Dask for Parallel Processing

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Dask

- Dask is a library to do parallel computing in Python
- Two main components
  - Data collections/types
  - Task scheduling functionality with parallel backends

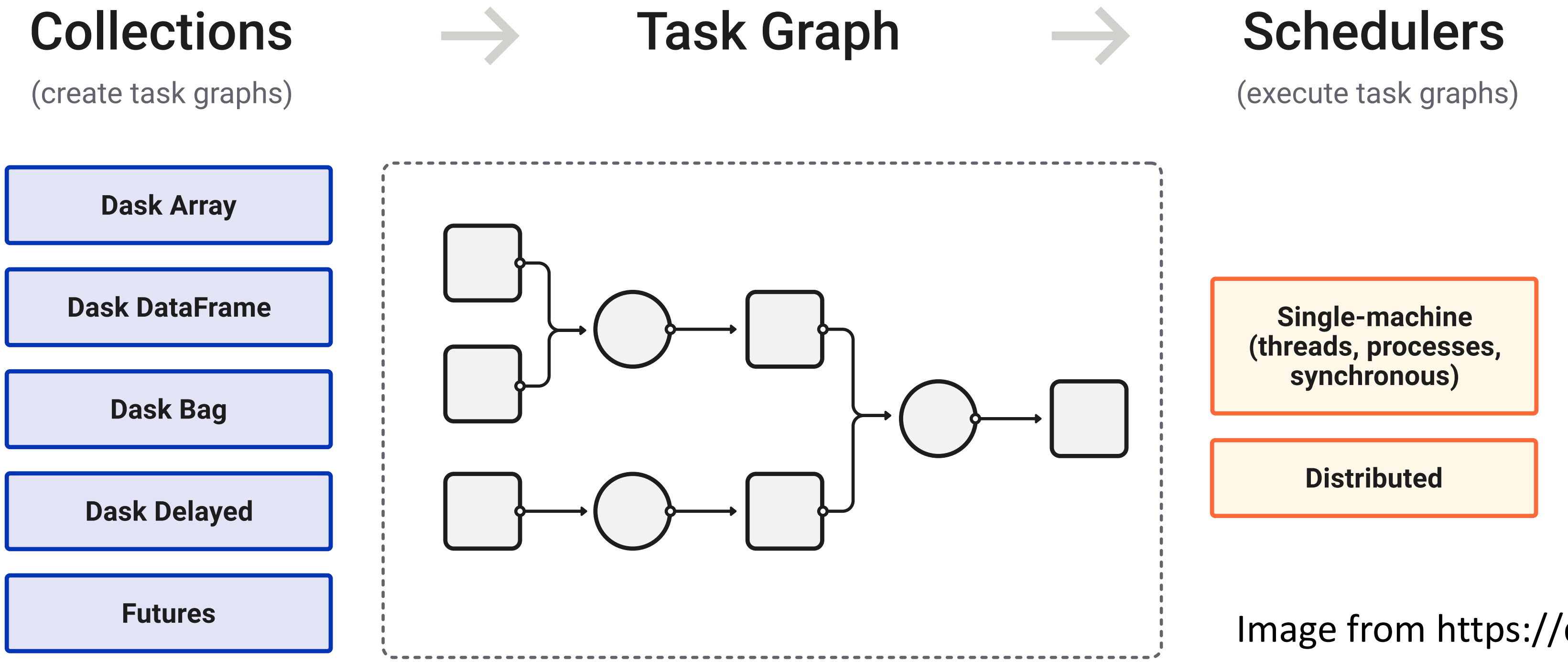
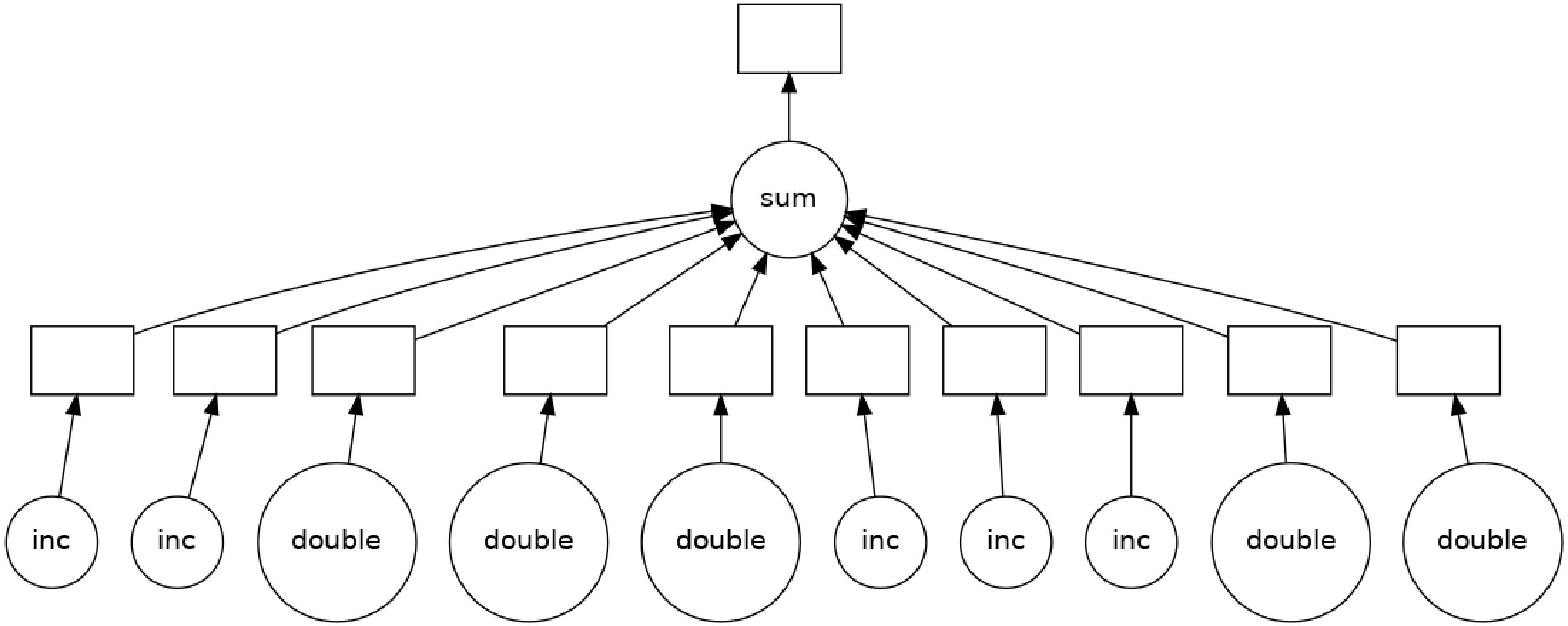


Image from https://docs.dask.org/en/latest/

Parallel computing

- Split work into tasks to be undertaken
- Schedule those tasks on available compute resources
- Execute the task schedule

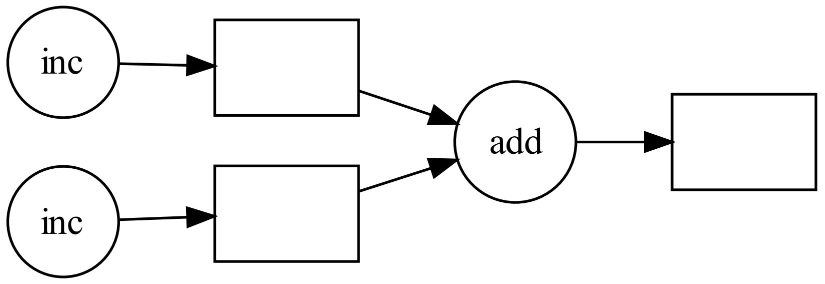


Collections/data types

- Array
  - n-dimensional array (similar to numpy arrays)
  - Out-of-memory functionality
- DataFrame
  - pandas DataFrame functionality
  - 2-d table/spreadsheet
- Bag
  - Unstructured data types
  - Python iterators
- Dask functionality allows all of these to be distributed across compute nodes but still processed as if local

Direct parallelisation

- `dask.delayed` interface
  - Construct custom parallelization
  - Dask task graph functions
- dask `Futures` functionality
  - Enable immediate task generation
  - Sidesteps delayed evaluation
- Data movement functions
  - `gather`, `scatter`, or realise data from futures
- Coordination/synchronisation functionality
  - Queues, Variables, Locks, etc…



Dask Array

- Create array with chunk size
  - `import dask.array as da`
  - `x = da.random.random((10000, 10000), chunks=(1000, 1000))`
- Many ways to create arrays
  - Random

```
random.binomial(n, p[, size, chunks])
random.normal([loc, scale, size, chunks])
random.poisson([lam, size, chunks])
random.random([size, chunks])
```

    - https://docs.dask.org/en/stable/array-api.html#random
  - numpy arrays

```
import numpy as np
import dask.array as da
np_array = np.ones((10000,10000))
x = da.from_array(np_array, chunks=(1000, 1000))
```

    - Input must have a `.shape`, `.ndim`, `.dtype` and support numpy-style slicing
      - https://docs.dask.org/en/stable/generated/dask.array.from_array.html#dask.array.from_array

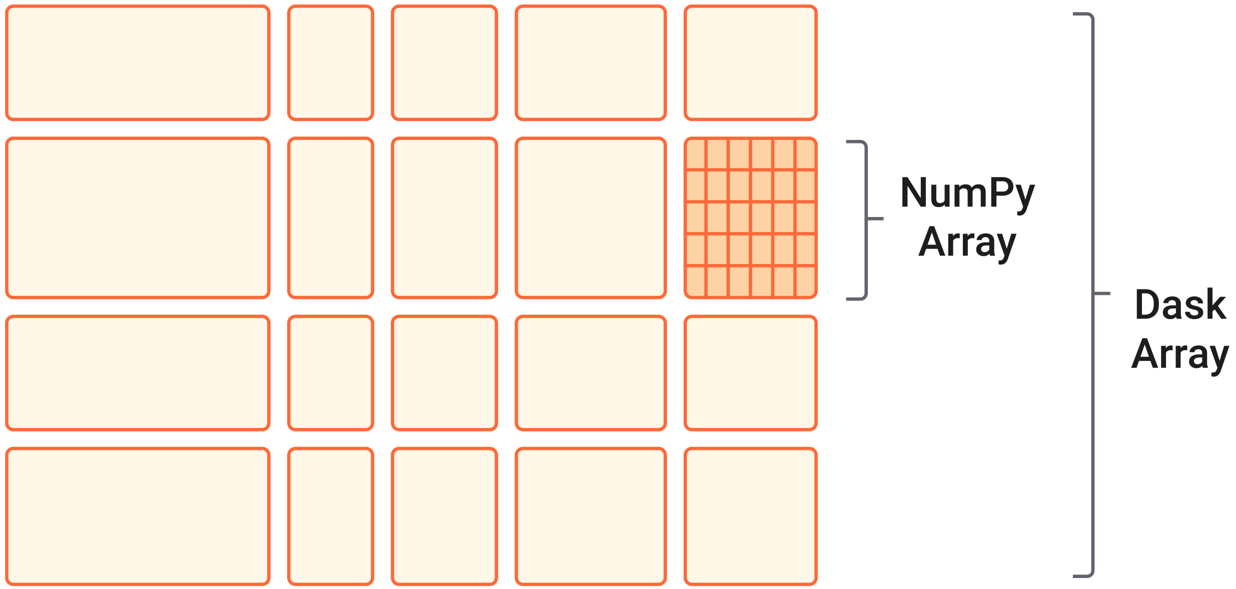


Image from https://docs.dask.org/en/stable/array.html/

Dask Array

- From files
  - `.npy` are numpy binary files
  - `.zarr` are binary files designed for blocked/chunked and compressed data
  - Load groups of files into a single array
  - `dask.array.from_npy_stack(dirname, mmap_mode='r')`
  - `dask.array.from_zarr(url, component=None, storage_options=None, chunks=None, name=None, inline_array=False, **kwargs)`
- From dask arrays
  - `concatenate`: create single dimension array from existing arrays
  - `stack`: create new dimension of data with existing arrays
- `delayed`
  - From delayed functions that return things that dask arrays can be constructed from
- Remember, tasking means everything is lazy

Array

- Dask supports a range of numpy like functionality:
  - Arithmetic and scalar mathematics: +, *, exp, log, ...
  - Reductions along axes: sum(), mean(), std(), sum(axis=0), ...
  - Tensor contractions / dot products / matrix multiply: tensordot
  - Axis reordering / transpose: transpose
  - Slicing: x[:100, 500:100:-2]
  - Indexing along single axes with lists or NumPy arrays: x[:, [10, 1, 5]]
  - Array protocols like __array__ and __array_ufunc__
  - Some linear algebra: svd, qr, solve, solve_triangular, lstsq
- Dask Array lacks the following features:
  - Much of np.linalg has not been implemented
  - Arrays with unknown shapes do not support all operations
  - Sorts are not fully supported
  - tolist
  - Iterators can be ineffcient
- Full API is at: https://docs.dask.org/en/stable/array-api.html

Dask DataFrame

- Create like a standard pandas dataframe

```
import dask.dataframe as dd
df = dd.read_csv('mydata.csv')
```

  - Can also specify blocksize (chunks)

```
dask.dataframe.read_csv(urlpath, blocksize='default', lineterminator=None, compression='infer', sample=256000, sample_rows=10, enforce=False, assume_missing=False, storage_options=None, include_path_column=False, **kwargs)
```

  - Many ways to create dataframes
  - https://docs.dask.org/en/stable/dataframe-create.html#
  - From files/data sources

```
read_csv(urlpath[, blocksize, ...])
read_parquet(path[, columns, filters, ...])
read_hdf(pattern, key[, start, stop, ...])
read_orc(path[, engine, columns, index, ...]
read_json(url_path[, orient, lines, ...])
read_sql_table(table_name, con, index_col..)
read_sql_query(sql, con, index_col[, ...])
read_sql(sql, con, index_col, **kwargs)
read_table(urlpath[, blocksize, ...])
read_fwf(urlpath[, blocksize, ...])
```

  - https://docs.dask.org/en/stable/array-api.html#random
  - From dask objects

```
from_delayed(dfs[, meta, divisions, prefix, ...])
from_dask_array(x[, columns, index, meta])
dask.bag.core.Bag.to_dataframe([meta, ...]
```

  - From other objects
    - `from_bcolz(x[, chunksize, categorize, ...])`
    - `from_array(x[, chunksize, columns, meta])`

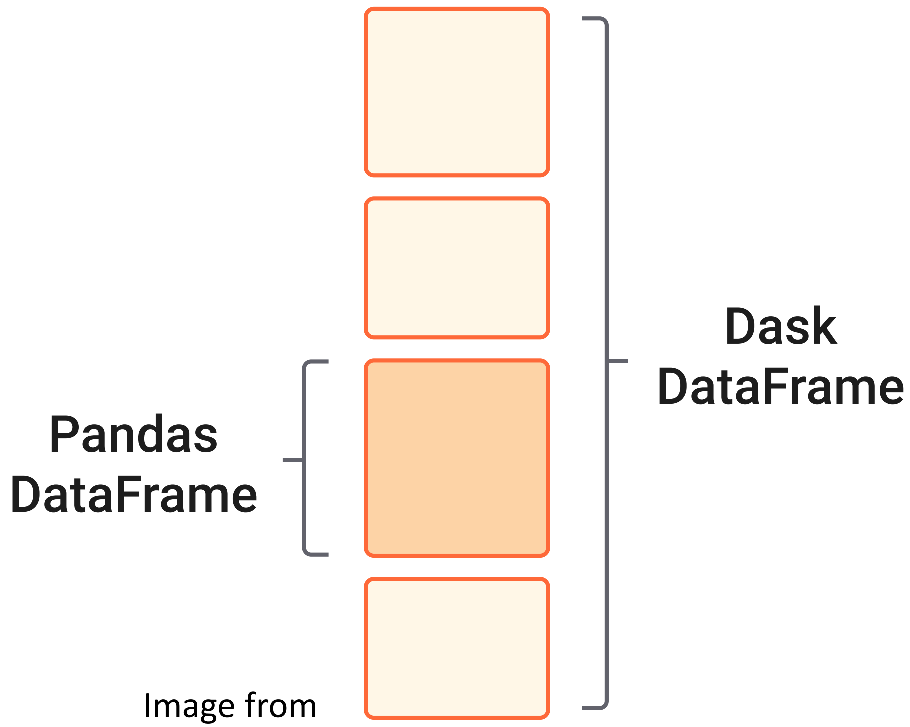


Image from
https://docs.dask.org/en/stable/dataframe.html

DataFrames

- DataFrames cover part of the pandas API:
  - Independent operations:
    - Element-wise operations: df.x + df.y, df * df
    - Row-wise selections: df[df.x > 0]
    - Loc: df.loc[4.0:10.5]
    - Common aggregations: df.x.max(), df.max()
    - Is in: df[df.x.isin([1, 2, 3])]
    - Date time/string accessors: df.timestamp.month
  - Group operations:
    - groupby-aggregate (with common aggregations): df.groupby(df.x).y.max(), df.groupby('x').max()
    - groupby-apply on index: df.groupby(['idx', 'x']).apply(myfunc), where idx is the index level name
    - value_counts: df.x.value_counts()
    - Drop duplicates: df.x.drop_duplicates()
    - Join on index: dd.merge(df1, df2, left_index=True, right_index=True)
    - Join with Pandas DataFrames: dd.merge(df1, df2, on='id')
    - Element-wise operations with different partitions / divisions: df1.x + df2.y
    - Date time resampling: df.resample(...)
    - Rolling averages: df.rolling(...)
    - Pearson’s correlation: df[['col1', 'col2']].corr()
  - Group operations requiring data reordering
    - Set index: df.set_index(df.x)
    - groupby-apply not on index (with anything): df.groupby(df.x).apply(myfunc)
    - Join not on the index: dd.merge(df1, df2, on='name')

DataFrames

- DataFrame has the following limitations:
  - Setting a new index from an unsorted column is expensive
  - Many operations like groupby-apply and join on unsorted columns require setting the index, which as mentioned above, is expensive
  - The Pandas API is very large. Dask DataFrame does not attempt to implement many Pandas features or any of the more exotic data structures like NDFrames
  - Operations that were slow on Pandas, like iterating through row-by-row, remain slow on Dask DataFrame
- Full API is https://docs.dask.org/en/stable/dataframe-api.html

Dask Bag

- Bag is like a list or set
  - Unordered collection of data with repeats, i.e. `{1, 2, 2, 3}`
  - Immutable
- Operations
  - **`map, groupby, filter, fold, etc…`**
  - Full API https://docs.dask.org/en/latest/bag-api.html
- Parallelise simple computations
  - unstructured or semi-structured data
  - i.e. text data, log files, JSON records, or user defined Python objects.
- Implemented using multi-processing (not threads)
  - Reduces communication efficiency between bag elements

Bag

- Creating bags:
  - `from_sequence(seq[, partition_size, npartitions])`
  - `from_delayed(values)`
  - `from_url(urls)`
  - `range(n, npartitions)`
  - `read_text(urlpath[, blocksize, compression, ...])`
  - `read_avro(urlpath[, blocksize, ...])`
  - `DataFrame.to_bag([index, format])`
- Bag operations
  - `Bag.accumulate(binop[, initial])`

```
import dask.bag as db
from operator import add
b = db.from_sequence([1, 2, 3, 4, 5], npartitions=2)
b.accumulate(add).compute()
```

  - `Bag.all(split_every=None)`
  - `Bag.any(split_every=None)`
  - `Bag.count([split_every])`
  - `Bag.max([split_every])`
  - `Bag.min([split_every])`
  - `Bag.msum([split_every])`

```
import dask.bag as db
bool_bag = db.from_sequence([True, True, False])
bool_bag.all().compute()
```

Bag

- `Bag.reduction(perpartition, aggregate[, ...])`
- `Bag.random_sample(prob, random_state=None)`
- `Bag.filter(predicate)`

```
def iseven(x):
    return x % 2 == 0
import dask.bag as db
b = db.from_sequence(range(5))
list(b.filter(iseven))
```

- `Bag.groupby(grouper[, method, npartitions, ...])`

```
import dask.bag as db
b = db.from_sequence(range(10))
iseven = lambda x: x % 2 == 0
dict(b.groupby(iseven))
```

- `Bag.foldby(key, binop[, initial, combine, ...])`
  - Combined `reduction` and `groupby`
  - Efficient parallel split-apply-combine tasks.
- Bags can't be changed
  - Immutable
- Arrays and DataFrame are faster than Bags
- Bag `groupby` is slow.
  - `foldby` faster alternative if possible

delayed

- Direct task graph creation
  - Delay python functions

    `dask.delayed(func)(inputs…)`
  - Code annotation

    `@dask.delayed`
  - `compute` still required to complete
- Delay function specifics matter
  - `dask.delayed(f(x, y))`
    - Calculates `f` first then delays the output
  - `dask.delayed(f)(x, y)`
    - Enables lazy evaluation
- Don’t delay other dask functionality

```
def inc(x):
    return x + 1

def double(x):
    return x * 2

def add(x, y):
    return x + y

data = [1, 2, 3, 4, 5]

output = []
for x in data:
    a = inc(x)
    b = double(x)
    c = add(a, b)
    output.append(c)

total = sum(output)
```

```
import dask
…
…
output = []
for x in data:
    a = dask.delayed(inc)(x)
    b = dask.delayed(double)(x)
    c = dask.delayed(add)(a, b)
    output.append(c)

total = dask.delayed(sum)(output)
total.compute()
```

```
import dask

@dask.delayed
def inc(x):
    return x + 1

@dask.delayed
def double(x):
    return x * 2

@dask.delayed
def add(x, y):
    return x + y

data = [1, 2, 3, 4, 5]

output = []
for x in data:
    a = inc(x)
    b = double(x)
    c = add(a, b)
    output.append(c)

total = dask.delayed(sum)(output)
total.compute()
```

Futures

- Futures provide more complex functionality to build arbitrary task graphs
  - Similar to `delayed`, but tasks executed as soon as available
- Create task:

```
Client.submit(func, *args[, key, workers, ...])
Client.map(func, *iterables[, key, workers, ...])
Future.result([timeout])
```

- Move data:

```
Client.gather(futures[, errors, direct, ...])
Client.scatter(data[, workers, broadcast, ...])
```

Futures

```
from dask.distributed import Client
client = Client()  # start local workers as processes
# or
client = Client(processes=False)  # start local workers as threads
def inc(x):
    return x + 1

def add(x, y):
    return x + y

a = client.submit(inc, 10)
b = client.submit(inc, 20)
c = client.submit(add, a, b)
c.result()
futures = client.map(inc, range(1000))
```

Parallelisation

- Dask generally defaults to threaded parallelisation
  - Single node
  - Maximum cores available
  - Dask array and dataframe
- Bag uses the multiprocessing scheduler by default
- Threads are lightweight workers for the main process (program)
  - Easy to parallelise
  - Share data easily between workers
  - Often doesn’t scale up to all cores efficiently
- Processes are heavier weight workers (copies of the main program)
  - More scope for independent work
  - More heavy weight in startup costs
  - Explicit communication needed between workers if required

Dask scheduling

- Scheduling choices can be modified by the user
- Default is generally threading:
```
import dask
dask.config.set(scheduler='threads')
```
  - Works well for Array, DataFrame, and Delayed
  - Relies on threading, so native python code will be restricted by the GIL
- Can change to processes:
```
import dask
dask.config.set(scheduler='processes’)
```
  - No GIL issues but slower for inter-task communications
- More advanced scheduling can be done using distributed
```
from dask.distributed import Client
client = Client()
```
  - Defaults to processes
```
client = Client(processes=False)
```
  - Might require `distributed` to be installed (not part of core dask install)
- Distributed can do single node or multi node
  - asynchronous API (Futures)
  - Has a dashboard
  - Improved data locality functionality for multi process work

Dask scheduling

- Can customise amount of resources and scheduler
  - Per run basis:
    ```
    x.sum().compute(scheduler='processes’)
    ```
  - As a context:
    ```
    with dask.config.set(scheduler='threads'):
        x.compute()
    ```
  - Globally:
    ```
    dask.config.set(scheduler='threads’)
    ```
  - Number of workers
    ```
    from multiprocessing.pool import ThreadPool
    dask.config.set(pool=ThreadPool(8))
    ```
  - Distributed scheduler
    ```
    client = Client(processes=False, n_workers=4)
    ```

Distributed scheduler

- Distributed `Client`

```
from dask.distributed import Client
client = Client(...)
df.x.sum().compute()
```

- Local cluster (single node)

```
from dask.distributed import Client, LocalCluster
cluster = LocalCluster()
client = Client(cluster)
df.x.sum().compute()
```

- `dask_jobqueue` provides batch system interfaces

```
HTCondorCluster([n_workers, loop, security, ...])
LSFCluster([n_workers, loop, security, ...])
MoabCluster([n_workers, loop, security, ...])
OARCluster([n_workers, loop, security, ...])
PBSCluster([n_workers, loop, security, ...])
SGECluster([n_workers, loop, security, ...])
SLURMCluster([n_workers, loop, security, ...])
```

- `dask_mpi` provides MPI launch interfacing

```
from dask_mpi import
initialize
initialize()
from dask.distributed import Client
Client = Client()
mpirun -np 4 python my_client_script.py
```

  - Or

```
mpirun -np 4 dask-mpi --scheduler-file ~/dask-scheduler.json
from dask.distributed import Client
client = Client(scheduler_file='~/dask-scheduler.json’)
```

https://docs.dask.org/en/latest/deploying-hpc.html

Guiding principles

- If you don't need Dask, don't use it
  - Numpy array, panda dataframe, etc… all faster for small scale, in-memory
- Chunking/granularity important for performance
  - Too big chunks -> not enough parallelism
  - Too small chunks -> large parallelisation overhead
- `compute` as infrequently as possible
  - `compute` forces evaluation of the task graph
  - Might need multiple compute calls if task graph gets too big
- Mix threads and processes if doing larger parallelisation
  - Threads good for small scale parallelisation
- Load data with dask
- Persist datasets to memory when reduced

Dask on ARCHER2

- Dask is available in the cray-python
  - Threading/shared memory backends
- Distributed dask needs to be installed

```
module load cray-python
export PYTHONUSERBASE=/work/t01/t01/auser/.local
export PATH=$PYTHONUSERBASE/bin:$PATH
python -m pip install -user dask distributed -upgrade
python -m pip install --user dask-jobqueue --upgrade
```

- Currently need to submit from compute nodes
  - Dask runs a scheduler that needs connection from the workers

Threaded Dask on ARCHER2

- Running single node dask as normal job works fine
  - Default mode is threading
  - Requires process binding and thread placement to be sensible

```
#!/bin/bash
#SBATCH --job-name=my_job
#SBATCH --nodes=1
#SBATCH --tasks-per-node=1
#SBATCH --cpus-per-task=128
#SBATCH --partition=standard
#SBATCH --qos=short
#SBATCH --account=z19
#SBATCH --time=0:10:0
python dask-program.py
```

- Can also do an interactive run:

```
srun --nodes=1 --tasks-per-node=1 --cpus-per-task=128 --exclusive --partition=standard --qos=short
--reservation=shortqos --account=z19 --time=0:20:0 python dask-program.py
```

Distributed Dask on ARCHER2

```
from dask_jobqueue import SLURMCluster
cluster = SLURMCluster(cores=128,
                       processes=128,
                       memory='256GB',
                       queue='standard',
                       header_skip=['--mem'],
                       job_extra=['--qos="standard"'],
                       python='srun python',
                       project=‘t01’,
                       walltime="01:00:00",
                       shebang="#!/bin/bash --login",
                       local_directory='$PWD'
                       env_extra=['module load cray-python',
                                  'export PYTHONUSERBASE=/work/t01/t01/auser/.local/',
                                  'export PATH=$PYTHONUSERBASE/bin:$PATH',
                                  'export PYTHONPATH=$PYTHONUSERBASE/lib/python3.8/site-
packages:$PYTHONPATH'])
cluster.scale(jobs=2)    # Deploy two single-node jobs
from dask.distributed import Client
client = Client(cluster)  # Connect this local process to remote workers
import dask.array as da
x = da.random.random((10000, 10000), chunks=(1000, 1000))
mean = x.mean().compute()
```