Dask External Tasks

for HPC/ML In Transit Workflows

Amal Gueroudji
Julien Bigot
Bruno Raffin
Robert Ross

HP-C/DA Workflows

Machine Learning is everywhere now!

- Data analytics more and more equates to ML-based HPDA
- Streaming & task-based tools, often in Python, such as Dask

Numerical simulation is not dead!

- We still need to produce the data
- Fortran is dying? Long live C++ & MPI (+X?) for parallel processing

Two worlds, two languages, two sets of tools that **need coupling!**

Dask distributed?

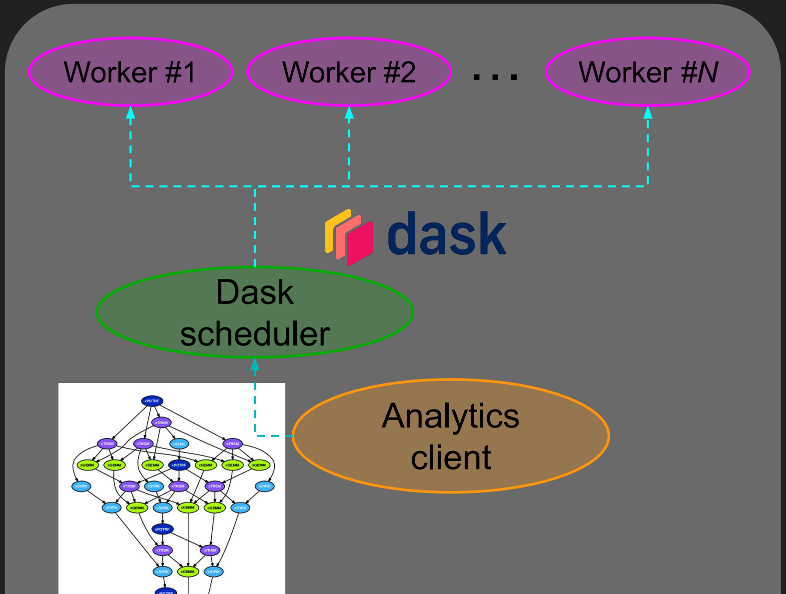
A Python distributed runtime

Scheduler/workers (+client) model to run work (each on its own process/node)

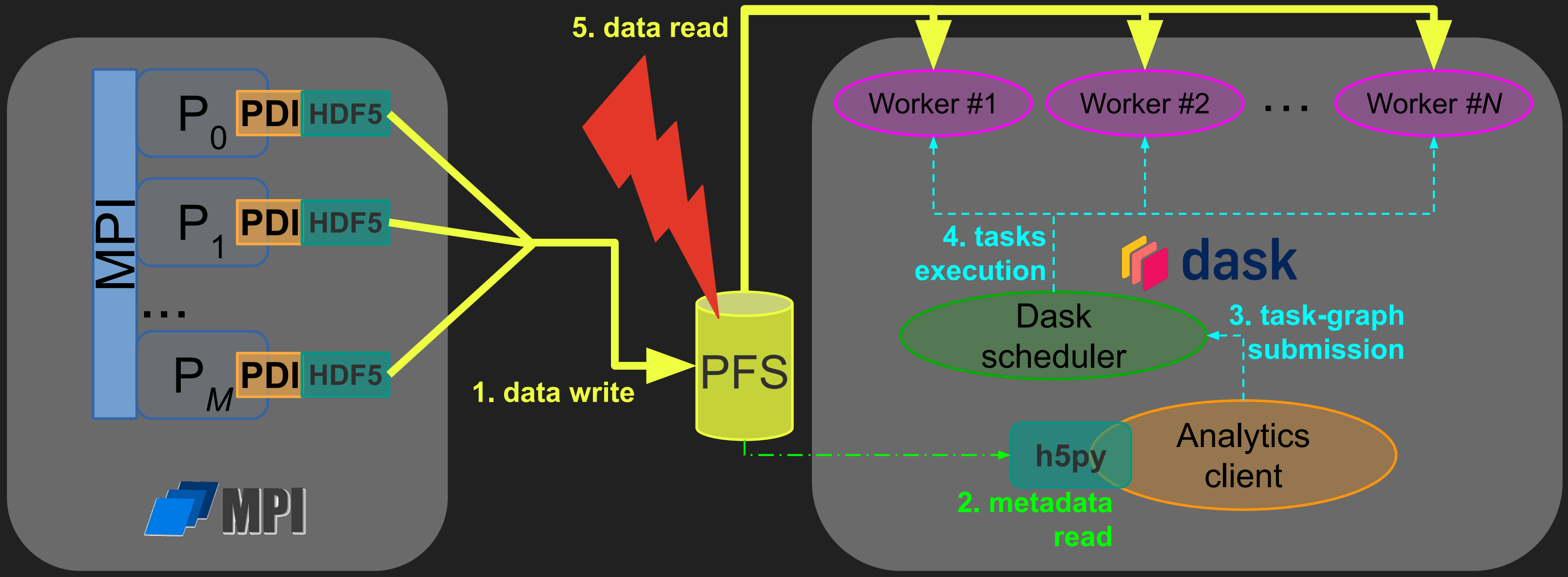
A task-based model to describe work

Many APIs ported on top of dask

- Numpy => distributed Arrays
- SciPy
- Scikit-learn
- Pandas => distributed Dataframes
- ...

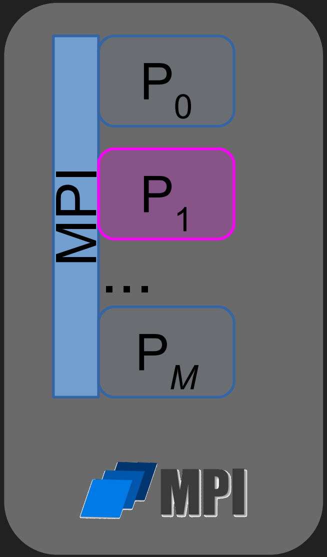


Dask for post hoc analytics



File-system IO performance is an issue

In situ analytics



Simulation…disk…analytics legacy workflow

- Hit the disk **performance bottleneck**!

Solution: in situ analytics use the network instead

- Run simulation & analytics concurrently
- Often dedicate some MPI ranks for analytics
  - MPI Communicator system is perfect for that
  - Eg: one per node
  - Or in transit with dedicated nodes

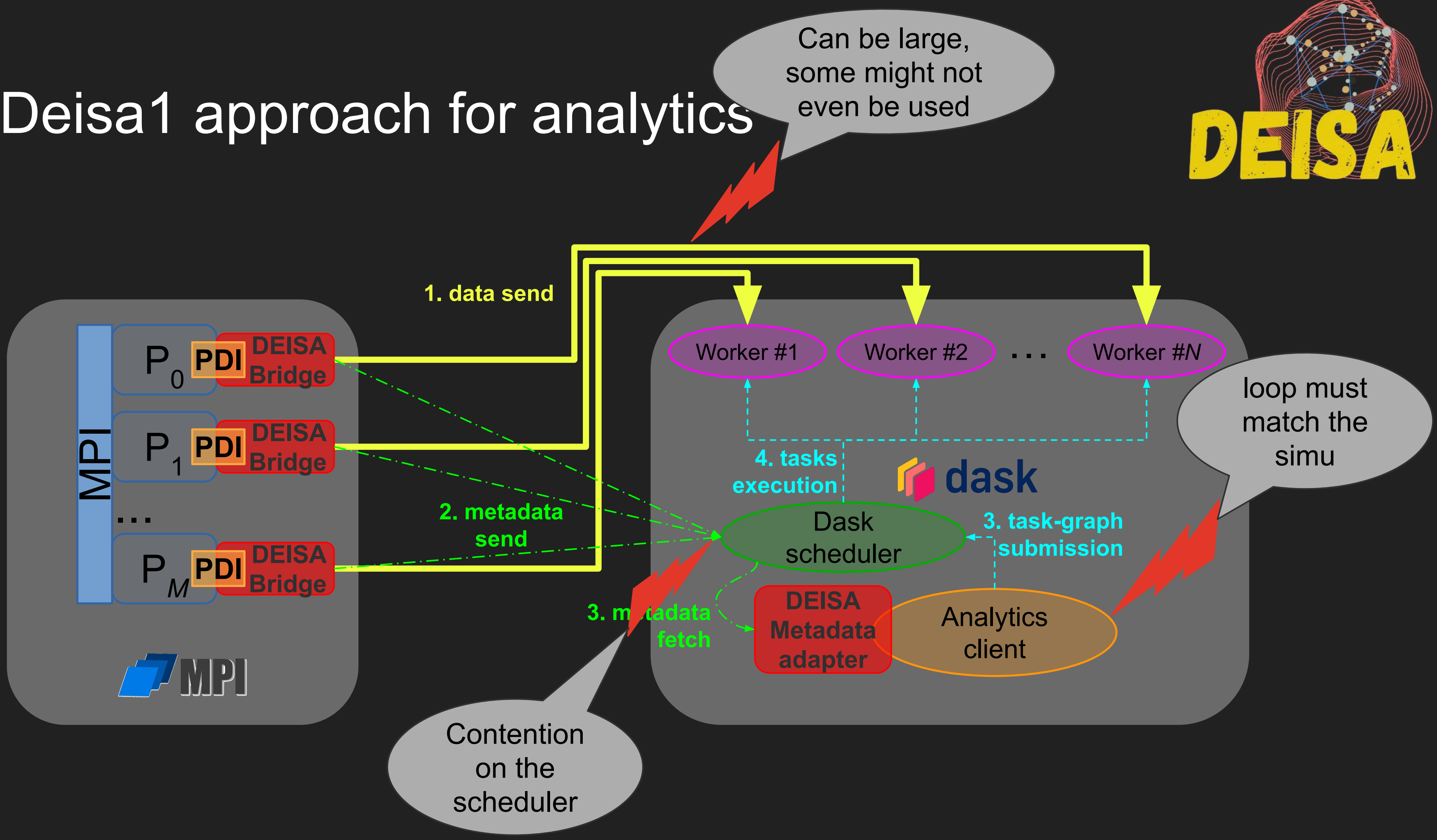
But… MPI is not well suited for HPDA

Can we do better? => **Deisa!**

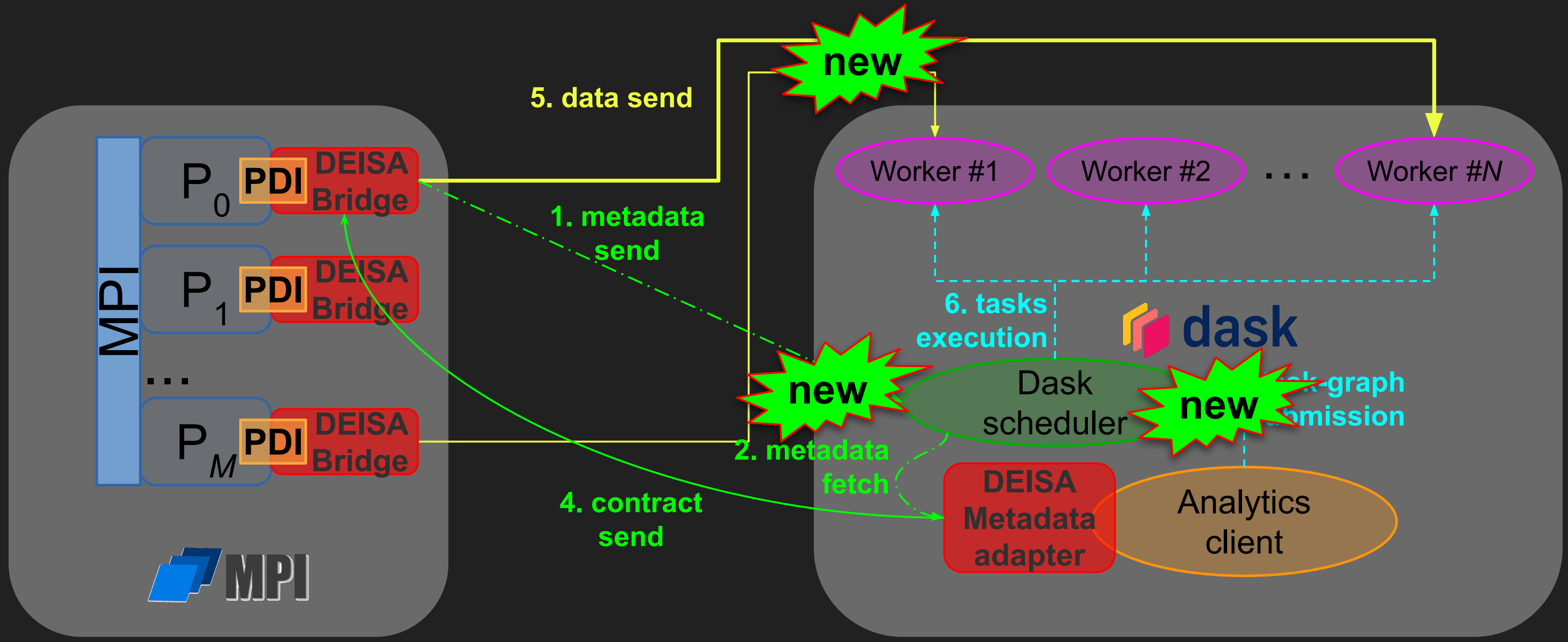
DEISA

A. Gueroudji, J. Bigot and B. Raffin, "DEISA: Dask-Enabled In Situ Analytics," *2021 IEEE 28th International Conference on High Performance Computing, Data, and Analytics (HiPC)*, Bengaluru, India, 2021, pp. 11-20

The Deisa1 approach for analytics



Introducing now: Deisa3 with External tasks



What is an external task

- Represents data that will be produced later
  - By an external tool that is not under Dask scheduler control
- Introduce a new state in tasks state machine: *external*
- Support a new client call & scheduler RPC to create external tasks
  - The user chooses a UID (key)
  - Adding new parameters to Dask `Future.__init__` with default value for compatibility
  - Sets the task state to *external*
- Support a new client call & worker RPC to provide external tasks data
  - The user lists UIDs & provide data values
  - Adding new parameters to Dask `scatter`
  - Transition the task state from *external* to *memory*

Evaluation

Irene supercomputer skylake partition @ CEA TGCC, France

- 1,653 nodes, each 2 Intel Skylake CPUs × 24-cores @ 2.7 GHz, 180 GB memory
- 100Gb/s EDR Pruned fat tree InfiniBand network
- Lustre parallel file system (300GB/s)

Simple 2D Heat PDE solver mini-app

Principal Component Analysis based data analytics (Imported from a production code requirement)

- Unsupervised tool to reduce dimensionality
- Available in Scikit-learn & Dask-ML (based on SVD)

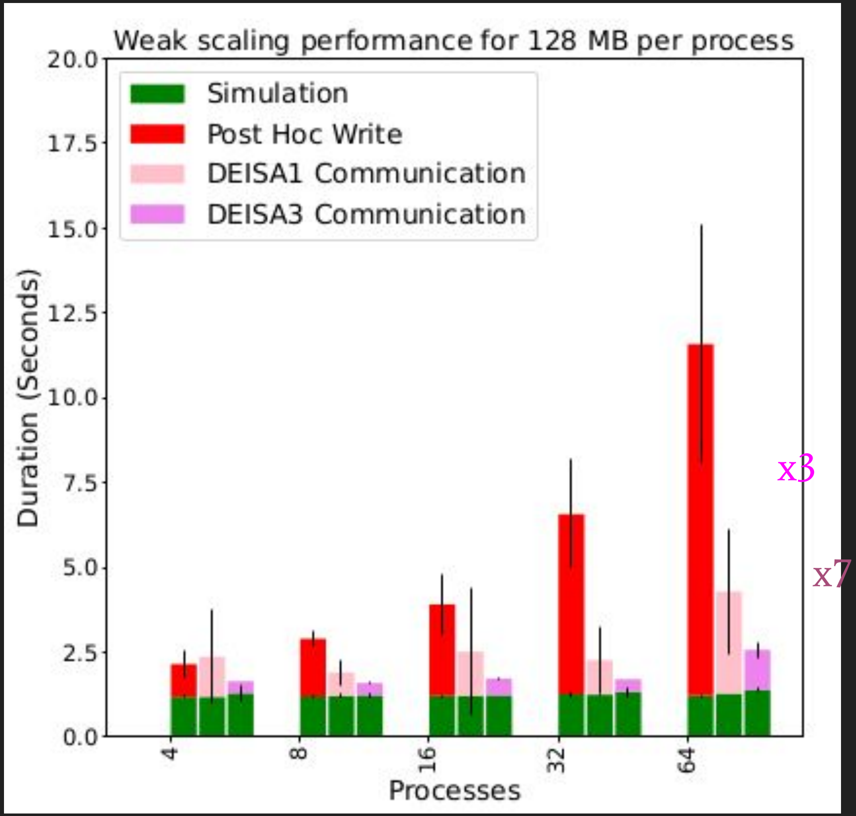
Incremental PCA

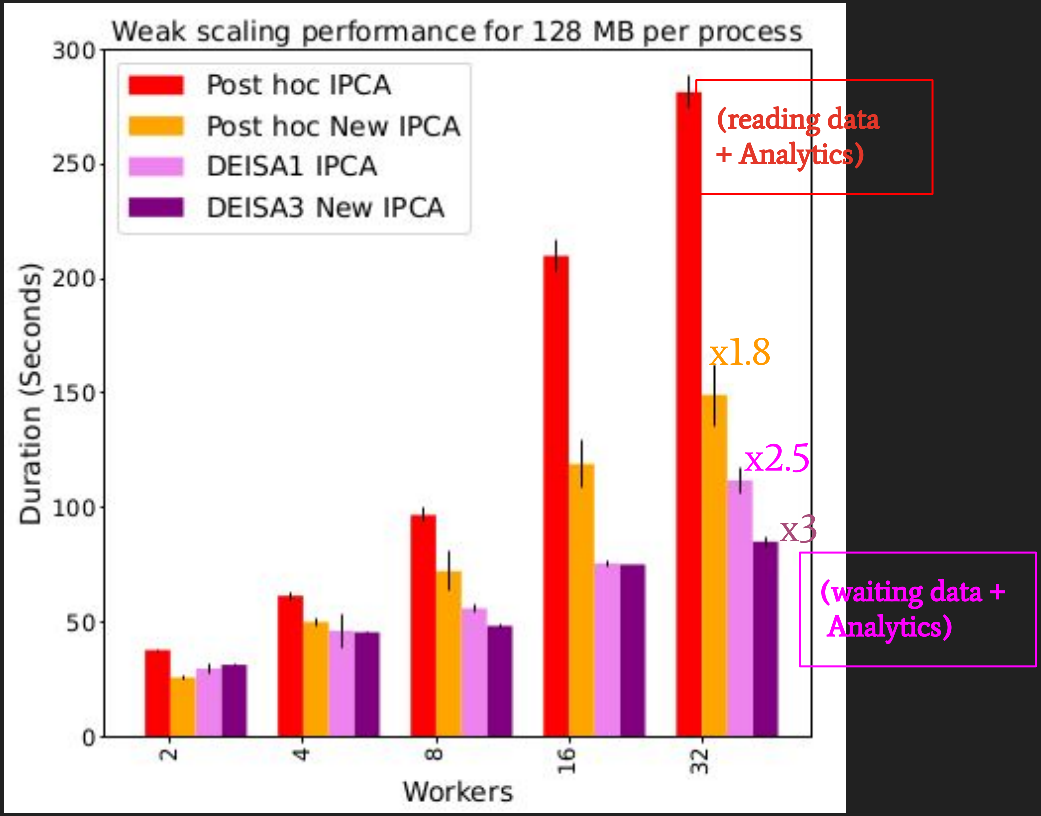
PCA needs all data in memory, single task

- Incremental PCA works on data minibatches
  - constant memory complexity
  - multiple tasks
- Dask-ML offers an IPCA
  - different API than PCA
- Implemented a new version of IPCA
  - API compatible with Dask-ML PCA

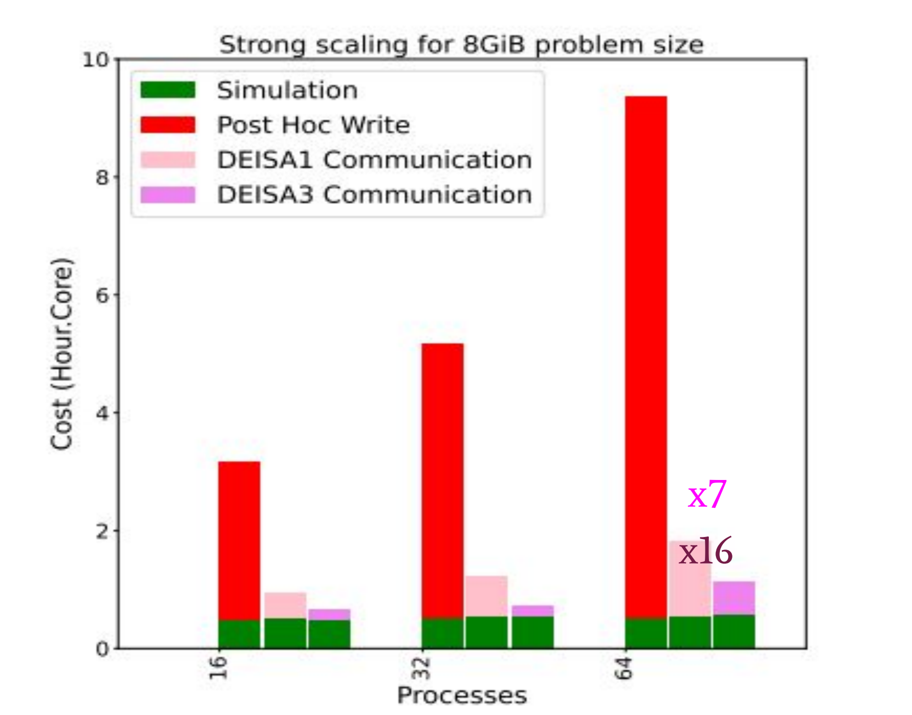
```python
from dask_ml.decomposition import InSituIncrementalPCA
from dask_interface import Deisa
# Initialize the Deisa
Deisa = Deisa(scheduler_info, config_file)
client = Deisa.get_client()
# Get data descriptor as a list of Deisa arrays object
arrays = Deisa.get_deisa_arrays()
# Filter data
gt = arrays["global_t"][...]
arrays.validate_contract()
ipca=InSituIncrementalPCA(n_components=2,copy=False,
        svd_solver='randomized')
ipca = ipca.fit(gt, ["t", "X", "Y"], ["X"], ["Y"])
# Submit the task graph to the scheduler
explained_variance ,singular_values  = client.persist([
        pca.explained_variance_ , pca.singular_values_])

# ...
```

Weak Scalability

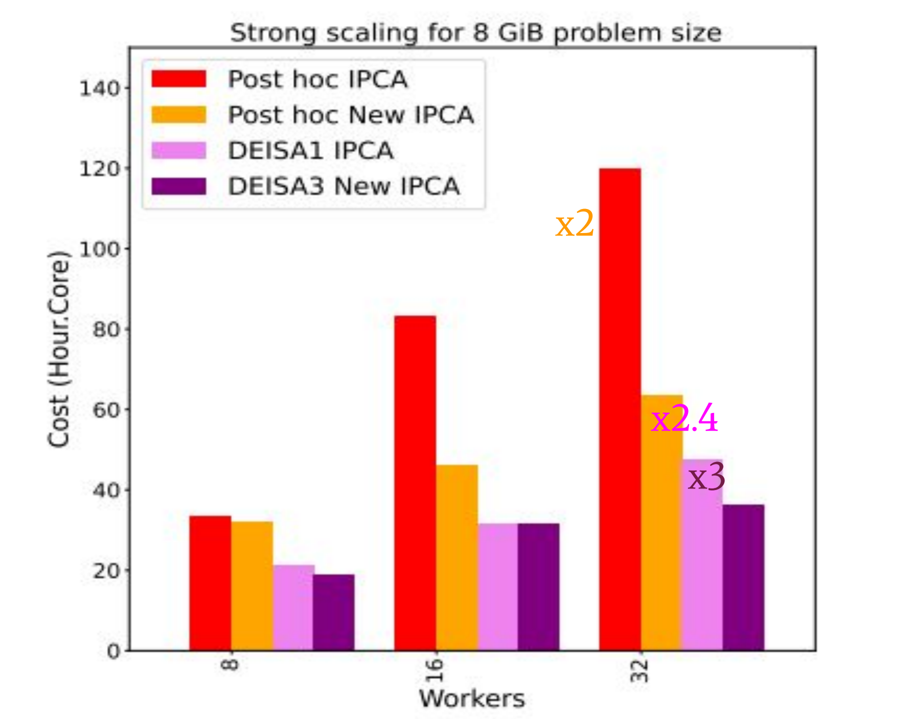




Strong scalability (in hour.core)



(c) Strong scaling results represented in hour-core for an 8 GiB problem size



(c) Strong scaling results represented in hour-core for a 8 GiB problem size

Variability over iterations and processes

Communication time

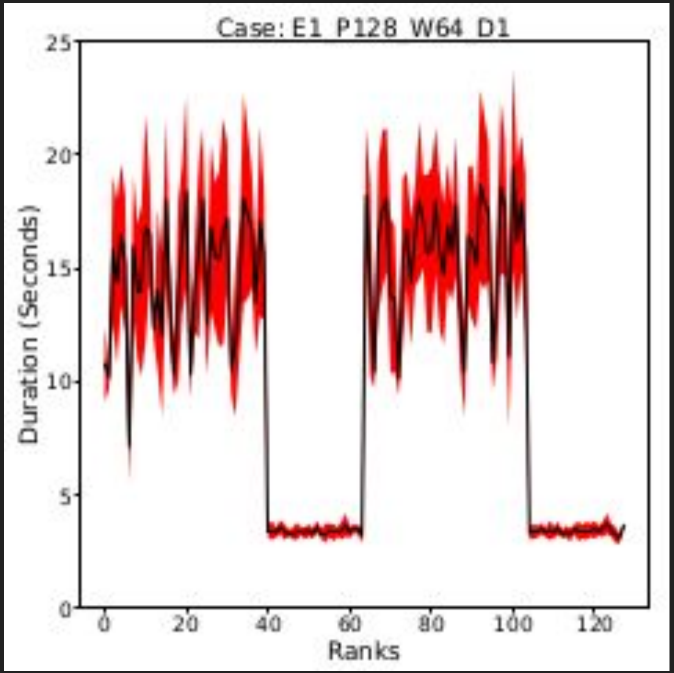
- by MPI rank
- averaged over iterations
- std dev in red

High node allocation impact

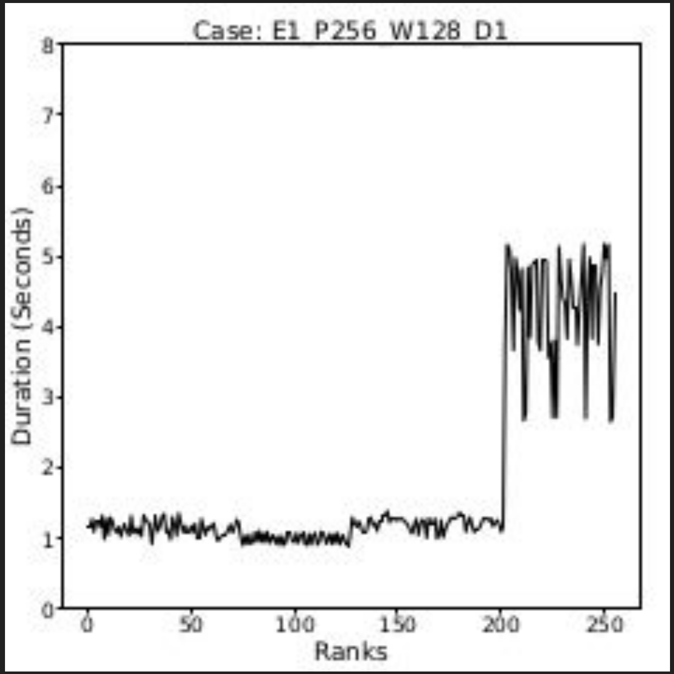
- Pruned fat tree

DEISA1 has high noise

- Scheduler contention
- Wait for laggers
- Impact perf



DEISA1
lots of metadata



DEISA3
less metadata

Deisa3 based on external tasks

Metadata sent from simulation to dask ahead of time

- A single task-graph constructed encompassing all time-steps
  - Requires the addition of the “external tasks” concept to dask
- Time is a dimension like any other
  - More expressivity (e.g. one graph for time derivative)
- Reduced metadata transfer
  - Less contention on the scheduler
- Contracts
  - Detect data actually required by the graph, do not transfer useless data
  - Better performance

To conclude

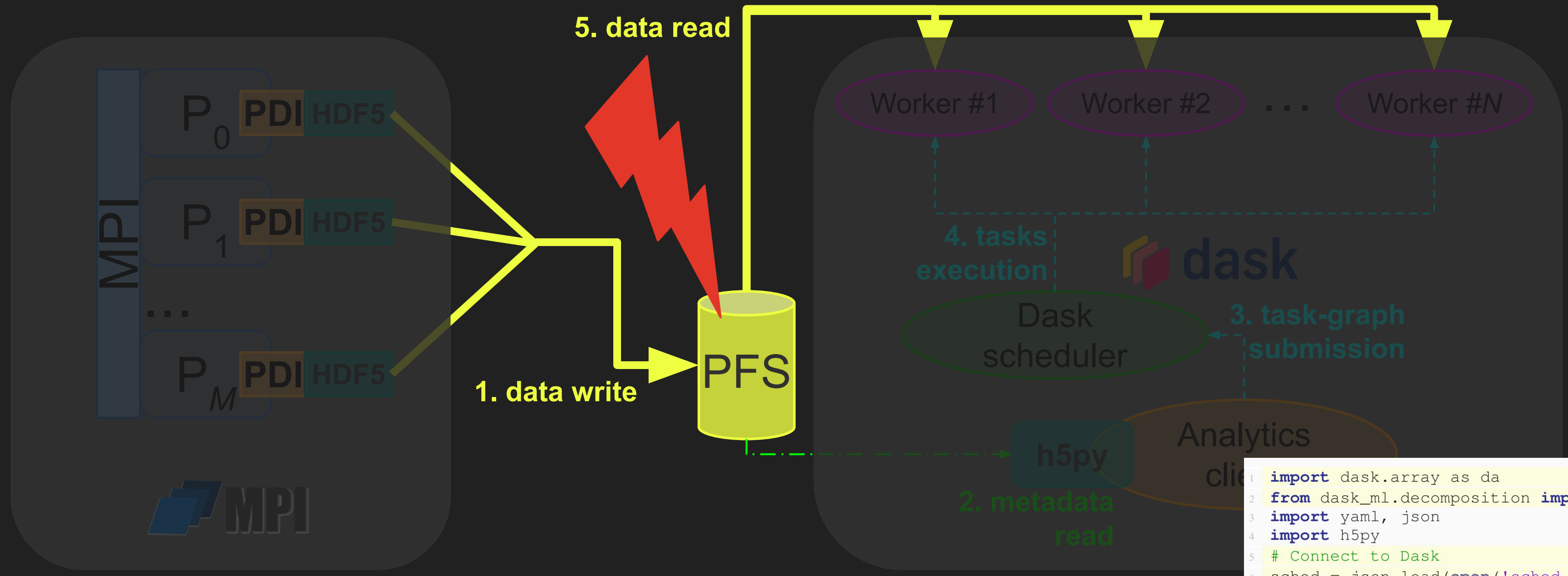
A work to support in-transit HPC/ML workflows : MPI + Dask = Deisa

- Added external tasks in Dask
  - Makes Deisa3 possible: single-graph, contracts, less contention
  - A concept useful beyond Deisa!
- Implemented a new IPCA in Dask-ML
- Evaluated an in situ Heat2D / PCA workflow
  - Outperforms plain Dask by a high margin
  - Solves performance issues of Deisa1

Now working to

- Bring external tasks to Dask main branch & make them available to the world
- Move to a workflow with production simulation & more complex ML-analytics

Dask for post hoc analytics




```python
import dask.array as da
from dask_ml.decomposition import IncrementalPCA
import yaml, json
import h5py
# Connect to Dask
sched = json.load(open('sched.json'))
client = dask.distributed.Client(sched["address"])
# load the simulation configuration
simu = yaml.load(open('simulation.yml'))
# Build a lazy array descriptor from HDF5
gtemp = h5py.File('data.hdf5',mode='r')['gtemp']
gtemp = da.from_array(gtemp, chunks=(1,4096,4096))
for step in range(0, simu['timesteps']):
  pca = IncrementalPCA(n_components=2, copy=False,
                       svd_solver='randomized')
  pca.fit(gtemp[step,:,:])
  print(pca.explained_variance_)
```

File-system IO performance is an iss