Lecture 13:

Introduction to Parallel Computing and CUDA

Markus Hohle

University California, Berkeley

Machine Learning Algorithms

MSSE 277B, 3 Units

Fall 2025

Outline

- **Parallel Processing**
- **Using Map**
- **Using Process**
- **CUDA & PyTorch**

Outline

- Parallel Processing

- Using Map

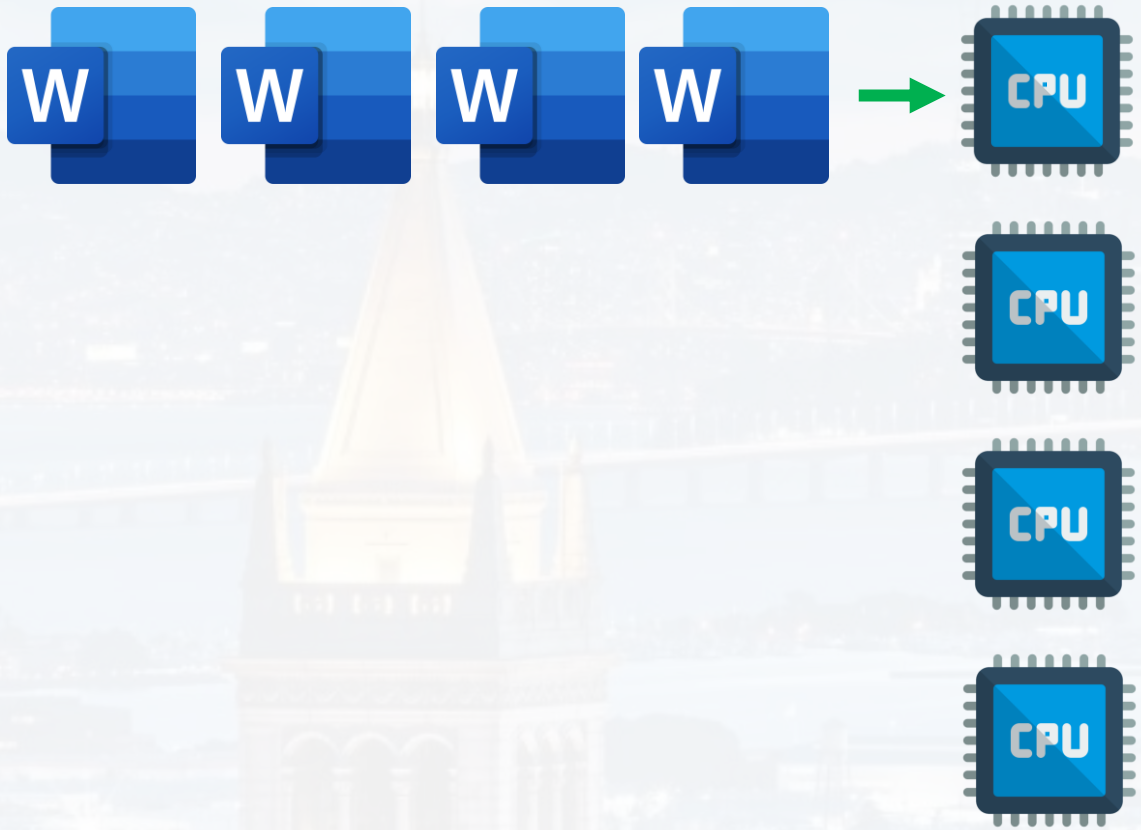
- Using Process

- CUDA & PyTorch

Parallel & CUDA:

even for moderate models and data: → computational limits

standard:



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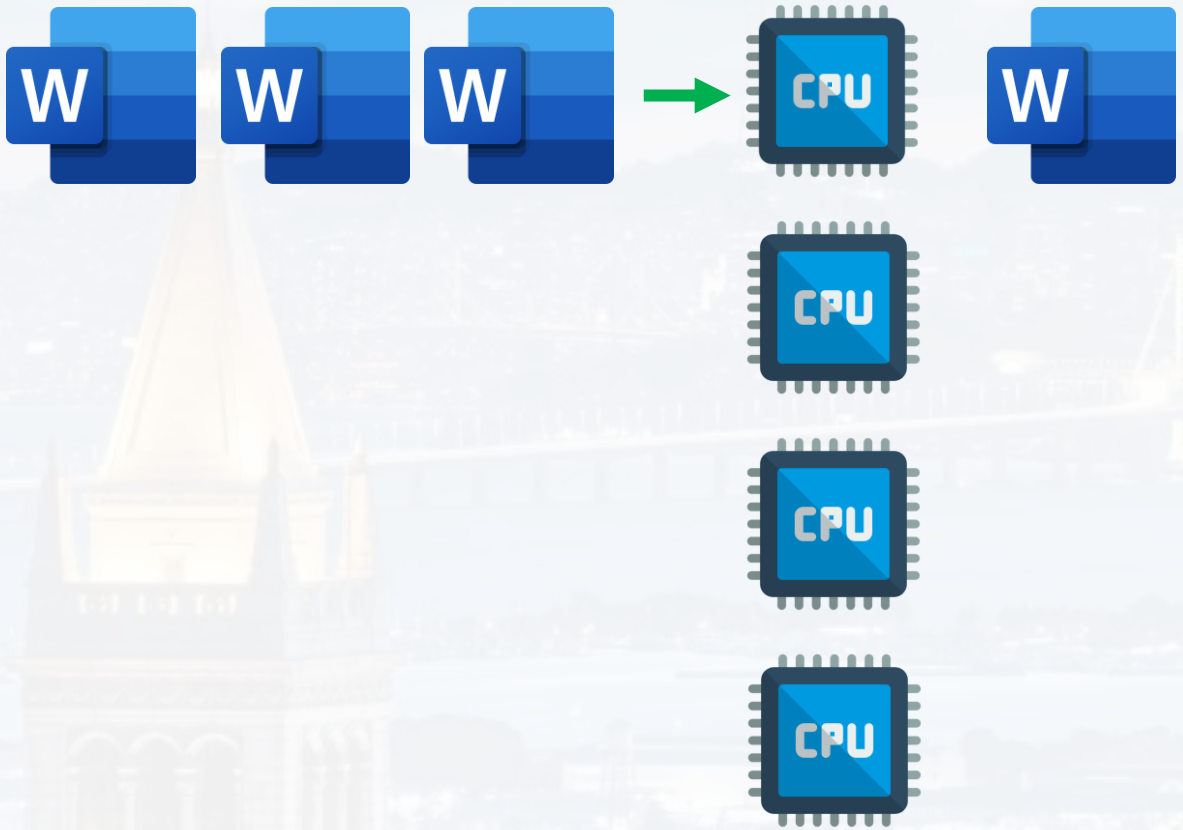

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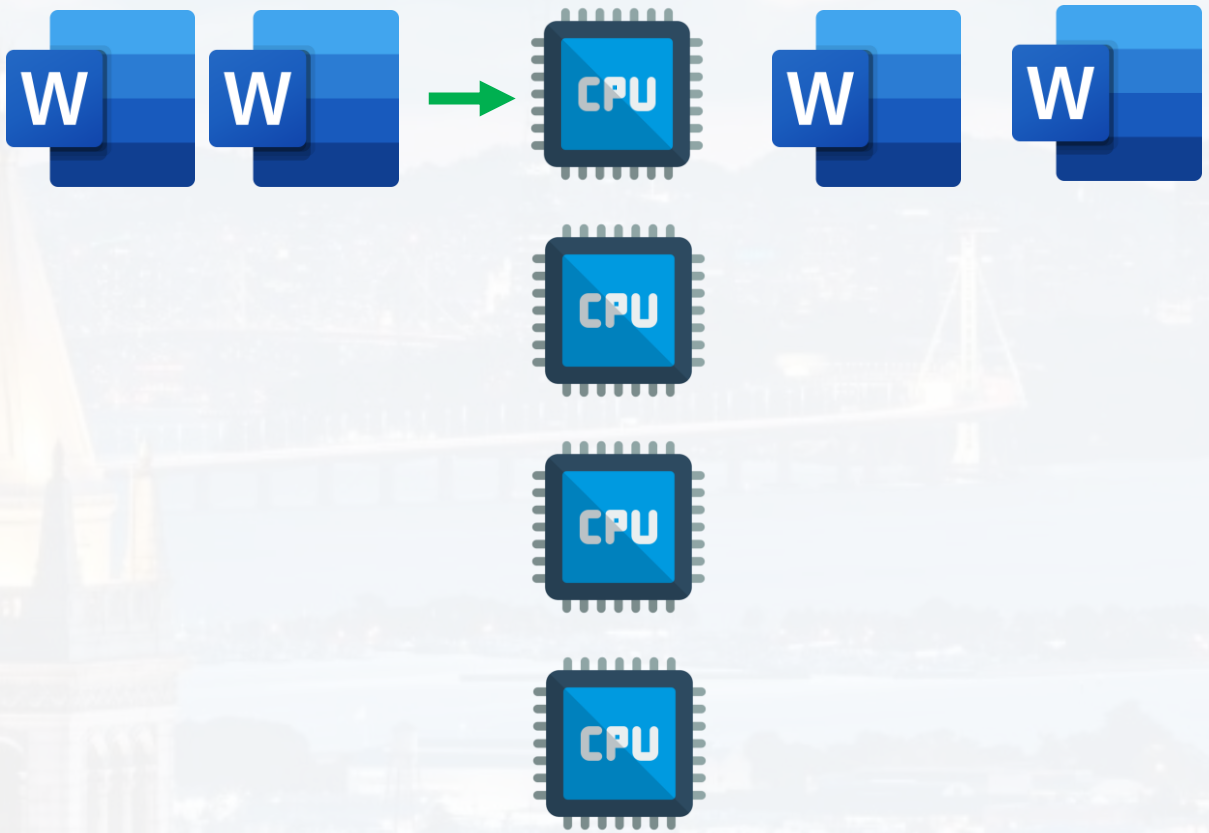

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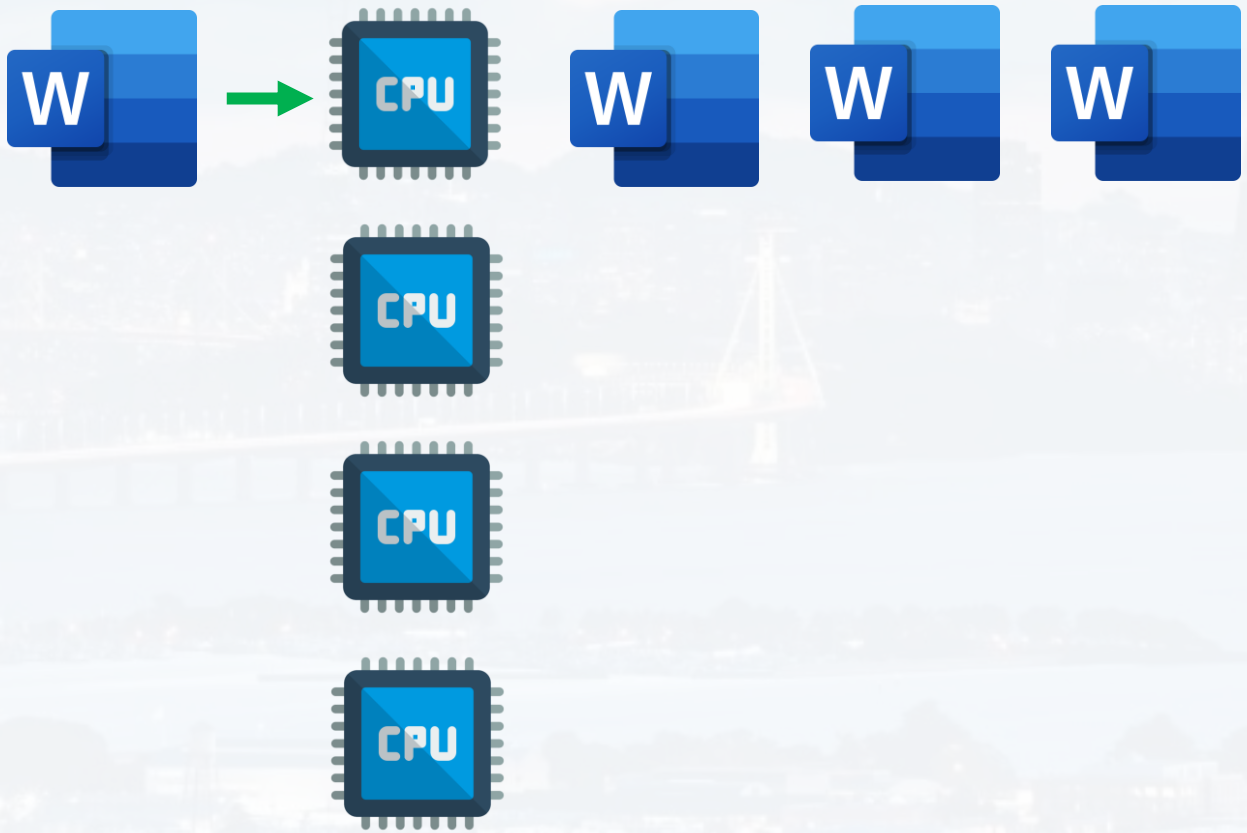

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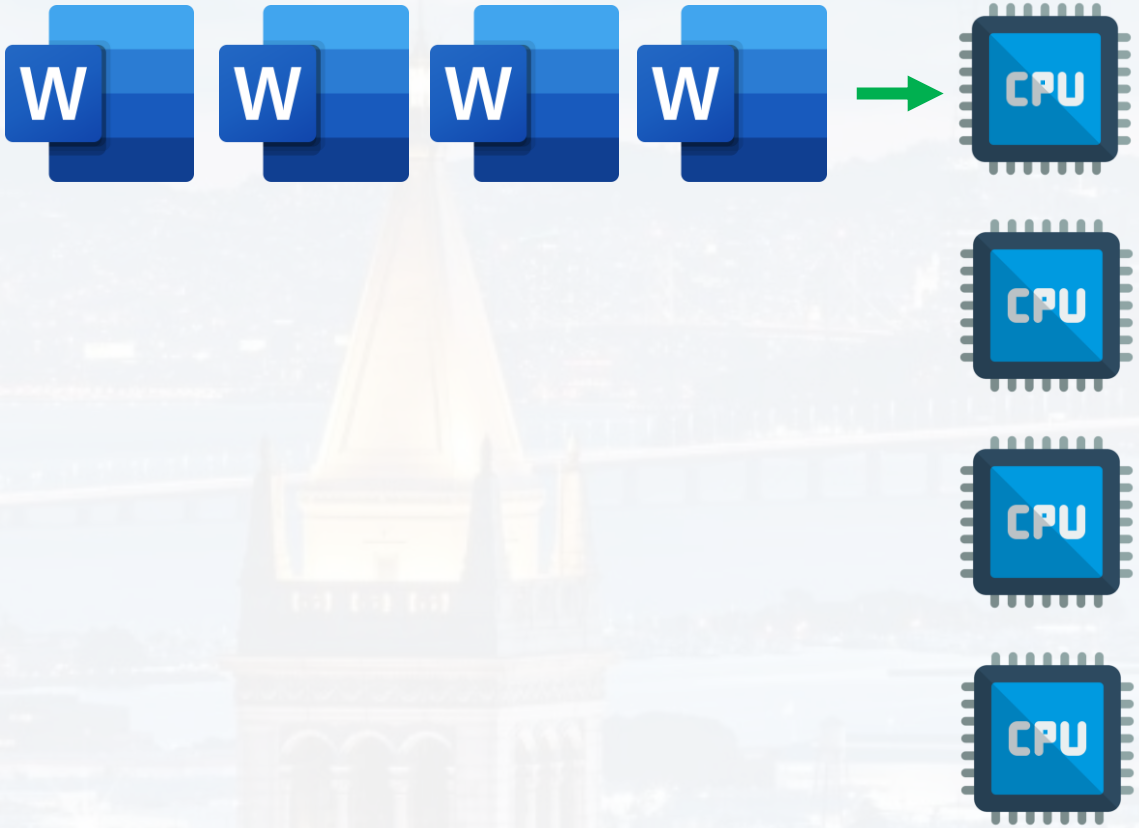
same program, but different instances:

- eg. reading different files, and perform the same analysis
- frequency grid search (different sub intervals)



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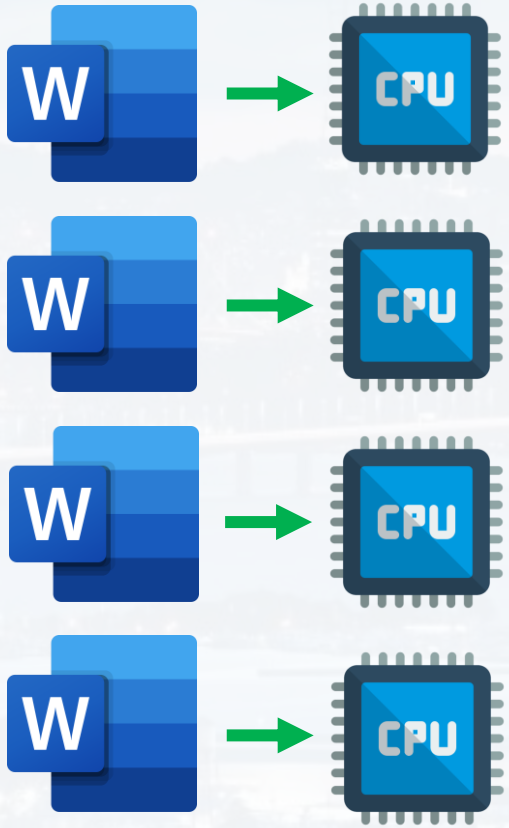

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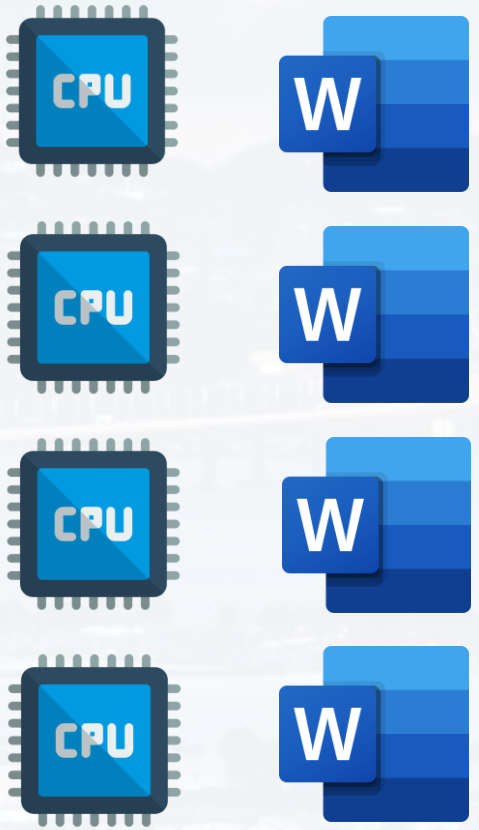

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same program, but different instances:

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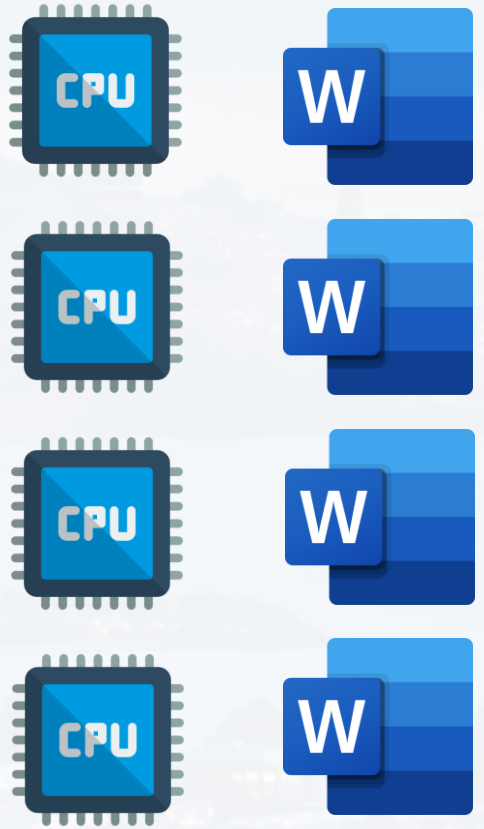
```
import multiprocessing as mp

Processes = [mp.Process(target = MyFun, args = (List,))\
             for List in list_filenames]
```

```
for p in Processes:
        p.start()
```

allocating processes to CPUs

```
for p in Processes:
        p.join()
```

running and finishing processes



Parallel & CUDA:

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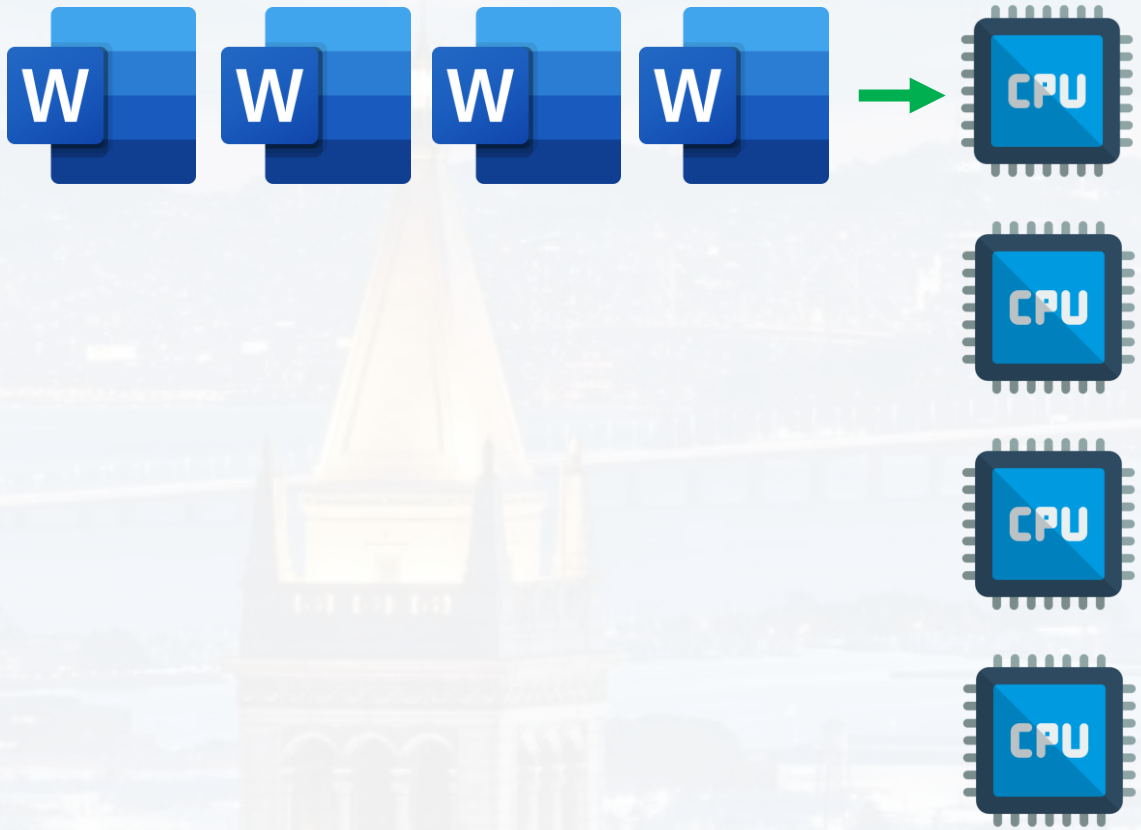
parallelizing the process itself: - eg. a non vectorized function in a for loop



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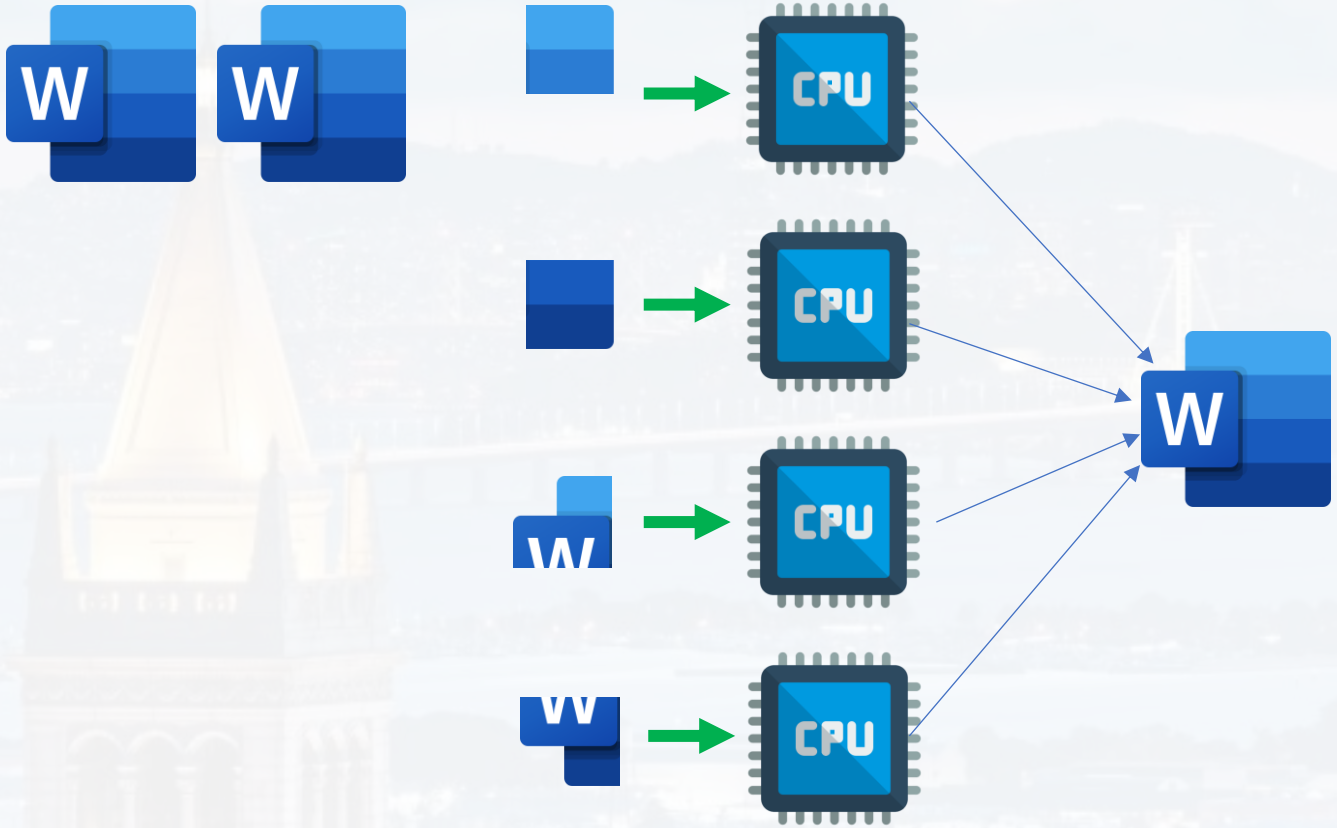

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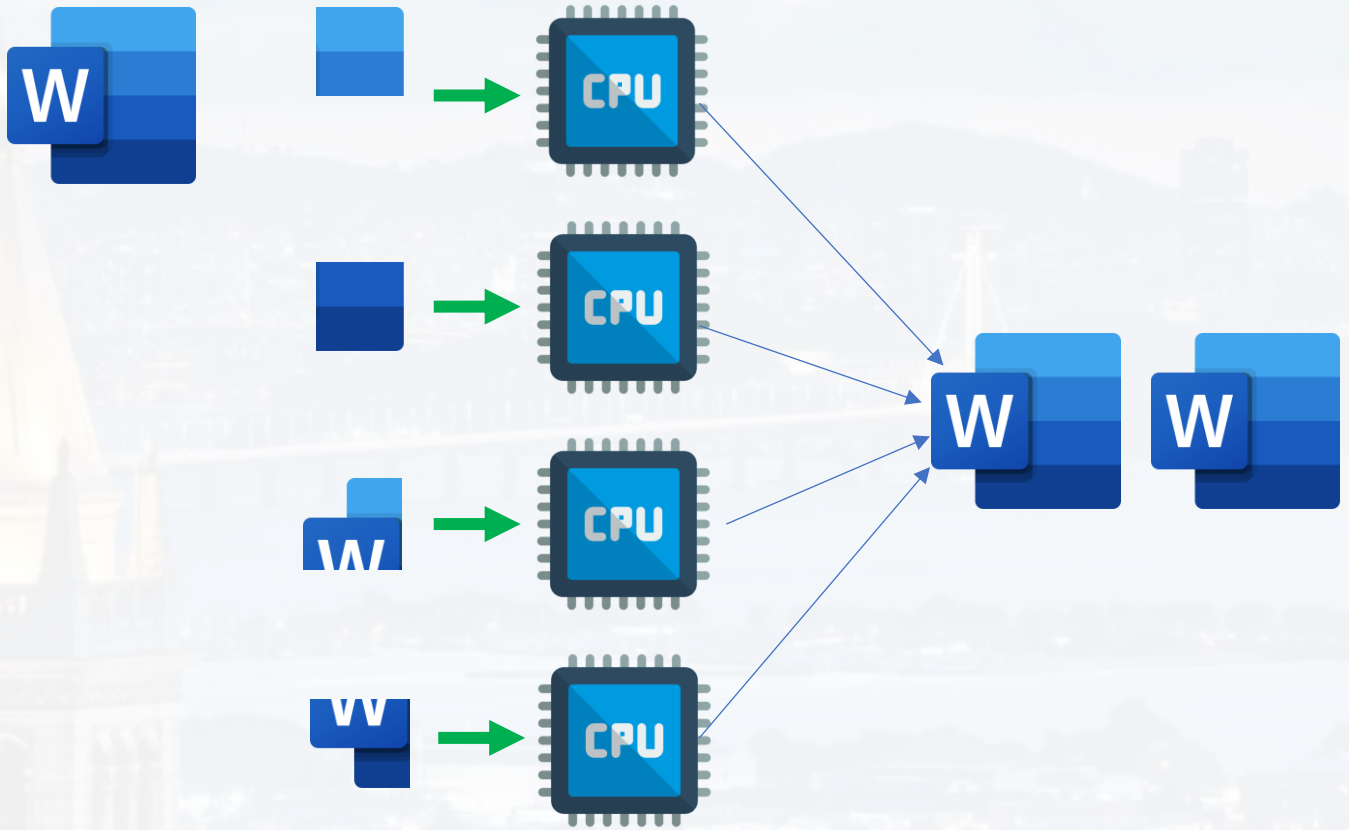

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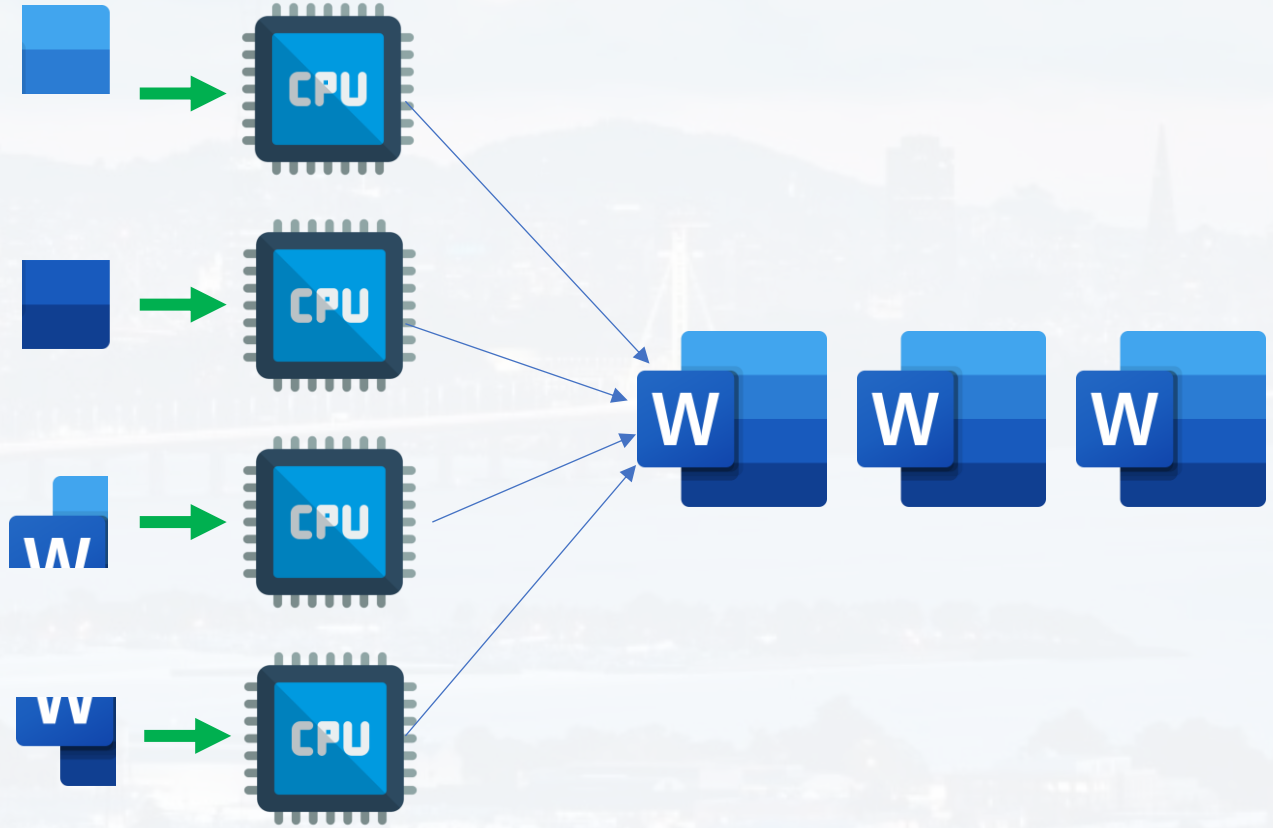
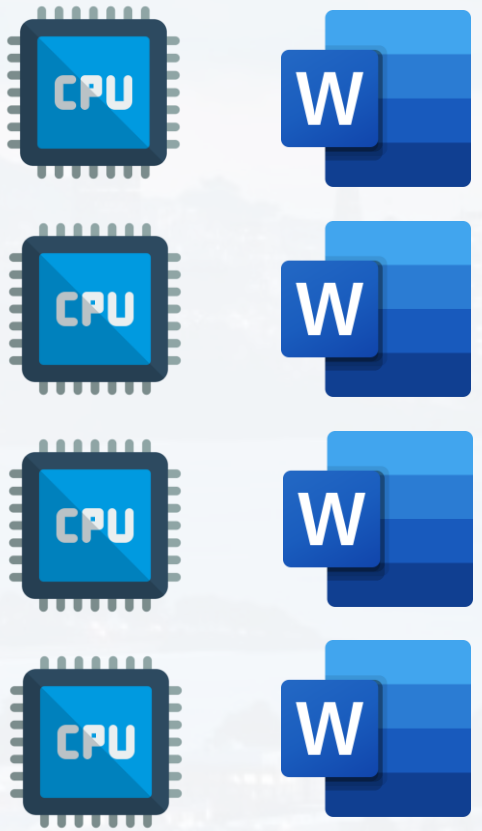


even for moderate models and data: → computational limits

parallelizing the process itself: - eg. a non vectorized function in a for loop

```
import multiprocessing as mp


with mp.Pool(processes = len(list_filenames)) as pool:
        All = pool.map(MyFun, list_filenames)

return All
```

combined output

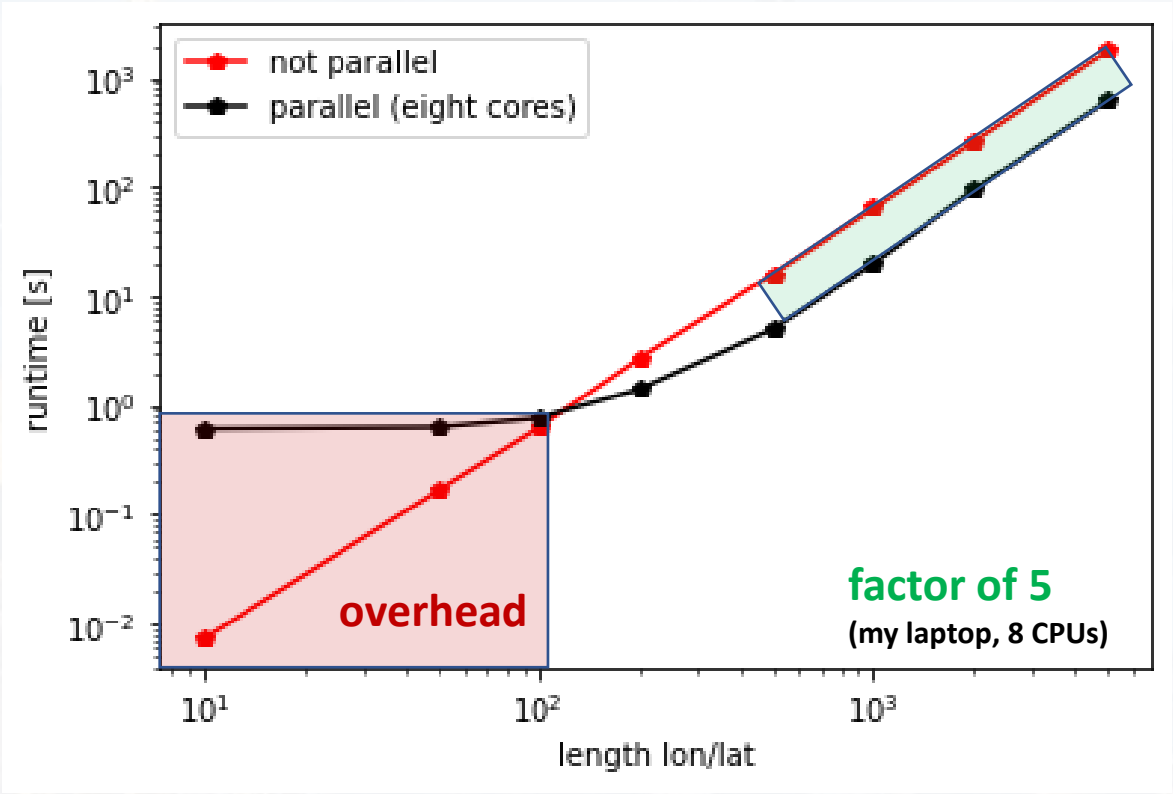


Parallel & CUDA:

parallelizing the process itself: - eg. a non vectorized function in a for loop

same program, but different instances: - eg. reading different files, and perform the same analysis
- frequency grid search (different sub intervals)

note: preparing and coordinating the different processes takes time → **overhead**

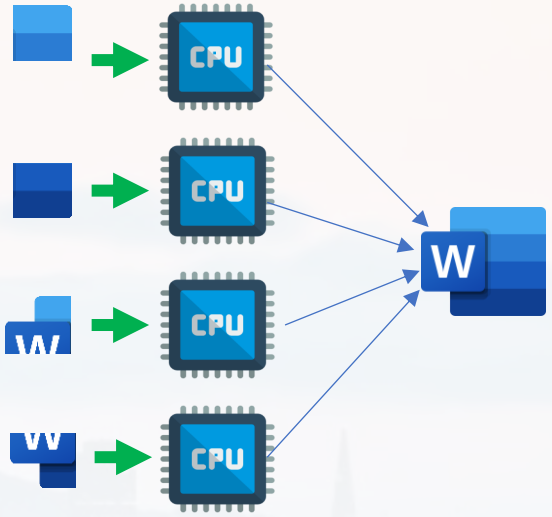


parallelizing two nested for loops

Outline

- Parallel Processing
- **Using Map**
- Using Process
- CUDA & PyTorch

example1: reading excel files, extracting some content and combing it.




```
import multiprocessing as mp
```

a) writing a function that does one thing at the time

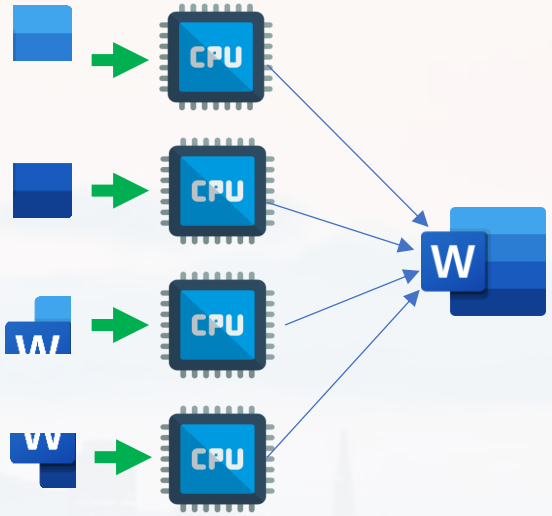
```
def MyFun(filename: str) -> np.array:
    #reads huge data set
    data = pd.read_excel(filename)
    return np.array(data.time)
```

b) writing a **main** function that calls the first function using **map**

```
def Parallel(self, list_filenames: list) -> list:

        with mp.Pool(processes = len(list_filenames)) as pool:
                All = pool.map(MyFun, list_filenames)

        return All
```

Parallel & CUDA:

example1: reading excel files, extracting some content and combing it.



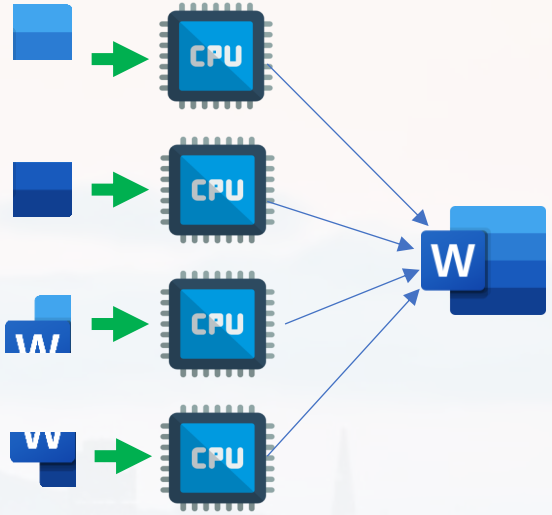
check out the function Map.py

```
from Map import *

globals()['MyFun'] = my_timer(MyFun)

MAP                = Parallel_MAP()
```

```
In [7]: out  = MyFun(list_filenames[0])
Total runtime: 26.93699999997625 seconds

In [8]: out1 = MAP.Serial(list_filenames)
Total runtime: 151.76500000001397 seconds

In [9]: out2 = MAP.Parallel(list_filenames)
Total runtime: 49.14100000000326 seconds
```

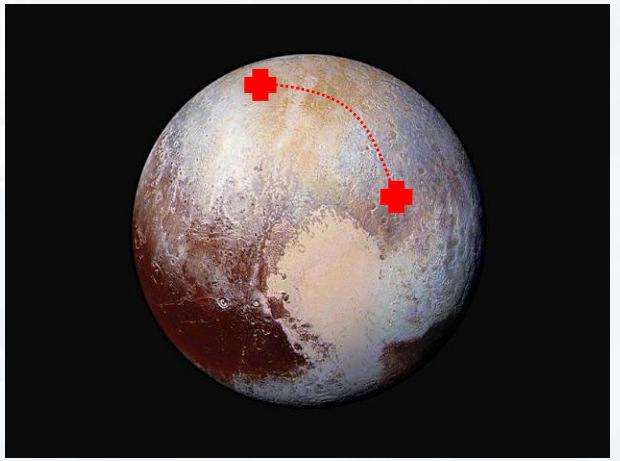
example2: parallelizing a non vectorized function.

`geodesic` from `GeoPy` can take only **one pair of coordinates** at the time




```
coords1 = (lon[i],lat[i])
coords2 = (lon[j],lat[j])

d       = geodesic(coords1, coords2).m

distance[i,j] = d
distance[j,i] = d
```

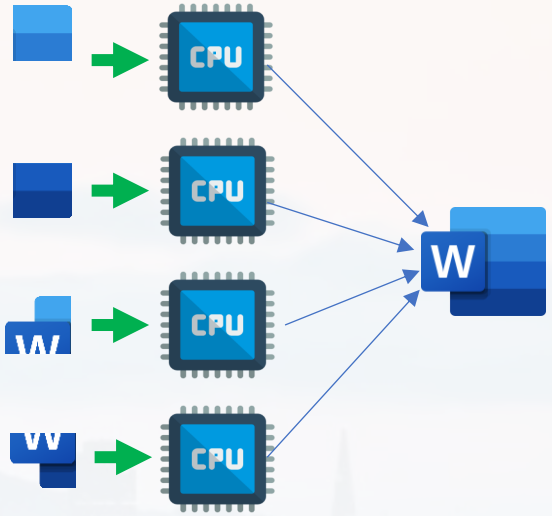
an example of a non vectorized method



$$d^2s = R^2dv^2 + R^2sin^2v\,d\phi^2$$

example2: parallelizing a non vectorized function.

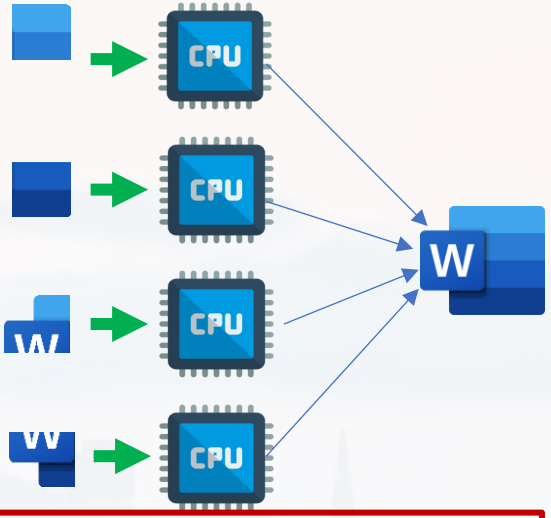
a) writing a function that does one thing at the time




```
from geopy.distance import geodesic

def calculate_distance(args):

    i, j, lat, lon = args

    coords1 = (lon[i], lat[i])
    coords2 = (lon[j], lat[j])

    d = geodesic(coords1, coords2).m

    return i, j, d
```

example2: parallelizing a non vectorized function.

b) writing a **main** function that calls the first function using **map**




```
import numpy as np
from multiprocessing import Pool
from calculate_distance import calculate_distance

def DistanceGeoParallel(lat, lon):

        n        = len(lat)
        distance = np.zeros((n, n))

        args_list = [(i, j, lat, lon) for i in range(n) for j in range(i+1, n)]

        with Pool() as pool:
            results = pool.map(calculate_distance, args_list)

        for i, j, d in results:
            distance[i, j] = d
            distance[j, i] = d

        return distance
```

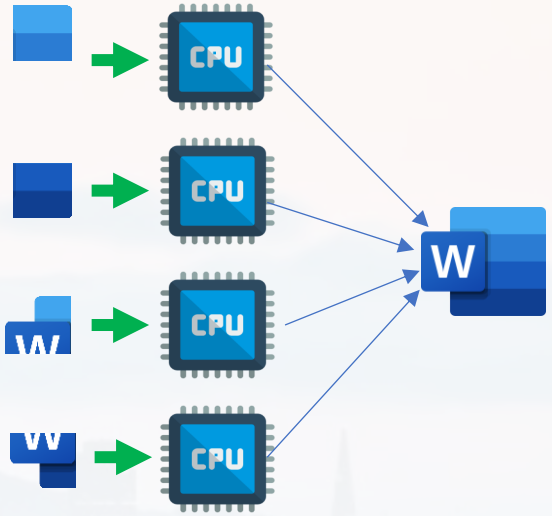
calling subroutine

creating list of all variables and indices **(be careful: j starts at i+1 for symmetry reasons!)**

actual parallelization

check out:

```
from multiprocess import cpu_count
cpu_count()
```



- calling CPUs via `Pool` **itself takes time** and creates **overhead**
  → only effcient for larger runtimes
- processes have to be **independent** *(i.e. calculating distances, linear algebra, see also AI)*
- functions have to be **independent** *(function A **is not** a subroutine of B)*
- processes should not contain `lambda` or `map`

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- Parallel Processing
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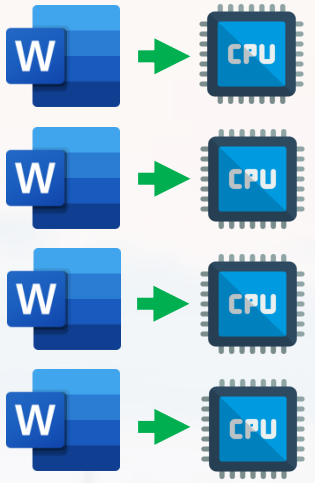
example: reading excel files and saving them as csv.




```
import multiprocessing as mp
```

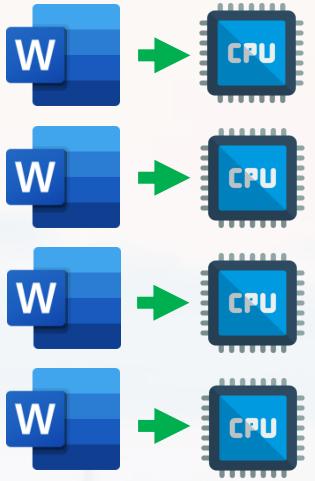
a) writing a function that does one thing at the time

```
def MyFun(filename: str):
    #reads & saves huge data set
    data = pd.read_excel(filename)
    data.to_csv('Data_set_' + str(time.monotonic()).replace('.','-') + '.csv'))
```

adding a time stamp to the output file name

b) writing a **main** function that calls the first function using Process

example: reading excel files and saving them as csv.



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for p in Processes:
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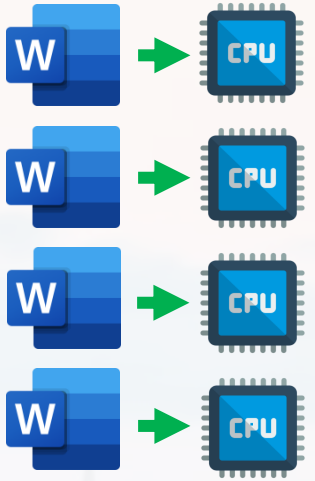
running and finishing processes

example: reading excel files and saving them as csv.



check out the function `Process.py`

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out  = MyFun(list_filenames[0])
Pro.Serial(list_filenames)
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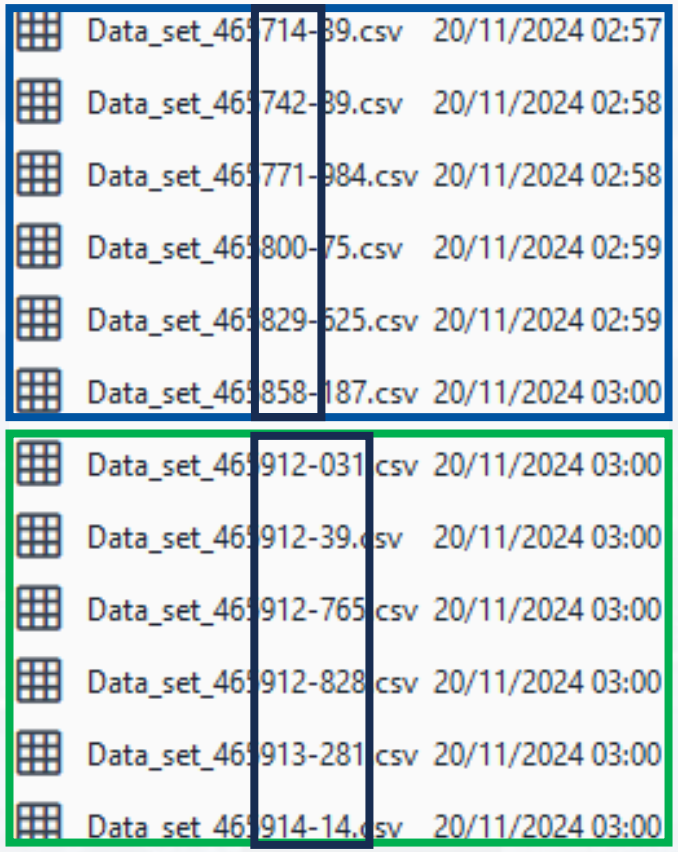
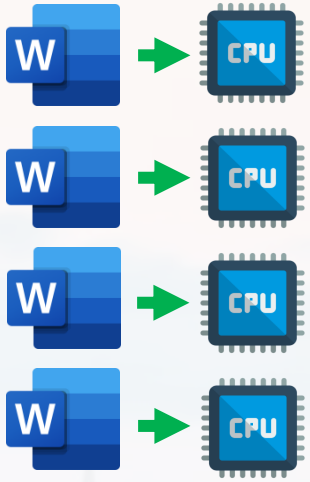
```
Total runtime: 27.703000000003772 seconds
Total runtime: 172.03099999995902 seconds
Total runtime: 57.407000000000652 seconds
```

example: reading excel files and saving them as csv.



every 30 seconds

every 0.3 seconds

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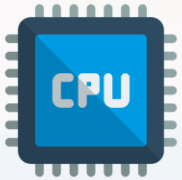
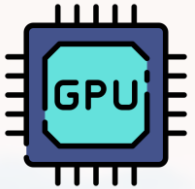
Parallel & CUDA:



training AI

→ mainly matrix operations
→ GPUs are a lot better at it!



CUDA is the link of your GPU to Python (PyTorch)

check, if graphic card is on list

check your graphics device:

→ Windows command shell prompt

→ type `nvidia-smi`

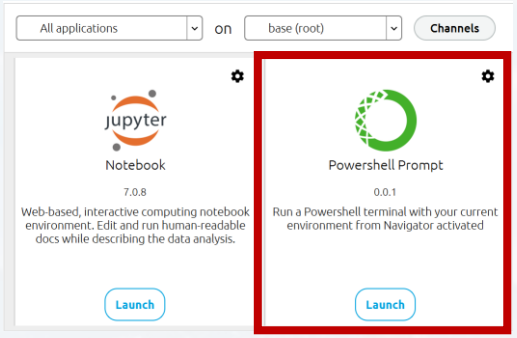
→ press *Enter*

```
(base) C:\Users\MMH_user>nvidia-smi
Tue Jan 16 20:09:26 2024
+---------------------------------------------------------------------------------------+
| NVIDIA-SMI 537.79                 Driver Version: 537.79       CUDA Version: 12.2     |
|-----------------------------------------+----------------------+----------------------+
| GPU  Name                     TCC/WDDM  | Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |         Memory-Usage | GPU-Util  Compute M. |
|                                         |                      |               MIG M. |
|=========================================+======================+======================|
|   0  NVIDIA GeForce MX450         WDDM  | 00000000:01:00.0 Off |                  N/A |
| N/A   49C    P0              N/A /   9W |      0MiB /  2048MiB |      0%      Default |
|                                         |                      |                  N/A |
+-----------------------------------------+----------------------+----------------------+

+---------------------------------------------------------------------------------------+
| Processes:                                                                            |
|  GPU   GI   CI        PID   Type   Process name                            GPU Memory |
|        ID   ID                                                             Usage      |
|=======================================================================================|
|  No running processes found                                                           |
+---------------------------------------------------------------------------------------+
```

Installing CUDA

conda environment




```
C:\WINDOWS\System32\Win
(base) PS C:\Users\MMH_user>
```

```
C:\WINDOWS\System32\Win
(base) PS C:\Users\MMH_user> conda create --name CUDAenv
```

```
C:\WINDOWS\System32\Win
(base) PS C:\Users\MMH_user> conda activate CUDAenv
```

```
(base) PS C:\Users\MMH_user> conda activate CUDAenv
(CUDAenv) PS C:\Users\MMH_user> conda install -c pytorch pytorch
Channels:
 - pytorch
```

Installing CUDA

cuda toolkit

```
(CUDAenv) PS C:\Users\MMH_user> conda install -c anaconda cudatoolkit
```

check libraries

→ type: `conda list`

```
(CUDAenv) PS C:\Users\MMH_user> conda list
# packages in environment at C:\Users\MMH_user\anaconda3\envs\CUDAenv:
#
# Name                    Version                   Build  Channel
blas                      1.0                         mkl
bzip2                     1.0.8                h2bbff1b_6
ca-certificates           2024.7.2             haa95532_0
cudatoolkit               11.8.0               hd77b12b_0
expat                     2.6.2                hd77b12b_0
filelock                  3.13.1           py312haa95532_0
intel-openmp              2023.1.0          h59b6b97_46320
```

Installing CUDA

usually, a few libraries are missing

check again graphics card:	type in anaconda	**nvidia-smi**
check libraries:	type in anaconda	**conda list cudnn** **conda list cudatoolkit** **conda list torch**
	if not:	**conda install <library>**
check Python:	type in anaconda	**python** **import torch** **torch.cuda.is_available()**
open Spyder	run in Spyder	**pip install** (see the commented line in `CheckMyCuda.py`)

Installing CUDA

usually, a few libraries are missing

CheckMyCuda.py

```
import torch

def test_cuda():
    print("PyTorch version: ", torch.__version__)
    print("CUDA version: ", torch.version.cuda)
    print("CUDA Available: ", torch.cuda.is_available())
    if torch.cuda.is_available():
        print("Number of GPUs: ", torch.cuda.device_count())
        print("GPU Name: ", torch.cuda.get_device_name(0))

if __name__ == "__main__":
    test_cuda()
```

```
PyTorch version:  2.3.1+cu118
CUDA version:  11.8
CUDA Available:  True
Number of GPUs:  1
GPU Name:  NVIDIA GeForce MX450
```

Parallel & CUDA:

The key part in PyTorch is to set all matrices and the model **to the device (CPU or GPU)**

```
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print("Using device:", device)
```

```
In [13]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
    ...: print("Using device:", device)
Using device: cuda
```

Congratulation! If you see this, you are ready to go!

Parallel & CUDA:

The key part in PyTorch is to set all matrices and the model **to the device (CPU or GPU)**

```
In [13]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
    ...: print("Using device:", device)
Using device: cuda
```

Torch objects like **`model`** or **`torch.tensor`** have the property **`.to`**

```
TrainX = torch.tensor(TrainX, dtype = torch.float32)
TrainY = torch.tensor(TrainY, dtype = torch.float32)
```

turning `numpy array` into `torch.tensor`

```
TrainX = TrainX.to(device)
TrainY = TrainY.to(device)
```

allocating objects to the device

```
model  = model.to(device)
```

Parallel & CUDA:

The key part in PyTorch is to set all matrices and the model **to the device (CPU or GPU)**

```
In [13]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
    ...: print("Using device:", device)
Using device: cuda
```

When running the training, we need to **synchronize** between GPU (for training the model) and CPU (for everything else)…

```
torch.cuda.synchronize()

        #training loop
        for epoch in range(n_epochs):
                outputs = model(TrainX)

                ... #do stuff...

torch.cuda.synchronize()
```

Parallel & CUDA:

The key part in PyTorch is to set all matrices and the model **to the device (CPU or GPU)**

```
In [13]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
    ...: print("Using device:", device)
Using device: cuda
```

When running the training, we need to **synchronize** between GPU (for training the model) and CPU (for everything else)…

…and later detach the model from the GPU

```
PredY = model(TestX).detach().to('cpu').numpy()
```

check out script **HowToRun.py**

that runs the **same LSTM model** for Keras and PyTorch

```
n_neurons  = 100
n_epochs   = 200
dt_past    = 30
dt_futu    = 10
n_features = 1
n_sample   = 1

n_stack    = 3
```

number of stacked LSTM

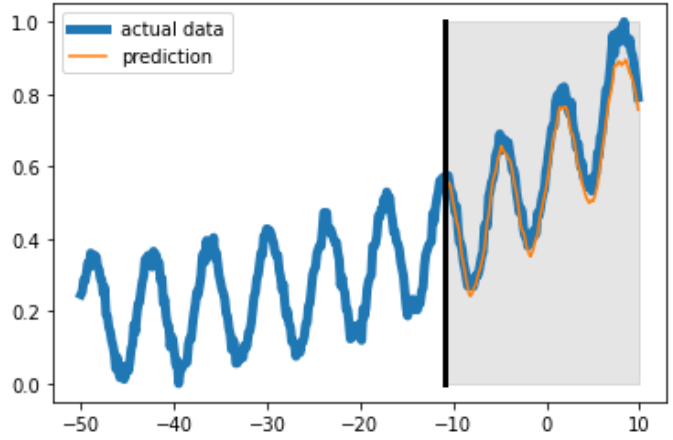
Parallel & CUDA:

check out script **HowToRun.py**

that runs the **same LSTM model** for Keras and PyTorch

```
n_neurons  = 100
n_epochs   = 200
dt_past    = 30
dt_futu    = 10
n_features = 1
n_sample   = 1

n_stack    = 3
```



Lenovo T14, NVIDIA GeForce MX450:

Keras LSTM (CPU):	**300 sec**
PyTorch (CPU):	11 sec
PyTorch (GPU):	**3 sec**

Thank you very much for your attention!