Imperial College
London

Parallel simulations and using clusters
Fluidity Training Course 2014

Michael Lange

AMCG, Imperial College London

6th November 2014

AMCG

Parallel Simulations

Large simulations require more than a laptop

- ▶ Fluidity runs in parallel via MPI
- ▶ Optional: OpenMP threading for hybrid runs
  - ▶ Configuration option `--enable-openmp`

- ▶ Fluidity runs on various clusters
  - ▶ Imperial College: CX1, CX2 (Intel)
  - ▶ UK national supercomputer: Archer (Cray CX30)
  - ▶ ANU/NCI: Raijin (Fujitsu Primergy)

Parallel Simulations

How to run Fluidity in parallel:

- ▶ No changes to the .flml required!
  - ▶ Optional: Remove fields from output
    (.stat and .vtu)

- ▶ Need to decompose the mesh
  - ▶ Tools provided:
    flredecomp, ~~fldecomp~~
  - ▶ Build both with: `make fltools`
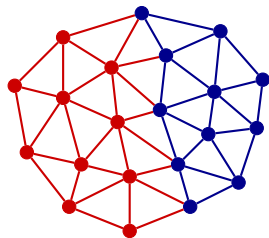
Mesh decomposition

Mesh decomposition before the run:

- `mpiexec -n 4 flredecomp -i 1 -n 4 serial parallel`
  - Needs to be run in parallel!
  - Decomposes mesh named in `serial.flml`
  - Creates new parallel setup: `parallel.flml`

- Now run this on 4 processors:
  `mpiexec -n 4 fluidity parallel.flml`

Mesh decomposition

Mesh decomposition with checkpoints:

- Switch on checkpointing!
    - `/io/checkpointing` in .flml

- `mpiexec -n 8 flredecomp -i 4 -n 8 par_4 par_8`
    - Needs to be run on max(-i, -o) processes
    - Enables re-starting on more/fewer processes

- Run as before:
  `mpiexec -n 8 fluidity par_8.flml`

AMCG

Archer

```
#!/bin/bash --login
#PBS -l walltime=01:00:00
#PBS -N jet_sim
#PBS -l select=2
#PBS -A n01-IC1

# Load Fluidity environment
module swap PrgEnv-cray PrgEnv-fluidity

# Make sure any symbolic links are resolved to absolute path
export PBS_O_WORKDIR=$(readlink -f $PBS_O_WORKDIR)
cd $PBS_O_WORKDIR

# Workaround for python environment
export LD_LIBRARY_PATH=$ANACONDA_LIB:$LD_LIBRARY_PATH

# Decompose the mesh
aprun -n 48 -N 24 -d 1 -j 1 $FLUIDITYDIR/bin/flredecomp -i 1 -n 48 jet_sim set_sim_48

# Run simulation
aprun -n 48 -N 24 -d 1 -j 1 $FLUIDITYDIR/bin/fluidity -l -p -v2 jet_sim_48.flml
```