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.

Latest Development and Center Integration

The **signac** URI scheme standardizes *links* within and between data spaces.

Execution hooks allow consistent tracking of all operations that manipulate the data space.

Improved handling of **dynamically** growing data spaces to broaden support for **optimization** workflows.

The **operations log** will be used to generate graphs ingestible by **Qresp**.

Archived data spaces may be stored in and ingested from **Qresp** collections.

Resources

- Website: [http://www.signac.io](http://www.signac.io)
- Documentation: [https://signac-docs.readthedocs.io](https://signac-docs.readthedocs.io)
- Installation:  
  `$ conda install --c conda-forge signac`
  
  `$ pip install signac`

References and Acknowledgements

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4. Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109
5. Department of Physics, University of Michigan, Ann Arbor, MI 48109
6. Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109
7. Biointerfaces Institute, University of Michigan, Ann Arbor, MI 48109