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Design of a Scientific Data Analysis Support Platform

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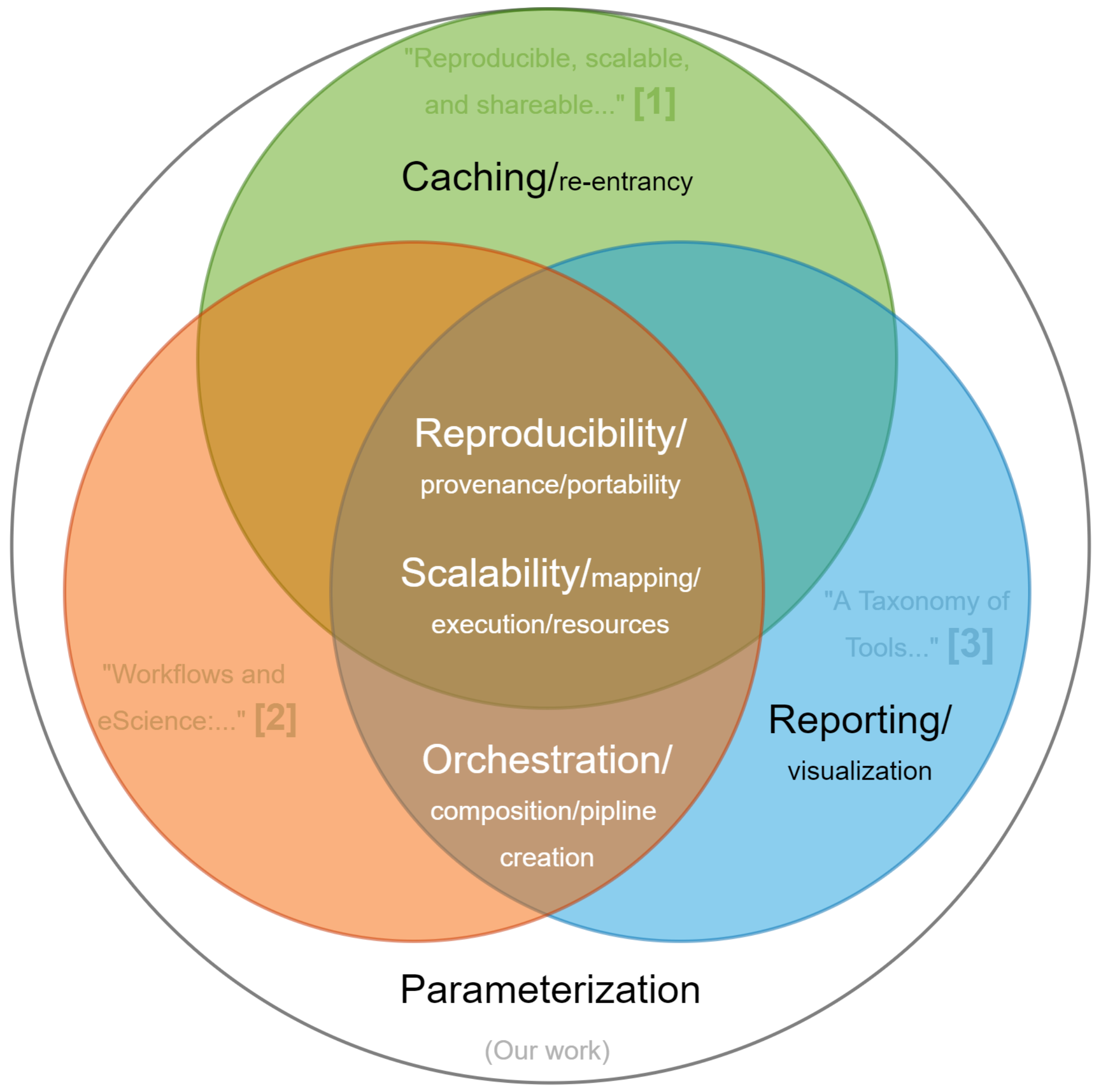
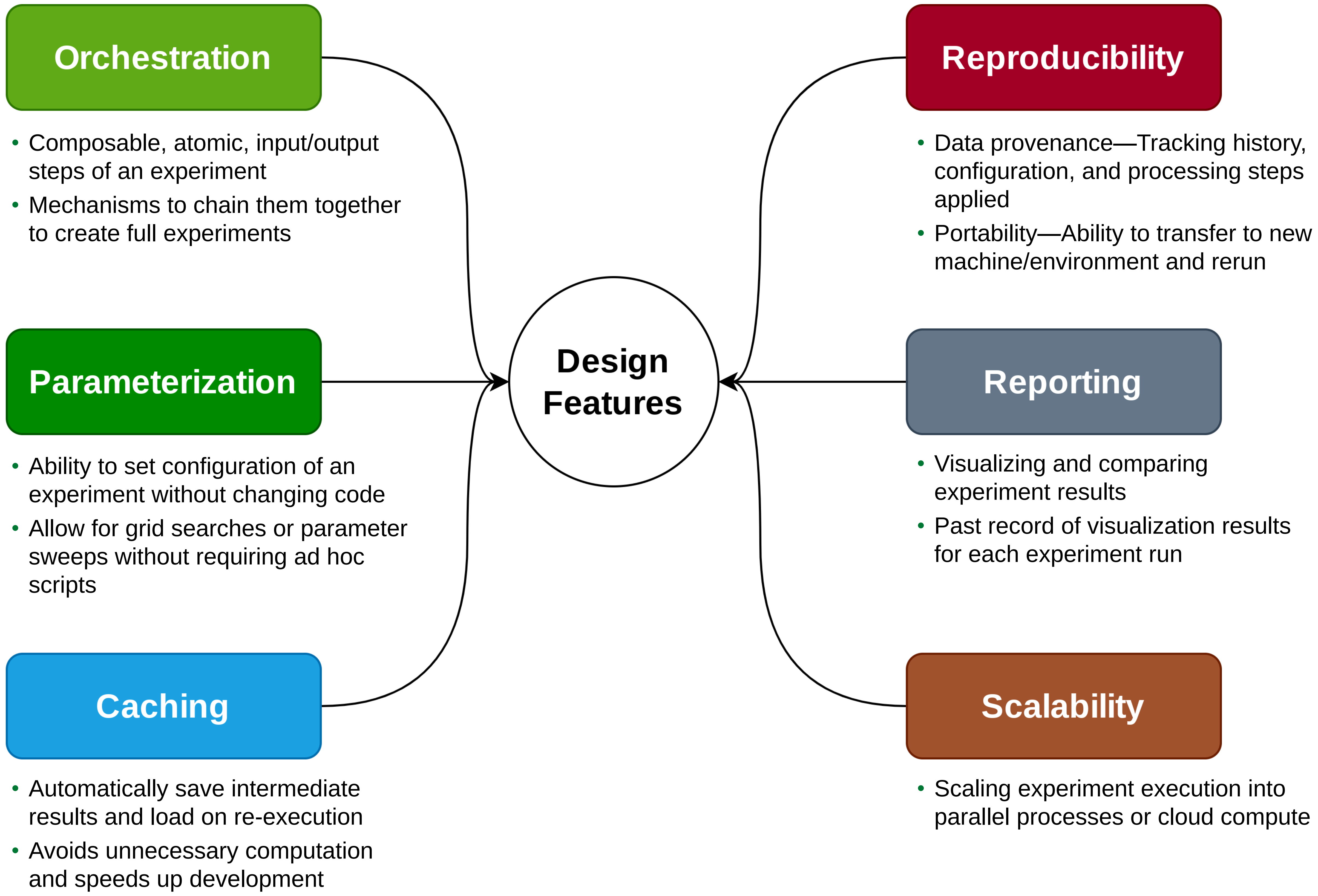
Reproducibility Crisis

- Complexity in software, environments, and lack of good software engineering principles in scientific domains has led to a reproducibility crisis in many computational research–based fields
- Resolving this requires infrastructure that supports good scientific and software practices
- Our work
  - surveys the literature for necessary design features and proposes a combination
  - analyzes design features of existing tools and proposes a new open-source tool, Curifactory

Concepts from Literature

- FAIRness principles
- Software engineering principles (testing, version control, agile)
- Compiled suggested design features from three other works on workflow/experiment management systems [1,2,3]


"Reproducible, scalable, and shareable..." [1]
Caching/re-entrancy
Reproducibility/ provenance/portability
Scalability/mapping/ execution/resources
"A Taxonomy of Tools..." [3]
"Workflows and eScience:..." [2]
Orchestration/ composition/pipline creation
Reporting/ visualization
Parameterization
(Our work)



Design Features

Orchestration

- Composable, atomic, input/output steps of an experiment
- Mechanisms to chain them together to create full experiments

Parameterization

- Ability to set configuration of an experiment without changing code
- Allow for grid searches or parameter sweeps without requiring ad hoc scripts

Caching

- Automatically save intermediate results and load on re-execution
- Avoids unnecessary computation and speeds up development

Reproducibility

- Data provenance—Tracking history, configuration, and processing steps applied
- Portability—Ability to transfer to new machine/environment and rerun

Reporting

- Visualizing and comparing experiment results
- Past record of visualization results for each experiment run

Scalability

- Scaling experiment execution into parallel processes or cloud compute

Existing Tooling

- DVC— Git-like interface for versioning datasets. Every compute input/output is a file, and caching/provenance is free
- MLFlow—STRONG MLOps tool, supporting entire data science life cycle, includes a powerful reporting dashboard and distributed computing
- Sacred—Allows parameterization directly in Python functions, user specification of observers for tracking metadata and artifacts
- Kedro—Ability to deploy to clusters, excellent web dashboard reporting and experiment visualization, ability to export entire project to docker container

	Orchestration	Parameterization	Caching	Provenance	Portability	Reporting	Scalability
DVC	▨	▨	🟩	▨	▨	▨	▨
MLFlow		▨	🟨	🟩	🟩	🟩	🟩
Sacred	▨	🟩	🟨	🟩	▨	▨	
Kedro	▨	▨	🟨	▨	🟩	🟩	🟩
Curifactory	▨	🟩	🟩	🟩	🟩	▨	▨

https://github.com/ORNL/curifactory

Curifactory

- **Orchestration**—Atomic level abstraction "stage," a function with defined inputs and outputs. Stages chained/composed into experiment scripts
- **Parameterization**—Parameters defined and instantiated in Python scripts, allowing inheritance, composition, looping
- **Caching**—Stages provide easy mechanism to store and reload every output to disk. Re-running same experiment will reload rather than recompute
- **Reproducibility**—Metadata tracked every run. Ability to create full store of an experiment containing all information, output report, and every intermediate artifact. Ability to build docker container for specific run
- **Reporting**—Every run outputs HTML report with metadata and user-definable graphics
- **Scalability**—Runs with multiple parameter sets can be run in multiple processes
- Published with BSD-3 clause license, available on PyPI and GitHub

References

[1] Laura Wratten, Andreas Wilm, and Jonathan Göke. Reproducible, scalable, and shareable analysis pipelines with bioinformatics workflow managers. Nature Methods 18(10):1161–1168, October 2021. doi:10.1038/s41592-021-01254-9.

[2] Ewa Deelman, Dennis Gannon, Matthew Shields, and Ian Taylor. Workflows and e-Science: An overview of workflow system features and capabilities. Future Generation Computer Systems, 25:524–540, May 2009. doi:10.1016/j.future.2008.06.012.

[3] Luigi Quaranta, Fabio Calefato, and Filippo Lanubile. A Taxonomy of Tools for Reproducible Machine Learning Experiments.

Acknowledgments

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