Parallel Analysis with Dask

> *Ever wondered why your Python script is taking so long to finish?*

Often in our daily work as researcher we process large amounts of data. The processing is usually done using utilities like `Python` or `NCL` which are, by default, not parallelized. On the other hand models used to produce the data that we analyse are obviously parallelized using libraries like `OpenMP` or `MPI`. With the increasing volume of data produced by models it is becoming more and more necessary to parallelise the processing part of data analysis. This can be easily done with `Python` and the `Dask` (https://dask.org/) library.

> *Why Dask?*

`Dask` parallelise the processing of data by (1) dividing the arrays into chunks, which can be defined by the users, and (2) interfacing with the functions of `numpy`, `pandas` and `scikit-learn` which can then operate over these chunks. Every operation is decomposed in many sub-operations which can then be parallelised across different processors. For example in order to compute an average of an array Dask will divide the array into chunks, compute the average over all the individual chunks and then merge everything together. The interesting part of this process is that Dask can be adapted to run either on your laptop or on a cluster where more processors are available. This means that machines that have a limited amount of memory (for example a 'default' macbook used at MPI may have about 8 GB of RAM) can still operate onto array which would not fit into memory since operations are performed over chunks. In other words, you will be able to open files of e.g. 64 GB on a machine that has 8 GB of RAM. For more information check out the official website https://dask.org/.

In this guide we will use `Dask` to process data of the simulations conducted over Germany in the framework of the HD(CP)^2 project. The idea is that we don't want to move/copy **any** file to compute our final result, which will be just a time series of rain rate. But first of all we need to talk about the configuration.

Configuration

When using `Python` on Mistral one is advised to use `conda` to manage the installed packages. This page https://www.dkrz.de/up/systems/mistral/programming/python explains how to install `conda` and create a virtual environment where all the packages are installed. Assuming that our environment is called `my_base` to install all the necessary packages one needs to do

```
source activate my_base
conda install -c conda-forge dask xarray dask-jobqueue ipython pandas numpy
matplotlib
pip install dask-mpi
```

Note that we used `pip` to install `dask-mpi` since this is the only way to correctly link the MPI library needed to launch a job using `dask-mpi`. Later it will become clear why this is important.

You can use `Dask` either in `ipython` or in a jupyter notebook, which I find more convenient. DKRZ created a nice script to launch a jupyter notebook on Mistral which can be found here https://www.dkrz.de/up/systems/mistral/programming/jupyter-notebook. When working with Dask it is advisable to reserve an explicit node on the shared partition so that any potential node for the computation can be easily reached through the network. This can be done specifying the account that need to be used for the allocation of the node:

```
chmod a+x start-jupyter
./start-jupyter -u m300382 -A bm0682
```

As documented on the DKRZ website this script will read some configuration from a `jupyter_preload` file located in your home on Mistral. You should use that file to load your specific virtual environment to make sure that the notebook will have all the packages that you installed. For example

```
module unload anaconda2 anaconda3 netcdf_c python
module load anaconda2/bleeding_edge
export PATH=/work/mh0731/m300382/conda_envs/my_base/bin:$PATH
source /sw/rhel6-x64/conda/anaconda2-bleeding_edge/bin/activate my_base
export PYTHONNOUSERSITE=True
```

Unfortunately `jupyterhub` cannot be used at the moment with `Dask` as the necessary packages cannot be installed in the default environment and a user defined environment cannot be loaded in `jupyterhub`.

Main difference in the processing workflow

`Dask` employs *lazy* arrays. This is a fancy way of saying that array are never loaded into memory if they are not needed for some computation or you don't tell `Dask` to load. This avoid to fill up the memory of the machine and reduce waiting time for operations. This, however, means that most of time the only informations that you can see on a dask array are its shape and type. You should avoid as much as possible to load the array into memory and define all the operations that you want to perform on an array before launching the actual computation. For example

```
import xarray as xr
dset = xr.open_dataset('dataset.nc', chunks={'time':10}) # This is opened using dask
var3 = dset['var'] + dset['var2']
mean = var3.mean(axis=1)
mean = mean.compute()
```

In a normal `Python` session that does not use the option `chunks={'time':10}` the operations will be evaluated in every row, and the last one won't make any sense. When using `dask`, instead, no operation is performed until the command `mean.compute()` is evaluated.
To start the computation usually you should use the `.compute()` or `.persist()` methods. The

second one keep the result into memory (handy!) and gives you back the control of the python shell, so it is advisable to use. To load the data into memory you can instead use the `.values` or `.load()` attribute and method, respectively.

Using a distributed scheduler in Dask on Mistral

`Dask` is loaded automatically when using `xarray` so that maybe some of your computations were already done using it without you noticing. In fact `Dask` can automatically detect the machine computation capabilities and act accordingly. However, in our case we want to be able to use `Dask` with a *distributed* configuration. In simple words `Dask` will do computations using a *scheduler*, that is a process that take care of organising the work of many *workers* which in a cluster architecture are usually equivalent to the nodes. Scheduler and workers can be started on Mistral using different strategies.
The first, easiest one, employs `dask-jobqueue`.

```
from dask_jobqueue import SLURMCluster
cluster = SLURMCluster(queue='compute2', cores=36, memory='64 GB',
                       project='bm0682',
walltime='02:00:00',local_directory='/work/mh0731/m300382/dask/',
                      job_extra=['-o
/work/mh0731/m300382/dask/LOG_worker_%j.o',
                                 '-e
/work/mh0731/m300382/dask/LOG_worker_%j.o'])
```

What `SLURMCluster` does is to prepare many scripts which are then submitted automatically to the machine to reserve as many nodes as you want. You can check what the script looks like doing `print(cluster.job_script())`. To reserve 4 nodes you just have to *scale* the cluster and connect `Dask` to it

```
cluster.scale(4)

from dask.distributed import Client
client = Client(cluster)
```

What is amazing in this is that the distributed part of `Dask` can balance the load depending on how many nodes you have available, which you can easily change even afterwards by scaling again the cluster `cluster.scale(8)`. The drawback is that one job has to be submitted per node, which may be problematic depending on the resources of your group.

> ⚠ Remember to launch the jupyter notebook using the `-A` option so that you reserved a node on the machine otherwise the notebook won't be able to connect to the workers as `mistralpp` is not in the same network.

For this reason the jobs can be launched manually using `dask-mpi`, which is the second method displayed here. In order to do that you can use the following bash script:

launch_dask_distributed.sh

```
#!/bin/bash
#=============================================================================
# =====================================
# mistral batch job parameters
#-----------------------------------------------------------------------------
#SBATCH --account=bm0682
#SBATCH --job-name=dask
#SBATCH --partition=compute2
#SBATCH --workdir=/work/mh0731/m300382/dask
#SBATCH --output=/work/mh0731/m300382/dask/LOG_dask.%j.o
#SBATCH --error=/work/mh0731/m300382/dask/LOG_dask.%j.o
#SBATCH --exclusive
#SBATCH --time=02:00:00
#SBATCH --cpus-per-task=72
#SBATCH --mem=60G

rm -r worker-*
rm scheduler.json
rm global.lock
rm purge.lock

ulimit -c 0

# Environment settings to run a MPI parallel program
# compiled with OpenMPI and Mellanox HPC-X toolkit
# Load environment
module purge
module load defaults
module load intel/17.0.6
module load openmpi/2.0.2p2_hpcx-intel14
module list
# Settings for OpenMPI and MXM (MellanoX Messaging)
# library
export OMPI_MCA_pml=cm
export OMPI_MCA_mtl=mxm
export OMPI_MCA_mtl_mxm_np=0
export MXM_RDMA_PORTS=mlx5_0:1
export MXM_LOG_LEVEL=ERROR
# Disable GHC algorithm for collective communication
export OMPI_MCA_coll=^ghc

srun -l --cpu_bind=threads --distribution=block:cyclic --propagate=STACK /work/mh0731/m300382/conda_envs/my_base/bin/dask-mpi --no-nanny
```

just make sure to create a folder, in my case `/work/mh0731/m300382/dask`, where all the log and temporary files are store, and then launch the script as you would do `sbatch -N number_nodes launch_dask_distributed.sh`. `dask-mpi` will use `MPI` library just to communicate with the nodes and start many workers and a scheduler which are then connected together. Once everything is running smoothly you should connect to the scheduler using this simple snippet in your notebook

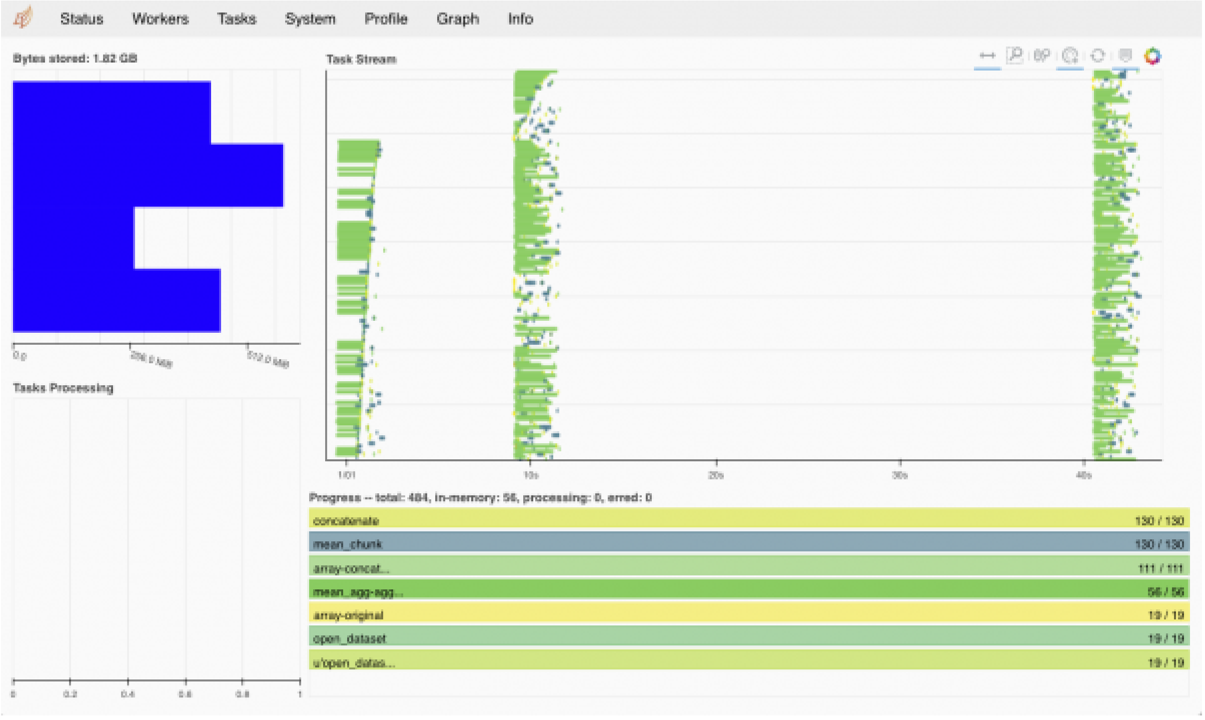
```
import json
data=[]
with open('/work/mh0731/m300382/dask/scheduler.json') as f:
    data = json.load(f)
scheduler_address=data['address']

from dask.distributed import Client
client = Client(scheduler_address)
```

Using this method only one job will be launched on the machine and you'll be more flexible in choosing a larger number of nodes.
Regardless of which method you use in the end you'll have a `client` object which `Dask` will use to distribute the computation. Once the client is started you can use the dashboard to check the status of your cluster and of the computation that you'll eventually launch. This can be usually reached on `localhost:8787` (8787 is the default port but it may vary) on your browser but since the scheduler lies on Mistral we have to make a ssh tunnel to make sure that this is locally accessible. Luckily this is quite easy:

```
ssh -N -L 8787:$1:8787 m300382@mistralpp.dkrz.de
```

where `$1` is the address of your scheduler which will be printed if you just do `client`. It should be something like `10.50.40.17`. If the address is ok when you type in your browser `http://localhost:8787` you should get something like this.



Progress -- total: 484, in-memory: 56, processing: 0, erred: 0

concatenate	130 / 130
mean_chunk	130 / 130
array-concat...	111 / 111
mean_agg-agg...	56 / 56
array-original	19 / 19
open_dataset	19 / 19
u'open_datas...	19 / 19

More info on how to use the dashboard can be found here http://docs.dask.org/en/latest/diagnostics-distributed.html.

Usage example

The example can be found on Mistral at `/work/mh0731/m300382/dask/dask_example.ipynb` (although it will probably be moved in the future).

Now that we have everything sorted out we can use the distributed computation to compute the average of rain rate over the entire domain of Germany for one of the days simulated (https://code.mpimet.mpg.de/projects/icon-lem/wiki/HDCP2_DE). We start by listing all the files that we need

```
import numpy as np
from glob import glob
import matplotlib.pyplot as plt
import xarray as xr
import dask.array as da
import pandas as pd

main_folder='/work/bm0834/k203095/ICON_LEM_DE/'
file_prefix='2d_cloud_day'
domain='DOM01'

folders=['20160529-default']
variable='rain_gsp_rate'

filenames=[]
for folder in folders:
filenames=filenames+(sorted(glob(main_folder+folder+'/DATA/'+file_prefix+'_'+domain+'*')))
```

And then read the single file and concatenate all together

```
temps=[xr.open_dataset(fn)[variable] for fn in filenames]
arrays=[da.from_array(t, chunks=(chunk_time, chunk_space)) for t in temps]
var=da.concatenate(arrays, axis=0)
```

Note again that until now **we didn't perform any computation** but just told Dask where the data should be found and what are the dimensions of the chunks. Just take one moment to appreciate how flexible and lightweight this is. Data may be scattered in different folders over the machine and without copying them we're just able to merge them and do computation, which will be parallelized automatically depending on how the data is organized.

We can start the computation by doing

```
mean = var.mean(axis=1).persist()
```

If you look into the dashboard you'll see all the chunks being processed, something like this.

dashboard.mp4

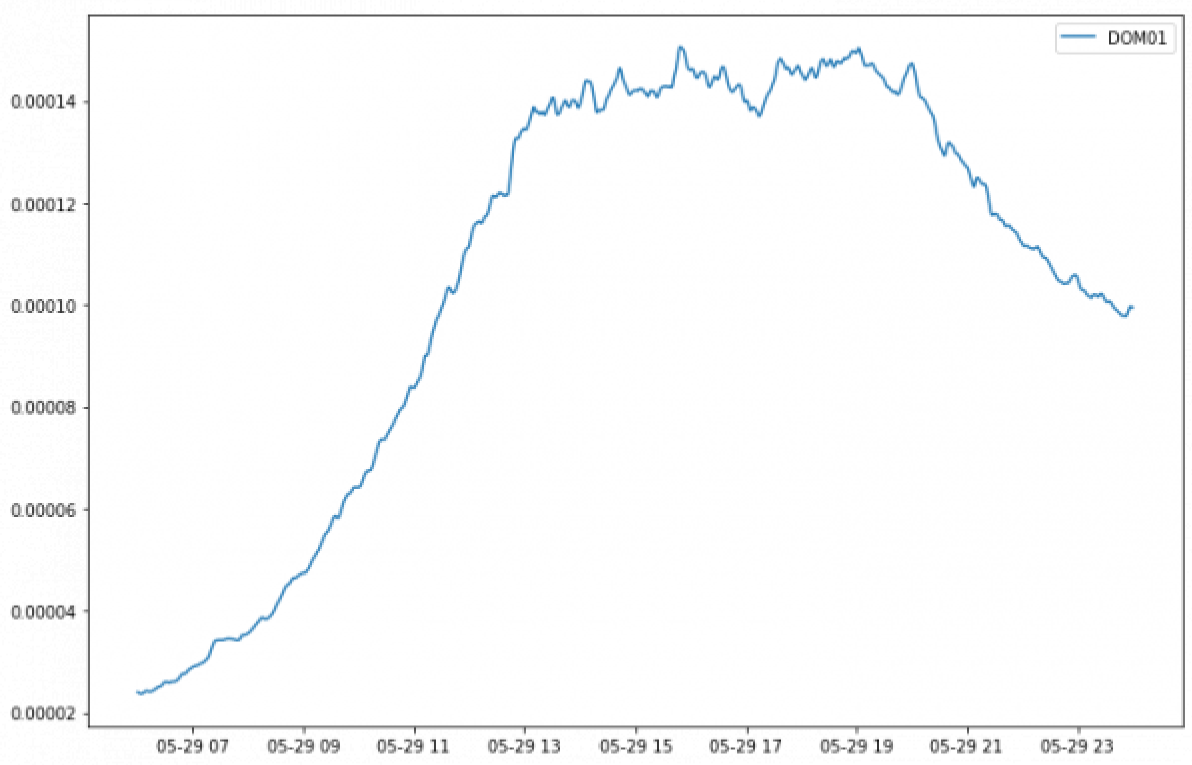
Once the computation is done you can save the result by loading into memory

```
mean = mean.compute()

array([2.4039342e-05, 2.3902332e-05, 2.3811526e-05, ..., 9.9697572e-05,
       9.9602083e-05, 9.9465833e-05], dtype=float32)
```

which we can then easily plot.

```
plt.figure(figsize=(12, 8))
time=pd.date_range(start='2016-05-29 06:00:00', end='2016-05-30 00:00:00',
periods=var.shape[0])
plt.plot(time, mean, label='DOM01')
plt.legend()
plt.show()
```



Instead of using `dask.array` we can merge the datasets using `xarray` directly but specifying the chunks size when loading the dataset. This should work most of the time and it is more flexible but fails if the input files are too large.

```
temps=[xr.open_dataset(fn, chunks={'time':50}) for fn in filenames]
dset = xr.concat(temps, dim='time')
dset[variable].mean(axis=1).compute()
```

Caveats/problems/suggestions

The first and most important:

> `Dask` is not always the answer. If your data fits into memory loading and processing the data with `Dask` will make everything slower. This is because when the dataset is not big the advantage of processing every chunk separately is overcomed by the intrinsic limited speed of transmitting the results of the computation between the workers. This is nothing new and the same problem that is encountered in parallel computation, the so-called scaling. So, as always, think before computing and processing!

`xr.open_mfdataset` can be used in place of `xr.open_dataset` to open multiple files BUT in this case every file will be loaded as single chunk with `Dask`. Thus the merged array will not be processed as one and the memory could get filled if the files are large. We do not advise to use this method.

Progress of a computation can be tracked also without the dashboard using the `progress` class of `dask.distributed`

`Dask` distributed can be run also on your laptop using the class `LocalCluster`.

`GRIB` files can be opened with `xarray` when `cfgrib` (https://github.com/ecmwf/cfgrib) is installed. Unfortunately `GRIB` files still remain `GRIB` files so they're not really flexible. So in theory you can use the method shown before also with grib files, but it will not always work. More importantly `DYAMOND` files are written in a compressed `GRIB2` format. Luckily the `eccodes` library shipped with `conda-forge` comes with the de-compression library installed but it will still hinder the performance of reading the files. So you may want to convert them to `netcdf` before analysing it. I know, it sounds stupid but it works.

> For a `xarray`-native workaround to the above issue with `grib1` output and `CDO` `stream.codes` files (found in `exp_id/log`), open `grb` files with `xr.open_mfdataset(engine=“cfgrib”)`, and rename variables based on `pd.read_fwf(stream.codes, sep=“\t”, header=None, names=[“param”,“nlev”,“varname”,“some1”,“some2”,“long_name_unit”], index_col=0)` looping over variables v and renaming based on `ds[v].attrs['GRIB_paramId']` as demonstrated in https://gist.github.com/aaronspring/bf5139a718bbd607dcb95a5222a9d0e8.

From:
https://wiki.mpimet.mpg.de/ - **MPI Wiki**

Permanent link:
https://wiki.mpimet.mpg.de/doku.php?id=analysis:pot_pourri:sapphire:dask_parallel_postprocessing

Last update: **2022/04/27 17:16**