Introductory OpenFOAM® Course

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Acknowledgements

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Today’s lecture

1. Running in parallel
2. Running in a cluster using a job scheduler
3. Running with a GPU

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Running in parallel

The method of parallel computing used by OpenFOAM is known as domain decomposition, in which the geometry and associated fields are broken into pieces and distributed among different processors.

- To decompose the domain we use the decomposePar utility. You also will need a dictionary named decomposeParDict which is located in the **system** directory of the case.
- OpenFOAM uses the public domain OpenMPI implementation of the standard message passing interface (MPI). Each processor runs a copy of the solver on a separate part of the domain mesh.
- Finally the solution is reconstructed to obtain the final result. This is done by using the reconstrucPar utility.

Running in parallel

Domain Decomposition

- The mesh and fields are decomposed using the decomposePar utility.
- The main goal is to break up the domain with minimal effort but in such a way to guarantee a fairly economic solution.
- The geometry and fields are broken up according to a set of parameters specified in a dictionary named decomposeParDict that must be located in the **system** directory of the case.
- In the decomposeParDict file the user must set the number of domains which the case should be decomposed into: usually it corresponds to the number of cores available for the calculation.
    - numberOfSubdomains 2;
- The user has a choice of six methods of decomposition, specified by the method keyword.
- On completion, a set of subdirectories will have been created, one for each processor. The directories are named processorN where N = 0, 1, 2, … Each directory contains the decomposed fields.

Running in parallel

Domain Decomposition

- **simple**: simple geometric decomposition in which the domain is split into pieces by direction.
- **hierarchical**: Hierarchical geometric decomposition which is the same as simple except the user specifies the order in which the directional split is done.
- **scotch**: requires no geometric input from the user and attempts to minimize the number of processor boundaries (similar to metis).
- **manual**: Manual decomposition, where the user directly specifies the allocation of each cell to a particular processor.

- **metis**: requires no geometric input from the user and attempts to minimize the number of processor boundaries.
- **parMetis**: MPI-based version of METIS with extended functionality.

Not supported anymore

Running in parallel

We will now run a case in parallel. From now on follow me.

- Go to the **$path_to_openfoamcourse/parallel_tut/rayleigh_taylor** folder. In the terminal type:
  - cd **$path_to_openfoamcourse/parallel_tut/rayleigh_taylor**
  - blockMesh
  - checkMesh
  - cp **0/**alpha1.org **0/**alpha1
  - funkySetFields -time 0
    (if you do not have this tool, copy the files located in the directory **0.init** to the directory **0**)
  - decomposePar
  - mpirun -np 8 interFoam -parallel
    (Here I am using 8 processors. In your case, use the maximum number of processor available in your laptop, for this you will need to modify the decomposeParDict dictionary located in the **system** folder)

Running in parallel

We will now run a case in parallel. From now on follow me.

- Go to the **$path_to_openfoamcourse/parallel_tut/rayleigh_taylor** folder. In the terminal type:
  - paraFoam -builtin

To directly post-process the decomposed case or

  - reconstructPar
  - paraFoam

To post-process the reconstructed case. More about post-processing in parallel in the next slides.

- Notice the syntax used to run OpenFOAM in parallel:
  - **mpirun -np 8 solver_name -parallel**

  where **mpirun** is a shell script to use the mpi library, **-np** is the number of processors you want to use, **solver_name** is the OpenFOAM solver you want to use, and **-parallel** is a flag you shall always use if you want to run in parallel.

Running in parallel

- Almost all OpenFOAM utilities for post-processing can be run in parallel. The syntax is as follows:
    - mpirun -np 2 utility -parallel
      (notice that here I am using 2 processors)

- When post-processing cases that have been run in parallel the user has three options:
    - Reconstruction of the mesh and field data to recreate the complete domain and fields.
        - reconstructPar
        - paraFoam

Running in parallel

- Post-processing each decomposed domain individually
  - paraFoam -case processor0

To load all processor folders, the user will need to manually create the file processorN.OpenFOAM (where N is the processor number) in each processor folder and then load each file into paraFoam.

- Reading the decomposed case without reconstructing them. For this you will need to:
  - paraFoam -builtin   (this will use a paraFoam version that will let you read a decomposed case or read reconstructed case)

Today's lecture

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Running in a cluster using a job scheduler

- Running OpenFOAM in a cluster is similar to running in a normal workstation with shared memory.
- The only difference is that you will need to launch your job using a job scheduler.
- Common job schedulers are:
    - Terascale Open-Source Resource and Queue Manager (TORQUE).
    - Simple Linux Utility for Resource Management (SLURM).
    - Portable Batch System (PBS).
    - Sun Grid Engine (SGE).
    - Maui Cluster Scheduler.
- Ask your system administrator the job scheduler installed in your system. Hereafter I will assume that you will run using PBS.

Running in a cluster using a job scheduler

- To launch a job in a cluster with PBS, you will need to write a small script file where you tell to the job scheduler the resources you want to use and what you want to do.

```
#!/bin/bash
#
# Simple PBS batch script that reserves 8 nodes and runs a
# MPI program on 64 processors (8 processor on each node)
# The walltime is 24 hours !
#
#PBS -N openfoam_simulation                          //name of the job
#PBS -l nodes=8:nehalem,walltime=24:00:00            //max execution time
#PBS -m abe -M joel.guerrero@unige.it     //send an email as soon as the job is launch or terminated

cd /lustre/ws1/ws/xicjoegi-joegi-0/xicjoegi-1.7.x/building/les_simu      //go to this directory

#decomposePar                                   //decompose the case, this line is commented

mpirun -np 64 pimpleFoam -parallel > log                       //run parallel openfoam
```

The green lines are not PBS comments. PBS comments use the numeral character (#)

Running in a cluster using a job scheduler

- To launch your job you need to use the qsub command (part of the PBS job scheduler). The command will send your job to queue.
    - qsub script_name

- Remember, running in a cluster is no different from running in your workstation. The only difference is that you need to schedule your jobs.
- Depending on the system current demand of resources, the resources you request and your job priority, sometimes you can be in queue for hours, even days, so be patient and wait for your turn.

Today’s lecture

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Running with a GPU

- The official release of OpenFOAM (version 2.1.x), does not support GPU computing.
- To test OpenFOAM's GPU capabilities, you will need to install the latest extend version (OpenFOAM-1.6-ext).
- To use your GPU with OpenFOAM, you will need to install the cufflink library. There are a few more options available, but I do like this one.
- You can download cufflink from the following link (as for 1/Jul/2012) : http://code.google.com/p/cufflink-library/
- Additionally, you will need to install the following libraries:
  - **Cusp:** which is a library for sparse linear algebra and graph computations on CUDA. http://code.google.com/p/cusp-library/
  - **Thrust:** which is a parallel algorithms library which resembles the C++ Standard Template Library (STL). http://code.google.com/p/thrust/

Running with a GPU

What is cufflink?

cufflink stands for Cuda For FOAM Link. cufflink is an open source library for linking numerical methods based on Nvidia's Compute Unified Device Architecture (CUDA™) C/C++ programming language and OpenFOAM®. Currently, the library utilizes the sparse linear solvers of Cusp and methods from Thrust to solve the linear Ax = b system derived from OpenFOAM's lduMatrix class and return the solution vector. cufflink is designed to utilize the course-grained parallelism of OpenFOAM® (via domain decomposition) to allow multi-GPU parallelism at the level of the linear system solver.

Cufflink Features

- Currently only supports the OpenFOAM-extend fork of the OpenFOAM code.
- Single GPU support.
- Multi-GPU support via OpenFOAM's course grained parallelism achieved through domain decomposition (experimental).

Running with a GPU

Cufflink Features

- A conjugate gradient solver based on Cusp for symmetric matrices (e.g. pressure), with a choice of
  - Diagonal Preconditioner.
  - Sparse Approximate Inverse Preconditioner.
  - Algebraic Multigrid (AMG) based on Smoothed Aggregation Precondtioner.
- A bi-conjugate gradient stabilized solver based on CUSP for asymmetric matrices (e.g. velocity, epsilon, k), with a choice of
  - Diagonal Preconditioner.
  - Sparse Approximate Inverse Preconditioner.
- Single Precision (sm_10), Double precision (sm_13), and Fermi Architecture (sm_20) supported. The double precision solvers are recommended over single precision due to known errors encountered in the Smoothed Aggregation Preconditioner in Single precision.

Running with a GPU

Running cufflink in OpenFOAM extend

Once the cufflink library has been compiled, in order to use the library in OpenFOAM one needs to include the line

```
libs ("libCufflink.so");
```

in your controlDict dictionary. In addition, a solver must be chosen in the fvSolution dictionary:

```
p
{
    solver              cufflink_CG;
    preconditioner      none;
    tolerance           1e-10;
    //relTol            1e-08;
    maxIter             10000;
    storage             1;//COO=0 CSR=1 DIA=2 ELL=3 HYB=4 all other numbers use default CSR
    gpusPerMachine      2;//for multi gpu version on a machine with 2 gpus per machine node
    AinvType        ;
    dropTolerance       ;
    linStrategy     ;
}
```

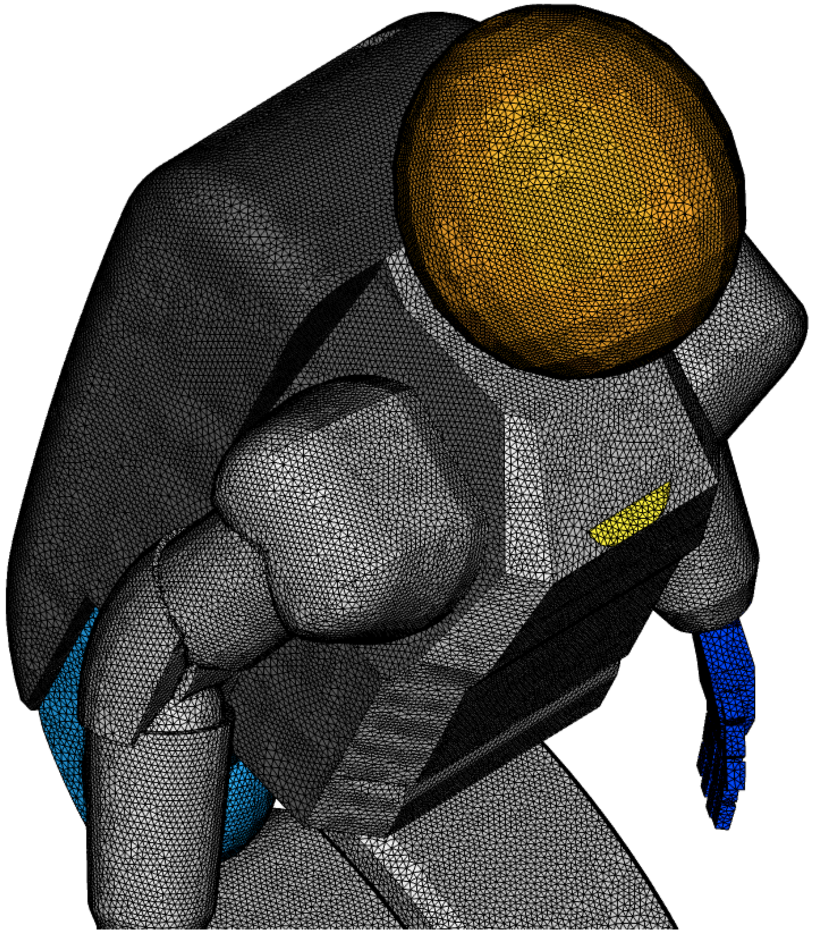
This particular setup uses an un-preconditioned conjugate gradient solver on a single GPU; compressed sparse row (CSR) matrix storage; 1e-8 absolute tolerance and 0 relative tolerance; with a maximum number of inner iterations of 10000.

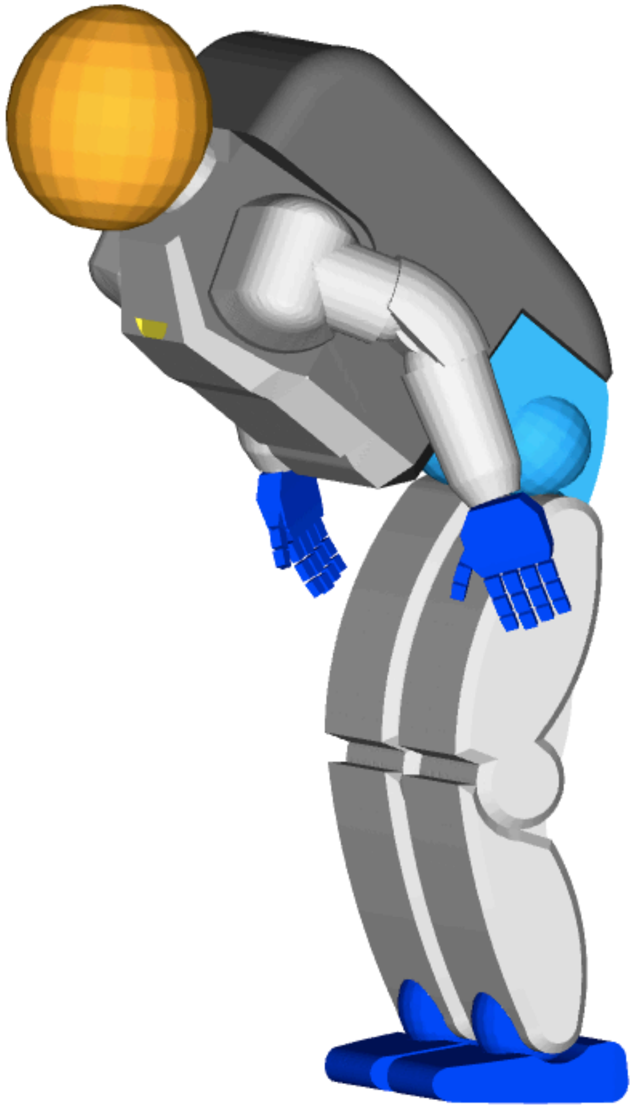
Mesh generation using open source tools

Additional tutorials

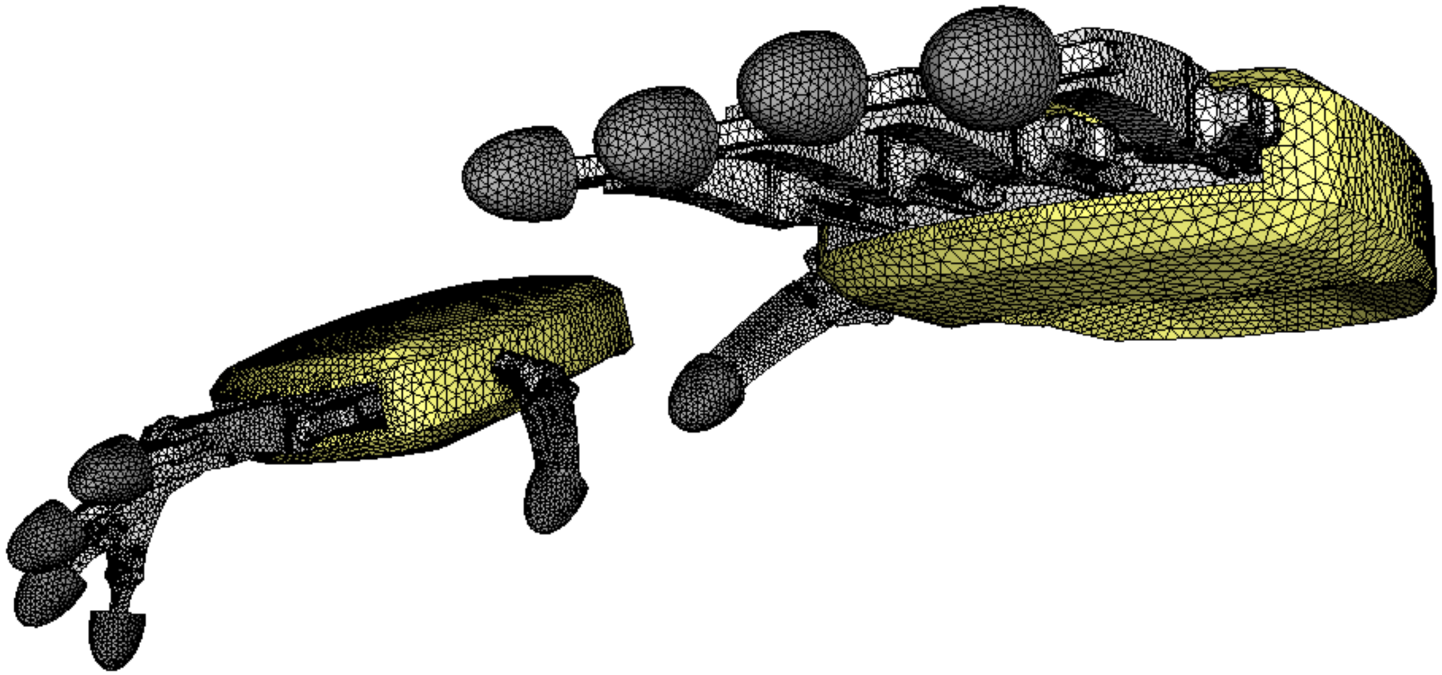
In the folder **$path_to_openfoamcourse/parallel_tut** you will find many tutorials, try to go through each one to understand how to setup a parallel case in OpenFOAM.

Thank you for your attention





Hands-on session



In the course's directory **($path_to_openfoamcourse)** you will find many tutorials (which are different from those that come with the OpenFOAM installation), let us try to go through each one to understand and get functional using OpenFOAM.

If you have a case of your own, let me know and I will try to do my best to help you to setup your case. But remember, the physics is yours.