High Performance Computing with Python

Implementing distance matrices with NumPy/SciPy, F2PY/Fortran90, CFFI/C and Dask

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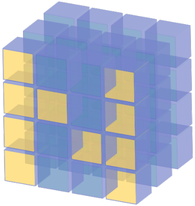
Lugano, 23-25.06.2021

NumPy is a Python library that adds support for large multi-dimensional arrays and matrices, along with a large collection of high-level mathematical functions to operate on these arrays.



- `numpy.ndarray`: a powerful N-dimensional array object
- Sophisticated functions often written in C
- Linear algebra, Fourier transform, and random number capabilities
- Tools for easy binding to Fortran code (F2PY)
- Compatibility with C

The **SciPy** library provides many user-friendly and efficient numerical routines for operations such as numerical integration, interpolation, optimization, linear algebra and statistics. SciPy builds on the `numpy.ndarray` and expands the set of mathematical functions included in NumPy

numpy.ndarray

```
>>> x = np.array([[0, 1, 2], [3, 4, 5], [6, 7, 8]], dtype=np.int8)
>>> x
array([[0, 1, 2],
       [3, 4, 5],
       [6, 7, 8]], dtype=int8)
```

`numpy.ndarray`

0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	1	0
0	0	0	0	0	0	1	1	0	0	0	0
0	1	0	0	0	0	0	0	0	1	0	1
0	0	0	0	0	1	1	0	0	0	0	0
0	1	1	1	0	0	0	0	1	0	0	0

`numpy.ndarray`

0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	1	0
0	0	0	0	0	0	1	1	0	0	0	0
0	1	0	0	0	0	0	0	0	1	0	1
0	0	0	0	0	1	1	0	0	0	0	0
0	1	1	1	0	0	0	0	1	0	0	0

`numpy.ndarray`

```
{'shape': (3, 3), 'strides': (3, 1),
 'dtypes': int8,  'ndim': 2, ...}
```

0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	1	0
0	0	0	0	0	0	1	1	0	0	0	0
0	1	0	0	0	0	0	0	0	1	0	1
0	0	0	0	0	1	1	0	0	0	0	0
0	1	1	1	0	0	0	0	1	0	0	0

numpy.ndarray

```
{'shape': (3, 3), 'strides': (3, 1),
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```

0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	1	0
0	0	0	0	0	0	1	1	0	0	0	0
0	1	0	0	0	0	0	0	0	1	0	1
0	0	0	0	0	1	1	0	0	0	0	0
0	1	1	1	0	0	0	0	1	0	0	0

- The memory block is called **data buffer**.
- The **metadata** is used to interpret the data buffer within the python context.
- The data buffer is stored in C order (row major) by default.
- All items in the array have the same data type.

`numpy.ndarray`

#	#	0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15	#	#

`numpy.ndarray`

Data buffer

#	#	0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15	#	#

NumPy representation

0	1	2	3
4	5	6	7
8	9	10	1
12	12	14	15

```
strides = (4, 1)
shape   = (4, 4)
dtype   = int8
```

`numpy.ndarray`

Data buffer

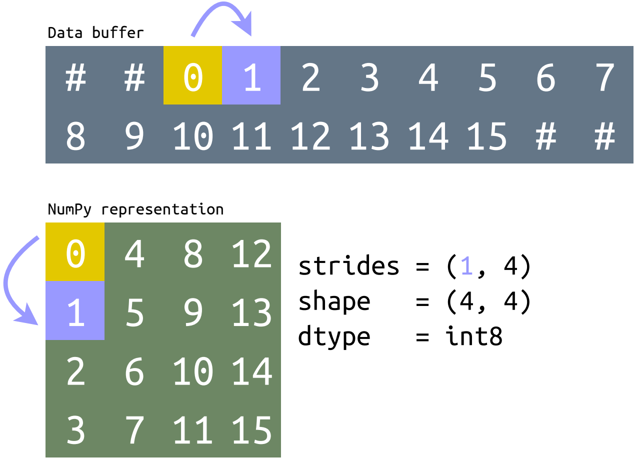
#	#	0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15	#	#

NumPy representation

0	4	8	12
1	5	9	13
2	6	10	14
3	7	11	15

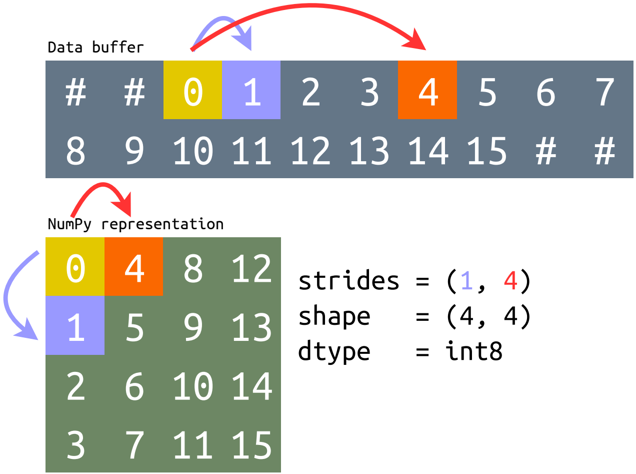
```
strides = (1, 4)
shape   = (4, 4)
dtype   = int8
```

`numpy.ndarray`



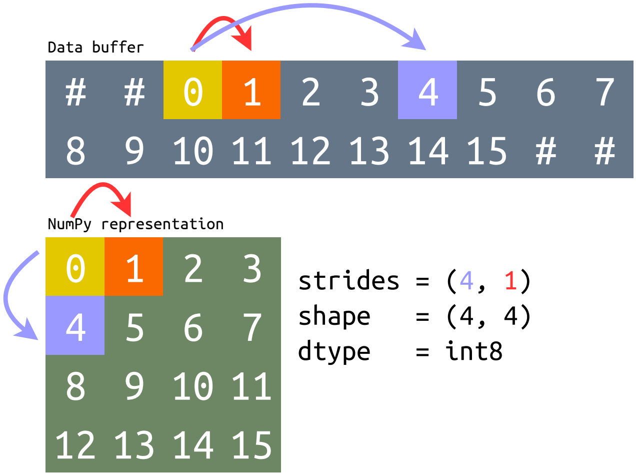

```
strides = (1, 4)
shape   = (4, 4)
dtype   = int8
```

`numpy.ndarray`




```
strides = (1, 4)
shape   = (4, 4)
dtype   = int8
```

`numpy.ndarray`

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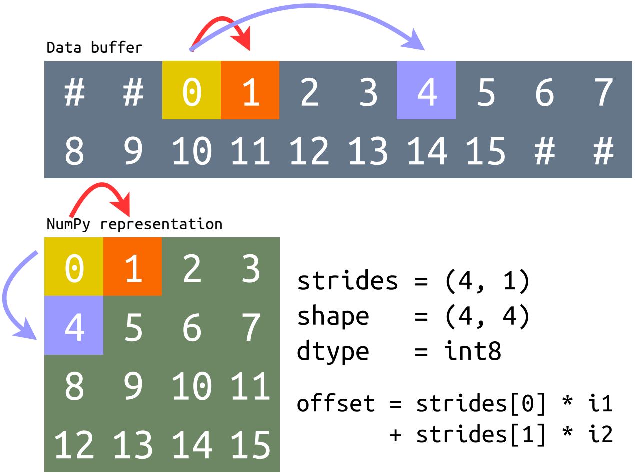
`numpy.ndarray`




```
strides = (4, 1)
shape   = (4, 4)
dtype   = int8

offset = strides[0] * i1
       + strides[1] * i2
```

[lab] `numpy.ndarray` internals

- Let's open the notebook `numpy/01-numpy-array-internals.ipynb` and go over the questions.

There are two parts:

- **Understanding strides**: a few arrays are given and you are asked to determine the corresponding strides (without looking at the `strides` attribute)
- **Metadata modification vs copying the data buffer**: some operations are given and we ask you to explain the results or differences in execution time. (Hint: Identify if new data is created or if the operations can be done with only a change of metadata)

Broadcasting

$$\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} + \begin{bmatrix} x_0 & x_1 & x_2 & \cdots & x_n \end{bmatrix}$$

$$(n, 1) \qquad\qquad (1, n)$$

Broadcasting

$$\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} + \begin{bmatrix} x_0 & x_1 & x_2 & \cdots & x_n \end{bmatrix} = \begin{bmatrix} y_0 + x_0 & y_0 + x_1 & \cdots & y_0 + x_n \\ y_1 + x_0 & y_1 + x_1 & \cdots & y_1 + x_n \\ y_2 + x_0 & y_2 + x_1 & \cdots & y_2 + x_n \\ \vdots & \vdots & \ldots & \vdots \\ y_n + x_0 & y_n + x_1 & \cdots & y_n + x_n \end{bmatrix}$$

$(n, 1)$ $(1, n)$ (n, n)

[lab] Broadcasting

- Let’s open the notebook `numpy/02-broadcasting.ipynb` and go over the cells and the questions. The goal of this notebook is to understand the broadcasting operations presented there.

Vectorization

- Use operations over the whole array instead of over single elements.

```
z = x * y          # x = np.array([...])
                   # y = np.array([...])
```

Vectorization

- Use operations over the whole array instead of over single elements.

```
z = x * y          # x = np.array([...])
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- When working with arrays, use *ufuncs* and general NumPy's functions.

```
x = np.exp(y)      # y = np.array([...])
z = np.dot(x, y)
```

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z = x * y            # x = np.array([...])
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```
x = np.exp(y)        # y = np.array([...])
z = np.dot(x, y)
```

- Adapt your solutions to use the two points above.

Euclidean distance matrix

$$d_{\mathsf{e}}\left(\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \dots & \dots & \dots \\ x_{n1} & x_{n2} & x_{n3} \end{bmatrix}, \begin{bmatrix} y_{11} & y_{12} & y_{13} \\ y_{21} & y_{22} & y_{23} \\ \dots & \dots & \dots \\ y_{n1} & y_{n2} & y_{n3} \end{bmatrix}\right) = \begin{bmatrix} \sum (x_{1i}-y_{1i})^2 & \sum (x_{1i}-y_{2i})^2 & \dots & \sum (x_{1i}-y_{ni})^2 \\ \sum (x_{2i}-y_{1i})^2 & \sum (x_{2i}-y_{2i})^2 & \dots & \sum (x_{2i}-y_{ni})^2 \\ \dots & \dots & \dots & \dots \\ \sum (x_{ni}-y_{1i})^2 & \sum (x_{ni}-y_{2i})^2 & \dots & \sum (x_{ni}-y_{ni})^2 \end{bmatrix}$$

Euclidean distance matrix

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Euclidean distance matrix

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Euclidean distance matrix

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Euclidean distance matrix

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Euclidean distance matrix

$$d_{\mathsf{e}}\left(\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \dots & \dots & \dots \\ x_{n1} & x_{n2} & x_{n3} \end{bmatrix}, \begin{bmatrix} y_{11} & y_{12} & y_{13} \\ y_{21} & y_{22} & y_{23} \\ \dots & \dots & \dots \\ y_{n1} & y_{n2} & y_{n3} \end{bmatrix}\right) = \begin{bmatrix} \sum(x_{1i}-y_{1i})^2 & \sum(x_{1i}-y_{2i})^2 & \dots & \sum(x_{1i}-y_{ni})^2 \\ \sum(x_{2i}-y_{1i})^2 & \sum(x_{2i}-y_{2i})^2 & \dots & \sum(x_{2i}-y_{ni})^2 \\ \dots & \dots & \dots & \dots \\ \sum(x_{ni}-y_{1i})^2 & \sum(x_{ni}-y_{2i})^2 & \dots & \sum(x_{ni}-y_{ni})^2 \end{bmatrix}$$

Euclidean distance matrix

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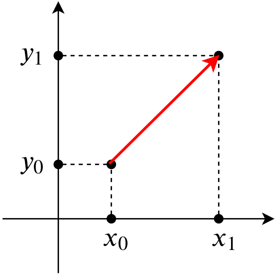
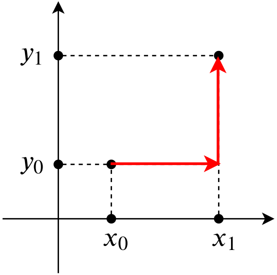
Euclidean distance matrix



$$d_e\left(\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \dots & \dots & \dots \\ x_{n1} & x_{n2} & x_{n3} \end{bmatrix}, \begin{bmatrix} y_{11} & y_{12} & y_{13} \\ y_{21} & y_{22} & y_{23} \\ \dots & \dots & \dots \\ y_{n1} & y_{n2} & y_{n3} \end{bmatrix}\right) =$$

$$\begin{bmatrix} \sum(x_{1i} - y_{1i})^2 & \sum(x_{1i} - y_{2i})^2 & \dots & \sum(x_{1i} - y_{ni})^2 \\ \sum(x_{2i} - y_{1i})^2 & \sum(x_{2i} - y_{2i})^2 & \dots & \sum(x_{2i} - y_{ni})^2 \\ \dots & \dots & \dots & \dots \\ \sum(x_{ni} - y_{1i})^2 & \sum(x_{ni} - y_{2i})^2 & \dots & \sum(x_{ni} - y_{ni})^2 \end{bmatrix}$$

Cityblock distance matrix



$$d_{\mathrm{cb}}\left(\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \dots & \dots & \dots \\ x_{n1} & x_{n2} & x_{n3} \end{bmatrix}, \begin{bmatrix} y_{11} & y_{12} & y_{13} \\ y_{21} & y_{22} & y_{23} \\ \dots & \dots & \dots \\ y_{n1} & y_{n2} & y_{n3} \end{bmatrix}\right) =$$

$$\begin{bmatrix} \sum |x_{1i} - y_{1i}| & \sum |x_{1i} - y_{2i}| & \dots & \sum |x_{1i} - y_{ni}| \\ \sum |x_{2i} - y_{1i}| & \sum |x_{2i} - y_{2i}| & \dots & \sum |x_{2i} - y_{ni}| \\ \dots & \dots & \dots & \dots \\ \sum |x_{ni} - y_{1i}| & \sum |x_{ni} - y_{2i}| & \dots & \sum |x_{ni} - y_{ni}| \end{bmatrix}$$

```python
def euclidean_distance_matrix(x, y):
    num_samples = x.shape[0]
    dist_matrix = np.empty((num_samples,
                            num_samples))
    for i, xi in enumerate(x):
        for j, yj in enumerate(y):
            diff = xi - yj
            dist_matrix[i][j] = np.dot(diff, diff)

    return dist_matrix
```

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```

- ✗ Use operations over the whole array instead of over single elements.
- ✓ When working with arrays, use ufuncs and general NumPy's functions.
- ✗ Adapt your solutions to use the two points above.

$$\sum_k (x_{ik} - y_{jk})^2 = (\vec{x}_i - \vec{y}_j) \cdot (\vec{x}_i - \vec{y}_j) = \vec{x}_i \cdot \vec{x}_i + \vec{y}_j \cdot \vec{y}_j - 2\vec{x}_i \cdot \vec{y}_j$$

$$\sum_k (x_{ik} - y_{jk})^2 = (\vec{x}_i - \vec{y}_j) \cdot (\vec{x}_i - \vec{y}_j) = \vec{x}_i \cdot \vec{x}_i + \vec{y}_j \cdot \vec{y}_j - 2\vec{x}_i \cdot \vec{y}_j$$

$\vec{x}_i \cdot \vec{y}_j \rightarrow$ `np.dot(x, y.T)` : Matrix product of $\{\vec{x}\}$ and $\{\vec{y}\}$

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$\vec{x}_i \cdot \vec{y}_j \rightarrow$ `np.dot(x, y.T)` : Matrix product of $\{\vec{x}\}$ and $\{\vec{y}\}$

$\vec{x}_i \cdot \vec{x}_i \rightarrow$ `np.einsum('ij,ij->i', x, x)` : A vector of elements $\sum_j x_{ij} x_{ij} \equiv \sum_j x_{ij}^2$

$\vec{y}_j \cdot \vec{y}_j \rightarrow$ `np.einsum('ij,ij->i', y, y)` : A vector of elements $\sum_j y_{ij} y_{ij} \equiv \sum_j y_{ij}^2$

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$\vec{x}_i \cdot \vec{y}_j \rightarrow$ `np.dot(x, y.T)`

$\vec{x}_i \cdot \vec{x}_i \rightarrow$ `np.einsum('ij,ij->i', x, x)[:, np.newaxis]`

$\vec{y}_j \cdot \vec{y}_j \rightarrow$ `np.einsum('ij,ij->i', y, y)[np.newaxis, :]`

```python
def euclidean_distance_matrix(x, y):
    x2 = np.einsum('ij,ij->i', x, x)[:, np.newaxis]
    y2 = np.einsum('ij,ij->i', y, y)[np.newaxis, :]
    xy = np.dot(x, y.T)

    return np.abs(x2 + y2 - 2. * xy)
```

[lab] Euclidean distance matrix with NumPy

- Let's open the notebook `euclidean-distance-matrix-numpy.ipynb` and check step by step what the function `euclidean_numpy` does:
  - What's the shape of the array resulting from the `np.einsum` operation? Why?
  - What's the effect of adding a new axis to an array with `[:, np.newaxis]`?
  - What's the effect of adding a new axis to an array with `[np.newaxis, :]`?
  - What's the effect of the sum `x2 + y2` in the `euclidean_trick` function?
  - Why is necessary to add a new axis?
- Run all cells and compare the execution times of the different approaches.

[lab] Profiling Python code

- Let's run together the notebook `profiling/01_line_profile.ipynb`.
- After that we run together the scripts `02_memprofiler.py` and `03_memprofiler.py`.

Cityblock distance matrix

$$\sum_k |x_{ik} - y_{jk}|$$

The trick we used for the Euclidean distance matrix doesn't work here!

F2PY is a Fortran to Python interface generator. It’s part of NumPy and also is available as a standalone command line tool `f2py` that’s installed with NumPy. It facilitates creating and building Python C/API extension modules that provide a connection between Python and Fortran.

[lab] Python binding with F2PY for a Cityblock distance matrix Fortran90 subroutine

- Let's go to the notebook `cityblock-distance-matrix-fortran.ipynb`.
    - Open a terminal and build the libraries.
    - Notice that the empty array is created with `order='F'` and that the `x` array containing the dataset is passed transposed.
    - You may try to build the libraries using the 'by hand' command described on the notebook. Make sure that you copy the `.so` files to the folder `metrics` to the directory level where the notebooks are running. Alternatively you could add the directory that contains the `.so` files to the `PYTHONPATH`.
- Run all cells and compare the execution times of the different approaches.
- While running the `%timeit` function calls, you may open a terminal and check with `top` that the function runs in multiple threads.

CFFI

CFFI (C Foreign Function Interface for Python) enables calling C code from Python without learning a third language, to be used as interface. CFFI interacts with almost any C code from Python, based on C-like declarations.

[lab] Python binding with CFFI for a Cityblock distance matrix C function

- Let's go to the folder `cityblock-cffi`.
  - Open a terminal and build the libraries following the instructions on the `README.md` file.
  - Notice that in this case two libraries are generated. A C library that contains the Cityblock distance matrix function and a python-importable library that's linked to it, which does the biding from C to Python.
  - You may create a notebook similar to the one with F2PY where you write a wrapper function for the `cbdm` C function. You can time it then and compare it to the NumPy implementation. While running the `%timeit` function calls, you may open a terminal and check with `top` that the function runs in multiple threads.

Dask is a flexible library for parallel computing in Python. It provides dynamic task scheduling optimized for computation as well as big data collections like parallel arrays, dataframes, and lists that extend common interfaces like NumPy and Pandas to larger-than-memory or distributed environments.

- `dask.delayed` can be used to parallelize custom algorithms by creating computational graphs.

```
# regular code        |   # with dask
x = func1(<args>)     |   x = dask.delayed(func1)(<args>)
y = func2(<args>)     |   y = dask.delayed(func2)(<args>)
z = func3(x, y)       |   z = dask.delayed(func3)(x, y)
                      |   #       x         y
                      |   #        \       /
                      |   #       func1  func2
                      |   #          \    /
                      |   #          func3
                      |   #            |
                      |   #            z
                      |   z.compute(scheduler='threads')
```

- `dask.delayed` can be used to parallelize custom algorithms by creating computational graphs.

```
list_delayed = [dask.delayed(func1)(<args>),
                dask.delayed(func2)(<args>),
                dask.delayed(func3)(<args>)]

dask.compute(*list_delayed, scheduler='threads')
```

- `dask.array` implements a subset of the NumPy array interface using blocked algorithms, cutting up the large array into chunks of small arrays.
- `dask.bag` parallelizes computations across a large collection of generic Python objects.
- `dask.dataframe` is a large parallel DataFrame composed of many smaller Pandas DataFrames which may live on disk for larger-than-memory computing on a single machine or a cluster.

[lab] Simple Dask graphs

- Let's run the notebook `dask/01-dask-intro.ipynb`.
  - The goal is the go over the cells and questions and annotate the code with `dask.delayed` to make the execution lazy.
  - Before running predict how much time it will take.
  - The processor on Piz Daint's 'gpu' nodes have 24 threads. Try a number of tasks higher and lower than 24 a see what happens.

[lab] Cityblock distance matrix with SciPy and Dask

- Let's run the notebook `dask/02-exercise-cityblock-distance-matrix-scipy.dask.ipynb`.
- `scipy.spatial.distance.cdist` can be used to compute the cityblock distance matrix. It is fast but doesn't use OpenMP threads. We can easily write a distributed Cityblock distance matrix function based on `cdist` with the help of Dask.
  - Same as the previous exercise, go over the cells and annotate the code to execute it lazily. This time you have to go over the notebook and find what needs to be changed.
  - While timing `cdist` check with `top` that it runs on a single thread.
  - Why is it relevant for the implementation of such distributed function that `cdist` runs on a single thread?
  - Check that when we create the list of delayed functions the execution is deferred to when `compute` is called.
- Run all cells and compare the execution times of the different approaches.
- While running the `%timeit` function calls, you may open a terminal and check with `top` that the new distributed function is runnig in multiple threads.

[lab] `dask.delayed` threads vs processes

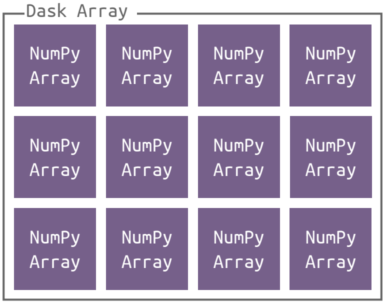
- Let’s run the notebook `dask/06-dask-processes-vs-threads.ipynb`.
  - Run the notebook and reply the questions.

Dask array

0	1	2	3
4	5	6	7
8	9	10	11
12	13	14	15

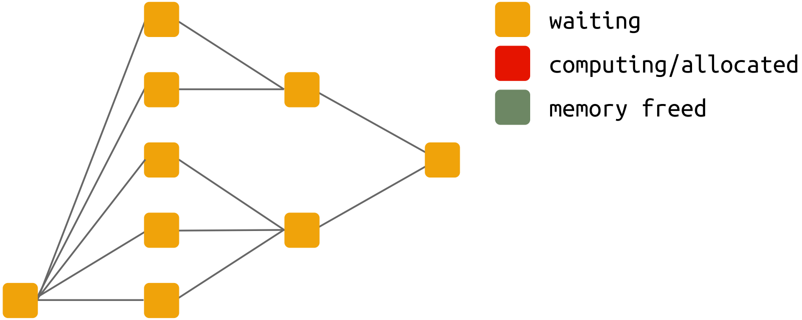
Dask array

0	1	2	3
4	5	6	7
8	9	10	11
12	13	14	15

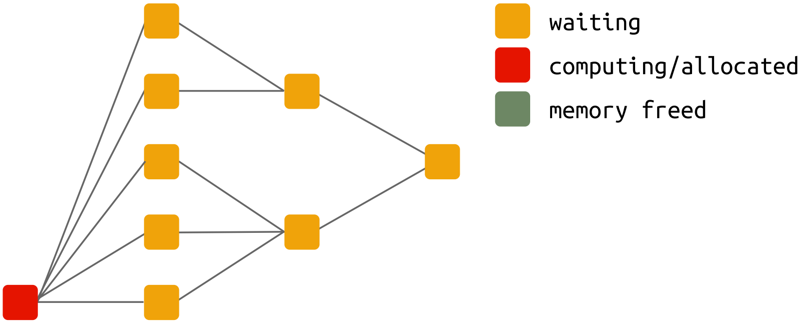


- A Dask array consists of many NumPy arrays arranged into a grid
- Those NumPy arrays may live on memory, disk or remote machines
- `dask.array` implements many of the numpy functions but in block-wise fashion and are executed through a graph.
- For equal sizes, operations on Dask arrays are in general slower than the corresponding NumPy ones.

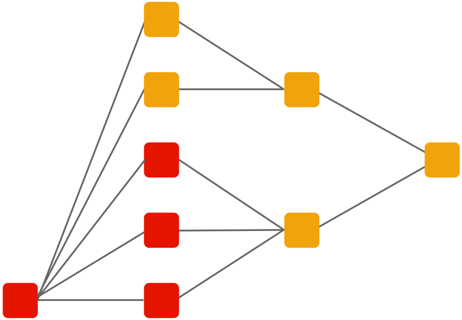
`dask.array` graph



`dask.array` graph



`dask.array` graph

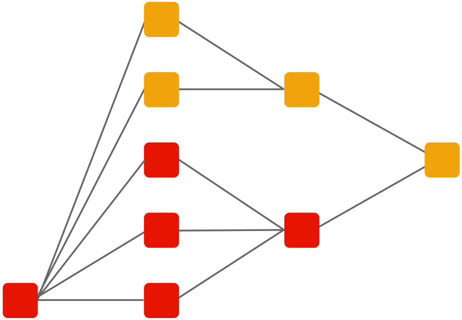


waiting

computing/allocated

memory freed

`dask.array` graph

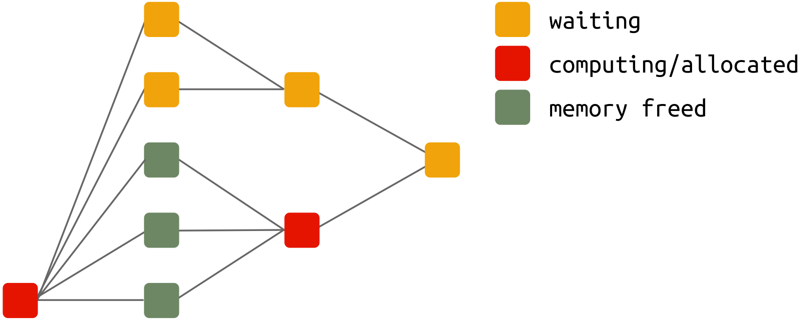


waiting

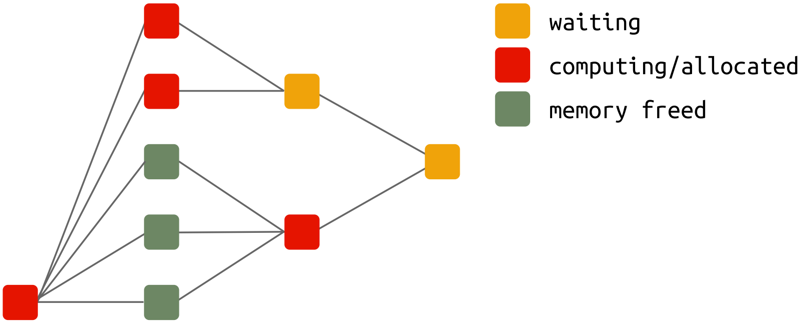
computing/allocated

memory freed

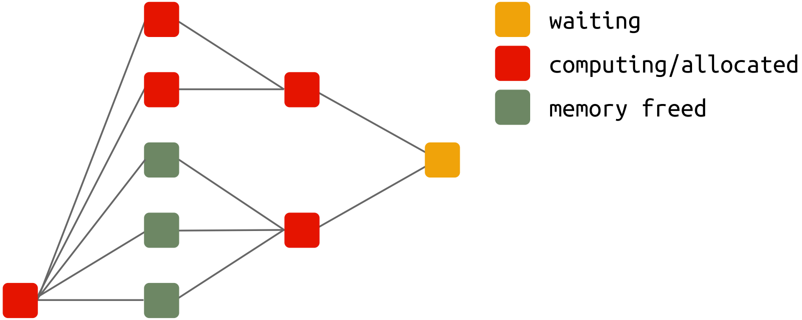
`dask.array` graph



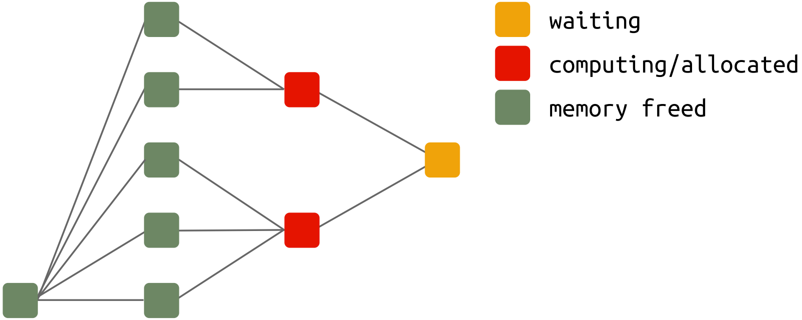
`dask.array` graph



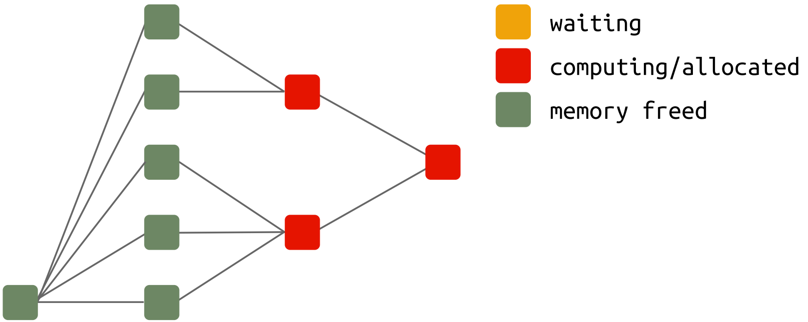
`dask.array` graph



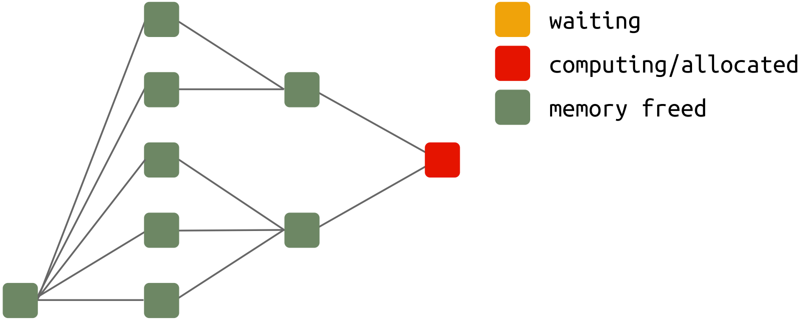
`dask.array` graph



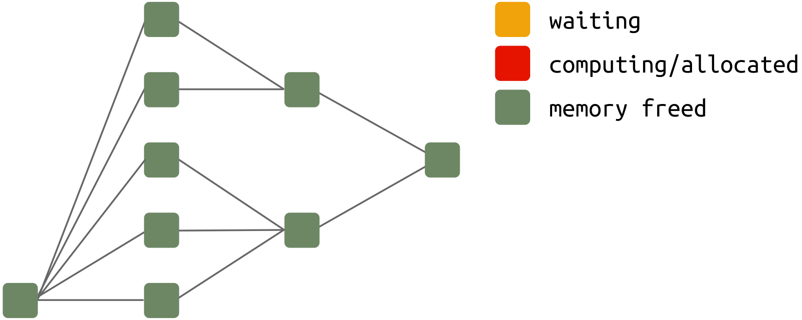
`dask.array` graph



`dask.array` graph

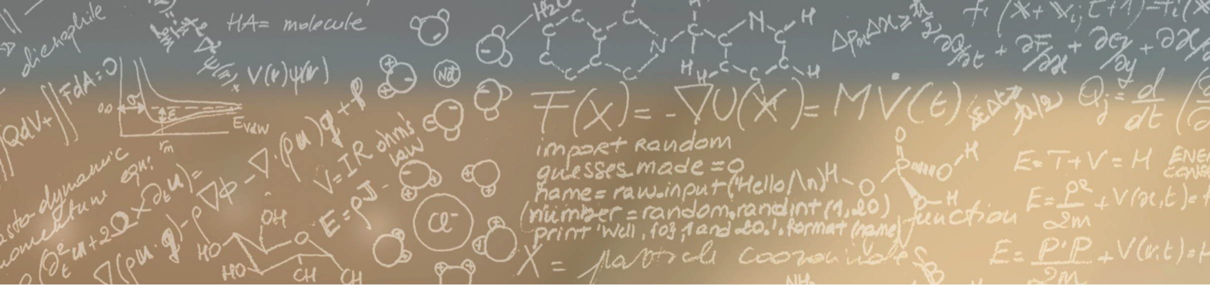


`dask.array` graph



[lab] Dask arrays

- Let's run together the notebooks `dask/03-dask-array.ipynb` and `04-dask-array-from-file.ipynb`



Thank you for your attention!

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