Packing Experiments for Sharing and Publication

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The Need for Computational Reproducibility

- The standard of having reproducible experiments, a long tradition in natural science, has not been adopted for computational experiments.
- Researchers often have to rely on figures, plots and tables presented in papers, which loosely describe the results. Consequently, these results are difficult to reproduce, leading to a credibility crisis in computational science [1].
- There are two main reasons why reproducibility is often not adopted:
  - Authors find it difficult to generate a compendium for their experiment,
  - Reviewers and collaborators have difficulties trying to reproduce and verify the results, even when the compendium is available.

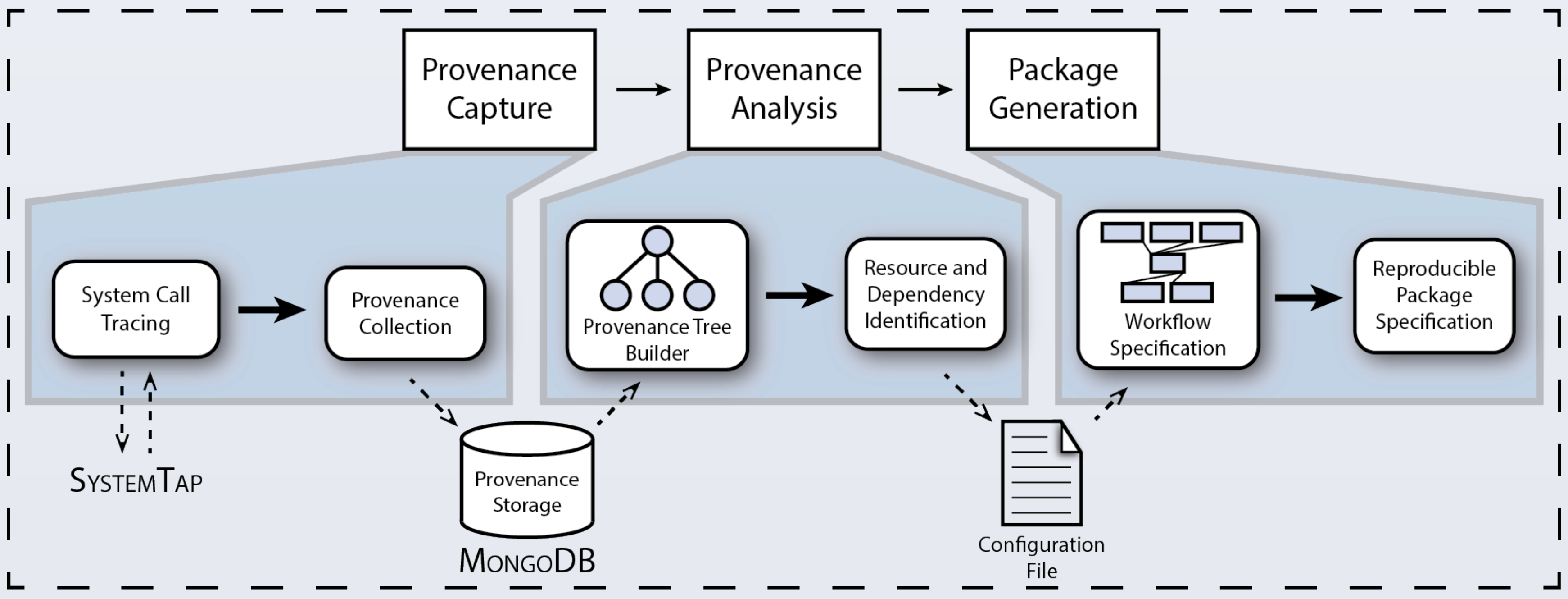
ReproZip

ReproZip is a *general* tool for packing reproducible research that

- tracks operating system calls and creates a *reproducible package* from *command-line executions*, in the author's environment *E*, with all the required files to run the experiment (***packing* step**). Authors do not need to port their experiment to a specific tool.
- generates a workflow specification to help reviewers and collaborators explore and verify the results, facilitating the review process.
- extracts files and workflow on another environment *E'* (***unpacking* step**).

Packing Experiments

Packing Step



Provenance Capture

- ReproZip transparently captures the provenance of the execution of the experiment. It uses SystemTap [2] to trace system calls and capture all the required information to correctly reproduce the experiment.
- The execution trace is stored in MongoDB [3], a NoSQL database

Provenance Analysis

- ReproZip uses the trace data to create a *provenance tree*. Each node in the tree stores information about an OS process, such as *files read*, *files written* and *command-line arguments* – if a process *p* spawns a process *p'*, an edge is inserted between their corresponding nodes.
- The provenance tree is traversed to identify *programs*, *input files*, *output files* and *dependencies*.

Package Generation

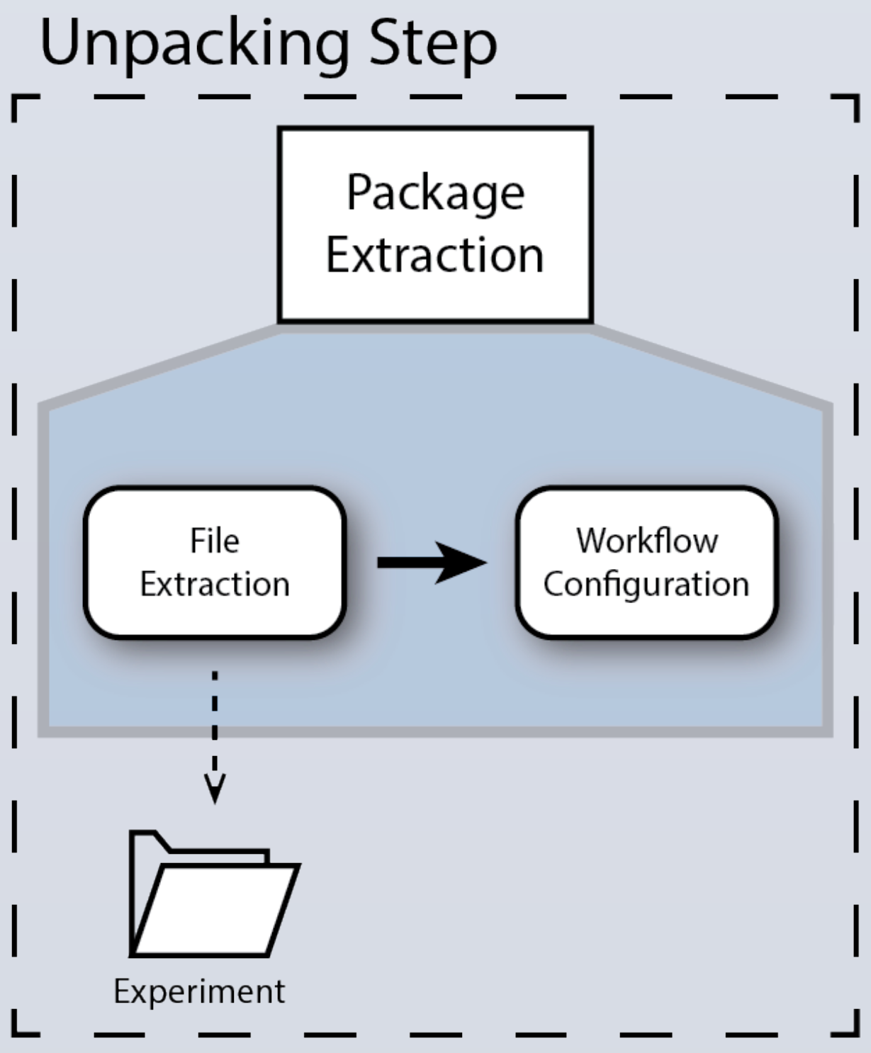
- The identified binaries and files are used to derive a workflow specification for the experiment.
- All the required files, together with the workflow, are packed on the author's environment *E* using the *original* directory structure.

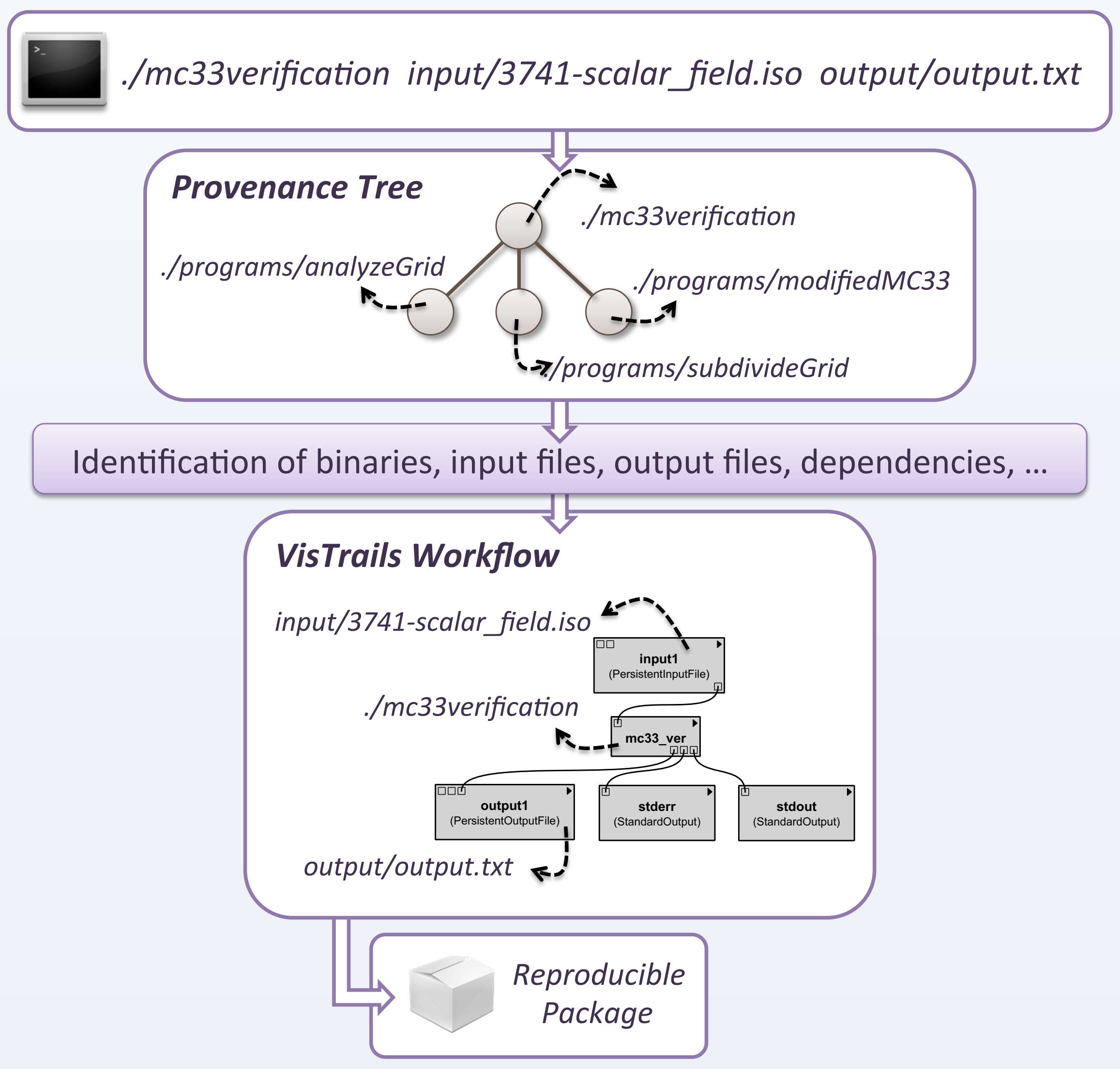
Unpacking Experiments

Package Extraction

- Given a reproducible package generated on environment *E*, ReproZip extracts all the files in a single directory on environment *E'*, without interfering with this environment.
- The workflow is automatically configured to point to the correct files inside the unpacked directory.
- Paths defined in environment variables for the experiment are adjusted to use the experiment directory in *E'*.

Unpacking Step



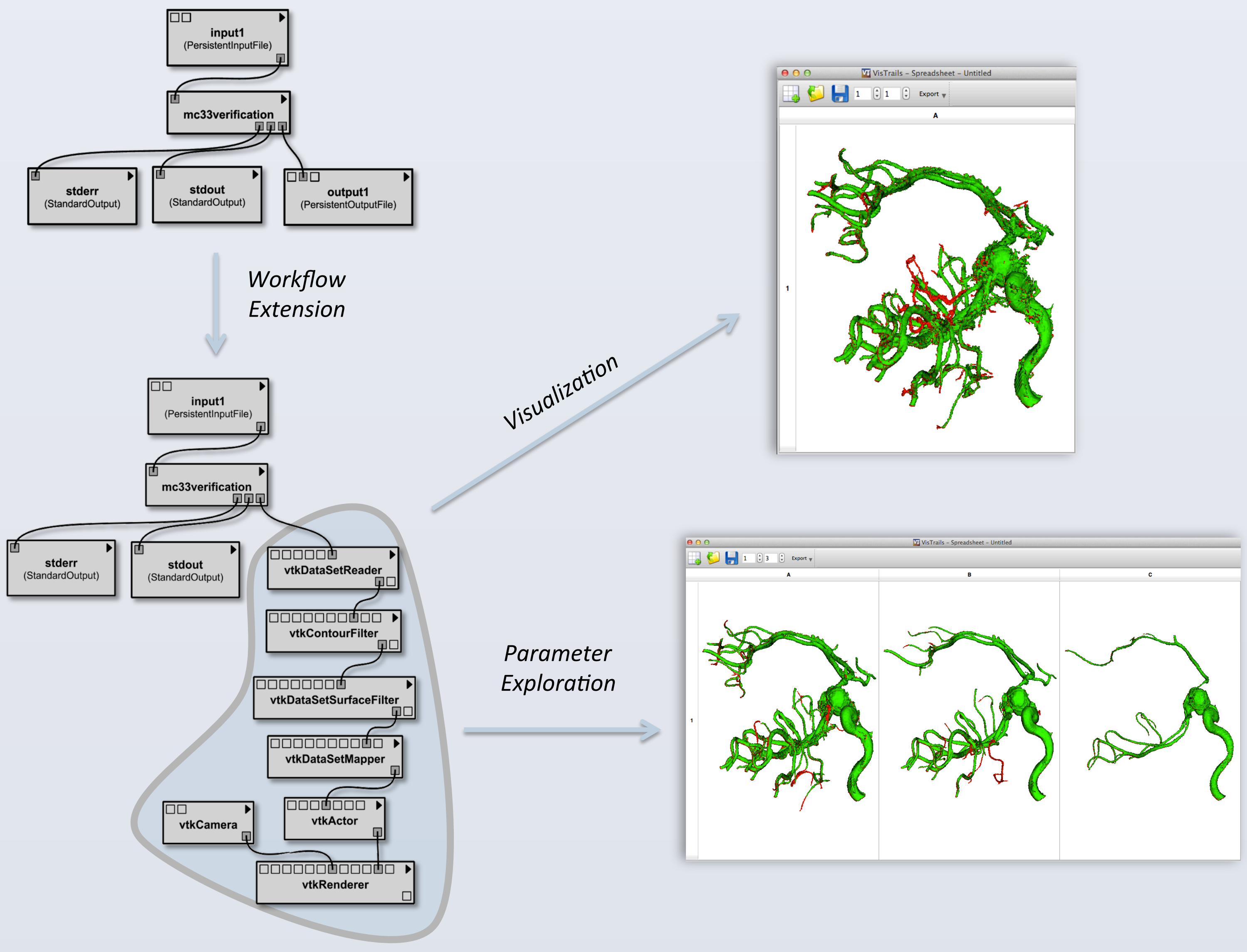


```
./mc33verification  input/3741-scalar_field.iso  output/output.txt
```

Packing an experiment on topological correctness of marching cubes [4]

Verification and Exploration

- Users may run the experiment from the command line and examine the results.
- ReproZip also creates a workflow specification that can be run within VisTrails [5]. By using this workflow: (1) experiment execution is straightforward; (2) a visual representation helps the reviewer to understand and explore the experiment; (3) users can try different parameters, as well as perform parameter sweeps and compare the results side by side; (4) users can extend the original experiment and perform additional analyses; and (5) the provenance of the verification process is automatically captured by VisTrails



Verifying the topological correctness of a marching cubes algorithm. The reviewer can extend the workflow to visualize the results; they may also verify the robustness of the algorithm by exploring different isosurface values using the parameter sweep feature of VisTrails.

Acknowledgments

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