

# PYTHON AND HIGH-PERFORMANCE COMPUTING

A decorative background graphic on the right side of the slide. It features a series of concentric, overlapping hexagonal patterns that create a sense of depth and movement, resembling a stylized representation of a hexagonal lattice or a honeycomb structure. The colors are light gray and white, blending into the background.

# Efficiency

- ➡ Python is an interpreted language
  - no pre-compiled binaries, all code is translated on-the-fly to machine instructions
  - byte-code as a middle step and may be stored (.pyc)
- ➡ All objects are dynamic in Python
  - nothing is fixed == optimisation nightmare
  - lot of overhead from metadata
- ➡ Flexibility is good, but comes with a cost!

# Parallelisation strategies for Python

- ➡ Global Interpreter Lock (GIL)
  - CPython's memory management is not thread-safe
  - no threads possible, except for I/O etc.
  - affects overall performance if threading
- ➡ Message-passing is the Way to Go to achieve true parallelism in Python
- ➡ Other alternatives include e.g. process-based “threading”
  - fork independent processes that have a limited way to communicate

# Embedding compiled code in Python

- ➡ One can also embed compiled code in a Python program
  - C is straightforward
  - Fortran is possible
- ➡ Implemented as wrappers around the compiled code
  - write code in C
  - write special wrappers in C
  - compile them into a shared object (.so)
  - use in Python just like a native module

# Agenda

## Thursday

9:00-9:15	Python and HPC
9:15-10:00	NumPy – fast array interface to Python
10:00-10:30	Exercises
10:30-11:00	Coffee Break
11:00-11:30	Vectorized operations & broadcasting
11:30-12:00	Exercises
12:00-13:00	Lunch break
13:00-13:30	Advanced indexing, I/O, and misc utilities
13:30-14:30	Exercises
14:30-15:00	Coffee Break
15:00-16:00	Visualisation with Python
16:00-17:00	Exercises

## Friday

9.00-9.45	MPI introduction
9:45-10:30	MPI and Python – mpi4py
10.30-11.00	Coffee break
11:00-12:00	Exercises
12.15-13.00	Lunch break
13.00-13:30	Multiprocessing, i.e. process-based "threading"
13:30-14:30	Exercises
14.30-15.00	Coffee break
15.00-15.30	C extensions – integrating efficient C routines in Python
15:30-16:30	Exercises
16:30-17:00	Summary of Python HPC strategies

Martti Louhivuori // CSC – IT Center for Science Ltd.

Python in High-Performance Computing

April 21-22, 2016 @ University of Oslo



All material (C) 2016 by the authors.

This work is licensed under a **Creative Commons Attribution-NonCommercial-ShareAlike 3.0**

Unported License, <http://creativecommons.org/licenses/by-nc-sa/3.0/>