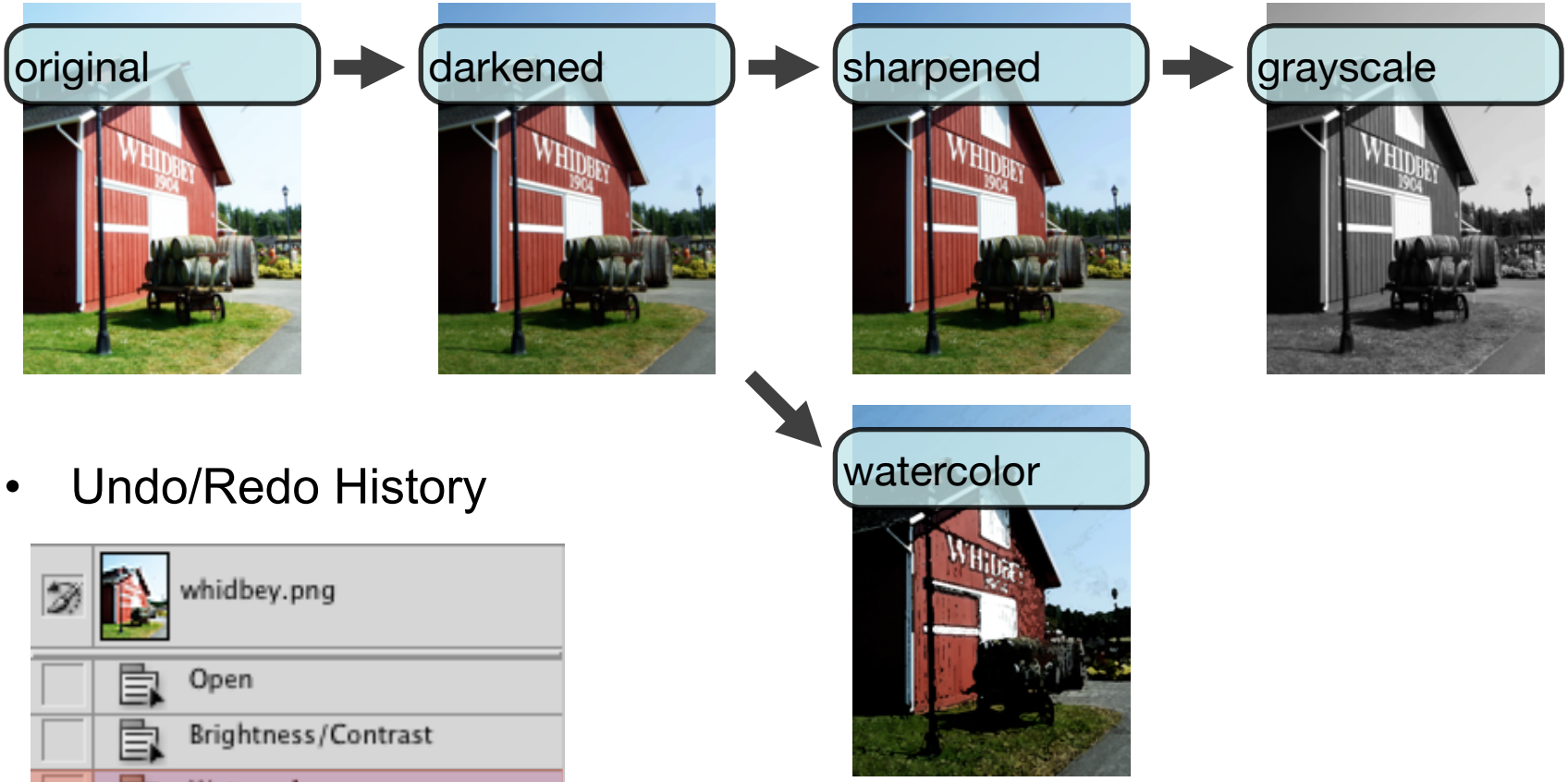
- Provenance: the **lineage** of data, a computation, or a visualization
- **Provenance is as (or more) important as the result!**
- Old solution:
  - Lab notebooks
- New problems:
  - Large volumes of data
  - Complex analyses
  - Writing notes doesn't scale



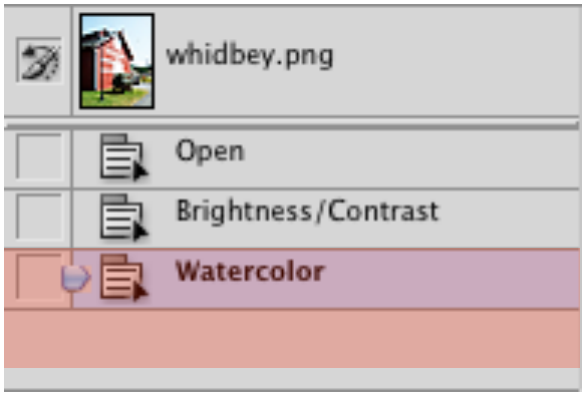
[DNA Recombination, Lederberg]

Simple Provenance Example: Photo Editing

- User Actions



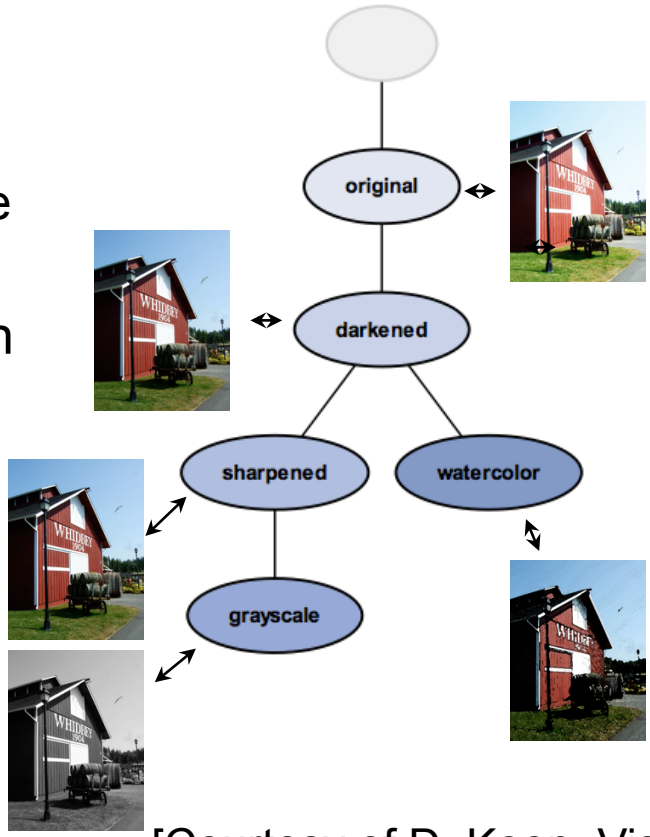
- Undo/Redo History



[Courtesy of D. Koop, VisTrails]

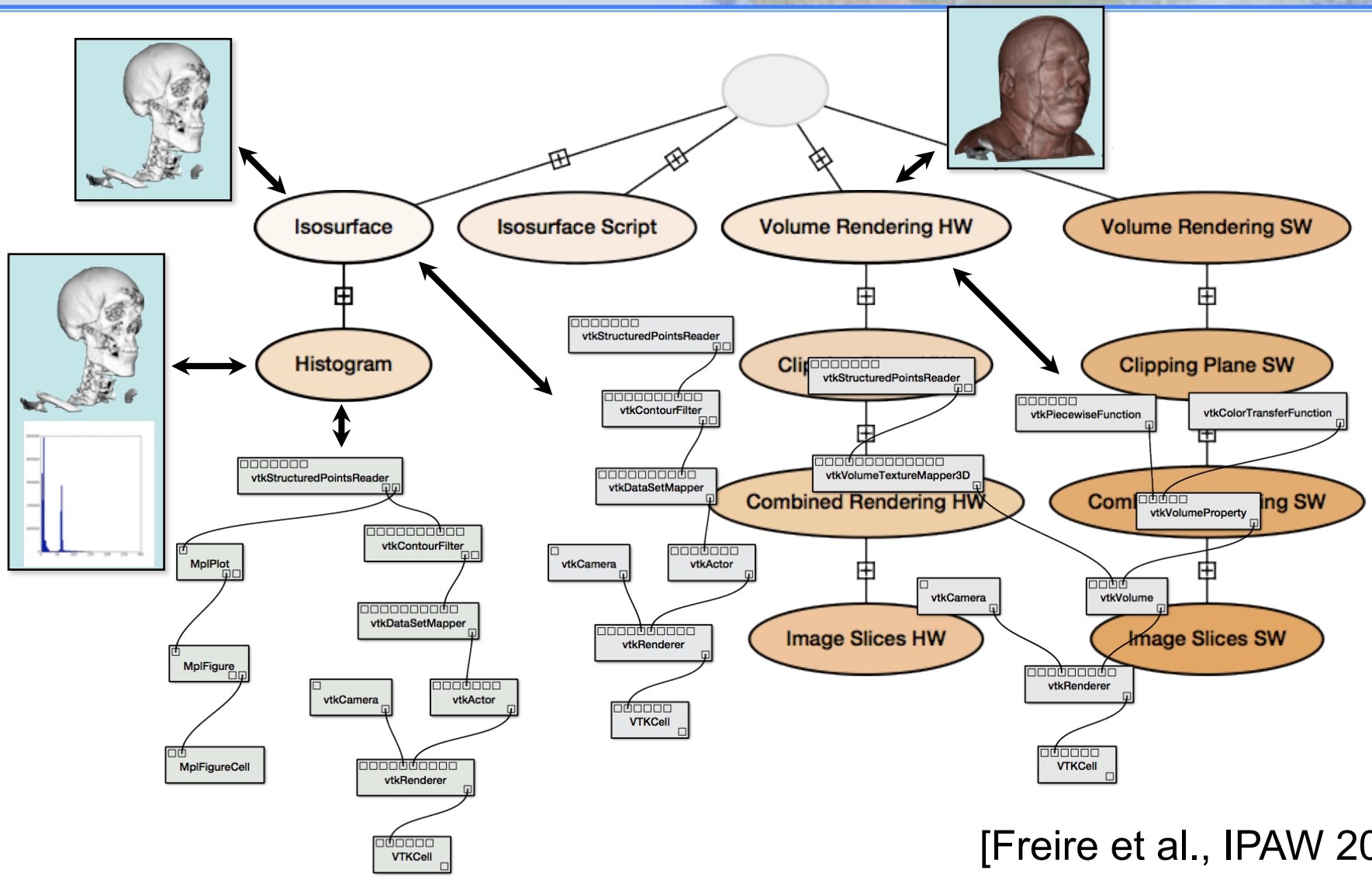
VisTrails Change-based Provenance

- Undo/redo stacks are linear!
- We lose history of exploration
- Old Solution: User saves files/state
- VisTrails Solution:
  - Automatically & transparently capture entire history as a tree
  - Users can tag or annotate each version
  - Users can go back to any version by selecting it in the tree



[Courtesy of D. Koop, VisTrails]

Change-based Provenance



[Freire et al., IPAW 2006]

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The VisTrails System

- Comprehensive **provenance** infrastructure for computational tasks
- Focus on **exploratory** tasks in collaborative environment
  - **Collaborative** design of scientific processes
  - Interactive parameter space exploration
- **Transparently** tracks provenance of the discovery process—from data acquisition to visualization
  - The **trail** followed as users generate and test hypotheses
  - Users can refer back to any point along this trail at any time
- Leverage provenance to **streamline exploration**

VisTrails: Specifications

- Open-source, freely downloadable system (www.vistrails.org)
- Multi-platform: users on Mac, Linux, and Windows
- User's guide, wiki, and mailing list
- Many users in different disciplines and countries
- You can try it **today** and be up and running in **minutes** (takes a little longer on some Linux systems because you have to build some dependencies)
- You can explore all examples from today's demo – they are part of the VisTrails distribution.

Now, let's try a demo

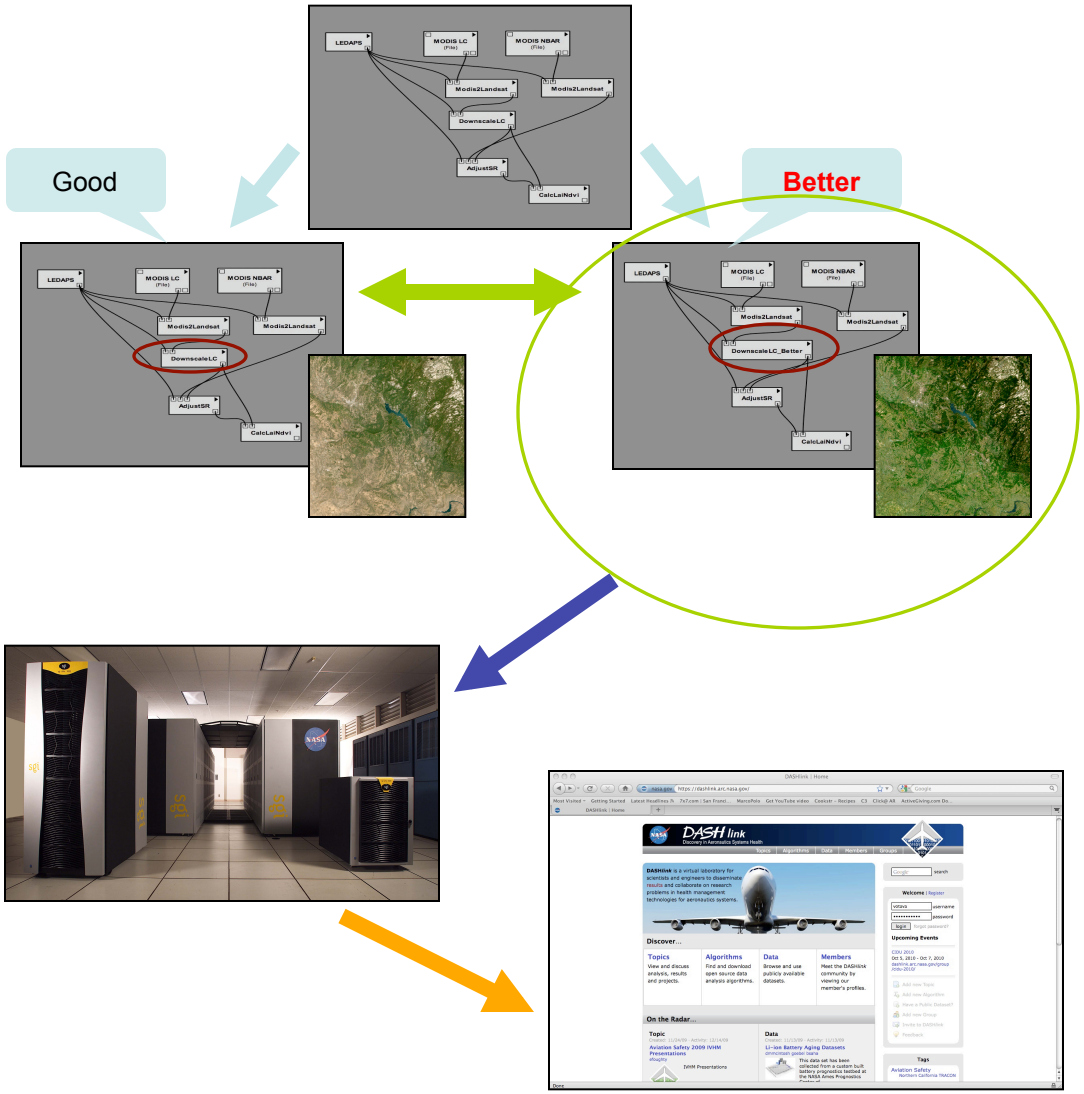
NEX Goal:
Collaborative Process Design and Knowledge Capture

Process Design

Iterative Refinement/
Distributed Collaboration

Full-scale Execution

On-Line Result Sharing and
Process Re-use

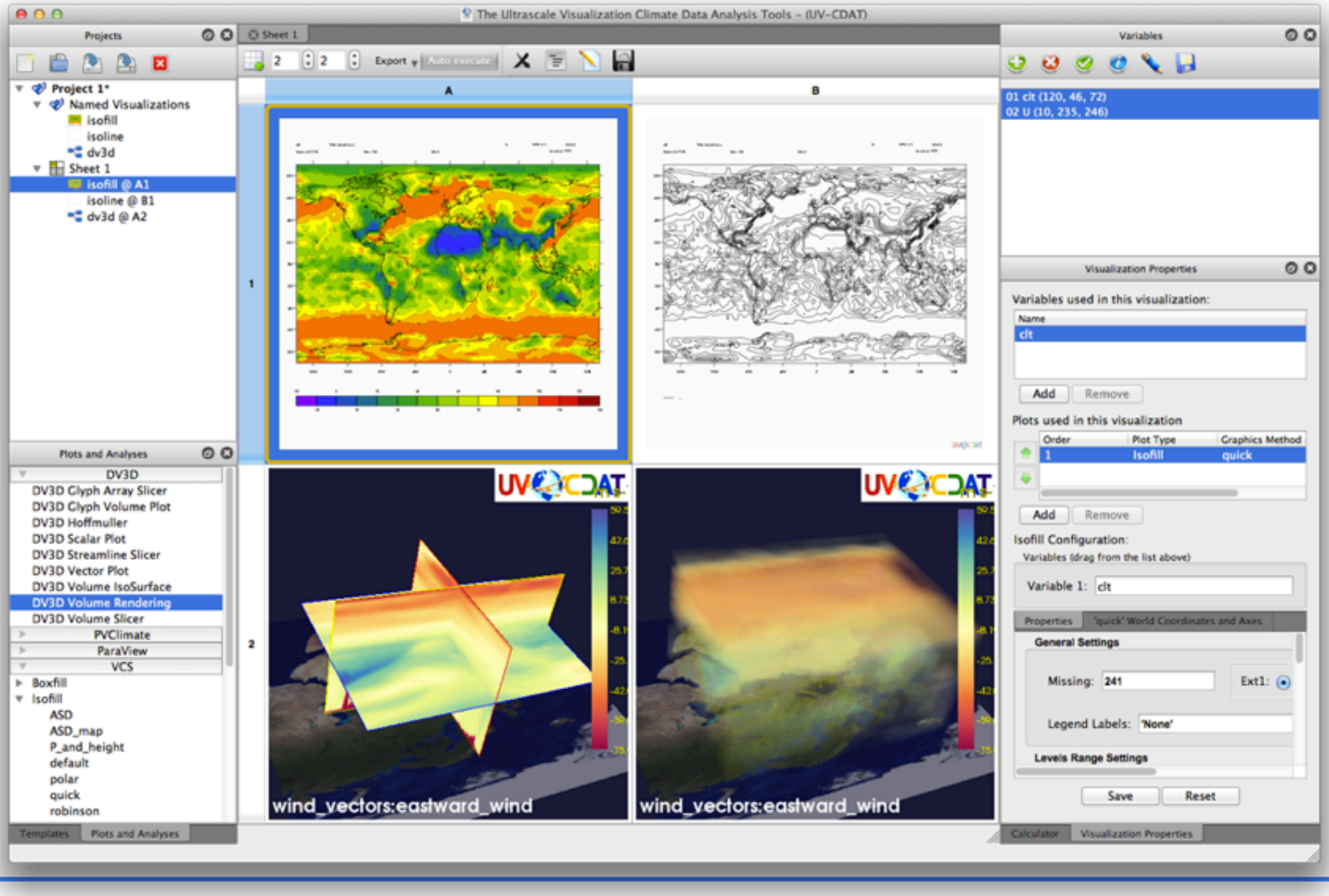


Additional NEX Integration

- Integration of VisTrails components with NEX semantic components
  - Bringing together provenance and semantics
- Developing workflow engine to interface with the Pleiades supercomputer
  - Running VisTrails on large scale problems, not just exploration any more

Example of VisTrails Integration: UV-CDAT

Ultrascale Visualization – Climate Data Analysis Tools (Lawrence Livermore)



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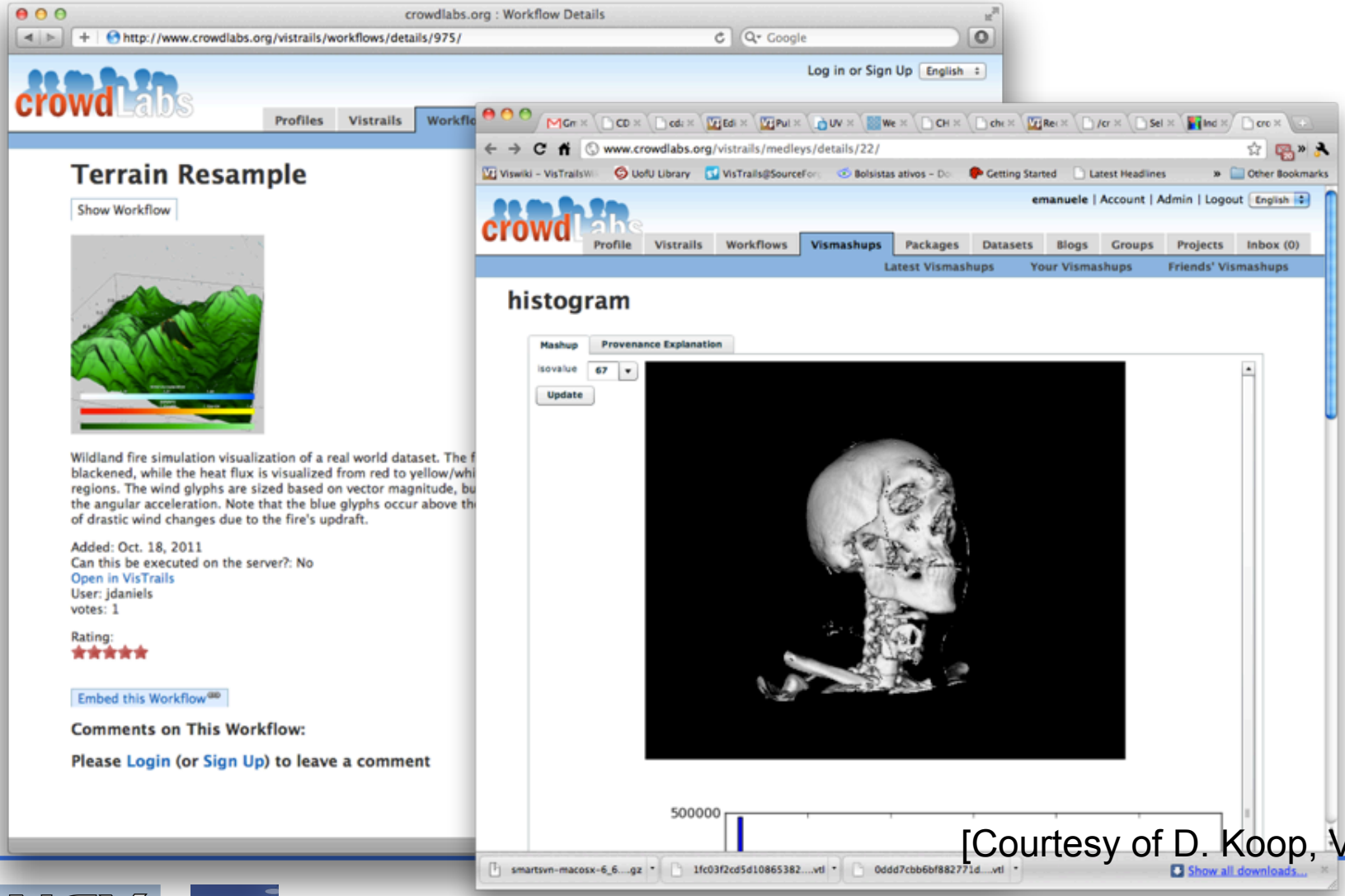
VisTrails Collaboration Site: crowdLabs

Planned integration with the NEX portal



[Courtesy of D. Koop, VisTrails]

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Executable Papers

The ALPS project release 2.0:
Open source software for strongly correlated systems

http://adsabs.harvard.edu/abs/2011arXiv1101.2646B

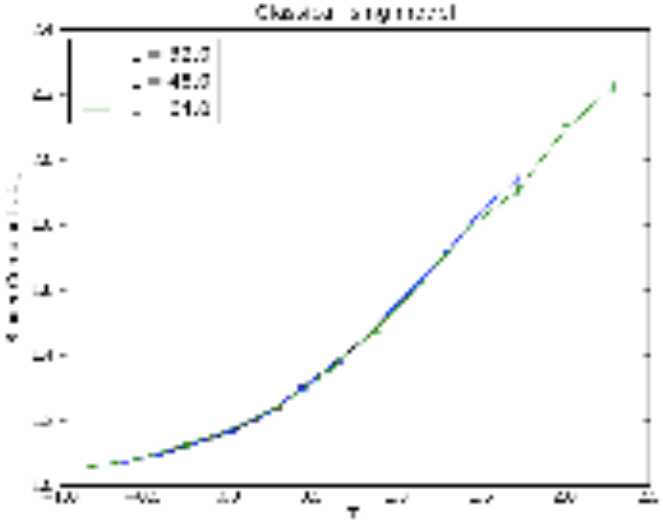

Figure 3. In this example we show a data collapse of the Binder Cumulant in the classical Ising model...

LaTeXcommand used to embed plot:

```
\vistrail[wfid=935,
  buildalways=false]{width=1.0\linewidth}
```

[Courtesy of D. Koop, VisTrails]

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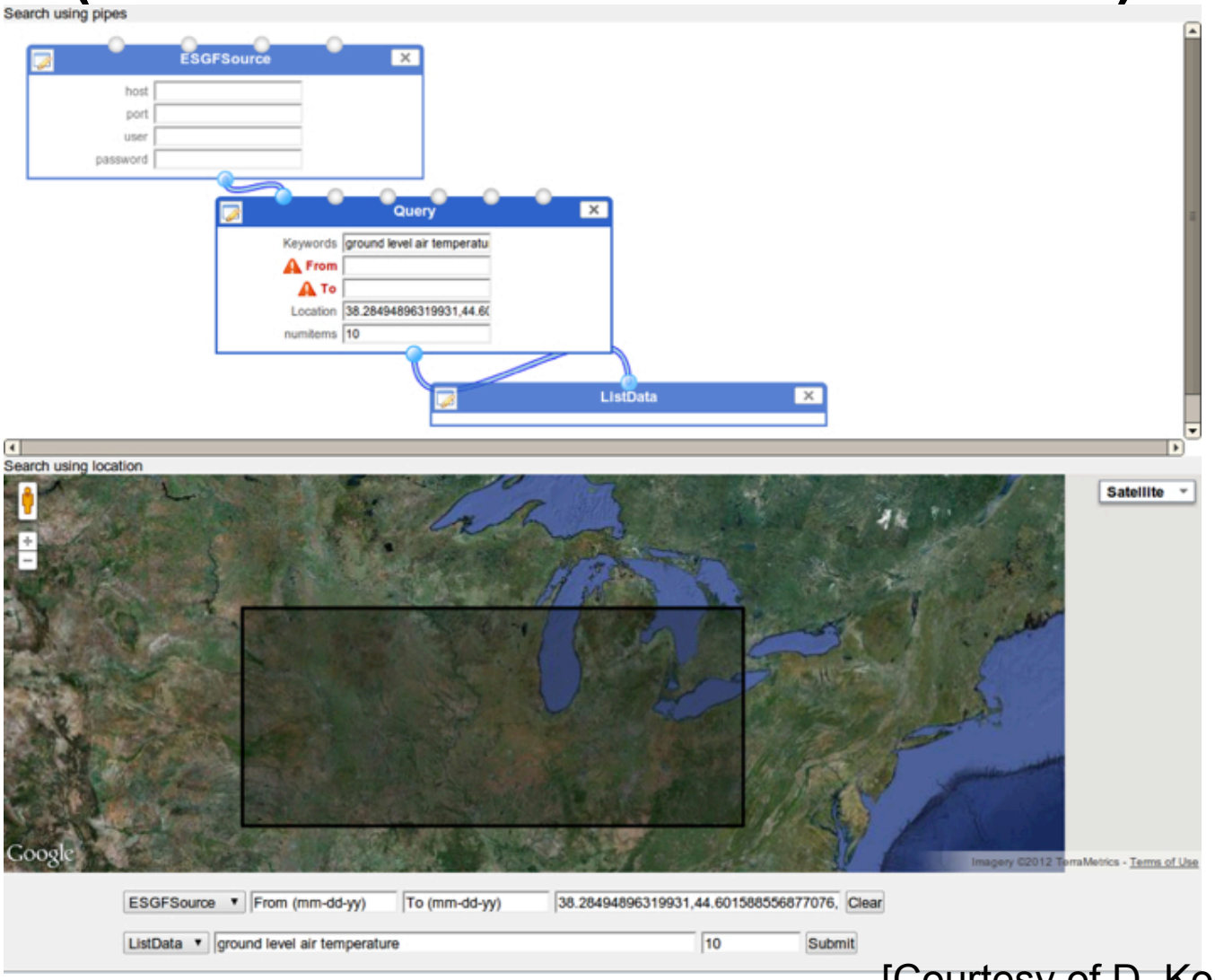
Future Work: ClimatePipes (web-based interface to VisTrails)



[Courtesy of D. Koop, VisTrails]

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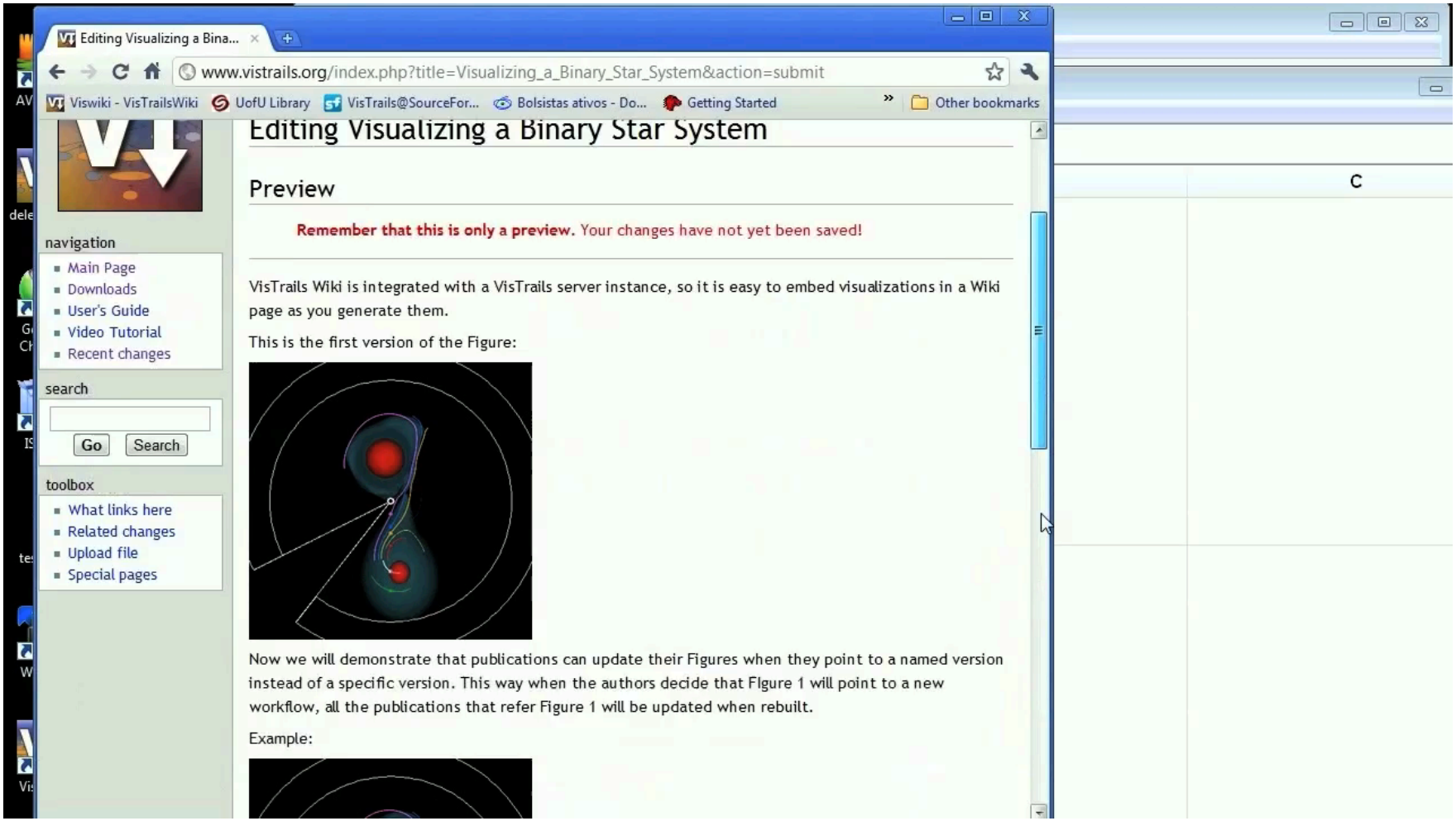
Web-based Publishing and Interaction



[Courtesy of D. Koop, VisTrails]

Scripting Support

```
import vt_setup

import core.api
vt = core.api.get_api()
text = vt.get_package("org.vistrails.text")
basic = vt.get_package("edu.utah.sci.vistrails.basic")
m1 = text.TextFile(value="/vistrails/climate/a.txt")
m2 = text.TextFile(value="/vistrails/climate/b.txt")
m3 = text.MergeFil
m3.addFile(m1.valu
m3.addFile = m2.va
m4 = basic.FileSin
m4.overwrite = Tru
m4.outputPath = "/vistrails/climate/c.txt"
m4.file = m3.outputFile
vt.tag_version("Merge2")
vt.execute()
vt.save_vistrail("/vistrails/climate/helloworld2.vt")
```

Provenance and Structure Automatic!

[Courtesy of D. Koop, VisTrails]

Final Thoughts on Reproducibility

- Workflow is just one of the components
  - It's a good start, but it is not enough
- Need to capture system information (OS, database, libraries) and configuration (versions, configuration options, …)
- Virtual machines play an important role
- Great reproducibility info

http://vgc.poly.edu/~juliana/talks/reproducibility-tutorial2012.pdf

Thank You

http://www.vistrails.org/