Open Data Science

WORKSHOP

13. - 16. June 2022

Prague, Czech Republic

Co-financed by the Connecting Europe Facility of the European Union

CTU CZECH TECHNICAL UNIVERSITY IN PRAGUE

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High performance computing in python

Jun 13, 2021: 13:30 - 15:00

https://bit.ly/3HfEim1

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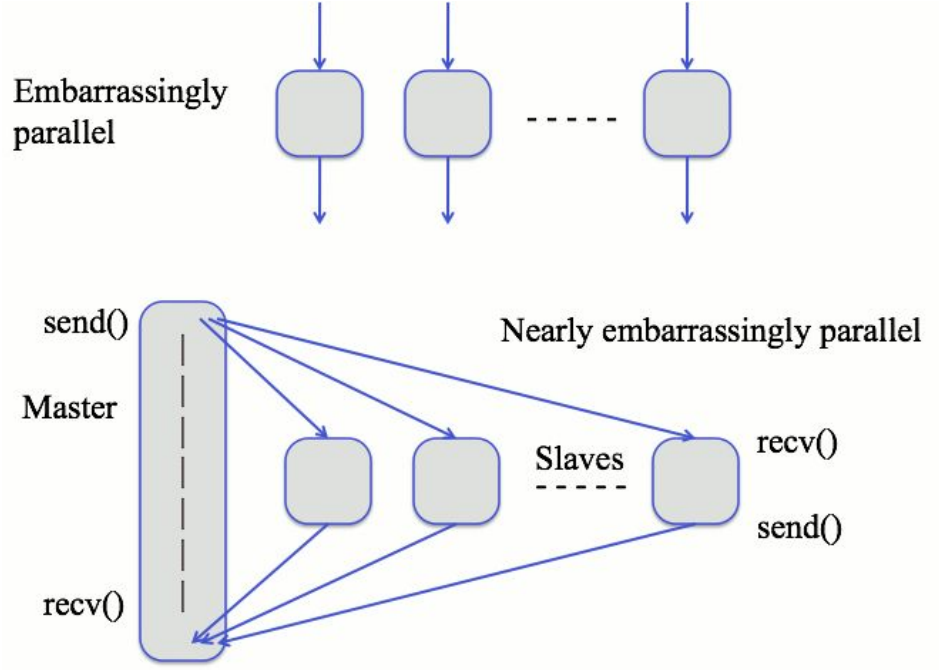
Introduction to ODSE datasets in Python - Outline

- Embarrassingly parallel problems
- Possibilities to optimize a raster processing workflow
- BLAS and LAPACK implementations
- Optimizing a temporal array reduction and a numeric operations

Embarrassingly parallel problems

- Can be divided into completely **independent** parts,
- Requires none or very little communication,
- **Nearly embarrassingly parallel** is an embarrassingly parallel computation that requires initial data to be distributed and final results to be collected in some way



Source: Embarrassingly Parallel Computations & Embarrassingly Parallel Algorithms

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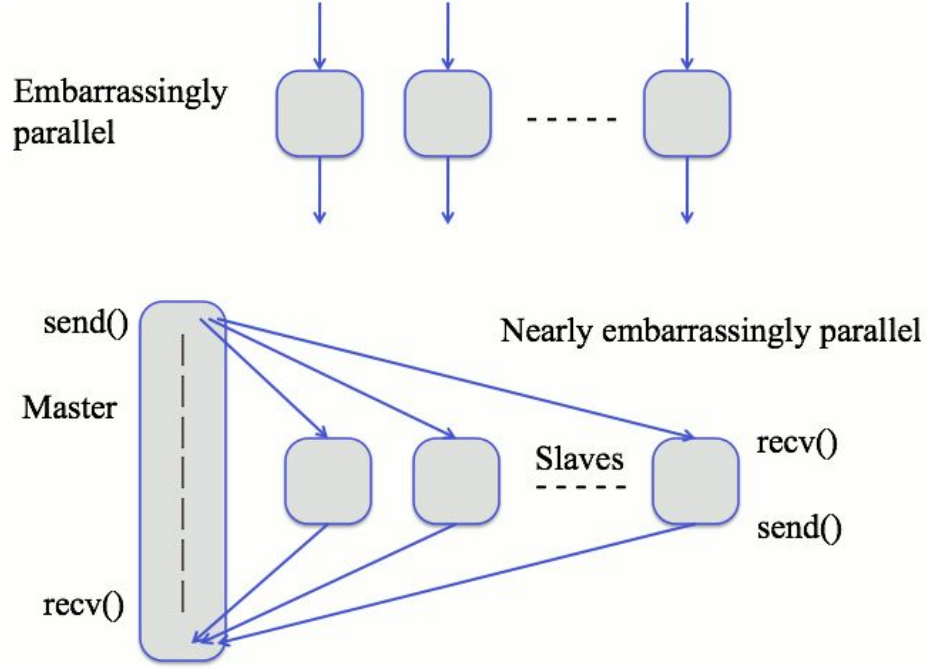

Raster processing

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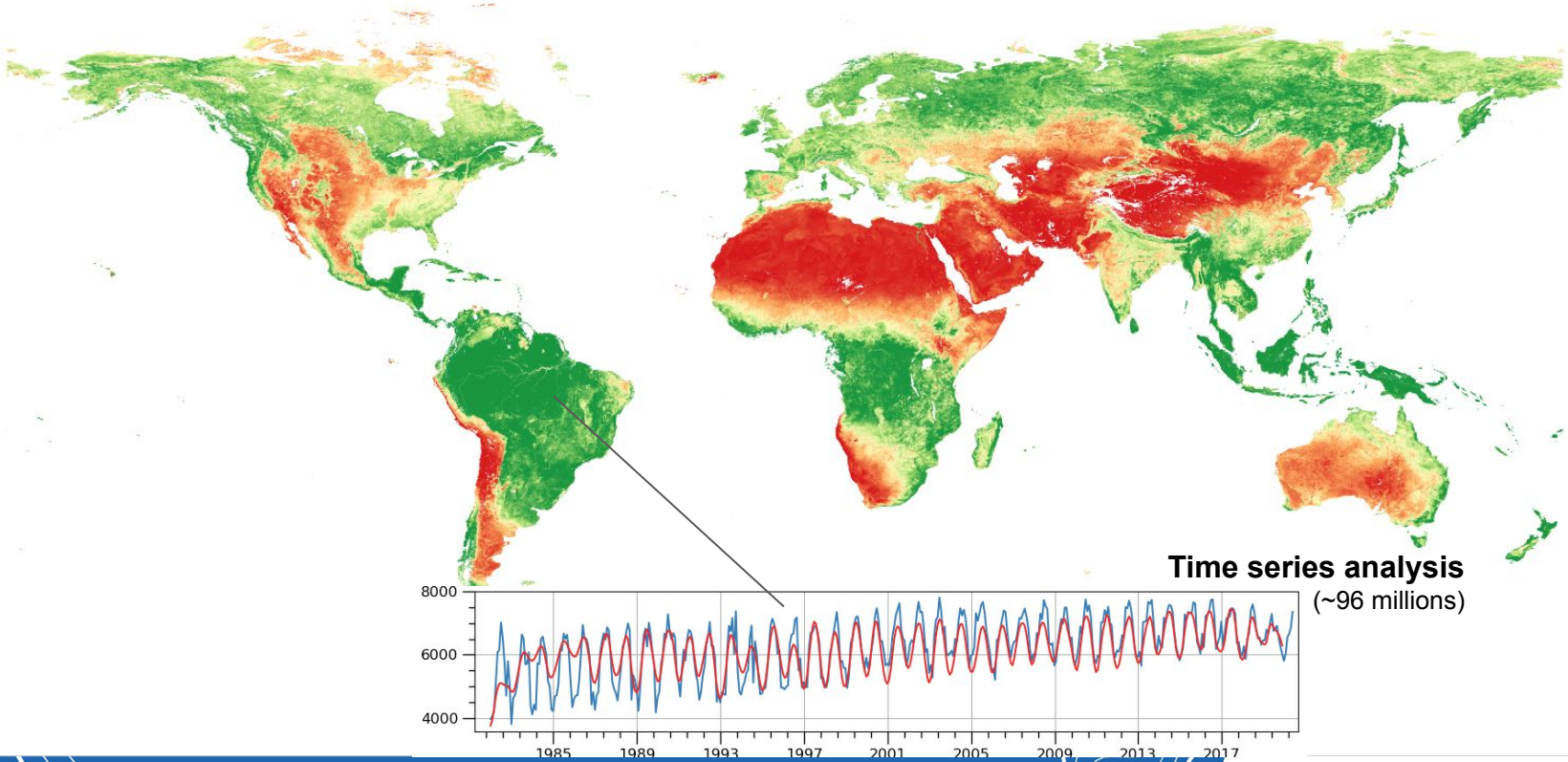
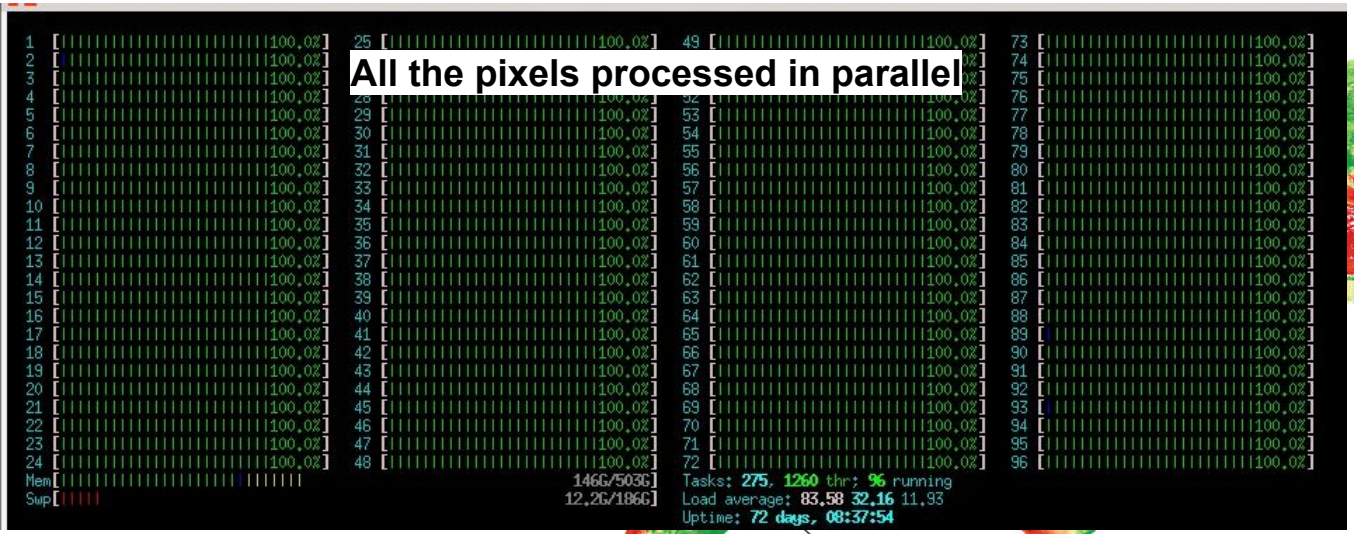
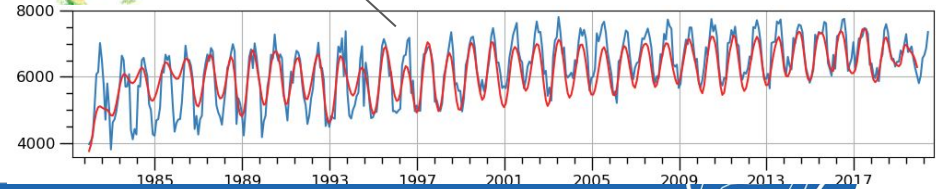
Embarrassingly parallel problems



Time series analysis
(~96 millions)

Embarrassingly parallel problems





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Possibilities to optimize a raster processing workflow

- Increase the number of CPU cores
- Improve data transfer speed
- Improve the processing code (new algorithms/functions):

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- Improve the processing code (new algorithms/functions):
  - Drop-in replacement
  - New code implementation

BLAS and LAPACK implementations

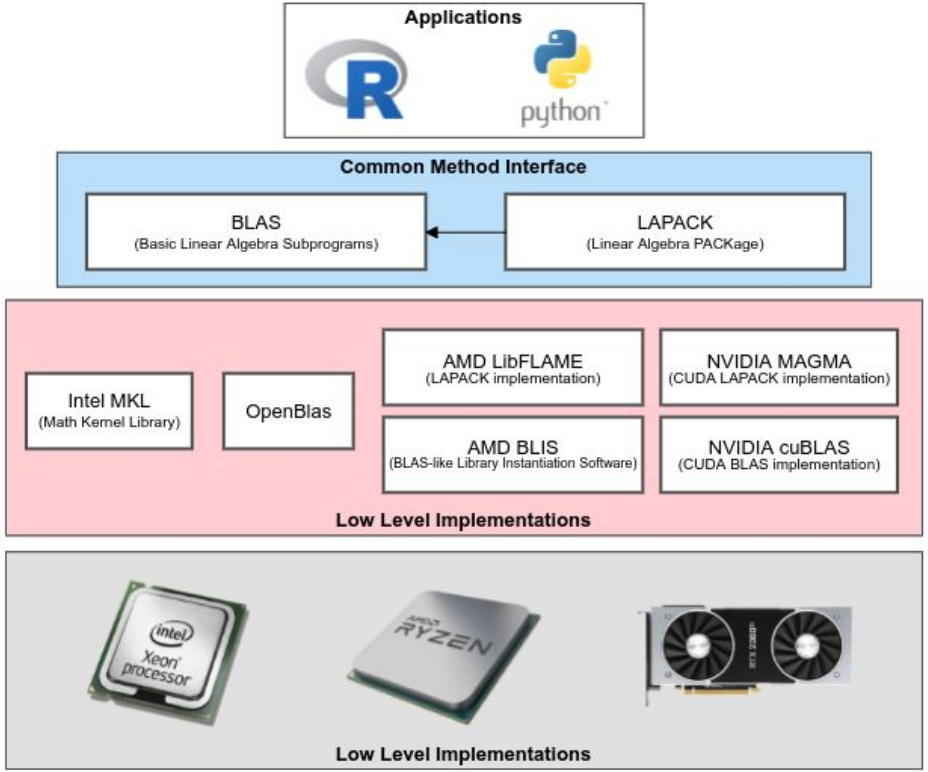
BLAS (Basic Linear Algebra Subprograms) is a C library to provide a set of routines for basic vector and matrix operations

LAPACK (Linear Algebra PAckage) Fortran 90 library to solve linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, singular value problems and the associated matrix factorization

Level 1 BLAS

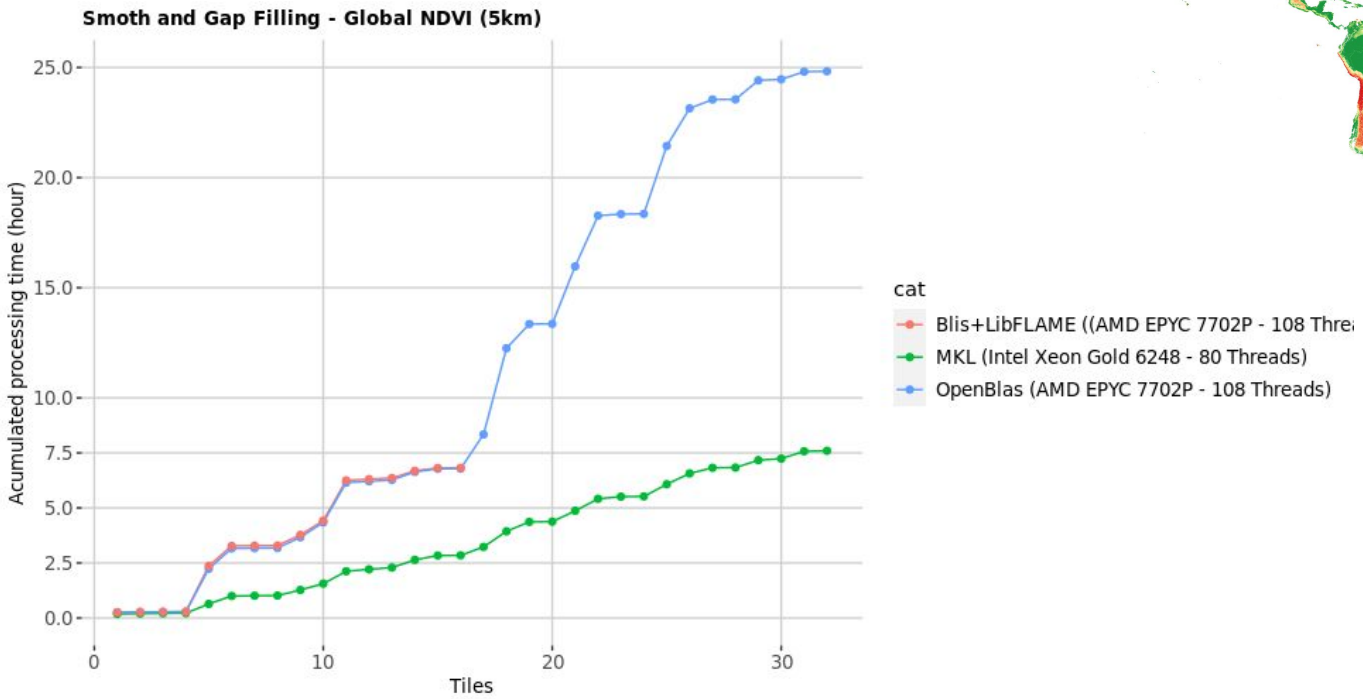
	dim	scalar	vector	vector	scalars	5-element array		prefixes
SUBROUTINE xROTG (					A, B, C, S)		Generate plane rotation	S, D
SUBROUTINE xROTMG(					D1, D2, A, B,	PARAM)	Generate modified plane rotation	S, D
SUBROUTINE xROT (	N,		X, INCX,	Y, INCY,	C, S)		Apply plane rotation	S, D
SUBROUTINE xROTM (	N,		X, INCX,	Y, INCY,		PARAM)	Apply modified plane rotation	S, D
SUBROUTINE xSWAP (	N,		X, INCX,	Y, INCY)			$x \leftrightarrow y$	S, D, C, Z
SUBROUTINE xSCAL (	N,	ALPHA,	X, INCX)				$x \leftarrow \alpha x$	S, D, C, Z, CS, ZD
SUBROUTINE xCOPY (	N,		X, INCX,	Y, INCY)			$y \leftarrow x$	S, D, C, Z
SUBROUTINE xAXPY (	N,	ALPHA,	X, INCX,	Y, INCY)			$y \leftarrow \alpha x + y$	S, D, C, Z
FUNCTION xDOT (	N,		X, INCX,	Y, INCY)			$dot \leftarrow x^T y$	S, D, DS
FUNCTION xDOTU (	N,		X, INCX,	Y, INCY)			$dot \leftarrow x^T y$	C, Z
FUNCTION xDOTC (	N,		X, INCX,	Y, INCY)			$dot \leftarrow x^H y$	C, Z
FUNCTION xxDOT (	N,		X, INCX,	Y, INCY)			$dot \leftarrow \alpha + x^T y$	SDS
FUNCTION xNRM2 (	N,		X, INCX)				$nrm2 \leftarrow \|x\|_2$	S, D, SC, DZ
FUNCTION xASUM (	N,		X, INCX)				$asum \leftarrow \|re(x)\|_1 + \|im(x)\|_1$	S, D, SC, DZ
FUNCTION IxAMAX(	N,		X, INCX)				$amax \leftarrow 1^{st} k \ni \|re(x_k)\| + \|im(x_k)\| = max(\|re(x_i)\| + \|im(x_i)\|)$	S, D, C, Z

BLAS and LAPACK implementations



BLAS and LAPACK implementations

MKL is 3x faster then OpenBlas



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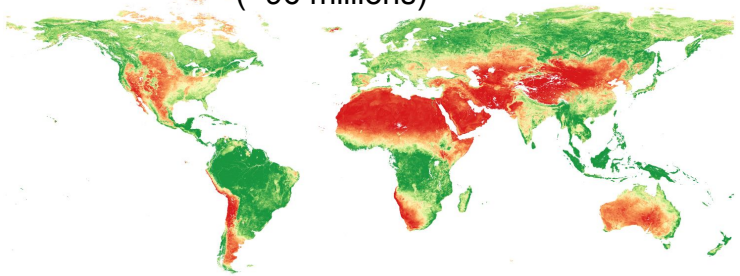
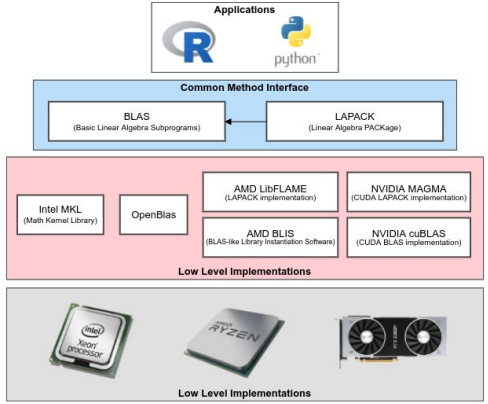


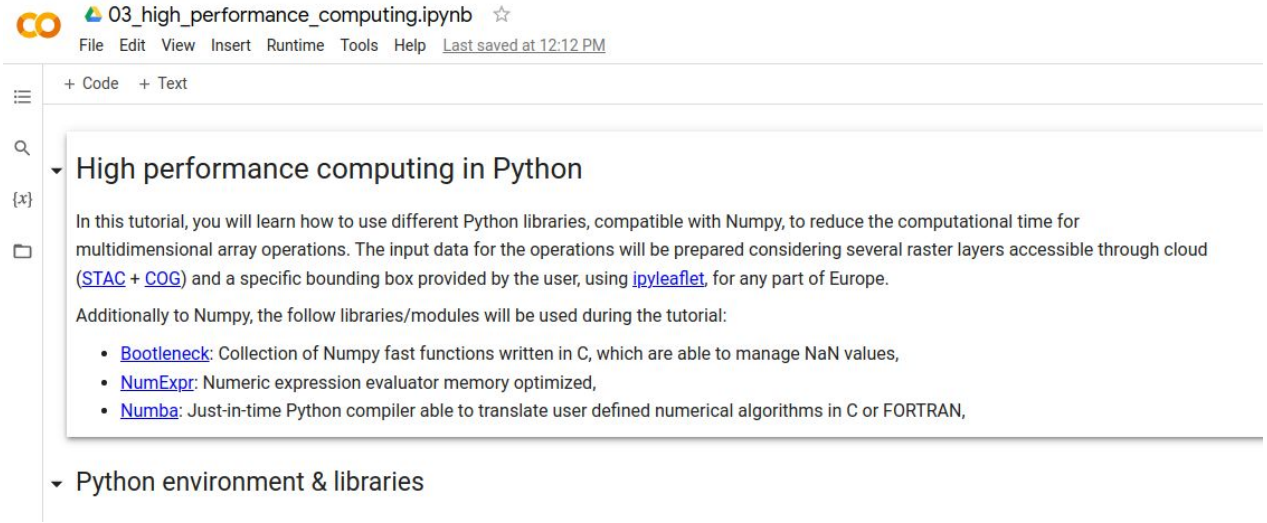


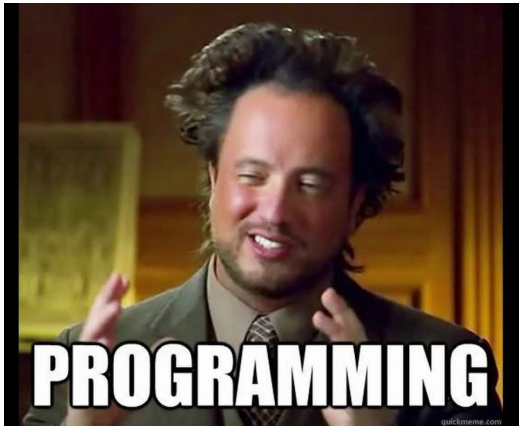
Open Data Science

Hands-on

https://colab.research.google.com/drive/1ekDvZB3Zz9Y7JE42YjN6U97S7oMjG39m

https://gitlab.com/geoharmonizer_inea/odse-workshop-2022/-/blob/main/python_training/03_high_performance_computing.ipynb





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