Imperial College London

Parallel simulations and using clusters

Fluidity Training Course 2014

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6th November 2014

Parallel Simulations

Large simulations require more than a laptop

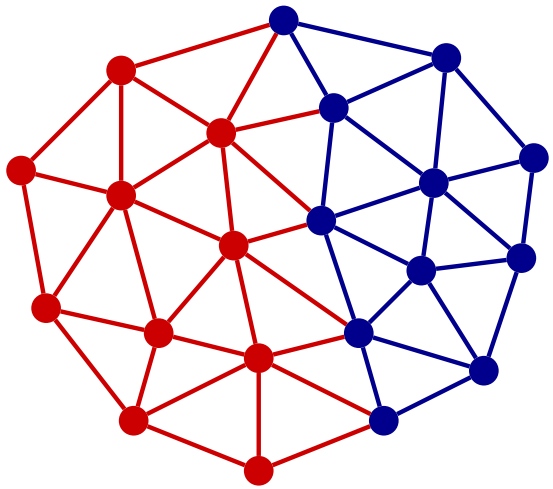
- Fluidity runs in parallel via MPI
- Optional: OpenMP threading for hybrid runs
  - Configuration option `--enable-openmp`

- 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!
  - Parallel compatible preconditioner (not eisenstat)
  - 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`

Running Fluidity on clusters

- Set up simulation on local machine!

- Install Fluidity on cluster
  - CX1/CX2: `module load fluidity`
  - Archer: instructions here
- Create `.pbs` submission script
  - Submit with `qsub`
- Copy results back to local machine
  - Visualisation as before

CX1

```
#!/bin/bash
#PBS -N pile
#PBS -l walltime=0:20:00
# Resource requirements
#PBS -l select=1:ncpus=8:mem=1550mb

module load fluidity

echo Working directory is $PBS_O_WORKDIR
cd $PBS_O_WORKDIR

mpiexec flredecomp -i 4 -o 8 flow_past_pile_50_checkpoint flow_past_pile_50_cp_n8

mpiexec fluidity -v2 -l flow_past_pile_50_cp_n8.flml
```

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

export FLUIDITYDIR=path/to/my/fluidity/install

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