# Highly flexible and fully reproducible computational workflows with signac

Carl S. Adorf[1], Vyas Ramasubramani[1], Bradley D. Dice[2], and Sharon C. Glotzer[1,2,3,4]

1. Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109
2. Department of Physics, University of Michigan, Ann Arbor, MI 48109
3. Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109
4. Biointerfaces Institute, University of Michigan, Ann Arbor, MI 48109

## Introduction

The **signac** framework[1]

- provides the infrastructure for the rapid development and execution of computational investigations
- simplifies collaboration on shared data spaces
- integrates well with high-performance computing cluster environments
- is tested and available for Python 2.7 and 3.4+ via pip and conda-forge
- is free and open-source (BSD-3-Clause License)

## Overview

A **signac** data space is organized within a managed directory on the file system, called the *workspace*. Data points are stored in separate subdirectories, each containing all data and metadata associated with that point, including its defining *state point* information.

Computational workflows are implemented with **signac-flow** and can be executed either on the local workstation or in HPC cluster environments with a scheduling system.

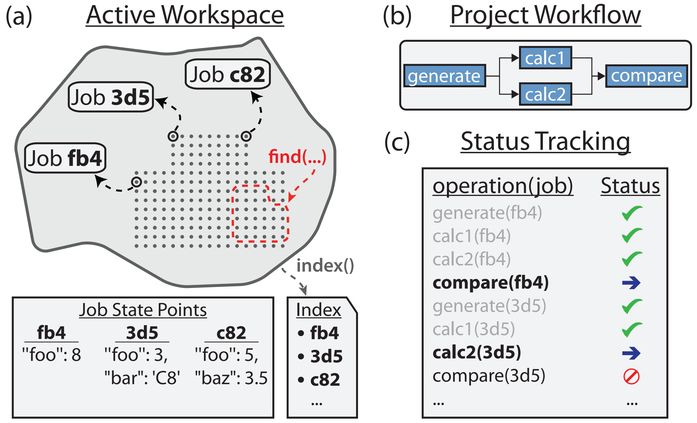
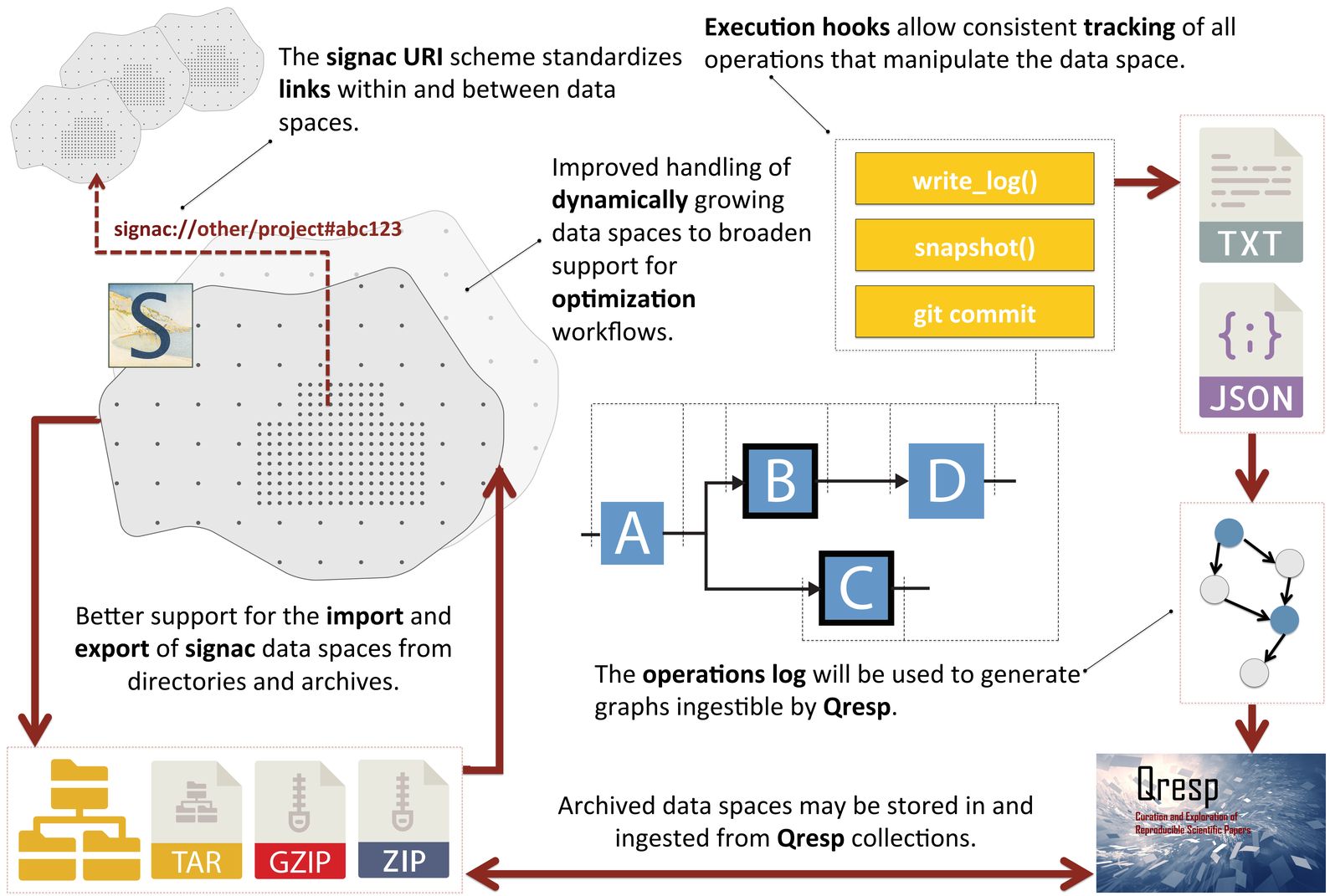



*Figure from reference [2].*

## Latest Development and Center Integration






## Resources

- Website: http://www.signac.io
- Documentation: https://signac-docs.readthedocs.io
- Installation:

```
$ conda install -c conda-forge signac
or
$ pip install signac
```

## References and Acknowledgements

1. C. S. Adorf, P. M. Dodd, V. Ramasubramani, and S. C. Glotzer, “Simple data and workflow management with the signac framework,” Comput. Mater. Sci., vol. 146, pp. 220–229, 2018.
2. V. Ramasubramani, C. S. Adorf, P. M. Dodd, B. D. Dice, and Sharon C. Glotzer, “signac: A Python framework for data and workflow management,” Proc. 17th Python Sci. Conf., pp. 91–98, 2018.

Development supported by MICCoM, as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Subcontract No. 6F-30844. Project conceptualization and implementation supported by the National Science Foundation, Award # DMR 1409620. Bradley Dice acknowledges support from the National Science Foundation Graduate Research Fellowship under Grant No. 1256260 DGE.