TaPP'13

ReproZip

Using Provenance to Support Computational Reproducibility

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Reproducibility

Good science requires reproducibility

> *"If I have seen further, it is by standing on the shoulders of giants."*
> *Isaac Newton*

Computational experiments require *reproducibility*

A program *P* running on computational environment *E* at time *T* is said to be *reproducible* if it yields the same answer on environment *E'* at time *T'* > *T*

Computational Reproducibility

Few computational experiments are reproducible

Why?

Author

How to encapsulate my experiment?
What should be included?
Too many dependencies…
Too many files to keep track…
Sigh.

We need **provenance**

- Description of the data
- Specification of the experiment
- Description of the environment

Computational Reproducibility

Manually tracking provenance is rarely feasible

Description of computational environment is *hard* to capture: It is *time consuming* and *error prone*

> *"authors have complained that the process* ***requires too much work for the benefit derived****"*
>
> Bonnet et al, SIGMOD Record 2011

> ***"Insufficient time*** *is the main reason why scientists do not make their data and experiment available and reproducible."*
> Carol Tenopir, Beyond the PDF 2 Conference

The process should be *simple* and *automatic!*

What tools are available to support reproducible experiments?

State of the Art

Domain-specific tools [GenePattern, Madagascar, Sumatra,…]

- Do not capture provenance of experiments that straddle multiple tools

Scientific workflow systems [VisTrails, Kepler, Taverna, …]

- Fail to capture provenance of the computational environment
- Do not support portability
- Users must integrate the software they need into these systems
  - Time consuming, and scientists do not have time to spare…

Configuration management tools [Chef, Puppet, Fabric]

- Recipes to configure machines may interfere with the target computational environment

State of the Art

- Virtual machines
  - Portable across multiple operating systems
  - Snapshots are usually *very* large
  - Users must port the experiment to a virtual machine: Again, time consuming
- System-level provenance capture
  - [Burrito, ES3, PASS] Describe how data products were derived *in detail*, but do not create an executable description to attain reproducibility and portability
  - [CDE] supports reproducibility
    - Lower overhead than a virtual machine: copy just what you need
    - Hard to further *explore* the experiment
    - Adds run-time overhead when executing the packaged experiment

Our Approach: ReproZip

Automatically and systematically captures required **provenance** of *existing* experiments

Uses captured provenance to:

- Create self-contained *reproducible packages* for the experiment
  - Include all the binaries, data and dependencies
- Derive a *workflow specification* for the experiment

Readers/reviewers can then extract the packages and execute the workflow to *reproduce* and *explore* the experiment

How does it work?

Packing Experiments

Computational Environment ***E***

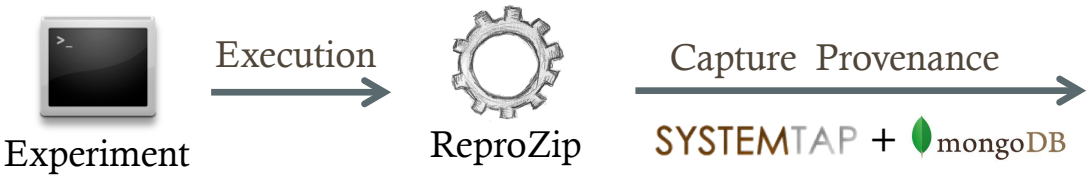
Experiment

Packing Experiments

Computational Environment ***E***

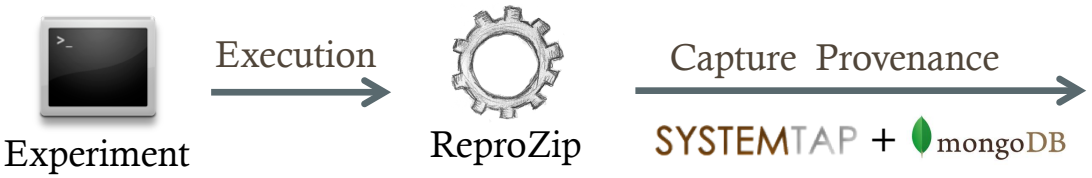
Packing Experiments

Computational Environment ***E***



Packing Experiments

Computational Environment ***E***



Packing Experiments

Computational Environment ***E***

Packing Experiments

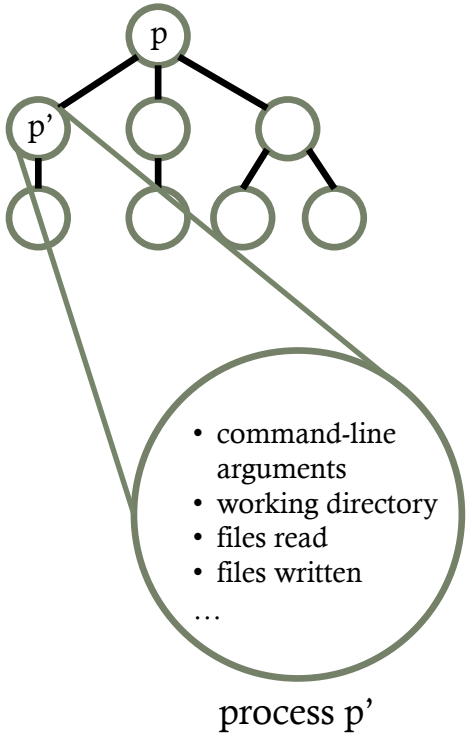
Computational Environment ***E***

Experiment

Execution

ReproZip

Capture of Provenance



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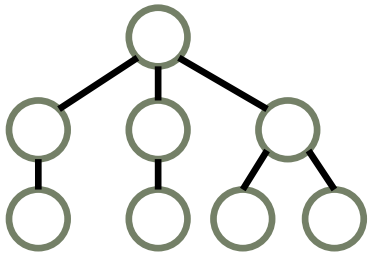

Provenance Tree

Identification of Necessary Components

Description of data

Input and output files

Description of experiment

Executable programs and steps

Description of environment

Environment variables, dependencies, …

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ReproZip

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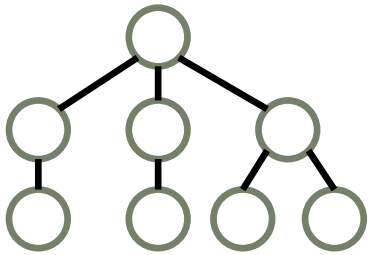

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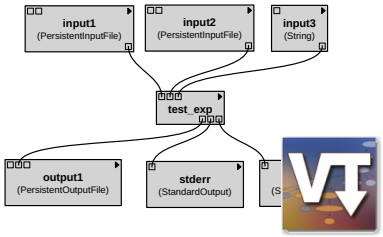
Specification of Workflow



VisTrails Workflow

Packing Experiments

Computational Environment ***E***

Experiment

Execution

ReproZip

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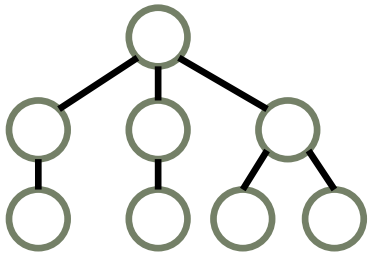

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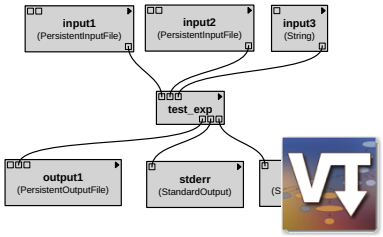


VisTrails Workflow

Reproducible Package

Verifying the Topological Correctness of Marching Cubes Algorithms

An example of making an experiment reproducible with ReproZip

Packing: Example

./mc33verification input/3741-scalar_field.iso output/output.txt

Original Command Line

Packing: Example

./mc33verification input/3741-scalar_field.iso output/output.txt

Original Command Line

python ~/reprozip/pack.py -e -c "./mc33verification input/3741-scalar_field.iso output/output.txt"

Packing with ReproZip

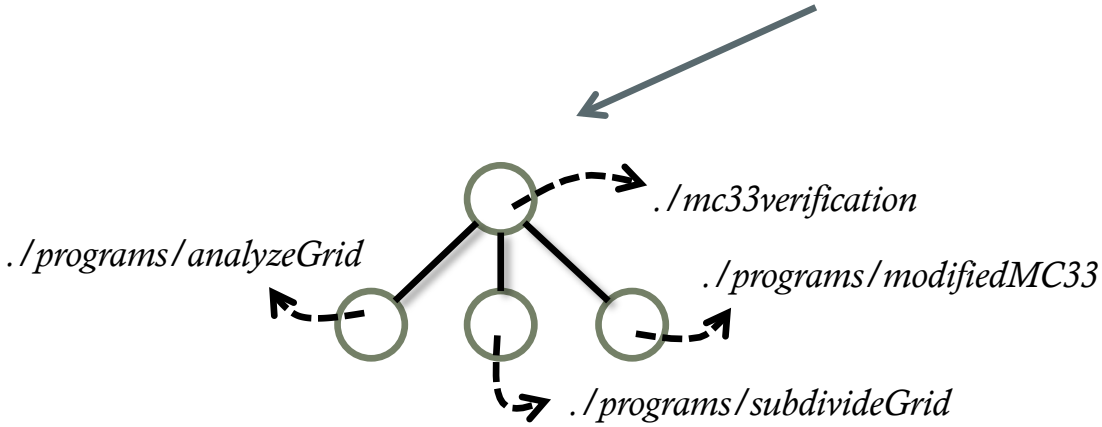
Packing: Capture Provenance

./mc33verification input/3741-scalar_field.iso output/output.txt

Original Command Line

python ~/reprozip/pack.py -e -c "./mc33verification input/3741-scalar_field.iso output/output.txt"

Packing with ReproZip



Provenance Tree

Packing: Configure Package

./mc33verification input/3741-scalar_field.iso output/output.txt

Original Command Line

python ~/reprozip/pack.py -e -c "./mc33verification input/3741-scalar_field.iso output/output.txt"

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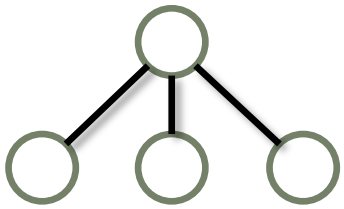

Provenance Tree

Configuration File

```
# Platform: Linux-3.2.0-32-generic-i686-with-Ubuntu-12.04-precise
# Processor: i686
# Number of CPUs: 1


* Original File *                                          * Size (KB) *   * Include? *

[main program]
/home/fernando/mc33/build/component_analysis                    7.55           Y

[other programs]
/home/fernando/mc33/build/others/vtkMarchingCubes              13.01           Y
/home/fernando/mc33/build/others/ModifiedMC33                 311.59           Y
/bin/sh                                                        97.93           Y
/bin/dash                                                      97.93           Y

[other input files]
/home/fernando/mc33/input/aneurism.iso                      65536.04           Y
/home/fernando/mc33/input/aneurism.vtk                      16384.19           Y

[dependencies]
/usr/lib/i386-linux-gnu/i686/cmov/libavutil.so.51.22.1        118.49           Y
/usr/lib/i386-linux-gnu/libkrb5support.so.0                    29.61           Y
/usr/lib/i386-linux-gnu/libkrb5support.so.0.1                  29.61           Y
/usr/lib/i386-linux-gnu/libroken.so.18.1.0                     82.46           Y
/usr/lib/i386-linux-gnu/libogg.so.0                            25.39           Y
```

Packing: Deriving Workflow Specification

python ~/reprozip/pack.py -g --name=mc33verification

Creating the reproducible package and the workflow

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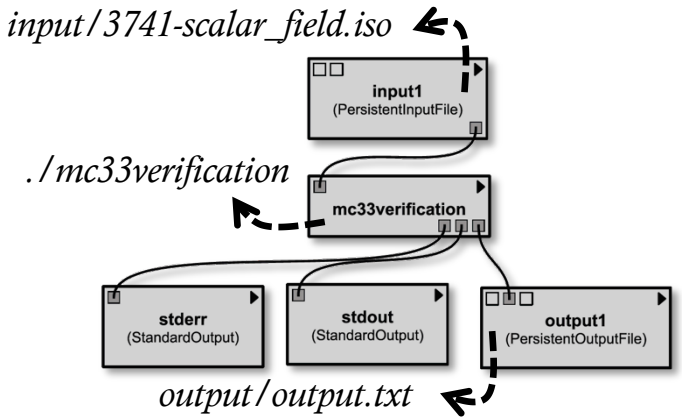
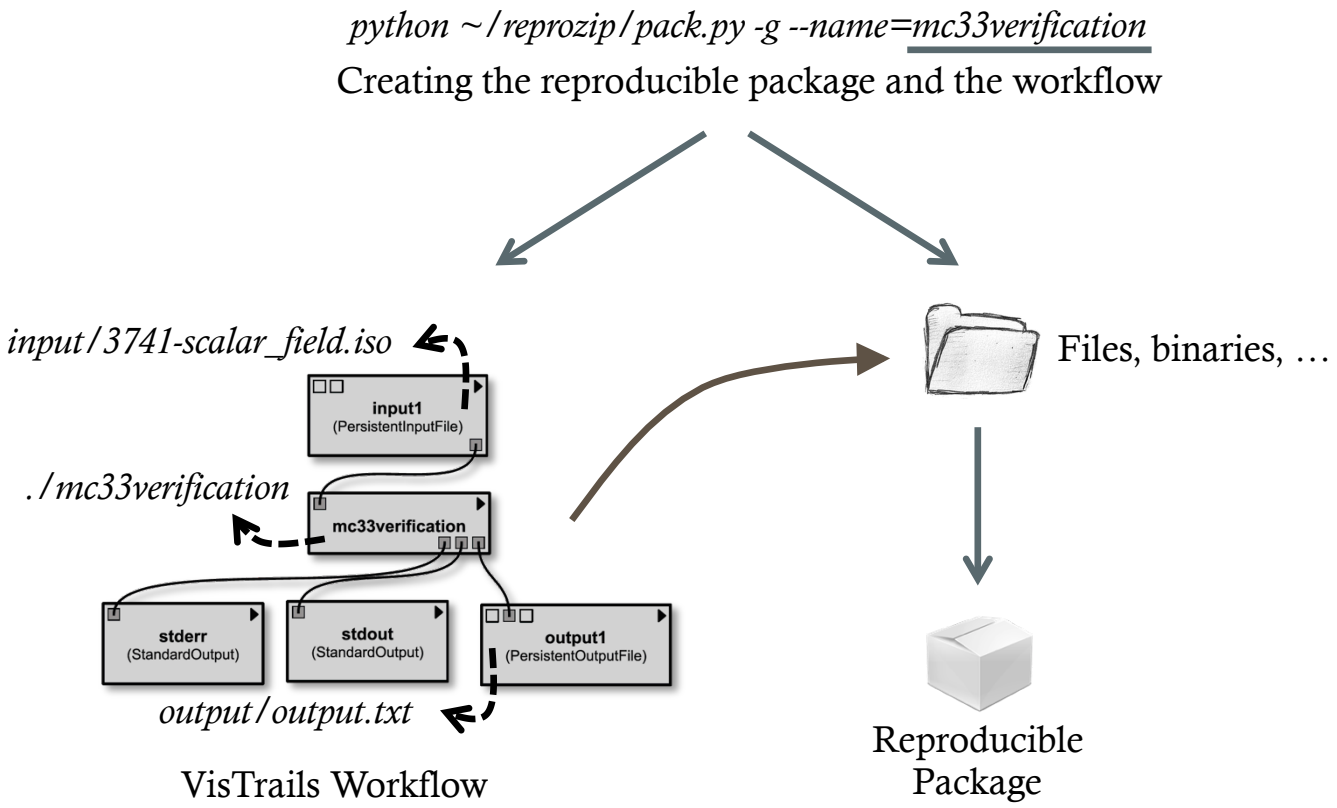
python ~/reprozip/pack.py -g --name=mc33verification

Creating the reproducible package and the workflow



VisTrails Workflow

Packing: Deriving Package



Unpacking Experiments

Computational Environment ***E'***

E' compatible with *E*

Reproducible Package

Unpacking Experiments

Computational Environment ***E'***

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Reproducible Package

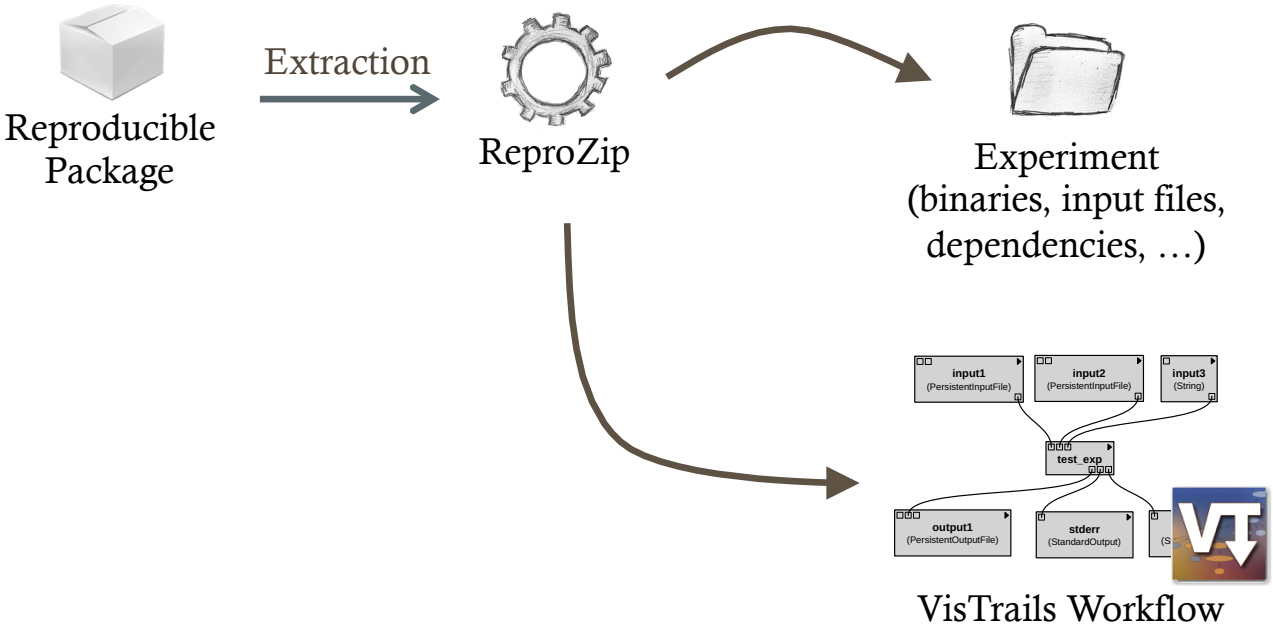
Extraction

ReproZip

Unpacking Experiments

Computational Environment ***E'***

E' compatible with *E*



Unpacking: Example

python ~/reprozip/unpack.py mc33verification

Unpacking experiment

Unpacking: Example

python ~/reprozip/unpack.py mc33verification

Unpacking experiment

./mc33verification

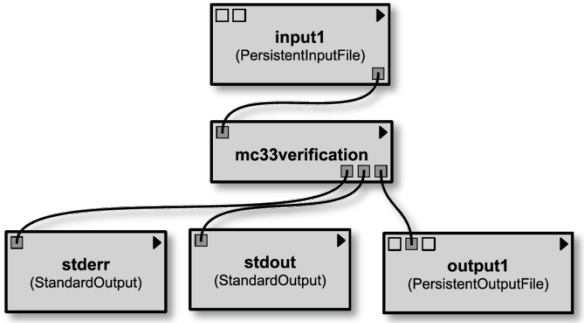
Verification and Exploration

Reproducibility of *deterministic* process

Two ways to reproducing the results:

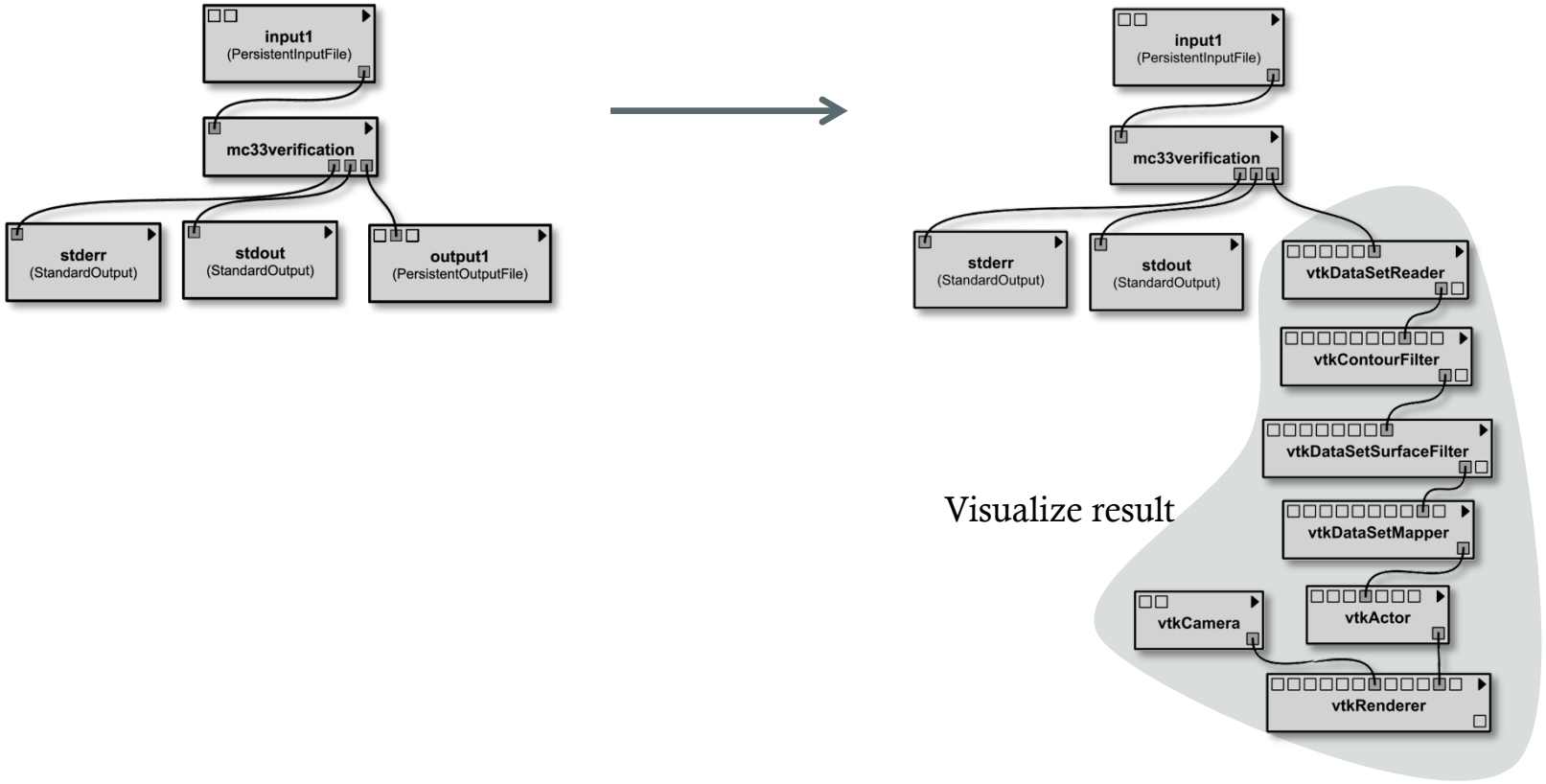
./mc33experiment/rep.exec

Command-line execution



VisTrails Workflow

Verification and Exploration



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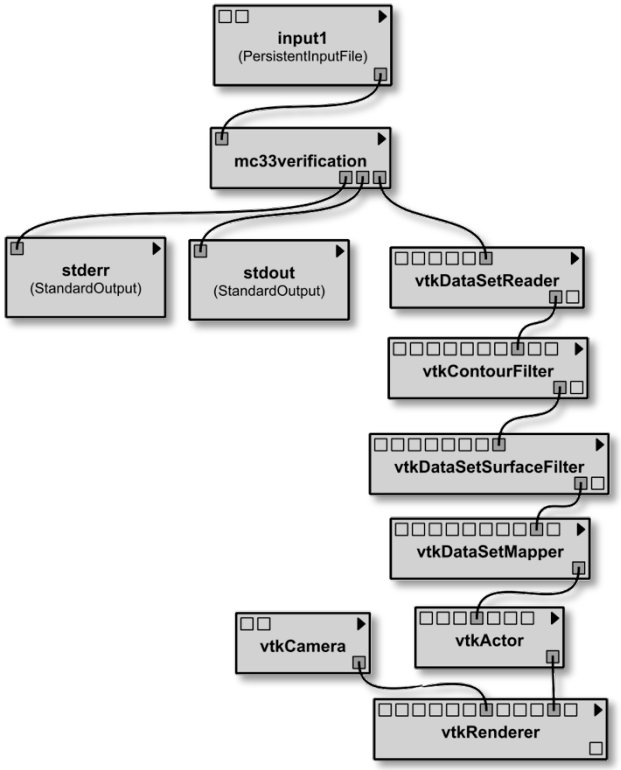
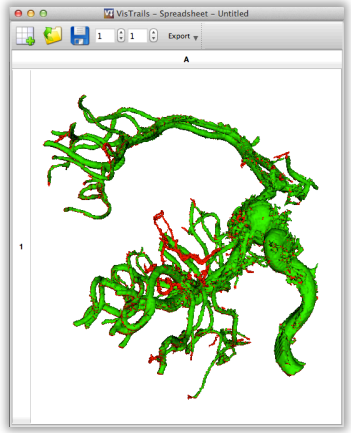
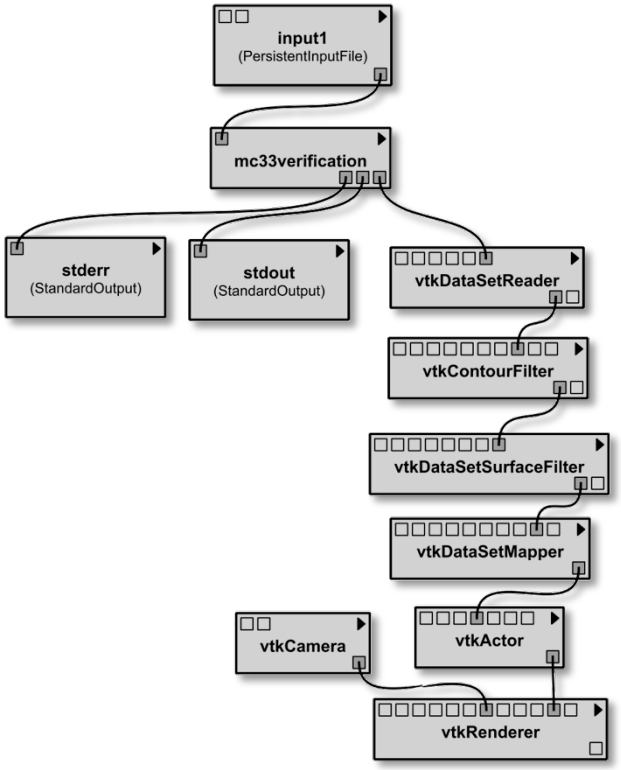
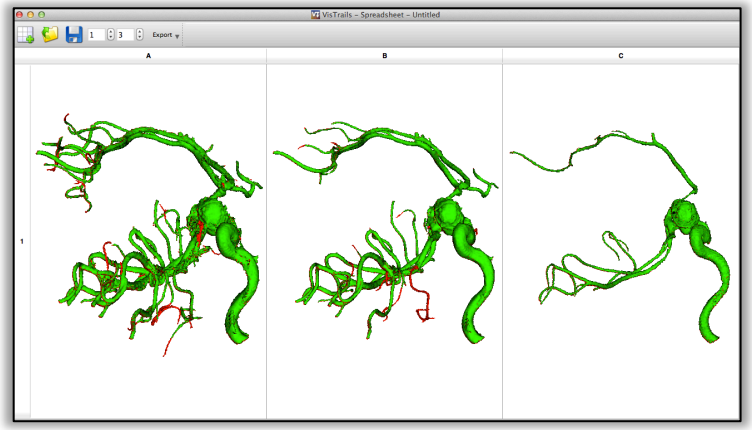




Visualization

Verification and Exploration





Parameter Exploration

Conclusion

ReproZip aims to simplify the creation of reproducible experiments

- It captures provenance and identifies the components needed to reproduce results
- Users can customize the package

Integrated with scientific workflows

- Scientists can reap the benefits without the cost
- Further explore the results and get review provenance for free

Limitations

- Works only on Linux
- Package may not run
  - If underlying software is incompatible with target environment---for this situation, we suggest the use of a VM
  - Executables that use hard-coded paths

Acknowledgments

- Claudio Silva and the VisTrails team
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Thank you!