Toward Understanding I/O Behavior in HPC Workflows

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DKRZ
DEUTSCHES KLIMARECHENZENTRUM

Argonne
NATIONAL LABORATORY

esiwace
CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

Universität Hamburg
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Overview

Motivation

Workflows & I/O Monitoring

Architecture

Demo

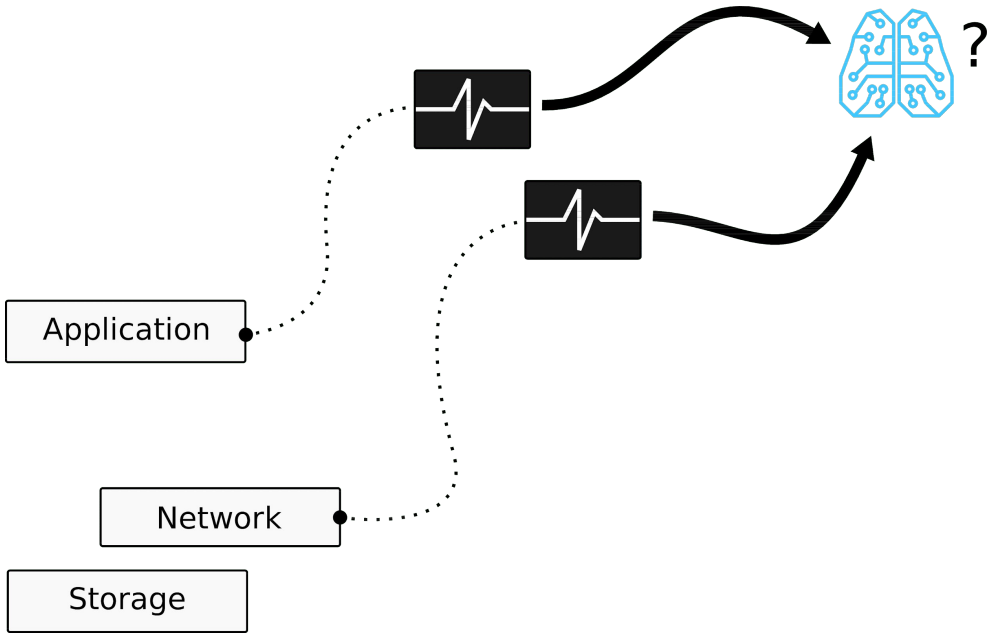
Outlook & Summary

Trying to add a missing link so we can move closer to realizing smarter systems...

Require **new interfaces** to preserve information about **structure of data**.

How to anticipate **user intentions** and **I/O behavior** of applications ?

Require **tools to observe and record** system activity as a basis to gain insight



Workflows a HPC Storage Perspective?

Workflows offer …

- … anticipatable future activity
- … implicit intent to be discovered
- … explicit intent description

Workflow Engines: Swift, Cylc, Tigres, etc.

Cylc, Swift-k, Fireworks

Job centric, with tasks and data targets. Tasks are distributed and possibly run on **remote systems**. Data products might be moved between sites.

Usually, a coarse granular dependency graph.

Swift-t, Tigres, Spark/RDD Lineage, QDO

A large **integrated** (MPI) application with many different tasks within the application. With **exascale** in mind and also closer to **in situ** enabled workflows.

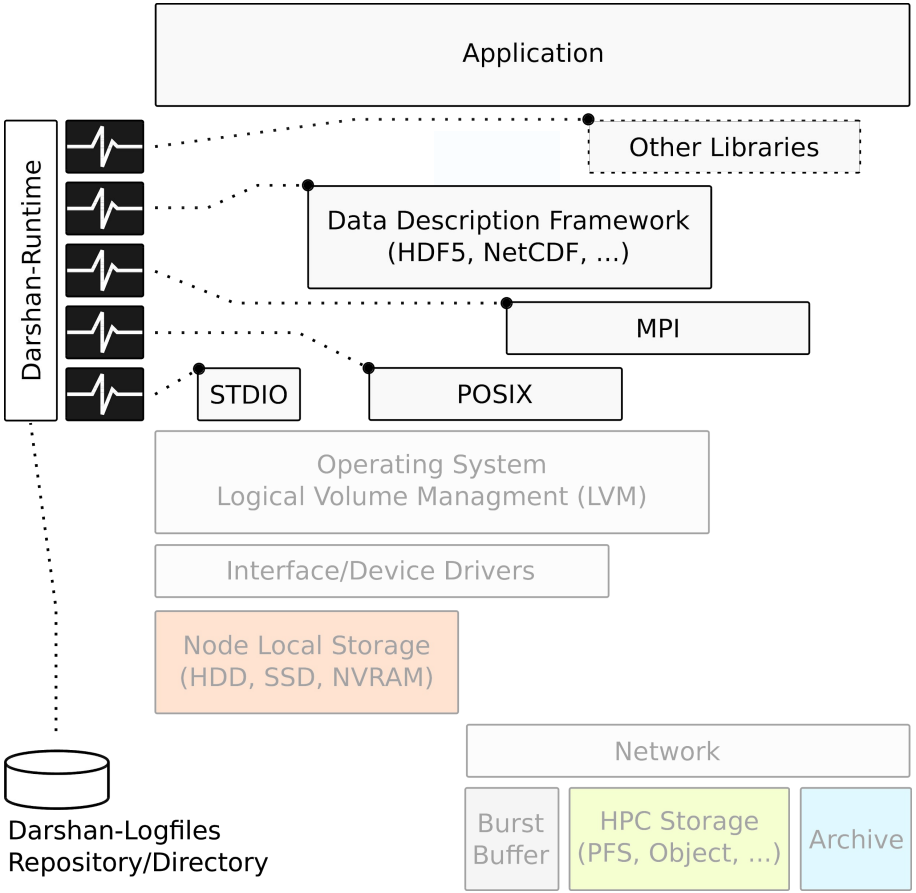
Closer to a programming language.

Holistic I/O Monitoring for HPC

Tracking at the Application/Library Layer

Total Knowledge of I/O in Data Centers

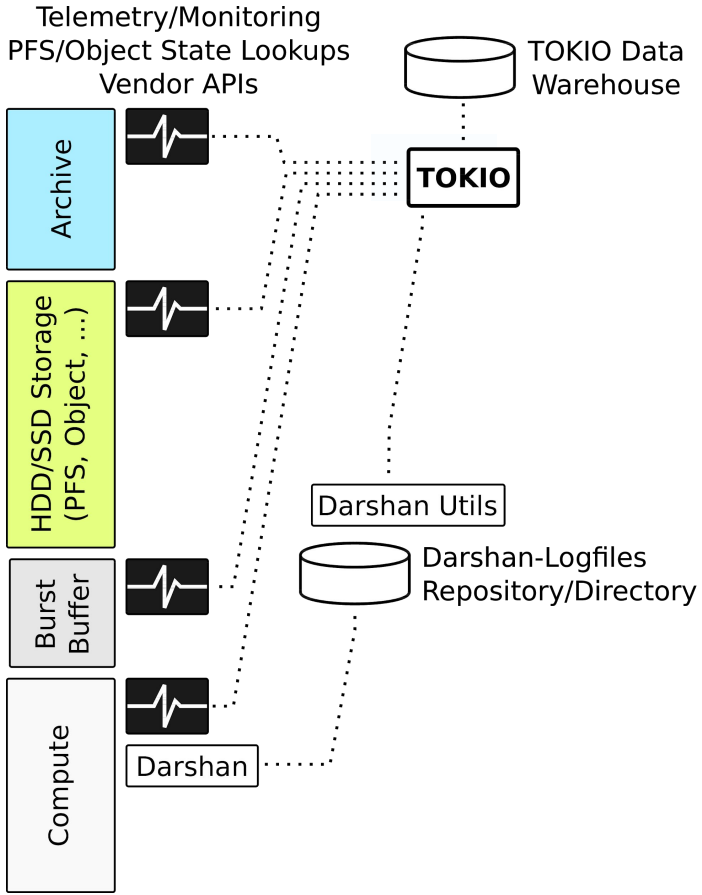
Darshan: Instrumentation at Library/Application Layer




```
$ export LD_PRELOAD=libdarshan.so
$ mpiexec -np 4 ./hellompi
```

[Darshan] HPC I/O Characterization Tool - https://www.mcs.anl.gov/research/projects/darshan/

TOKIO: Total Knowledge of Input/Output



Comprehensive capture of I/O activity

Support different storage services in data center

May require privileged access in many cases

[TOKIO] http://www.nersc.gov/research-and-development/tokio/

Toward Understanding Workflow I/O

Combine workflow descriptions with monitoring information from Darshan/TOKIO, etc.

Benefits:

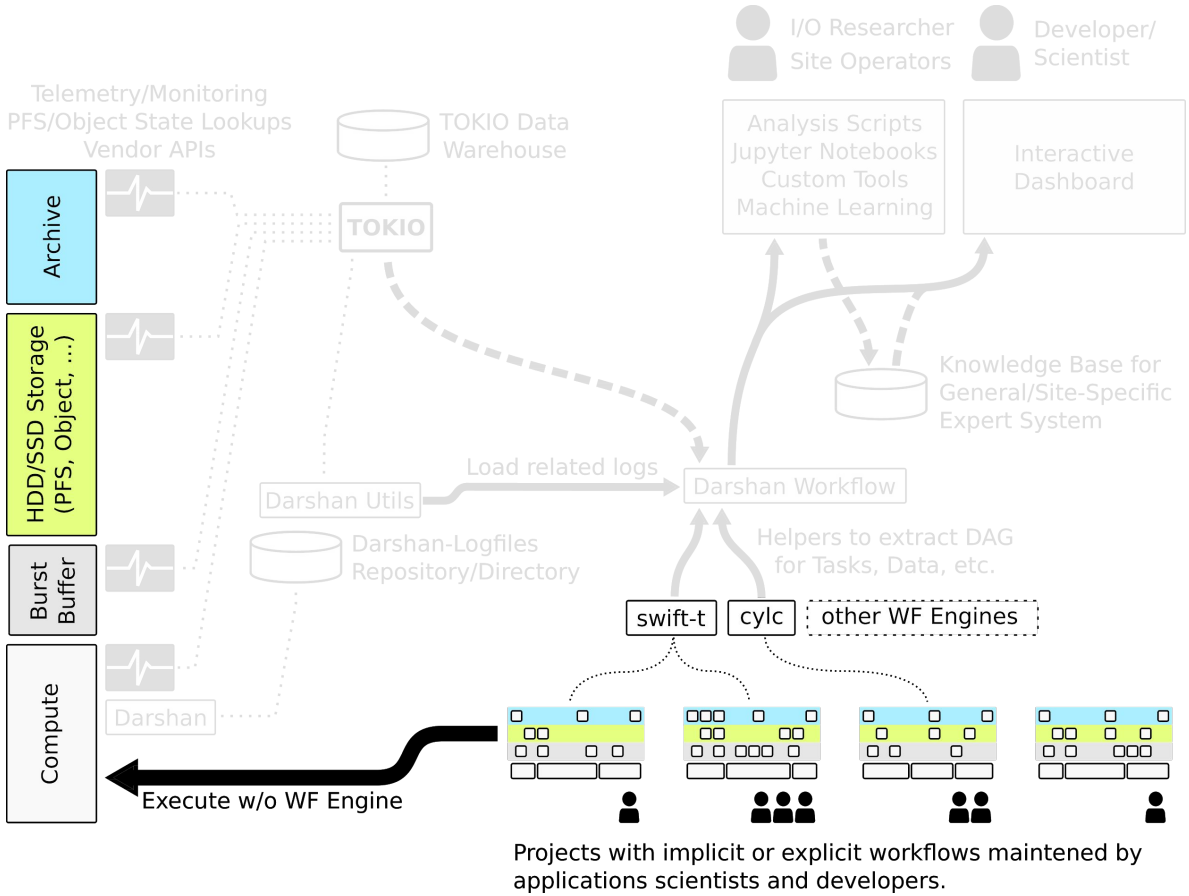
- Insight useful for operating decisions and system design
- Communication with users, relatable to their scientific process
- Source of information for smarter systems

Requirements:

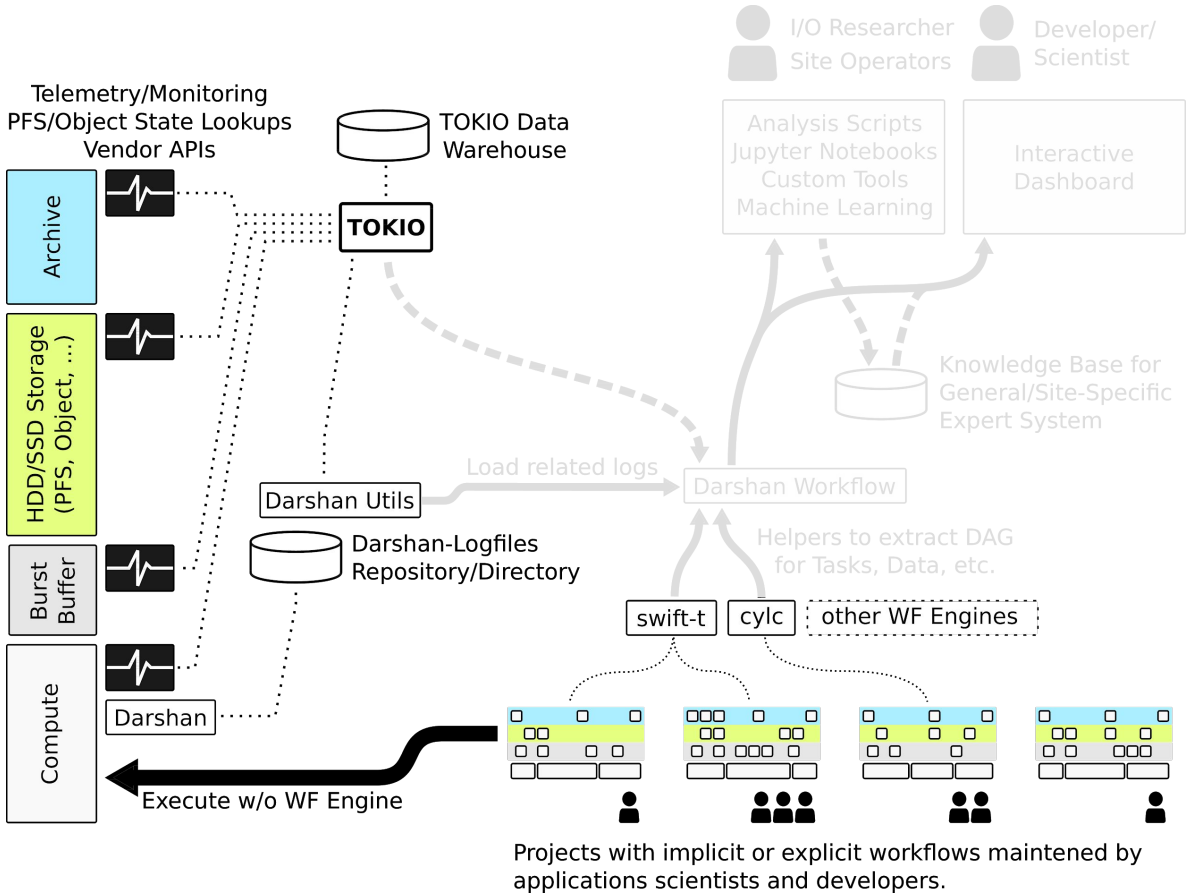
- Support multiple workflow engines as communities use different tools across difference sites

- Explore convenient toolchain for researchers and operators
- User facing component to communicate advice

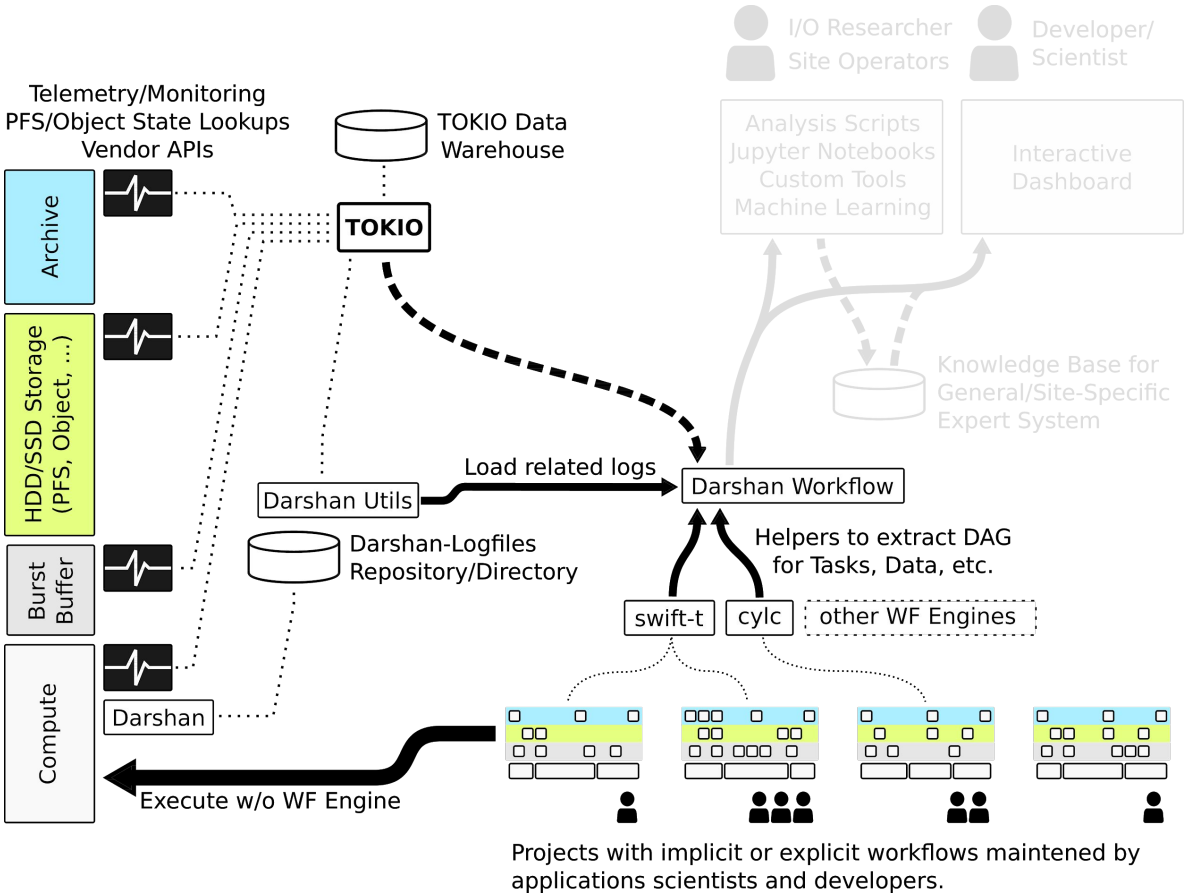
Architecture for Augmenting I/O in Workflows



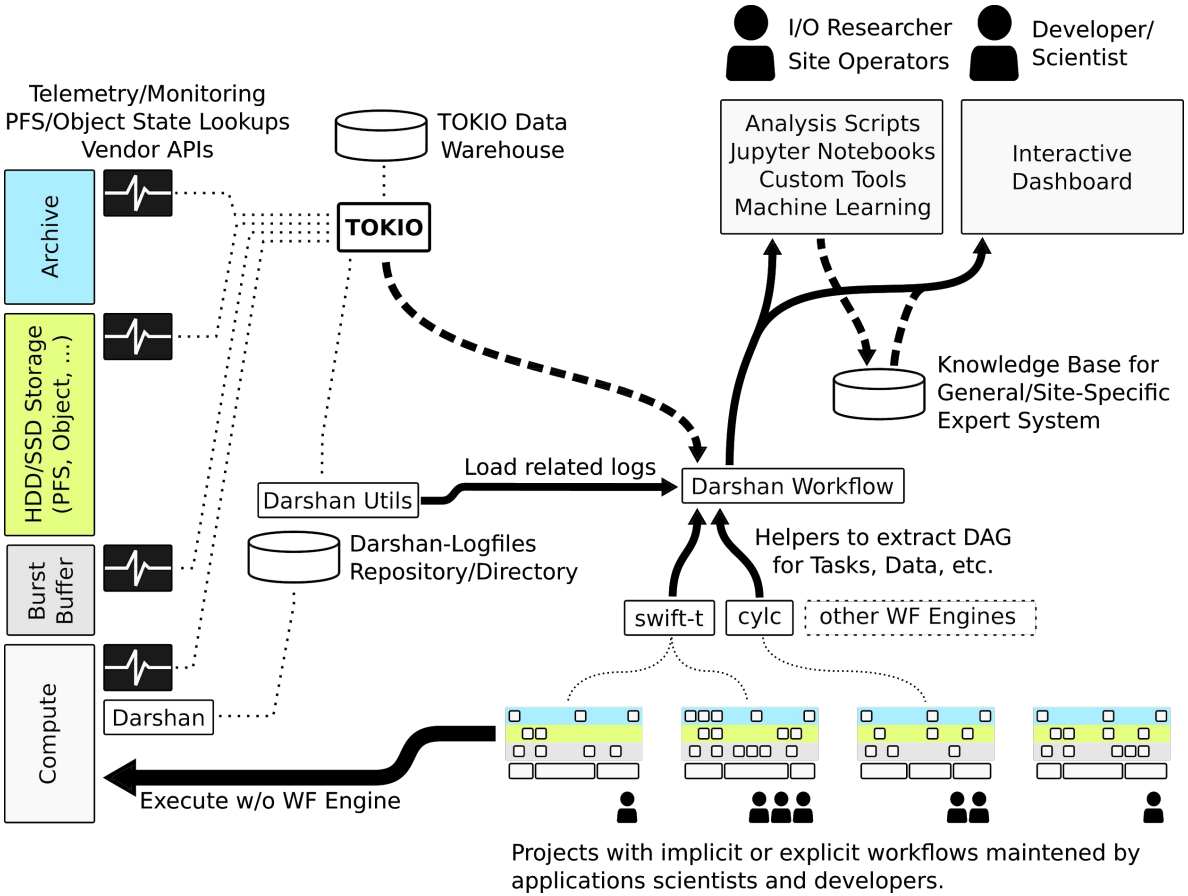
Architecture for Augmenting I/O in Workflows



Architecture for Augmenting I/O in Workflows



Architecture for Augmenting I/O in Workflows



Case Study
& Demonstration

Example Workflow

Research Perspective

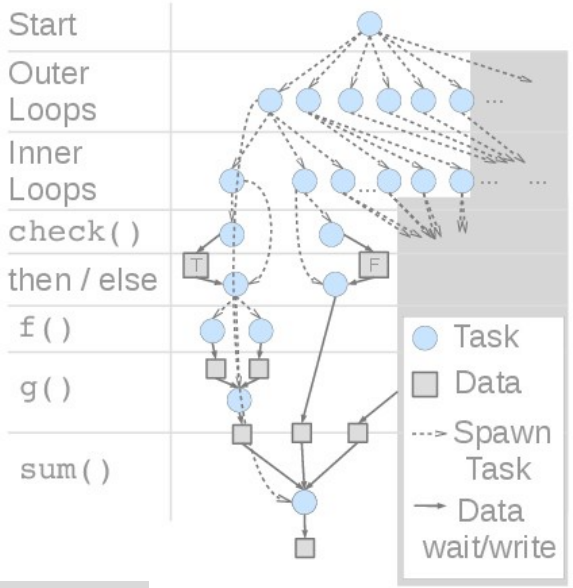
User Perspective

swift

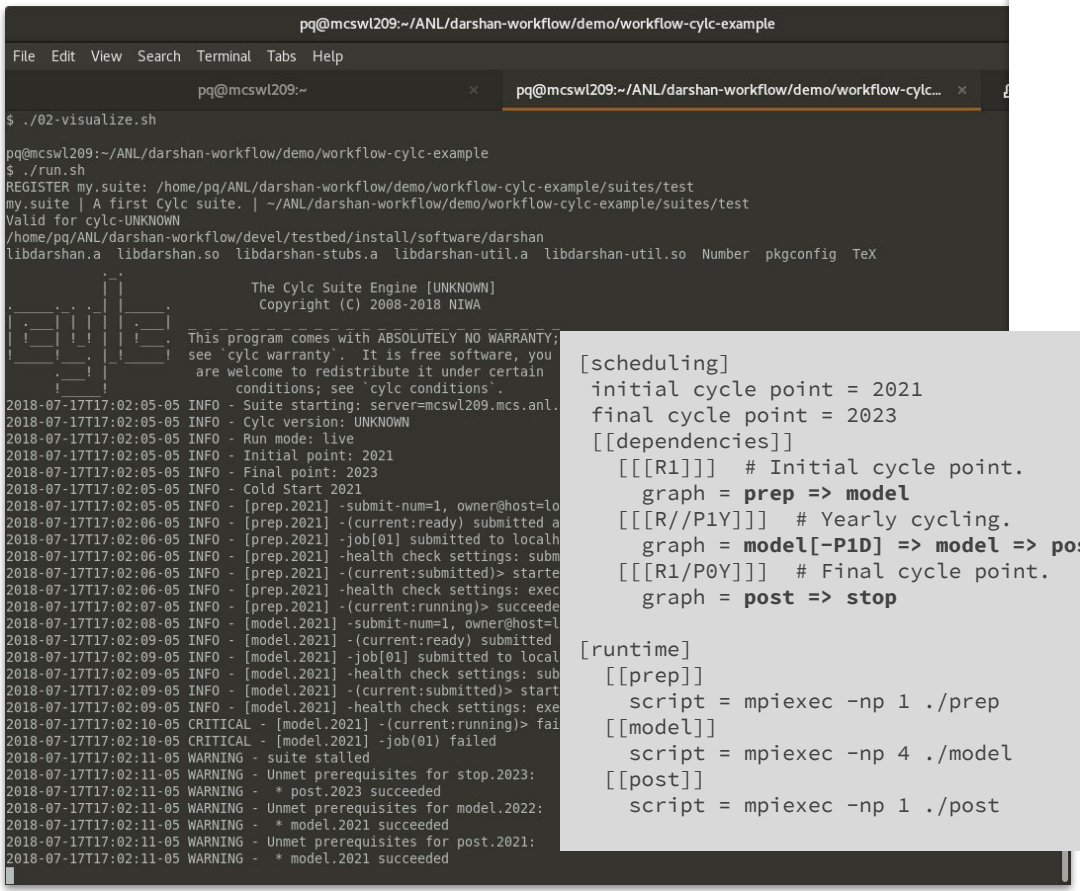
```
pq@mcswl209:~/ANL/darshan-workflow/demo/workflow-swiftt-ccgrid2013-example
File  Edit  View  Search  Terminal  Help
+/home/pq/ANL/darshan-workflow/devel/testbed/install/software/swiftt/stc/bin/swift-t:252> return 0
Swift/T
Compiling: workflow-launch+darshan.swift
       to: ./swift-t-workflow-launch+darshan.Bm4.tic
        /home/pq/ANL/darshan-workflow/devel/testbed/install/software/swiftt/stc/bin/stc -O 0 -V workflow-launch+darshan.swift ./swift
-t-workflow-launch+darshan.Bm4.tic
stc: using JVM: /usr/bin/java
Running:   ./swift-t-workflow-launch+darshan.Bm4.tic
       /home/pq/ANL/darshan-workflow/devel/testbed/install/software/swiftt/turbine/bin/turbine -n 5 -l -V ./swift-t-workflow-launch+
darshan.Bm4.tic
/usr/lib64/mpich/bin/mpiexec
[0]    0.000 WORK TYPES: WORK REPUT
[0]    0.000 WORKERS: 4 RANKS: 0 - 3
[0]    0.001 SERVERS: 1 RANKS: 4 - 4
[0]    0.033 global: u:HARD=<-8>
[0]    0.034 global: u:SOFT=<-7>
[0]    0.034 global: u:RANK=<-6>
[0]    0.034 global: u:NODE=<-5>
[0]    0.034 global: u:X=<-4>
[0]    0.034 global: u:Y=<-3>
[0]    0.034 global: u:A=<-2>
[0]    0.034 global: u:B=<-1>
[1]    0.024 function:swift:constants
[0]    0.035 function:swift:constants
[0]    0.035 allocated
[0]    0.035 store: <2
[0]    0.036 function:
[2]    0.036 function:
[3]    0.036 function:
[0]    0.036 allocated
[2]    0.037 allocated
[3]    0.036 allocated
[0]    0.036 allocated
[0]    0.036 store: <3
[1]    0.026 allocated
[0]    0.036 rule: <3>
[3]    0.037 store: <1
```

```
int X = 50, Y = 50;
int A[][];
int B[];

foreach x in [0:X-1] {
  foreach y in [0:Y-1] {
    if (check(x, y)) {           // mask a region which gets computed
      A[x][y] = g(f(x), f(y));   // compute result for this cell (a physics process)
    } else {
      A[x][y] = 0;               // default for skipped cells
    }
  }
  B[x] = sum(A[x]);              // compute some aggregate metric
}
```

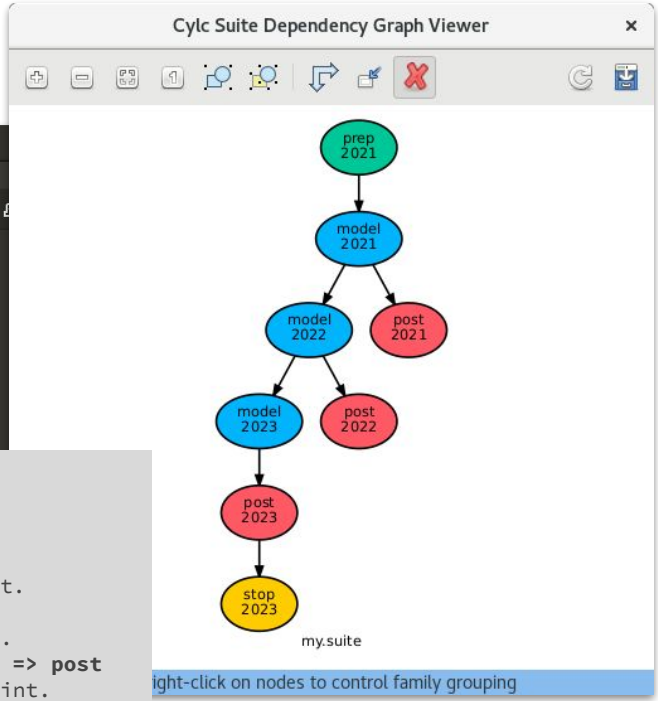


http://swift-lang.org




```
[scheduling]
 initial cycle point = 2021
 final cycle point = 2023
 [[dependencies]]
   [[[R1]]]  # Initial cycle point.
     graph = prep => model
   [[[R//P1Y]]]  # Yearly cycling.
     graph = model[-P1D] => model => post
   [[[R1/P0Y]]]  # Final cycle point.
     graph = post => stop

[runtime]
  [[prep]]
    script = mpiexec -np 1 ./prep
  [[model]]
    script = mpiexec -np 4 ./model
  [[post]]
    script = mpiexec -np 1 ./post
```



https://cylc.github.io/cylc/

Perspective for **I/O Research** and **Site Operating**?

Interactive Tools/Dashboards to ease navigating **overwhelming amounts of log data**, with “algebra”-like semantics for convenient aggregation of multiple tasks, data objects or pipelines.

Python Library for use in, e.g., **jupyter notebooks**, to draft/prototype/provide **templates** for more sophisticated and **reproducible** analysis.

JavaScript Packages (NPM) for visualisation/tools allowing easy **reuse** in custom tools , jupyter notebooks (widget plugins), and dashboards (e.g., Grafana).

Augmenting Workflow I/O with Darshan/TOKIO

Scientific discovery increasingly depends on complex workflows consisting of multiple phases and sometimes millions of parallelizeable tasks or pipelines. Typical workflows on HPC systems routinely require the pre-processing, generation by simulation and post-processing of data. Unfortunately, most workflow models focus on the scheduling and allocation of resources for tasks while the impact on storage systems remains a secondary objective.

By combining a workflow description (e.g., from a workflow engine like Swift or Cylc) with log data or telemetry information we can gain insight on the I/O behaivior of a complete workflow and then optimize applications, middleware and systems accordingly.

In [1]:
```
import darshan.workflow
```

In [2]:
```
# Load a workflow report
wf = darshan.workflow.load('data-workflow.json')
wf.data
```

Out[2]:

```
{'nodes': [{'id': 'model.2021',
   'label': 'model.2021',
   'x': 140.5,
   'y': -410.0,
   'data': {},
   'group': 'report'},
  {'id': 'model.2022',
   'label': 'model.2022',
   'x': 91.5,
   'y': -320.0,
   'data': {},
   'group': 'report'},
  {'id': 'post.2021',
   'label': 'post.2021',
   'x': 189.5,
   'y': -320.0,
   'data': {}},
  {'id': 'model.2023',
   'label': 'model.2023',
   'x': 42.5,
```


Inspecting a Workflow from Darshan

Darshan/TOKIO-workflow is build to ease interactive and automatic analysis of workflows with a focus on the I/O perspective. As such it explores a variety of convenience methods and common visualisations such as the `task_summary()` and `show_graph()` methods.

In [3]:
```
wf.tasks_summary()
```

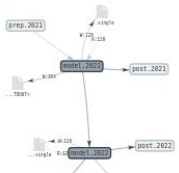
```
model.2021      Records: 2      Layers: POSIX, STDIO
model.2022      Records: 2      Layers: POSIX, STDIO
post.2021       Records: 0      Layers:
model.2023      Records: 2      Layers: POSIX, STDIO
post.2022       Records: 0      Layers:
post.2023       Records: 0      Layers:
stop.2023       Records: 0      Layers:
prep.2021       Records: 0      Layers:
```

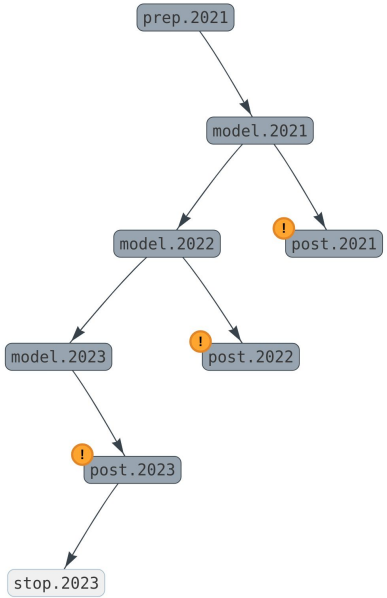
Displaying and Interacting with Workflow

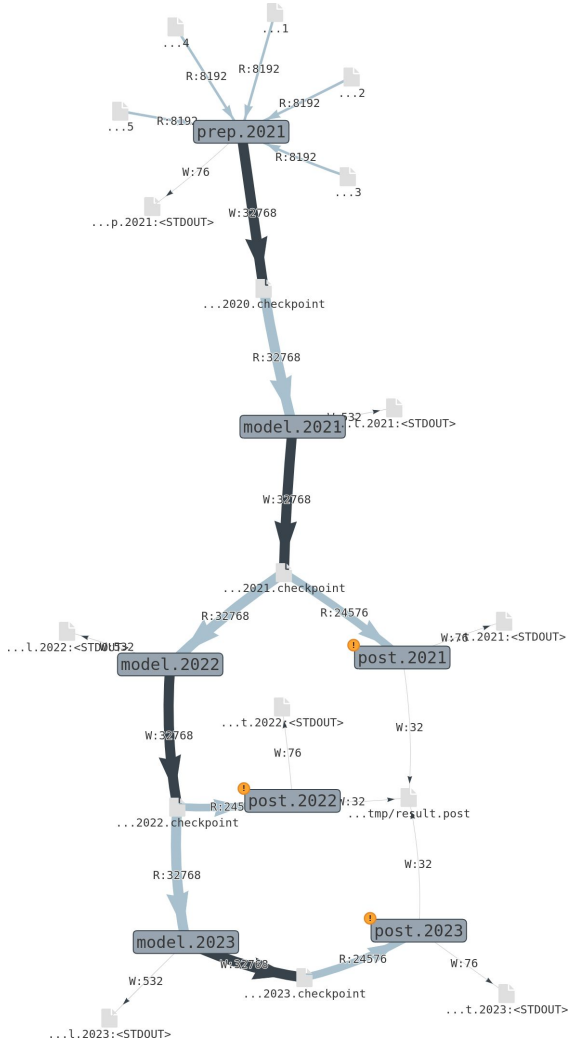
Jupyter Notebooks can be extended with custom widget, which allows to turn them into versatile tools for custom but powerful tools in I/O analysis. This is especially true for workflows, which generate a lot of log data so that interactive tools make data exploration more convienient.

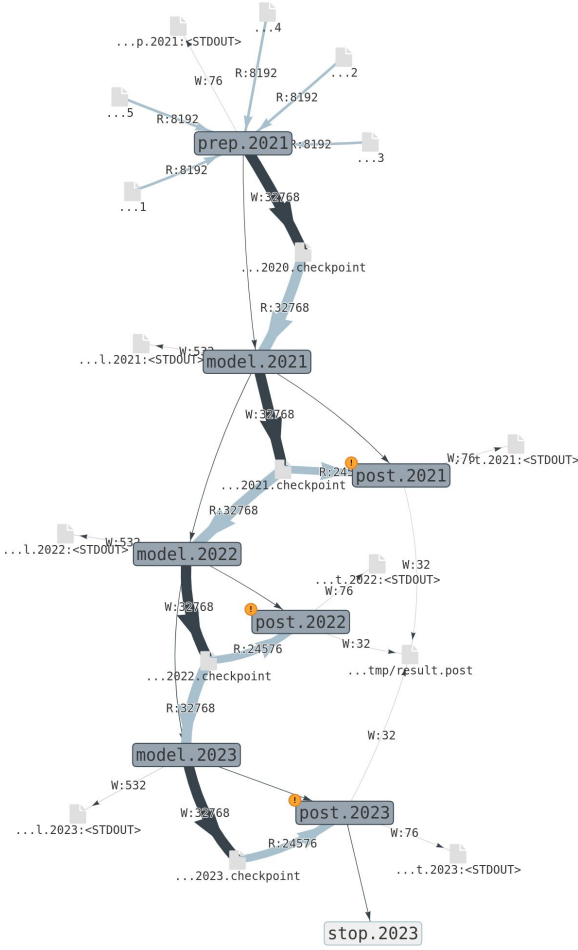
In [4]:
```
import darshan.ipywidgets.example as wfgraph
import json
wf.show_graph()
graph = wfgraph.HelloWorld()
graph
```

```
TODO: GRAPH IpythonWidget
```




prep.2021
model.2021
model.2022
post.2021
model.2023
post.2022
post.2023
stop.2023


...4
...1
R:8192
R:8192
...2
R:8192
...5
R:8192
prep.2021
R:8192
W:76
...3
...p.2021:<STDOUT>
W:32768
...2020.checkpoint
R:32768
model.2021
...t.2021:<STDOUT>
W:32768
...2021.checkpoint
R:32768
R:24576
...l.2022:<STDOUT>
model.2022
post.2021
...t.2021:<STDOUT>
...t.2022:<STDOUT>
W:32768
W:32
W:76
post.2022
...2022.checkpoint
...tmp/result.post
R:32768
W:32
model.2023
post.2023
W:532
R:24576
W:76
...2023.checkpoint
...l.2023:<STDOUT>
...t.2023:<STDOUT>


...p.2021:<STDOUT>
...4
W:76
R:8192
...2
R:8192
...5
R:8192
prep.2021
R:8192
...3
R:8192
...1
W:32768
...2020.checkpoint
R:32768
...l.2021:<STDOUT>
W:532
model.2021
W:32768
W:76
...t.2021:<STDOUT>
...2021.checkpoint
R:32768
...l.2022:<STDOUT>
W:532
model.2022
...t.2022:<STDOUT>
W:32
W:76
W:32768
post.2022
R:24576
W:32
...2022.checkpoint
...tmp/result.post
R:32768
W:32
model.2023
W:532
post.2023
...l.2023:<STDOUT>
W:32768
W:76
R:24576
...2023.checkpoint
...t.2023:<STDOUT>
stop.2023

Communication with Scientists/Developers

Maintain affinity to scientists perspective

- Stick to relationship of tasks/pipelines used by scientists/developers
- Use intuitiv presentation of data-flow by extending graph of workflow

Interactive to manage complexity

- 100s or 1000s of different tasks and files in a workflow
- Possibly, millions of log records per task (HTC, UQ)
- Make it easy to aggregate multiple log records

Integration with expert advice

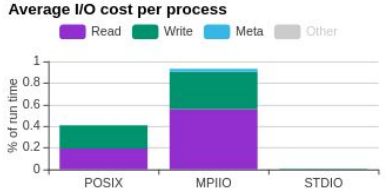
- Human in the loop
- Automatic advisories with machine learning (mid/long-term)

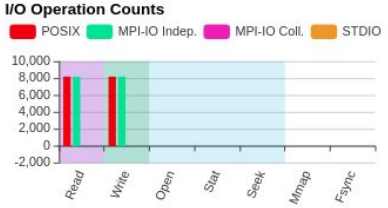
http://my.datacenter/workflow-io?worfklow_id=314159

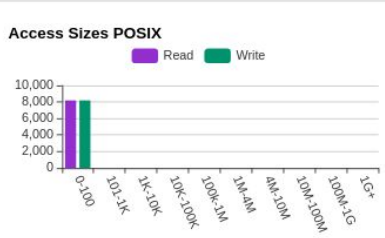
Workflow Overview

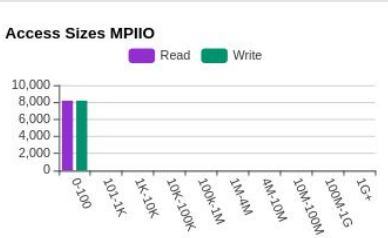
/home/pq/ANL/darshan-workflow/demo/workflow-cylc-example/model

jobid: 19911	uid: 1000	nproc: 4	runtime: 1 seconds









Most Common Access Sizes

(POSIX and MPI-IO)

Layer	Access Size	Count
POSIX	50013	14
POSIX	50007	14
POSIX	49986	9
POSIX	49998	9
MPI-IO	1020	212
MPI-IO	512	34

File Count Summary

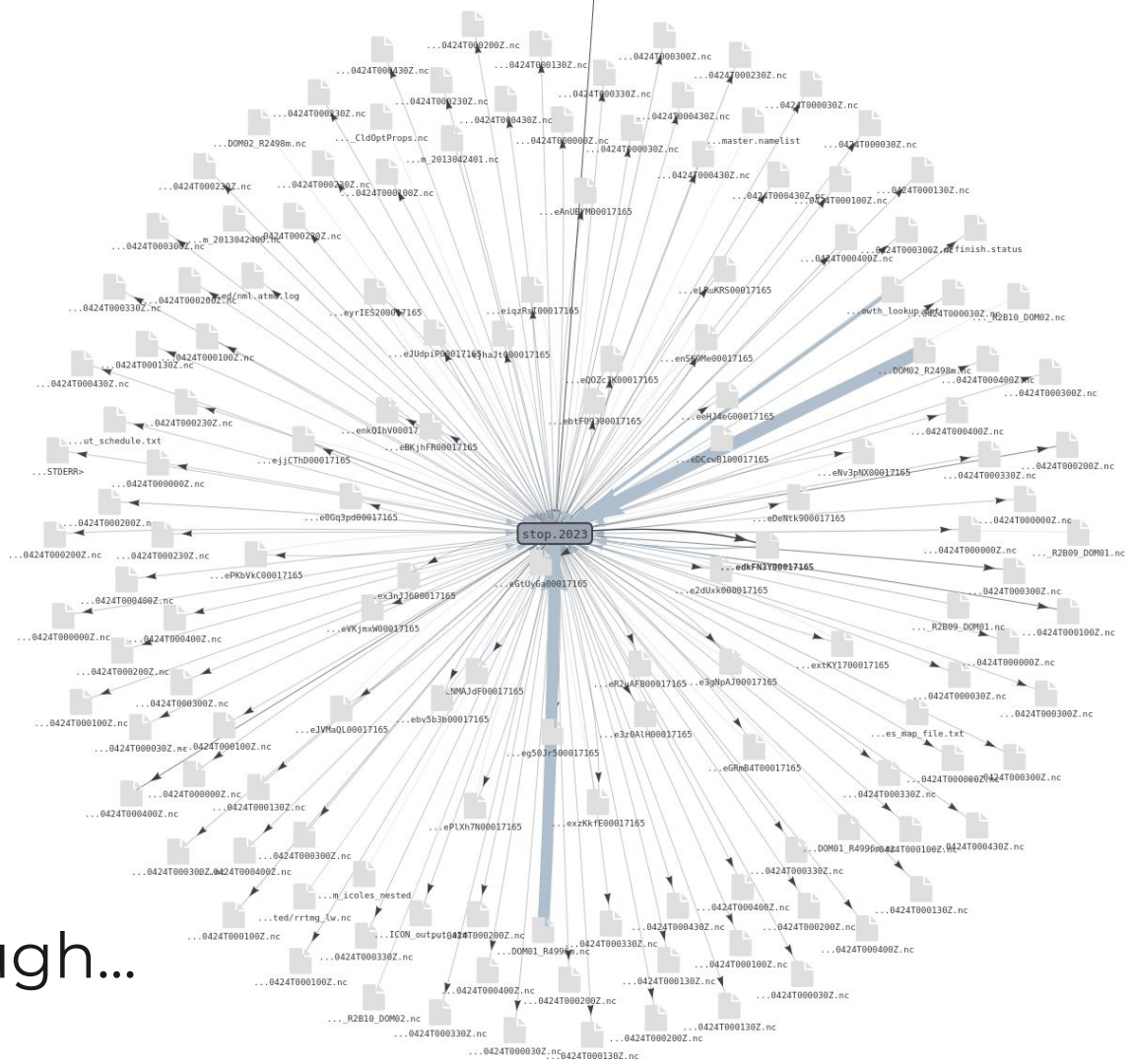
(estimated by POSIX I/O access offsets)

type	number of files	avg. size	max size
total opened	4	1.8M	7.2M
read-only files	0	0	0
write-only files	1	16K	16K
read/write files	3	2.4M	7.2M
created files	4	1.8M	7.2M

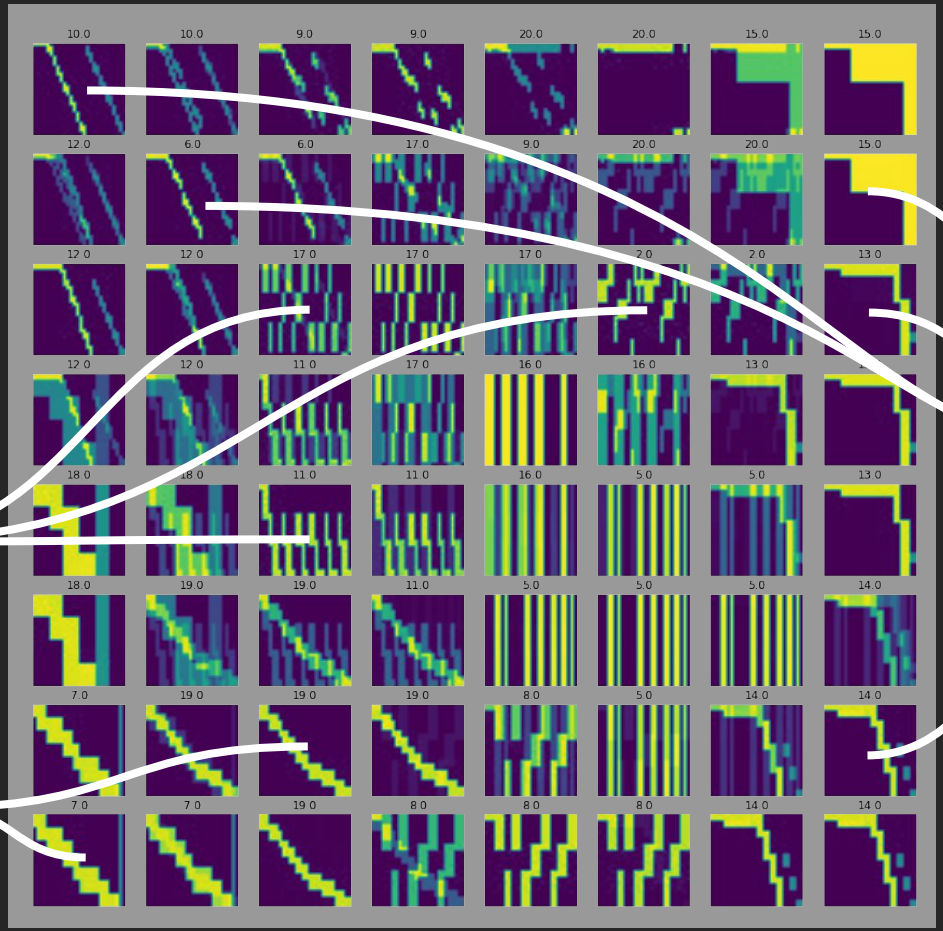
Logfiles:

Task: model.2021
model.2021: darshan-lo
Task: model.2022
model.2022: darshan-lo
Task: post.2021
post.2021: darshan-logs
Task: model.2023
model.2023: darshan-lo
Task: post.2022
post.2022: darshan-logs
Task: post.2023
post.2023: darshan-logs
Task: prep.2021
prep.2021: darshan-logs
Files
model.2021: /tmp/2020.
model.2021: /tmp/2021.
model.2021: <STDOUT:
model.2022: /tmp/2022.
model.2022: /tmp/2021.
model.2022: <STDOUT:
post.2021: /tmp/result.p
post.2021: /tmp/2021.ch
post.2021: <STDOUT>
model.2023: /tmp/2023.
model.2023: /tmp/2022.
model.2023: <STDOUT:
post.2022: /tmp/result.p
post.2022: /tmp/2022.ch
post.2022: <STDOUT>
post.2023: /tmp/result.p
post.2023: /tmp/2023.ch
post.2023: <STDOUT>
prep.2021: /tmp/file-raw.
prep.2021: /tmp/file-raw.
prep.2021: /tmp/file-raw
prep.2021: /tmp/2020.ch
prep.2021: /tmp/file-raw.
prep.2021: /tmp/file-raw
prep.2021: <STDOUT>

What a **real task**
might look like though...



Analyzing **Access Patterns**



Input Files

In this case diagnostic files otherwise not so clear

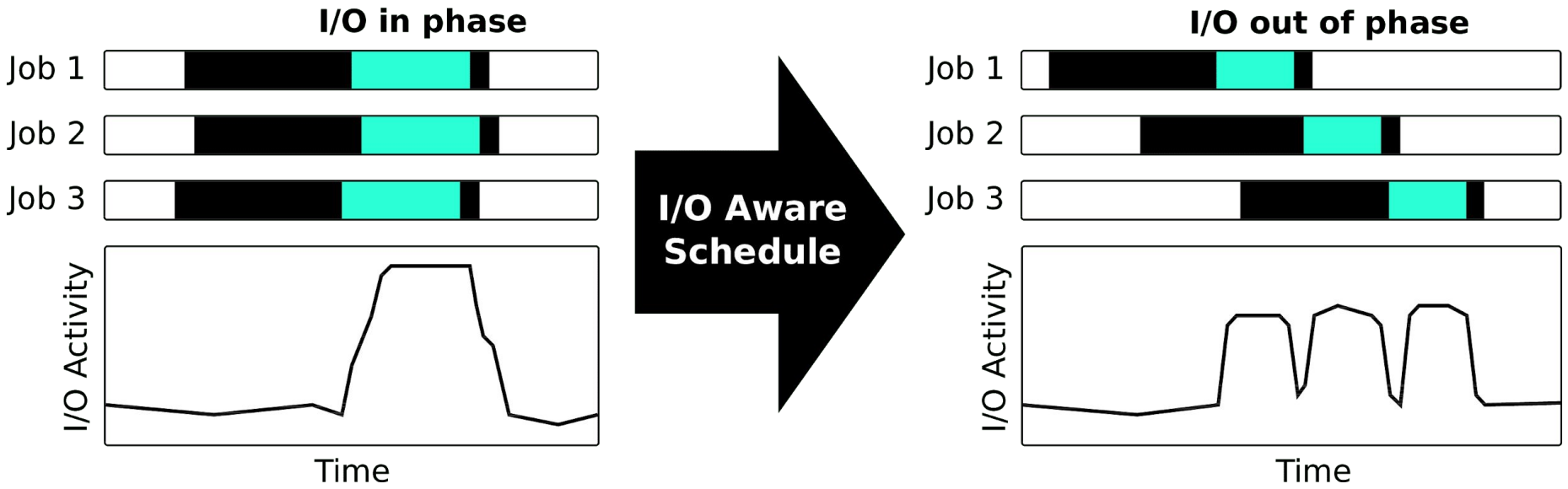
Output Files

Toward Adaptive I/O Systems

Influence **Job Scheduling** decisions

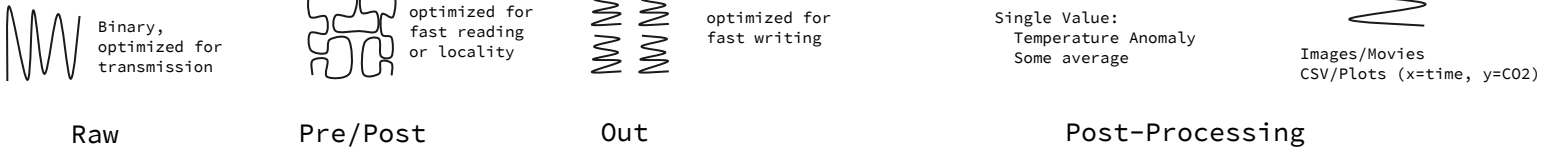
Support **I/O Middleware**
- Data Placement
- Transformations

Use Case 1: I/O-Aware Scheduling for Workflows

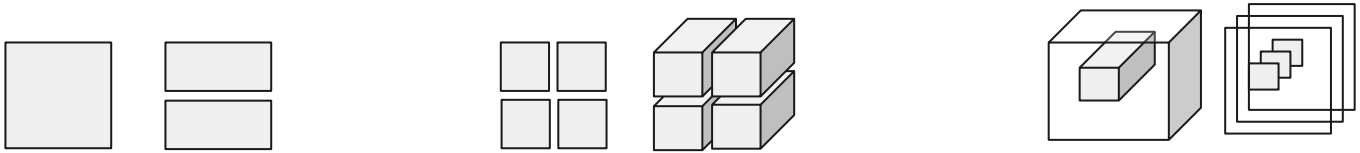


Use Case 2: Benefits for I/O Middleware (1/2)

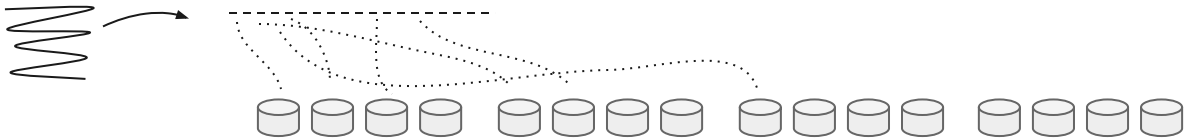
Data Representation



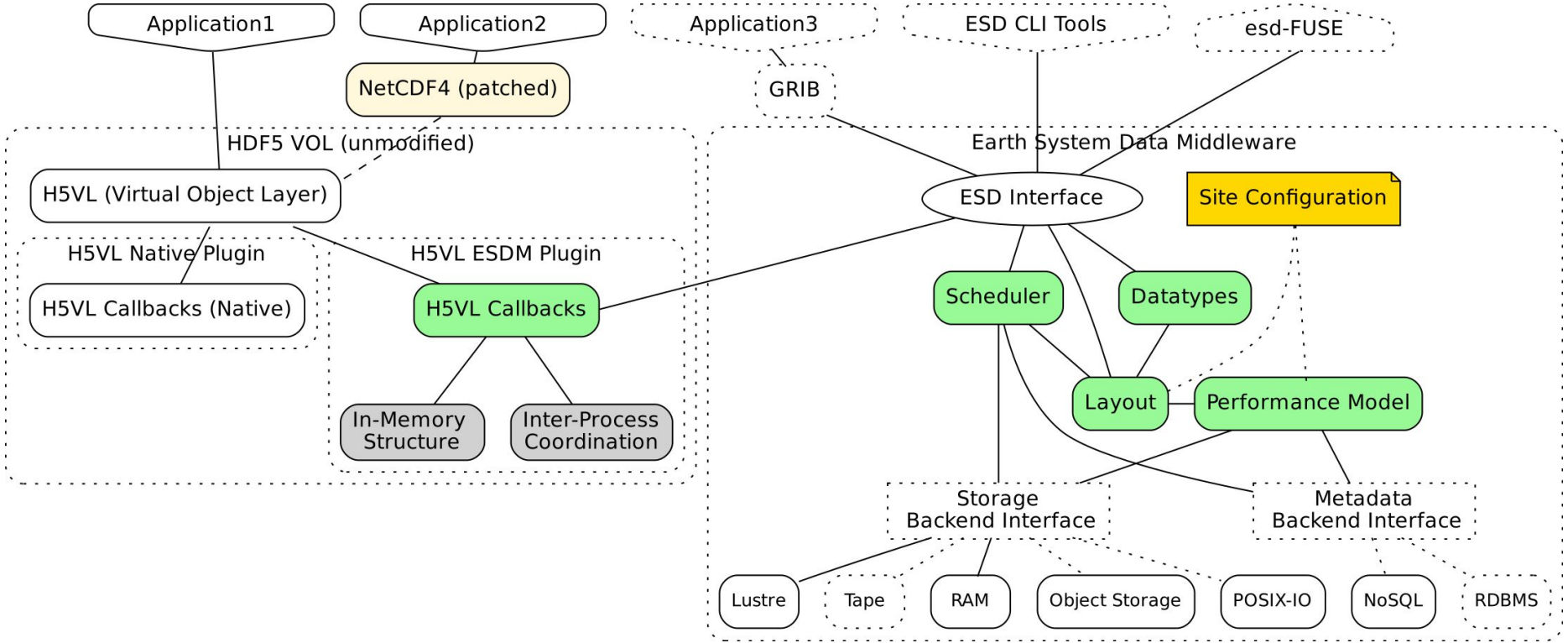
Domain Decomposition



Layout on Storage



Use Case 2: Benefits for I/O Middleware (2/2)



Discussion Summary

Requirements for Workflow Engines

Expose Context / DAGs of Workflows
Data/(file) notions
Reflection in execution runtime?

Requirements for Monitoring Solutions

Pick up context to allow associations
Support user-specific metadata with record
API to interact with monitoring toolkit
Allow counters per MPI Communicator

Requirements for Application Developers

Make intent explicit: use libs/DSL (e.g. HDF5)
Enable instrumentation with a subset of runs

Collect traces and logs for a training body.

Thank you!
Questions?

luettgau@dkrz.de

Disclaimer

This work was supported by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research, under Contract DE-AC02-06CH11357.

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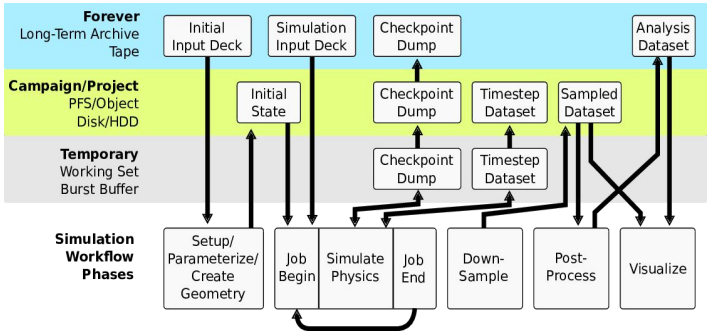
Appendix

Generic HPC Workflows

Example Climate Workflow

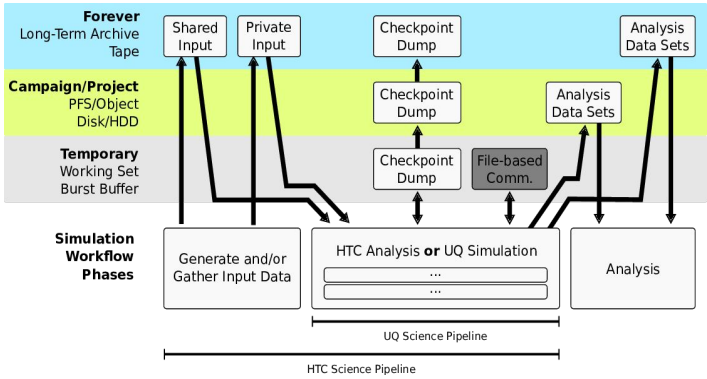
Common Scientific Workflows in HPC

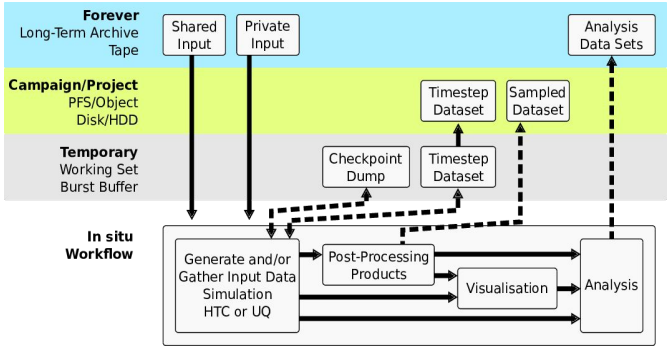
What makes a workflow?



SIM

UQ or HTC





in situ

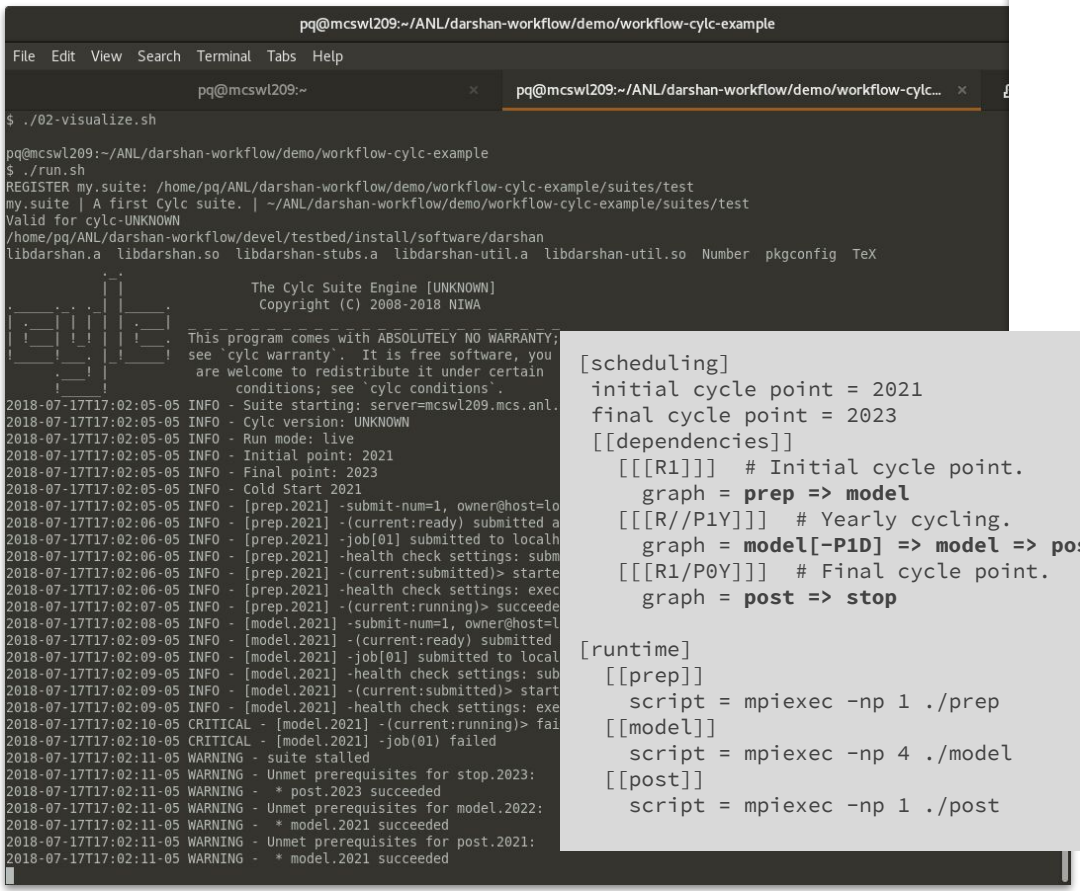
SIM and HTC/UQ are derived figures from [1]. For outlook on workflows refer to [2].

[1] LANL, NERSC, and SNL, “APEX Workflows.”, Whitepaper, Mar. 2016
Online: https://www.nersc.gov/assets/apex-workflows-v2.pdf

[2] E. Deelman *et al.*, “The future of scientific workflows,” *The International Journal of High Performance Computing Applications*, vol. 32, no. 1, pp. 159–175, Jan. 2018.

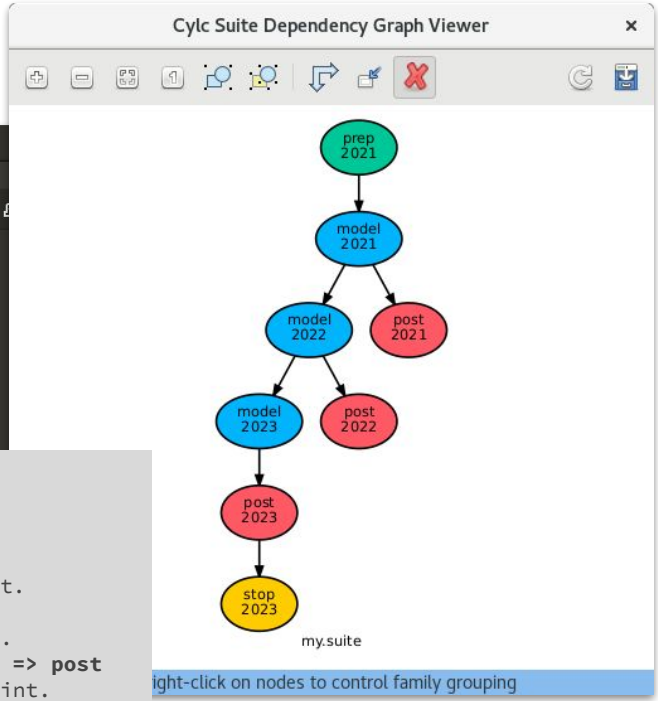
Data-Intensive Exascale Workflow: Climate Modeling

ICON is a climate model used by Researchers at Max-Planck and by the German Weather Service (DWD).
CDO is a pre/post-processing tool (climate operators) for NetCDF files.
ParaView is a popular visualisation toolkit built on top of VTK.




```
[scheduling]
 initial cycle point = 2021
 final cycle point = 2023
 [[dependencies]]
   [[[R1]]]  # Initial cycle point.
     graph = prep => model
   [[[R//P1Y]]]  # Yearly cycling.
     graph = model[-P1D] => model => post
   [[[R1/P0Y]]]  # Final cycle point.
     graph = post => stop

[runtime]
  [[prep]]
    script = mpiexec -np 1 ./prep
  [[model]]
    script = mpiexec -np 4 ./model
  [[post]]
    script = mpiexec -np 1 ./post
```



https://cylc.github.io/cylc/