The Last Resort: Mixed-language programming with MPI

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Motivation

A programme which has the source code written in more than one language. Why?

- Existing code is in a different language
- Speed
- e.g. f2py

But, if the parts are too large, it is difficult turn one of them into a subroutine.

Message Passing Interface (MPI)

MPI library is a set of commands that allow communicating between different processes

- Typically, it is used for communications between copies of the same programme to achieve parallel computing
 - "Single process, multiple data" (SPMD)
- Here, we execute more than one programme
 - "Multiple instructions, multiple data" (MIMD)

Requirements

In this demonstration, I show how a Python programme and a Fortran programme can communicate via MPI. Additionally, OpenMP is implemented to the Fortran programme.

- MPI Library (OpenMPI/MPICH)
- Fortran compiler, MPI wrapper (e.g. mpifort)
- mpi4py (docs)
- Use the 'colon notation' of mpiexec to execute multiple programmes (MIMD)
 (docs)

Summary

- Multiple large programmes can be joined together by MPI
 - Note array ordering (row-major vs column-major)
- They can run in parallel
- Extra cares may be required on computing cluster: e.g. slurm heterogenous job
- Mixed-language programming should be avoided if possible/worthwhile