

SoftWare InFrastructure and Technology for High Energy Physics

SWIFT-HEP WP5 Analysis Systems WP1 Data Management

Sam Eriksen & Timothy Noble

12th November 2024



Overview

- WP5 (Analysis Systems)
 - overview + roadmap
 - Current progress in WP5
 - Future for WP5

WP1 (Data + workflow management)

- overview
- Current progress in WP1
- Future for WP1

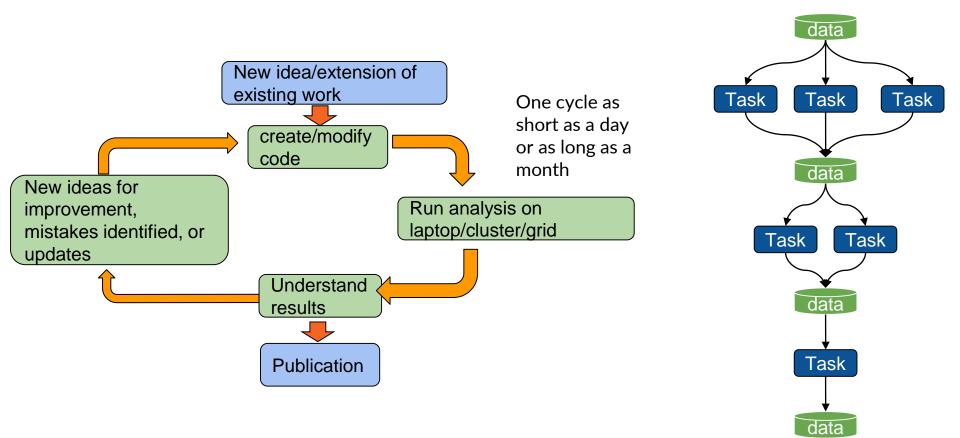
Previous updates

- March 2024
- November 2023
- September 2023
- <u>May 2023</u>
- March 2023
- February 2023

WP5: Analysis Systems

WP5: Analysis Systems Run analysis workloads optimally on distributed resources

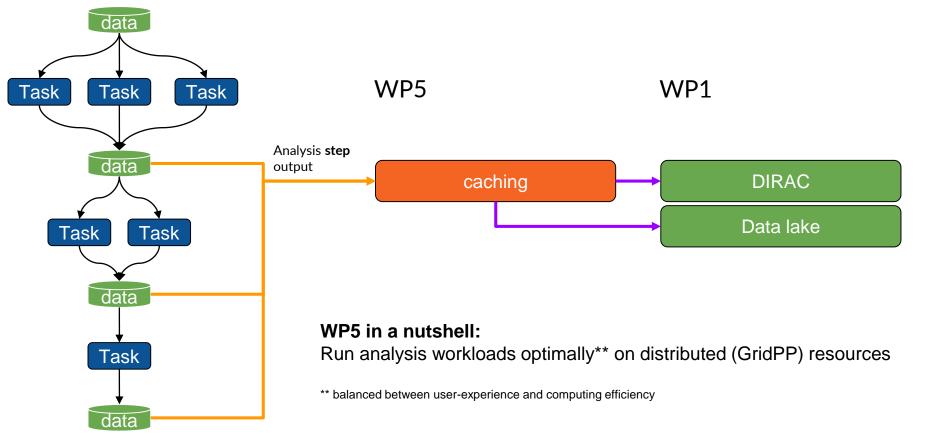




See talk by Luke Kreczko for some BIG Picture

Analysis Anatomy

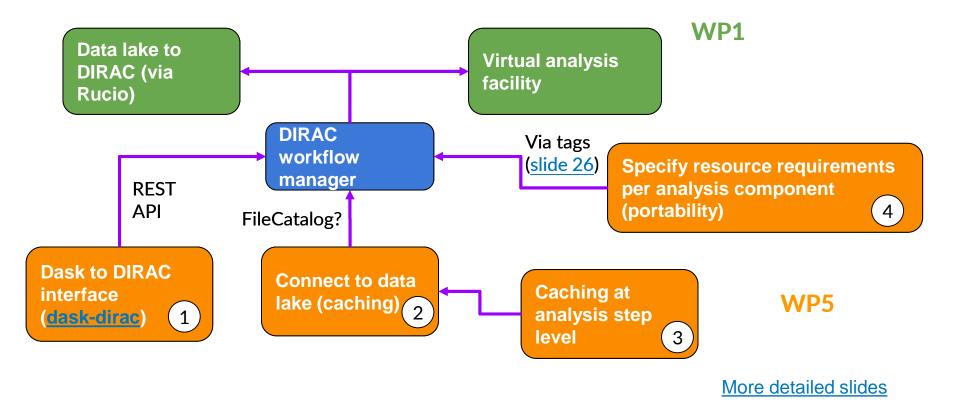




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WP5: Roadmap



Dask to DIRAC interface (dask-dirac)

- 2 Connect to data lake (caching)
 - Caching at analysis step level

3

4

- Add extension to dask
- Dask is able to parallelize any python code

• Add the ability to save output after dask instance has closed

- Avoid having to re-run analysis steps
- Persistent caching

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Specify resource requirements per analysis component (portability)

• E.g. Let some stages run on GPUs

See talk by Luke Kreczko for some future planning

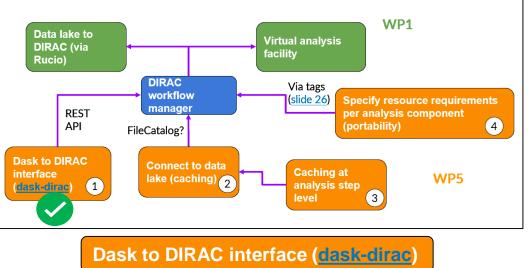
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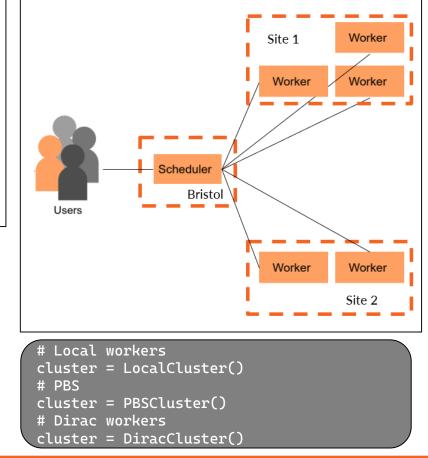
Where did we leave things at the last workshop

Where we left things last time

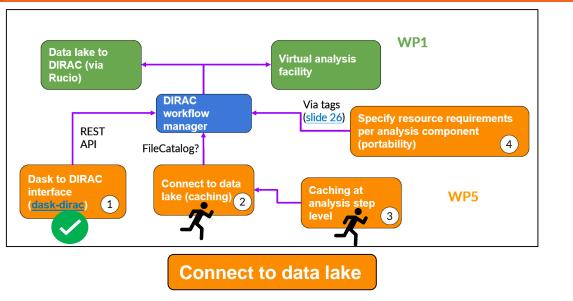




- Reliable dask-DIRAC interface
- Multi-site submission / fine control possible on distribution of workers
- Integrated with CMS AGC



Where we left things last time



- Interact with diracdev StorageElement via HTTP + x509
- gfal underneath
- Painful and wanted to move away from
- RUCIO via tokens was ideal

Caching at analysis step level

- Began looking at intermediate result caching using scheduler plugins
- Allows for tasks to be run when a worker connects/disconnects or transitions (e.g. from running to memory) a job
- Idea: perform check (ideally via RUCIO) if result exists before a task starts

What's happened since the last workshop



Connect to data lake

- Wanted to communicate with RUCIO via REST-API with tokens
 - Able to interact with RUCIO, but only with x509
 - Tokens generated from the OIDC-Agent and Rucio at least with the IRIS-IAM varied, to the point where Rucio would not accept the OIDC-Agent tokens. Investigation underway in association with James Walder from SKAO (Full token stack Rucio instance)
 - Token Authentication in Rucio is being redesigned by a token auth SIG
- We've parked progress on this until Tim has investigated further



Caching at analysis step level

Initial idea; dask plugins

Scheduler Plugins

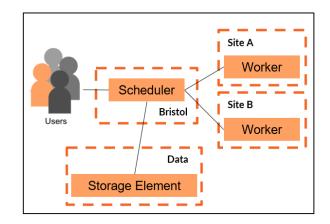
- Allows you to run custom Python code on scheduler when certain things happen
- Example;
 - Scheduler checks if output exists; if exists, load and don't run job, else, run job as normal
 - Workers send all data back to Scheduler which then perform 'saves'
 - Essentially intercepts result before it's passed to the user

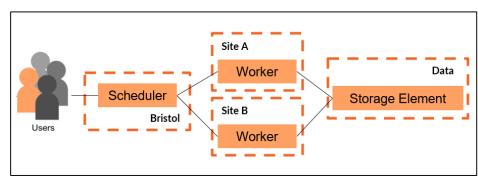
Worker Plugin

- Allows you to run custom Python code on all workers at certain event in the worker's lifecycle (such as when a process finishes)
- Example;
 - Workers check if output exists; if exists, load and don't run job, else run job as normal
 - In this case, workers interact with storage

Note

- Dask already does caching which does similar to the above, but we want persistency between dask sessions
- There's also the option for scheduler and worker plugins together





Caching at analysis step level

Initial idea; dask plugins

Worker Plugin - where did we get to

- Created examples to explore what information we can get from the worker at each stage
- Created worker plugin to show what in the worker directory

Problem

- This is only done when the worker is killed (or the plugin removed)
- Limited by access to analysis step information / would require interrupting the processes
- Very difficult to alter task graph on the fly

```
from distributed.diagnostics.plugin import WorkerPlugin
from distributed.diagnostics.plugin import forward_stream
import contextlib
import os
```

```
class ForwardOutput(WorkerPlugin):
```

| <pre>tabnine: test explain document ask def setup(self, worker): selfexit_stack = contextlib.ExitStack() selfexit_stack.enter_context(forward_stream("stdout", wor selfexit_stack.enter_context(forward_stream("stderr", wor selfexit_stack.enter_context(forward_stream("stderr"), wor self</pre> | |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|
| <pre>tabnine: test explain document ask def teardown(self, worker): print("{}: {} ".format(os.getcwd(), os.listdir(os.getcwd())</pre> |))) |

```
self._exit_stack.close()
```

| <pre>plugin = ForwardOutput()</pre> |
|------------------------------------------------------------|
| |
| |
| client.register_plugin(plugin, name='my-plugin') |
| √ 0.0s |
| <pre>'tcp://130.246.45.124:50000': {'status': 'OK'}}</pre> |





Caching at analysis step level

Initial idea; dask plugins

Scheduler Plugin - where did we get to

- Created examples to explore what information we can get from the scheduler at each stage
- Created example to check if a task (via hash) had already been run (in backup)

Workflow would be;

- Some kind of combination of scheduler and worker plugin
- Access task hash, check if it exists, and then replace with loading or saving data

```
class MyPlugin(SchedulerPlugin):
    def __init__(self):
        self.task_counter = 0
    def transition(self, key, start, finish, *args, **kwargs):
        if start == 'processing' and finish == 'memory':
            self.task_counter += 1
    def get_task_count(self):
        return self.task_counter
```

```
Executed at 2024.03.11 08:55:44 in 3n
```

| | i in range(10): x = client.submit(lambda x: x + 1, i) result = x.result() print(i, plugin.task_counter) |
|-------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------|
| | |
| 0 1 1 1 3 1 4 2 5 2 6 2 7 2 8 2 9 2 | 7 8 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 |



Caching at analysis step level

Initial idea; dask plugins

Problems with this approach

- Very hard to manipulate task graphs in this approach; hashes associated with tasks are only semi-deterministic -> change between dask sessions for the same code
- Very difficult to access individual steps in a task graph. Very coarse; approach was more limited to final task.

deterministic hash test

outputs = client.map(neg, [1,2,3])

′ 0.0s

Current time: 20:02:44 Tasks submitted: ['neg-cb23b95d4d96dbbf89cd1d672843469a

outputs = client.map(neg, [1,2,3])

Current time: 20:04:50 Tasks submitted: ['neg-3c404328af689f5d903f5dda07c47bd2'

Solution

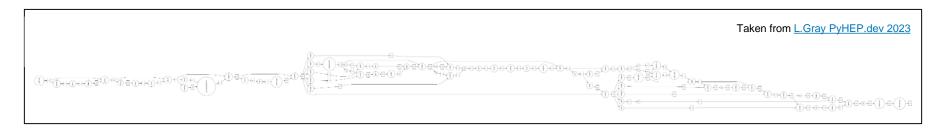
• Work on calculating hash that is independent of scheduler state and without plugins



Caching at analysis step level

Ways to interact with dask submission

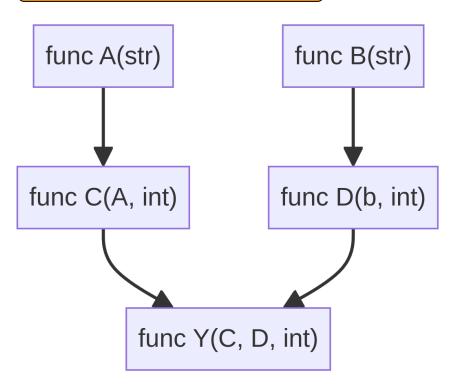
- client.get
- client.map (this is what CMS AGC uses)
- client.submit
- client.compute
- Find a common area where we can intercept the task graph and manipulate it
- Found <u>graph_to_futures</u>* where we have access to the full graph



*Actually, started with collections to dsk which only works with client.compute and developed a lot of this there before changing to _graph_to_futures



Caching at analysis step level

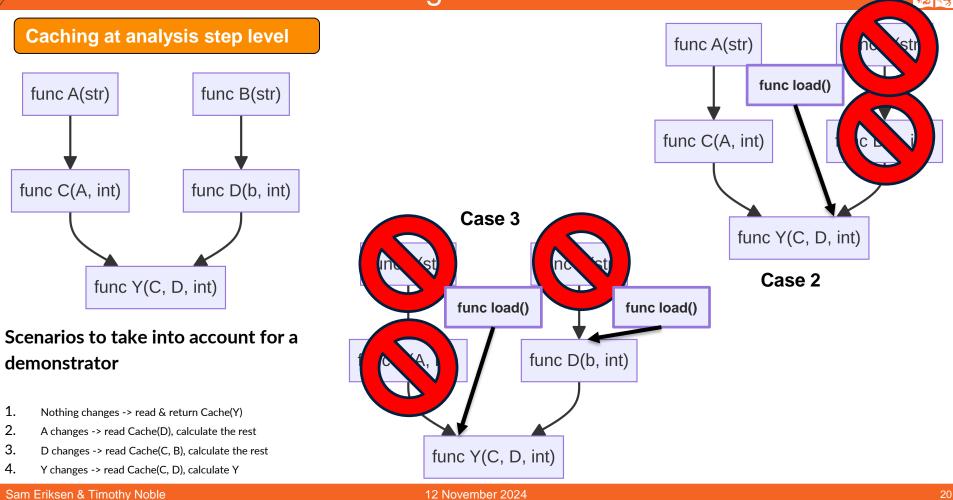


Scenarios to take into account for a demonstrator

- 1. Nothing changes -> read & return Cache(Y)
- 2. A changes -> read Cache(D), calculate the rest
- **3.** D changes -> read Cache(C, B), calculate the rest
- 4. Y changes -> read Cache(C, D), calculate Y

Requires

- 1. Probing task graph to work out output / input
- 2. Checking storage area for if it exists
- 3. Insert loading / saving stages into graph





Caching at analysis step level

Development State

 We've created a new dask client (<u>DiracClient</u>) which adds persistent caching functionality

```
For task in Tasks:
hash = calculate_task_hash(task)
hash_found = check_storage(hash)
if hash_found:
      task = load_from_storage(hash)
else:
      task = task + write_to_storage(hash)
```

Additional functionality in the works/what needs more thought;

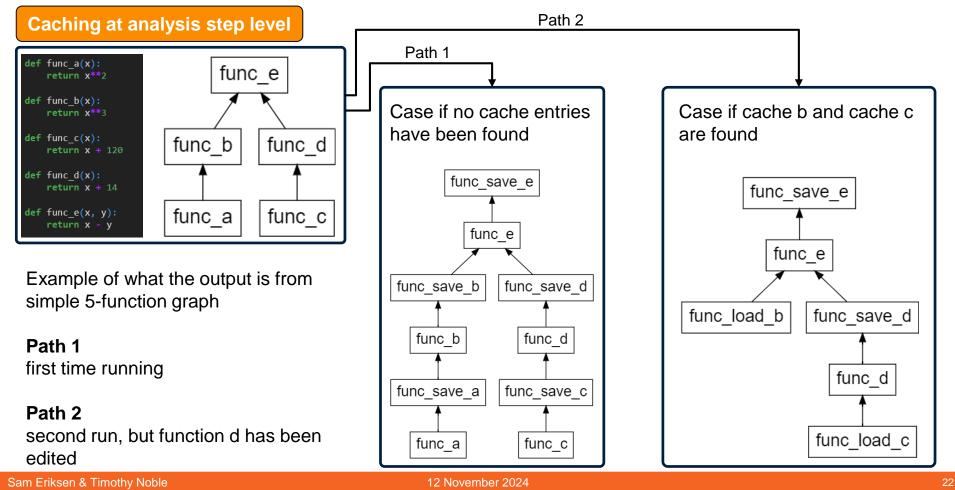
- Changeable location of Persistent Cache; want RUCIO and local options at the very least
- More work is needed to be compatible with CMS ACG; should wait for coffea-2024
- Default is to cache everything, good option to have but likely no ideal

```
class DiracClient(Client):
    """Client for caching dask computations"""
    def _graph_to_futures(
        self,
        dsk: dict[str, Any] | HighLevelGraph,
        *args: dict[str, Any],
        **kwargs: dict[str, Any],
        ***kwargs: dict[str, Any],
        / -> Any:
        if not isinstance(dsk, HighLevelGraph):
            dsk = HighLevelGraph.from_collections(id(dsk), dsk, dependencies={})
        info = dsk.to_dict()
        logging.debug(
            "Input dask graph:\n%s\n------\nperforming caching checks\n------"
            info,
        )
```

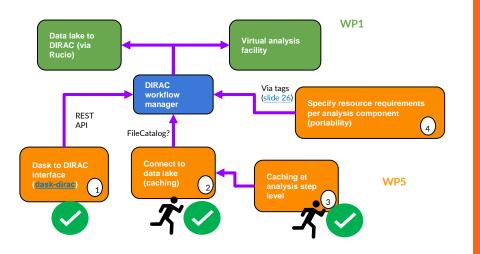
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Summary and plan going forward



We have a dask-dirac interface

- Workers are split across sites
- Effectively splits up work across these sites
- We have been looking at task graph manipulation
 - Found entry point giving fine-grain access to a graph
 - Implemented caching that persists between dask sessions
 - Avoid rerunning tasks where result exists
- Where are we going
 - Awaiting tokens
 - Awaiting ACG update -> coffea.2024

WP1: Data Management

WP1: Data Management Optimise the heterogeneous storage infrastructure across the UK

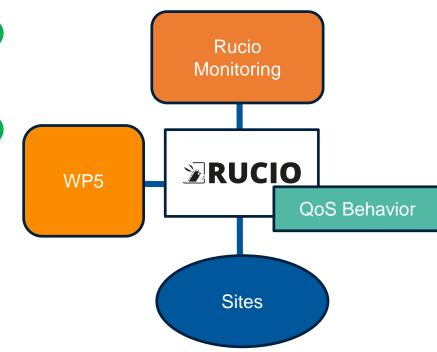
WP1: Data Management Overview



- Deploy a UK based prototype data lake
 - O Core sites
 - O S3 sites
 - O State-less storage
- Generate metrics for comparison of current to improvements made
- Implement Quality of Service behaviour and information

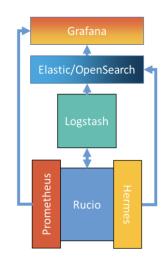
in Rucio

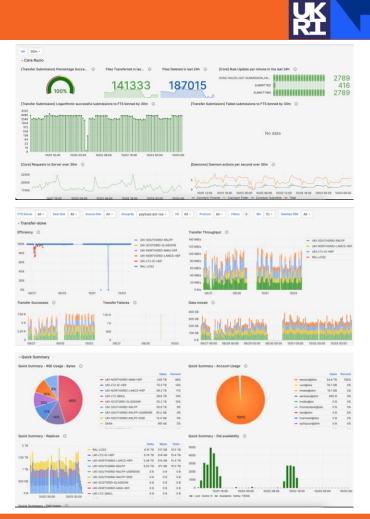
- O Develop Rucio to expand the levels of service it provides
- Create new behaviours in Rucio to enable improved data access
- Produce site recommendations on how to optimise data access and stateless storage
- Setup and test SSD storage endpoints to test and develop fast storage endpoints



Data Management developments

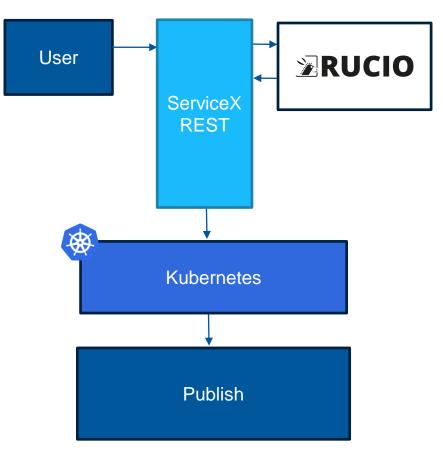
- Tim has redesigned and expanded upon <u>previously shown</u> <u>monitoring solution</u> to be production-ready (Deployed for astronomy experiment LSST), deployed with OpenSearch.
 - made these tools available to other communities by contributing deployment back to Rucio repositories (<u>Rucio workshop talk</u>)
- Takes 3 different data streams from Rucio, to be visualised in Grafana.
- Minimal design to ensure easy to maintain and deploy
- Allows for quantification of future developments





Data Management development plans

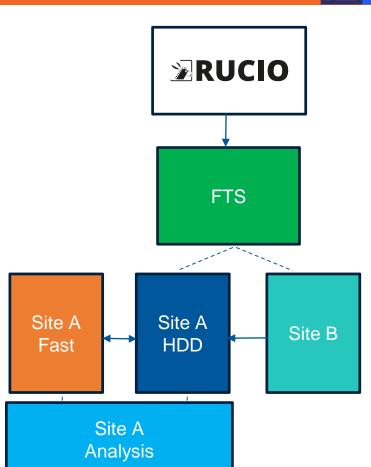
- Investigation of <u>ServiceX</u> (or other tools to optimise data access for analysis)
 - Developed by IRIS-HEP
 - Software that sits between the Storage and Analysis Facility (close to storage), and extracts a subset of data columns from whole files – rather than moving the whole file
 - Reduces the networking needs from storage to analysis
 - User requests a subset of data from file(s)
 - ServiceX queries Rucio for files
 - Job started in Kubernetes cluster to extract needed files and create a new one



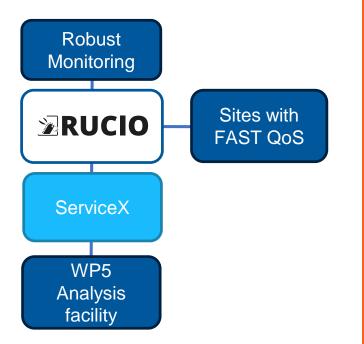
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Oata Management development plans

- Fast Storage
 - Sites provision Storage by Capacity, but not throughput or access rates
 - Issues will arise with larger data files and increased required data rates where storage endpoints provision more storage, but throughput does not scale at the same rate
 - Further coordination with Core Rucio team to develop Quality of Service to better serve Fast storage
 - Using file popularity to move data between Fast and Disk storage endpoints to ensure read/write needed for analysis



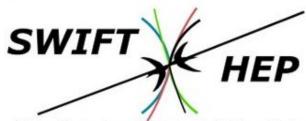
Data management summary and future plan



- Deployed Robust monitoring at RAL for SWIFT-HEP and at Stanford for LSST (improvements to one feed into the other)
- Approaching data management from Software and Hardware utilisation
- Further integrations with the Analysis facility to enable better data access
- Will develop Rucio to investigate the prioritization of fast storage as more fast storage pools are available in the UK now
- Will work with CERN liaisons to test deployment ServiceX at RAL to test data access improvements



Questions?



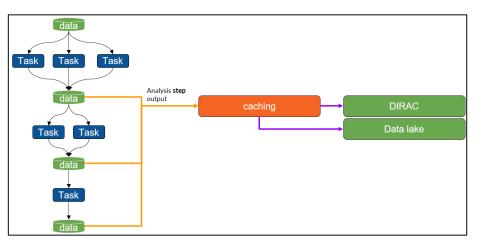
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Caching at analysis step level



What do we want to demonstrate

- Imagine a complex task that you want to run.
- If you know you are going to have to run this multiple times, but are only modifying one of the functions, you can think of a few ways to reduce the reprocessing;
- Most obvious would be to break up the graph and submit each task separately and save the outputs, and if you are rerunning, load the bits you haven't changed.
- We want that to automatically happen when you submit something.

Modifying a task graph: Practical example

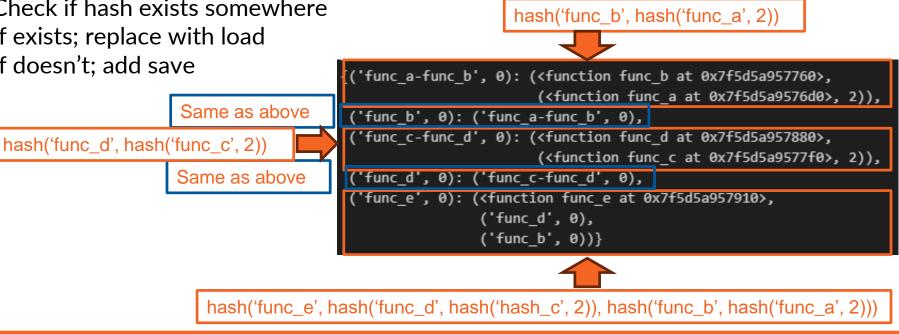


Caching at analysis step level

This is what we have to play with;

Task is:

- Calculate hash
- Check if hash exists somewhere
- If exists; replace with load
- If doesn't: add save



K Modifying a task graph: Practical Example

Caching at analysis step level

def func_a(x):
 return x**2

def func_b(x):
 return x**3

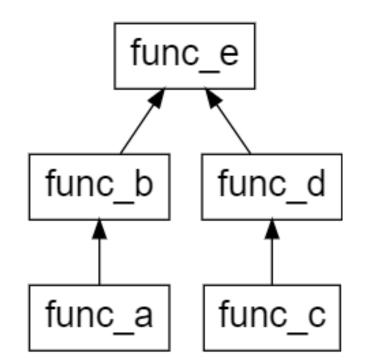
def func_c(x):
 return x + 120

def func_d(x):
 return x + 14

def func_e(x, y):
 return x - y

```
param_a = pd.DataFrame(np.array([2]))
param b = pd.DataFrame(np.array([2]))
layers = {
        ("func a", 0): (func a, param a),
    "func b": {
        ("func b", 0): (func b, ("func a", 0)),
        ("func_c", 0): (func_c, param_b),
        ("func_d", 0): (func_d, ("func_c", 0)),
        ("func_e", 0): (func_e, ("func_d", 0), ("func_b", 0)),
dependencies = {
    "func b": {"func a"},
    "func c": set(),
    "func e": {"func b", "func d"},
```

hlg = HighLevelGraph(layers, dependencies)



K Practical Example

Caching at analysis step level

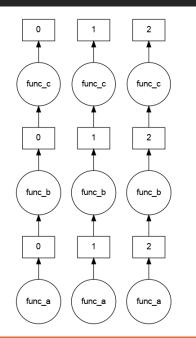
| {(ˈfunc_a-func_bˈ, 0): (<function 0x7f99bb6d3be0="" at="" func_save="">,</function> |
|-----------------------------------------------------------------------------------------------------|
| ************************************ |
| (<function 0x7f99bb6d3880="" at="" func_b="">,</function> |
| <pre>(<function 0x7f99bb6d3be0="" at="" func_save="">,</function></pre> |
| '0776ff206989787bf5a95a35b33716b797efcded6bf71a9e75c1897c5a7ea9ca4f9fb654fe3eba1ebcec7d7911b2dd16', |
| (<function 0x7f99bb6d37f0="" at="" func_a="">, array([2])))),</function> |
| ('func_b', 0): ('func_a-func_b', 0), |
| ('func_c-func_d', 0): (<function 0x7f99bb6d3be0="" at="" func_save="">,</function> |
| '4c082d6b9b9b918689b81a761abbaae92041057140553ca83e03c4665445a3e78b460e9f0eb8b205e0ef8cb4dd5567f7', |
| (<function 0x7f99bb6d3a30="" at="" func_d="">,</function> |
| <pre>(<function 0x7f99bb6d3be0="" at="" func_save="">,</function></pre> |
| 'f12ce0d8cd6105959827f329b79f2baca8767a4b436cdd843cf008ca50b0ae7754317a320740ecc96d739668308c9d2e', |
| (<function 0x7f99bb6d39a0="" at="" c="" func="">, array([2]))))),</function> |
| ('func d', 0): ('func c-func d', 0), |
| ('func e', 0): (<function 0x7f99bb6d3be0="" at="" func="" save="">,</function> |
| '4baeda9eda3c05b98d14b603cea2833cc5b4a3bf1e30cfca90dcaf4f24c9079ea33349840fb93b07c3585cf685dfb2d9', |
| (<function 0x7f99bb6d3ac0="" at="" e="" func="">,</function> |
| ('func d', 0), |
| ('func b', 0)))} |
| |

11 August 2022

* Practical Example

Caching at analysis step level

Create a Dask Array from the HighLevelGraph
array = Array(hlg, "func_c", shape=(3,), dtype=list, chunks=(1,))



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| {('func_a-func_b-func_c', 0): (<function 0x7efdccb7f6d0="" at="" func_c="">,</function> | |
|------------------------------------------------------------------------------------------|----|
| <pre>(<function 0x7efdccb7f640="" at="" func_b="">,</function></pre> | |
| <pre>(<function 0x7efdccb7f5b0="" at="" func_a="">, 2))</function></pre> |), |
| ('func_a-func_b-func_c', 1): (<function 0x7efdccb7f6d0="" at="" func_c="">,</function> | |
| <pre>(<function 0x7efdccb7f640="" at="" func_b="">,</function></pre> | |
| <pre>(<function 0x7efdccb7f5b0="" at="" func_a="">, 3))</function></pre> |), |
| ('func_a-func_b-func_c', 2): (<function 0x7efdccb7f6d0="" at="" func_c="">,</function> | |
| <pre>(<function 0x7efdccb7f640="" at="" func_b="">,</function></pre> | |
| <pre>(<function 0x7efdccb7f5b0="" at="" func_a="">, 4))</function></pre> |), |
| ('func_c', 0): ('func_a-func_b-func_c', 0), | |
| ('func_c', 1): ('func_a-func_b-func_c', 1), | |
| ('func_c', 2): ('func_a-func_b-func_c', 2)} | |

× Practical Example

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Caching at analysis step level

| ('func_a-func_b-func_c', 0): (<function 0x7efdccb7f6d0="" at="" func_c="">, (<function 0x7efdccb7f640="" at="" func_b="">, (<function 0x7efdccb7f5b0="" at="" func_a="">, 2))), ('func_a-func_b-func_c', 1): (<function 0x7efdccb7f6d0="" at="" func_c="">, (<function 0x7efdccb7f640="" at="" func_b="">,</function></function></function></function></function> | |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| (<function 0x7efdccb7f5b0="" at="" func_a="">, 3))),</function> | |
| ('func_a-func_b-func_c', 2): (<function 0x7efdccb7f6d0="" at="" func_c="">,</function> | |
| (<function 0x7efdccb7f640="" at="" func_b="">,</function> | |
| (<function 0x7efdccb7f5b0="" at="" func_a="">, 4))),</function> | |
| ('func_c', 0): ('func_a-func_b-func_c', 0), | |
| <pre>('func_c', 1): ('func_a-func_b-func_c', 1), ('func_c', 2): ('func_a-func_b-func_c', 2)} {('func_c', 2): ('func_a-func_b-func_c', 2)}</pre> ('func_a-func_b-func_c', 2) | |
| (<function 0x7fd85844cd30="" at="" func_b="">,</function> | |
| (<function 0x7fd858075870="" at="" func_a="">, 2)))</function> |), |
| <pre>('func_a-func_b-func_c', 1): (<function 0x7fd85844cdc0="" at="" func_c="">,</function></pre> | |
| (<function 0x7fd85844cd30="" at="" func_b="">.</function> | |
| (<function 0x7fd85844c9d0="" at="" func_a2="">,))),</function> | |
| <pre>('func_a-func_b-func_c', 2): (<function 0x7fd85844cdc0="" at="" func_c="">,</function></pre> | Γ. |
| (<function 0x7fd85844cd30="" at="" func_b="">,</function> | |
| (<function 0x7fd858075870="" at="" func_a="">, 4)))</function> |), |
| ('func_c', 0): ('func_a-func_b-func_c', 0), | |
| <pre>('func_c', 1): ('func_a-func_b-func_c', 1),</pre> | |
| <pre>('func_c', 2): ('func_a-func_b-func_c', 2)}</pre> | |
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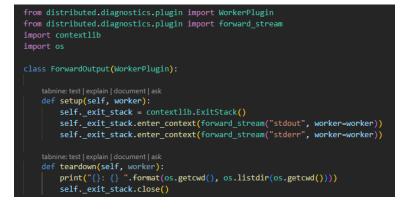
Worker Plugin example



Caching at analysis step level

Description

 When worker is shutdown/killed or the plugin is disconnected, the directory path and contents are displayed



| <pre>plugin = ForwardOutput()</pre> | |
|----------------------------------------------------------|---|
| √ 0.0s | |
| | |
| | |
| client.register_plugin(plugin, name='my-plugin') | |
| √ 0.0s | |
| | |
| {' <u>tcp://130.246.45.124:50000</u> ': {'status': 'OK'} | } |

Worker Plugin example

Caching at analysis step level

Description

 When worker is transitioning between states, the state is printed and the number of transitions are counted

| class ny | Program | workerp | cogin): |
|----------|---------|---------|----------|
| def | | _(self, | logger): |

```
self.worker = None
self.logger = logger
self.n_transitions = 0
```

```
def setup(self, worker):
    self.worker = worker
```

| state: | executing n_transitions: 223 |
|--------|------------------------------|
| state: | memory n_transitions: 224 |
| state: | released n_transitions: 225 |
| state: | forgotten n_transitions: 226 |
| state: | waiting n_transitions: 227 |
| state: | ready n_transitions: 228 |
| state: | executing n_transitions: 229 |
| state: | released n_transitions: 230 |
| state: | forgotten n_transitions: 231 |
| state: | memory n_transitions: 232 |
| state: | waiting n_transitions: 233 |

Scheduler Plugin example



Caching at analysis step level

Description

 Remove a task from the graph if it has already been executed

lass MySchedulerPlugin(SchedulerPlugin):

global previous_executed_tasks

tabnine: test | explain | document | ask

```
tasks_to_execute = []
```

```
for task in tasks:
    if task in previous_executed_tasks:
        print(f"Task {task} has already been executed - removing from task list")
        else:
            tasks to execute.append(task)
```

```
previous_executed_tasks.append(task)
```

tasks = tasks_to_execute
keys = set(tasks)

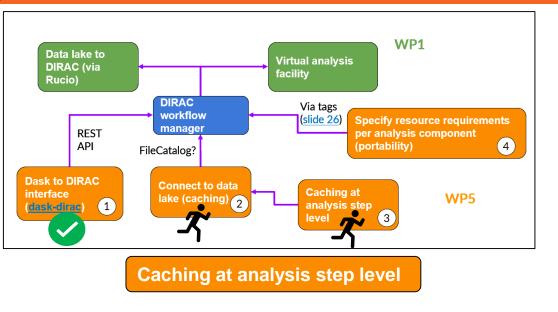
print(f"Tasks to be executed: {tasks_to_execute}")
print(f'keys: {keys}')

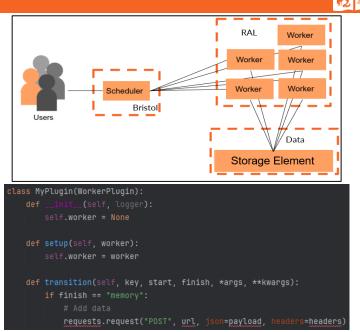
```
# Update the scheduler's tasks and keys
```

scheduler.tasks = {key: scheduler.tasks[key] for key in keys}
scheduler.unrunnable = {key: scheduler.unrunnable[key] for key in keys if key in scheduler.unrunnable}
print(f"scheduler tasks: {scheduler.tasks}")
print(f"scheduler unrunnable: {scheduler.unrunnable}")

tabnine:test|explain|document|ask
def transition(self, key, start, finish, *args, **kwargs):
 print("------")
 print(f'Task {key} is transitioning from {start} to {finish}")

Where we left things last time





- Began looking at intermediate result caching using scheduler plugins
- Allows for tasks to be run when a worker connects/disconnects or transitions (e.g. from running to memory) a job
- Idea: perform check (ideally via RUCIO) if result exists before a task starts