Workflow Orchestration for Material Science

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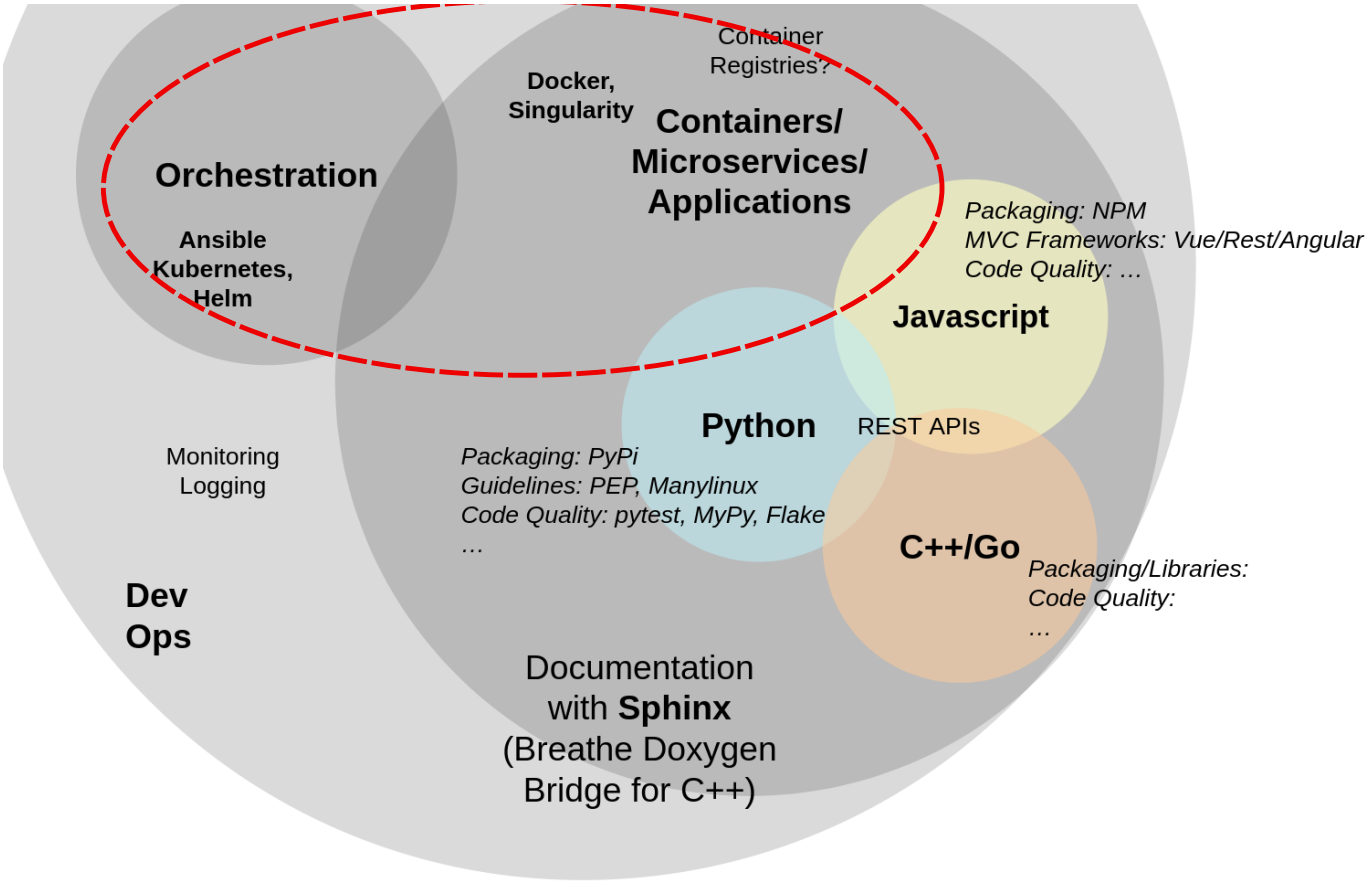
Overview

Workflow Orchestration on Cloud and HPC

Conclusion Remarks and Next steps


Container
Registries?
Docker,
Singularity
Containers/
Microservices/
Applications
Orchestration
Ansible
Kubernetes,
Helm
Packaging: NPM
MVC Frameworks: Vue/Rest/Angular
Code Quality: …
Javascript
Python
REST APIs
Monitoring
Logging
Packaging: PyPi
Guidelines: PEP, Manylinux
Code Quality: pytest, MyPy, Flake
…
C++/Go
Packaging/Libraries:
Code Quality:
…
Dev
Ops
Documentation
with Sphinx
(Breathe Doxygen
Bridge for C++)

Outline

Overview of Workflow Orchestration on Cloud and HPC

- Workflow containerisation
  - enable reproducibity
  - provide environment
  - portable
- Provision and orchestration of resources: compute, storage, network, etc.
- High Performance Storage

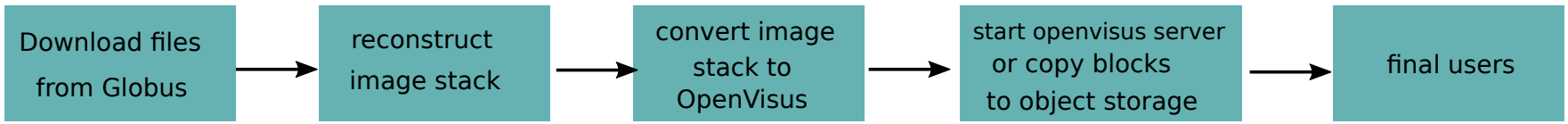


Figure: simplified workflow for material science

Resource Provision and Orchestration

Cluster deployment automation

- Provide easy access clusters.
- Ready to use

Smart scheduling

- Automatically identify the workload
- Decide the type of node to schedule: e.g. computation intensive, storage demanding, etc.?

Cluster Deployment Automation —Case study

Deployment Approches

- user-friendly interface: Jupyter Notebook
- Ansible: a software orchestration tool
- Python scripts
- bash scripts

Frameworks

- Kubernetes (k8s)— a widely-used container orchestrator
- Container engines, i.e Docker and/or Singularity

Automatic Cluster Deployment on Demand

—Chameleon Use case

Chameleon cluster: a large-scale, reconfigurable experimental platform hosted by the University of Chicago and TACC: bare-metal and VM nodes with root privileges.

Automation tools [1]

- Ansible Playbooks (yaml scripts)
- bash scripts

Cluster architecture

- one Ansible host
- A k8s cluster
  - one k8s login node (also the Ansible host)
  - one master node
  - one or multiple worker nodes

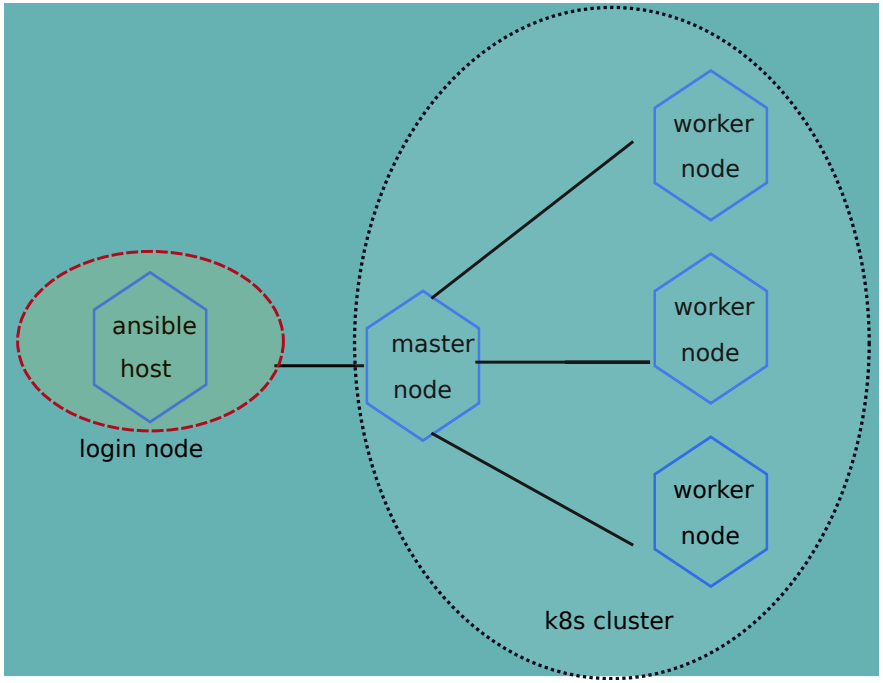
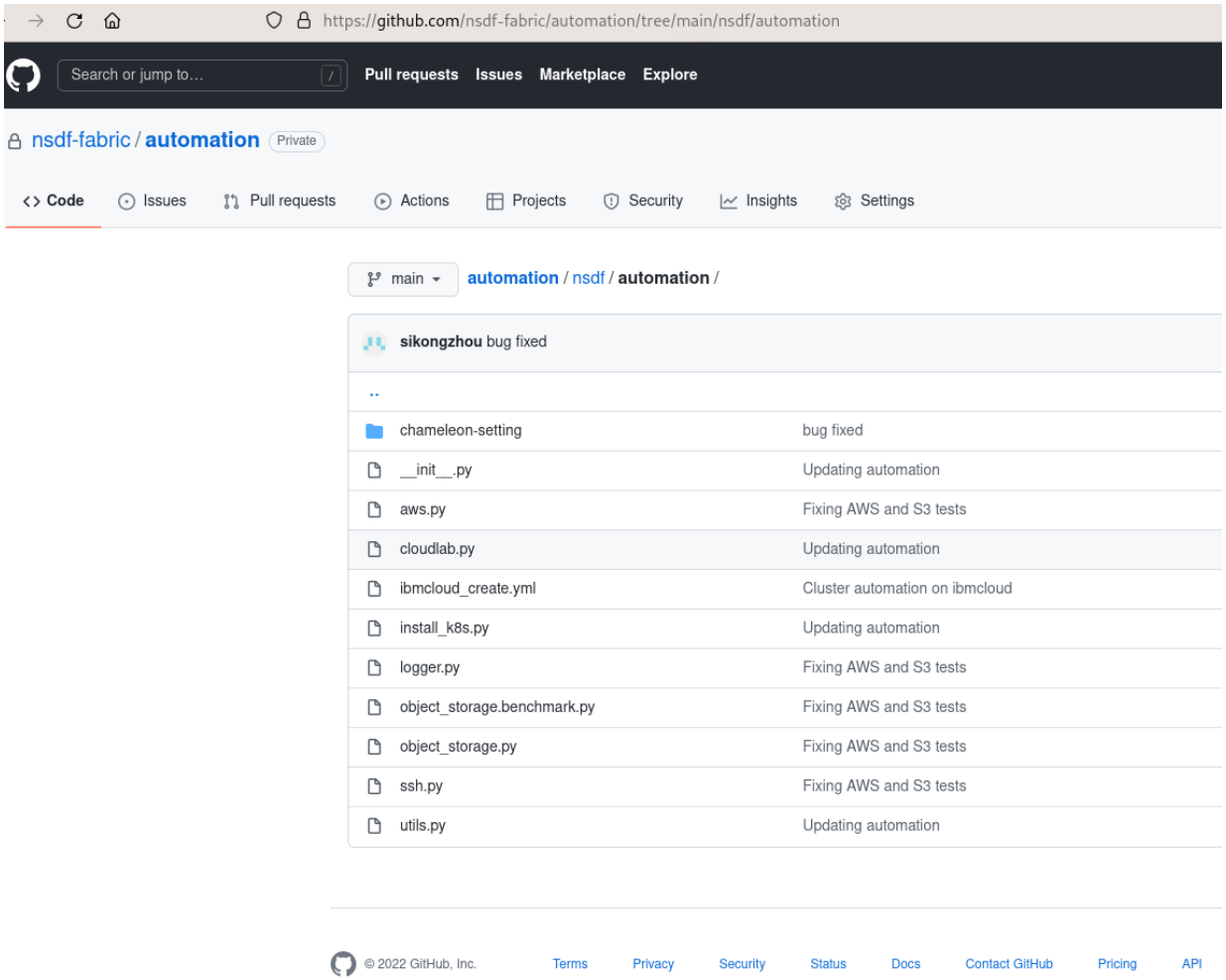


Figure: Our cluster arch on Chameleon

1. https://github.com/nsdf-fabric/automation/tree/main/nsdf/automation

Automatic Cluster Deployment on Demand



https://github.com/nsdf-fabric/automation/tree/main/nsdf/automation

High Performance Storage

Material science workflow requires:

1. Large data size
2. Fast data access

Storage Benchmarking

- Explore the state-of-the-art High-performance Storage Tech:
  - file storage
  - block storage
  - object storage
- Identify the suitable frameworks
- Identify the optimization technlogies.
  - Many threads/processes
  - Non-blocking
  - Hybrid
- benchmaking to analyse the storage throughput

Storage Benchmarking —A case study on Chameleon

```
=================================
                          Local-Path   vs              Longhorn    :            Change
IOPS (Read/Write)
        Random:          78,029 / 67,871   vs     20,538 / 13,723    :   -73.68% / -79.78%
    Sequential:          49,593 / 86,024   vs     25,332 / 23,434    :   -48.92% / -72.76%
  CPU Idleness:                      96%   vs                89%    :               -7%

Bandwidth in KiB/sec (Read/Write)
        Random:        344,901 / 402,383   vs    364,769 / 270,326    :    5.76% / -32.82%
    Sequential:        442,456 / 381,376   vs    419,740 / 280,534    :   -5.13% / -26.44%
  CPU Idleness:                      95%   vs                91%    :               -4%

Latency in ns (Read/Write)
        Random:        123,293 / 31,932   vs    411,993 / 336,327    :  234.16% / 953.26%
    Sequential:         36,896 / 32,565   vs    317,705 / 332,241    :  761.08% / 920.24%
  CPU Idleness:                      94%   vs                90%    :               -4%
```

Figure: Comparison of two types of storage: Local storage VS Longhorn on k8s evaluated with Kbench

- IOPS: IO operations per second. Higher is better
- Bandwidth: Throughput. Higher is better.
- Latency: The total time each request spent in the IO path. Lower is better.

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Concludsion and Next Steps

Summary

1. Workflow containerisation
2. Resource provision and orchestration
3. High performance storage
4. two case studies (preliminary results):
   - cluster deployment automation/orchestration on Chameleon
   - storage benchmarking

Next steps

- identify the bottleneck of the workflow
- workflow containerisation
- workflow automation

Feedbacks...

1. Processing time of your given amount of data
2. Which part of the workflow procedure is the bottleneck

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