PYTHON AND HIGH-PERFORMANCE COMPUTING

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

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Python in High-Performance Computing

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