EPFL

HPC for numerical methods and data analysis

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Matrices and vectors in Python and MPI

Exercise I Matrices in Python

Find an efficient way in Python to assign the following matrix:

$$M = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{bmatrix},$$

without entering manually each element (*hint*: create two row vectors and then combine them to form a matrix).
Suitably use the Python commands to:

a) extract the element in the first row, third column of A;

b) extract the entire second row of A;

c) extract the first two columns of A;

d) extract the vector containing all the elements of the second row of A except for the third element.

Exercise II Function in Python

We want to compute the function $f(x) = (\sqrt{1+x} - 1)/x$ for different values of x in a neighborhood of 0. We first notice that $f(x)$ can be equivalently written as $f(x) = 1/(\sqrt{1+x} + 1)$ and also as $f(x) = 1/2 - x/8 + x^2/16 - 5x^3/128 + o(x^4)$.
Create three function handles representing the above definitions of $f(x)$ (*hint*: the term $o(x^4)$ can be neglected in the computation) and, for each function handle,

a) evaluate $f(x)$ at $X = [10^{-10}\, 10^{-12}\, 10^{-14}\, 10^{-16}]$ using a `for` loop;

b) evaluate $f(x)$ at the same points given in a) using Python vector algebra;

c) display the results and comment on the importance of *round-off errors* for this example.

Exercise III Matrix-vector multiplication in Python

a) Consider the multiplication of a matrix $A \in \mathbb{R}^{m \times n}$ with a vector $v \in \mathbb{R}^n$. Write a Python file containing a script that:

- creates a matrix of dimension $m \times n$
- creates a vector of dimenstion n
- define a function that computes Av by using two nested loops

Exercise IV Matrix-vector multiplication with NumPy

a) Consider the same operation as in the previous exercice, the multiplication of a matrix $A \in \mathbb{R}^{m \times n}$ with a vector $v \in \mathbb{R}^n$. Compute matrix-vector multiplication by using numpy library:

- create a matrix of dimension $m \times n$, a vector of dimenstion n
- define a function that computes Av by using two nested loops
- compare the performance obtained for different values of m and n between the two nested loops code and the code using numpy library and draw a plot displaying the obtained performance

Exercise V Hello world with Python and MPI
Execute the following simple code on 4 processors several times.

```
from mpi4py import MPI
import numpy as np

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
print("I am rank = ", rank )
```

To execute this code, do

```
$ mpiexec -n 4 python script.py
```

Observe the order in which the prints take place.