Data Science with DASK

2nd MarDATA Block Course
“Advanced Scientific Programming”

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Agenda for today

- Overview of Dask's fundamental concepts
- First hands-on session on Dask basics
- Review of the key takeaways
- Excursion: Dask distributed deployments / tools
- Second hands-on session on Dask for machine learning
- Question / Answer Session

Let's also schedule breaks?

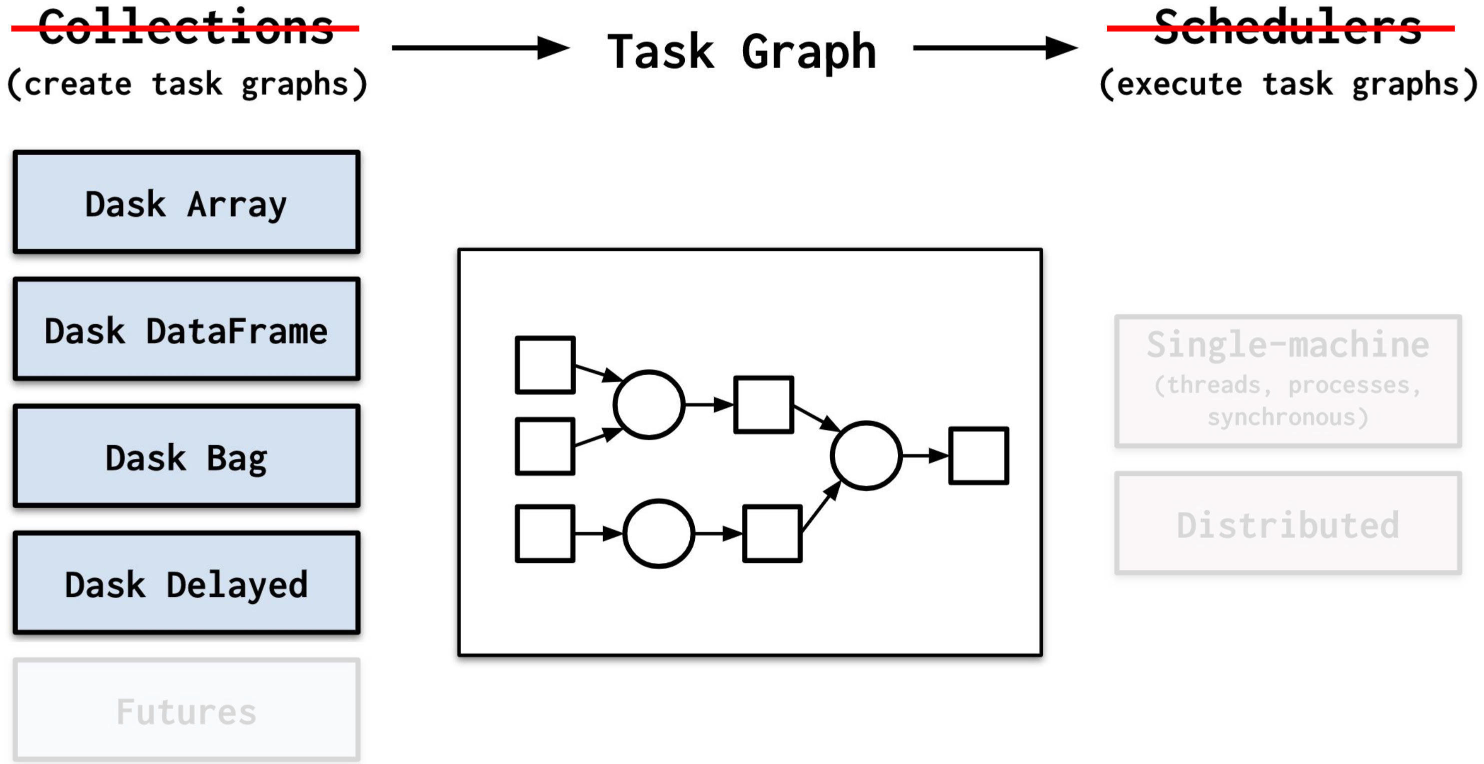
Aim of this course

We want you to understand the following:

- Dask is all about *task-graphs*.
- Dask provides various ways of *building task graphs*
  some of which can *replace existing toolboxes* like Numpy or Pandas.
- Dask provides various ways of executing task-graphs
  in *parallel* on a single machine or on *distributed clusters*.

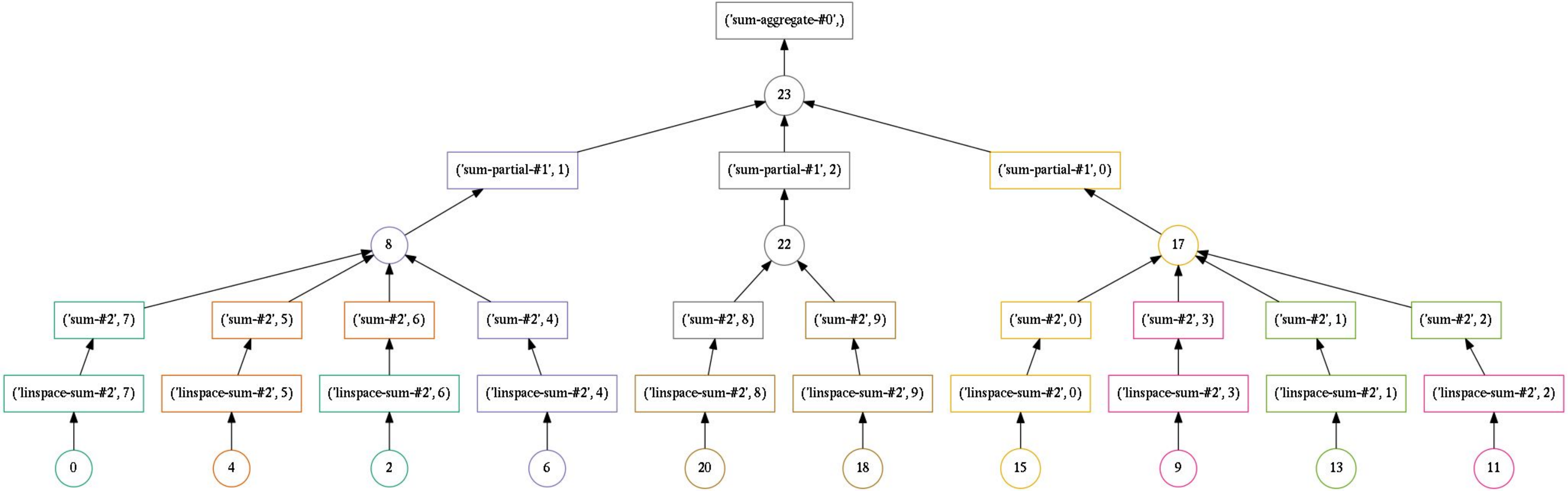
And: Know when *<u>NOT to use</u>* Dask!

Dask base concepts



from: https://docs.dask.org/en/latest/

Task graphs encode the flow of information



Your turn: *Can you find workflows / calculations you already know that can be described as a directed acyclic graph?*

Hands on

What is Dask *[30 minutes?]*

- Lecture-style overview of the core concept of Dask.
- Simple examples for explicitly building a task graph.

Creating task graphs *[60 minutes?]*

- Using Dask bag.
- Dask Dataframes.
- Dask Arrays.

Different ways of executing task graphs *[45 minutes?]*

- Get to know a simple application.
- Run the workflow on a single machine.
- Scale _out_ to multiple machines.

[Lunch ~ 12:30 - 13:00]

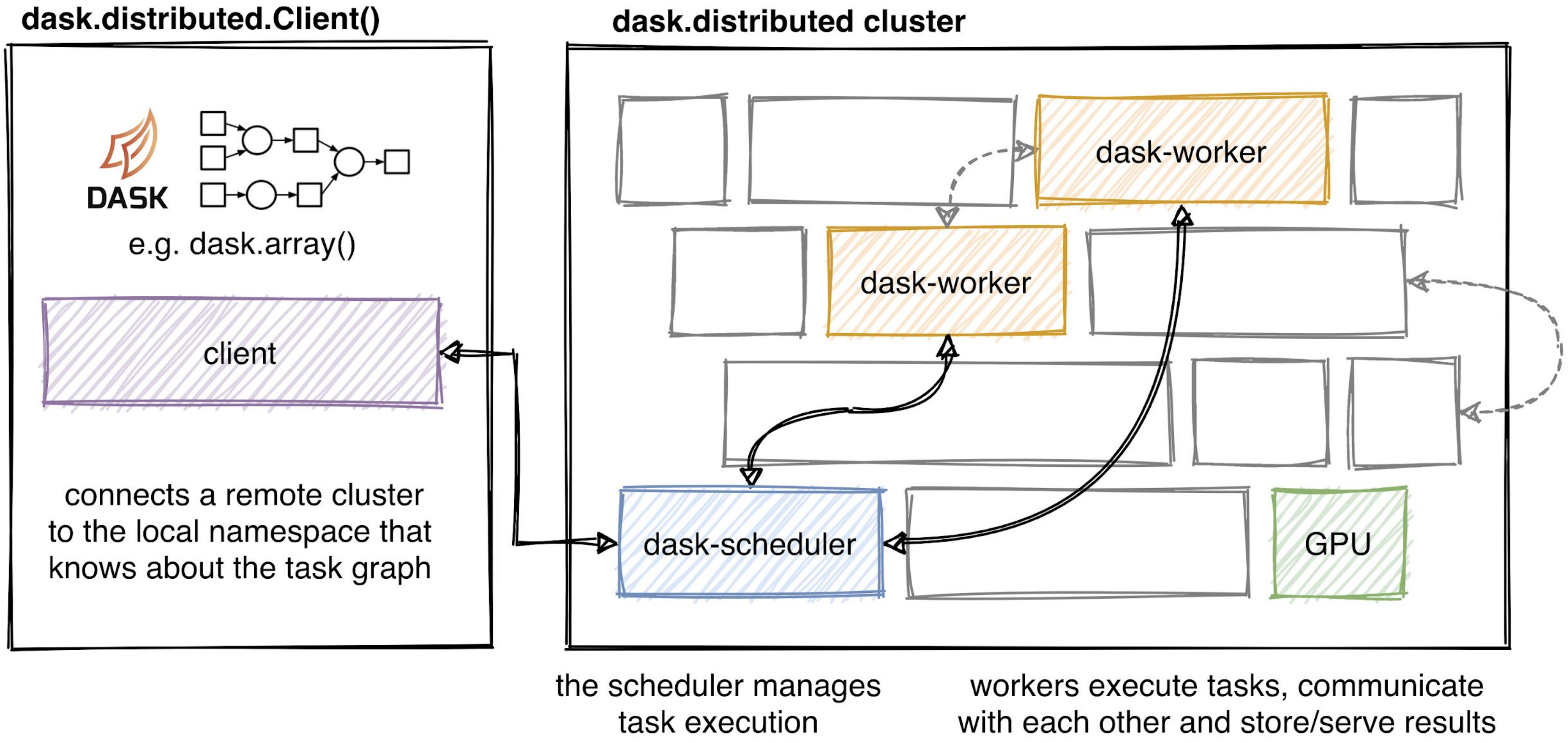
Parallelize machine learning with Dask *[45 minutes?]*

- Parallelize machine learning workloads.

→ https://github.com/mardatade/Course-Data-Science-with-Dask

Dask distributed scheduling

- For now, we have only worked with Dask single-machine schedulers.
- The necessary entities to go remote and to scale out are provided by the Dask distributed package (https://distributed.dask.org/en/latest/).
- Key strength of Dask: it is designed for the utilization of compute/memory resources of hundreds of separate machines in a common network.
- Let’s have a look now… and put together some machines manually!


dask.distributed.Client()
DASK
e.g. dask.array()
client
connects a remote cluster
to the local namespace that
knows about the task graph
dask.distributed cluster
dask-worker
dask-worker
dask-scheduler
GPU
the scheduler manages
task execution
workers execute tasks, communicate
with each other and store/serve results

Semi-Automatic Ways of Creating Dask Clusters

- For high-performance computers / other compute servers
    - Dask jobqueue: Manages clusters with a single-node granularity. Probably the most mature and most convenient of the HPC deployment solutions.
    - Dask MPI: Uses MPI to distribute scheduler and workers within an HPC job.
(but does not communicate via MPI!)
    - Dask SSH: Starts scheduler and workers on hosts you can access via SSH
    - Dask DRMAA: Uses DRMAA (a common interface to many different HPC scheduling softwares) for deploying Dask clusters.
- For cloud-computing platforms
    - Dask kubernetes: Creates and manages Dask clusters with Kubernetes
    - Dask cloudprovider: High-level tool that deploys clusters to (Amazon Web Services, Digital Ocean, Google Cloud Platform, Microsoft Azure).
    - Dask yarn: Deploys Dask clusters on Hadoop clusters.
    - Dask gateway: Provides Dask clusters via a web service / API.

… and counting

Summary: Key points to remember

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What's missing here?

- Dask as backend for other libraries
  - scikit-learn (partially covered here)
  - Xarray (labeled ndimensional arrays): http://xarray.pydata.org
  - Workflow management: https://prefect.io
- Actors
- Optimizing / tuning graphs
- Debugging
- Input / Output
- Resilience
- ...

Practical Problems

- Task graph should reflect <u>flow of information</u> between functions / methods rather than operations within calculations. Example high-order polynomial with a few coefficients is best wrapped into generalized ufuncs.
- Keep task graphs below a few 100.000 tasks, because scheduling takes time and resources.
- How to choose chunk sizes for Dask arrays?
- ...

Thank you!
What else do you want to know?