# OpenFOAM on HECToR

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#### Overview

- Project details
- Overview of OpenFOAM
  - Open-source comments
  - Applications and scientific benefits
  - Background of work
- Work plan outline and status
- Technical notes
  - Installation on HECToR
  - Changes to standard release
  - User information
    - Compilation information
    - Example batch scripts
- Future Plans
- Acknowledgements

- Distributed CSE Support project to provide the OpenFOAM toolbox functionality to HECToR users.
- Project overview
  - Install and test the core OpenFOAM solvers on HECToR
  - Benchmark a range of the OpenFOAM modules
    - identified as useful via UK CFD communities
  - Make OpenFOAM available to HECToR users
    - "how-to" guide
  - Disseminate the benchmark results
- Ultimately, make OpenFOAM, and relevant performance information, available on HECToR
- Presents HECToR to a new group of potential users and allow them to undertake larger, more complex simulations, in a more timely fashion.

#### Applications

# epco

#### Aerospace

- super- and hyper-sonic flow, ice deposition, etc
- Automotive
  - external noise, combustion, fuel injection, catalytic converters, etc
- Energy
  - fuel storage, heating/ventilation, etc
- Heavy industry:
  - bearings, pumps, etc
- Others
  - baking
  - polymer extrusion
  - ink-jets
  - crystal growth
  - climatic flows
  - etc.

#### **Overview of OpenFOAM**

- Open-source toolbox for CFD
  - C++ modules, with MPI calls for parallel inter-core communication
- Generic tools to simulate complex physics for
  - fluid flows involving chemical reactions, turbulence and/or heat transfer
  - solid dynamics
  - electromagnetism
  - pricing of financial options.
- Solvers
  - simulate specific problems in engineering mechanics
- Utilities
  - perform pre- and post-processing tasks ranging from simple data manipulations to visualisation and mesh processing
- Libraries
  - create toolboxes that are accessible to the solvers/utilities

#### **OpenFOAM** is open-source

- OpenFOAM is maintained by OpenCFD
  - OpenCFD provides contracted development, support and training for users of OpenFOAM.
- Any user can augment code to create customised applications for specific problems
  - i.e. turbo-machinery
- Some user-augmented versions are available via the OpenCFD
- These are referred to as 'development' versions
  - misnomer: more akin to 'augmented' versions
  - any new functionality in online development versions are not, in general, included in future releases
- Maybe open-source, but official code is written only by OpenCFD
  - plus one trusted external user.

#### Work plan



- The work plan is in three parts
  - WP1: install and test the core OpenFOAM solvers on HECToR
  - WP2: benchmark a variety of the modules available
  - WP3: publicise the results to the potential users.

- Note on visualisation
  - OpenFOAM GUIs present some difficult challenges
    - paraFOAM employs ParaView
      - HECToR's ParaView does not work for all users
    - post-processing and rendering burning cycles on login nodes?!
  - thus, focus is on core solvers
    - GUIs only being considered time permitting.

### WP1: Install and test OpenFOAM

- Identify a suitable subset of modules for installation
  - EPCC will liaise with the project co-PI Professor David Emerson to identify which solvers and modules should be the focus for this project.
  - Also includes polling the UK CFD community in general to find which modules are mainly being used, and specifically which would be useful to future researchers using HECToR.
  - Several consortia have expressed a strong interest in making use of OpenFOAM on HECTOR if it was available, including:
    - UK Applied Aerodynamics Consortium
    - UK Turbulence Consortium
- Create test cases
  - once the modules have been chosen, suitable test examples need to be created/obtained.
- Installation
  - the modules will be installed on HECToR
- Run tests and validate
  - the example test cases will be run to check the installation for correctness.

### WP1: Effort, Tasks and Outputs

- Effort: 3 months over 6 months
  - 1<sup>st</sup> April 2009 30<sup>th</sup> September 2009
- Tasks and status:
  - Task 1. Identify suitable subset of modules for testing
  - Task 2. Create tests
  - Task 3. Install remaining OpenFOAM modules
  - Task 4. Run tests and validate
  - Task 5. Revisit installation if required
- Outputs:
  - D1.1 Short report listing the modules chosen for testing and test cases
  - D1.2 Short report on the installation process

#### WP1: Current status

- Task1. Identify suitable subset of modules for testing
  - co-PI requested that the Tutorials Test Suite be employed
- Task 2. Create tests
  - Tutorials Test Suite needs extended to run in parallel
  - OpenCFD assisting
    - also giving general guidance with code
    - creating dam break 'cases'
      - 'Finest simulation' yet to be used for advertising purposes
- 3. Install remaining OpenFOAM modules
  - Done: all modules, bar GUIs, are installed.
    - Cray's assistance invaluable.
- 4. Run tests and validate
  - Some tutorials fail due to bugs in code
- 5. Revisit installation if required

#### WP2: Benchmarking

- Effort: 2 months
  - 1<sup>st</sup> October 2009 31<sup>st</sup> January 2010
- Task 1: Create benchmark models/tests
  - the benchmark models will ideally follow on from the test cases created in the first work package.
- Task 2: Generate the benchmark data
  - demonstrate the scaling of the parallel OpenFOAM modules
  - give idea of the limits on the size of models which can be simulated
  - Scaling and performance improvements, compared with serial runs, will be measured.
  - Optimal runtime parameters will be identified for the different models based on the results
- Output:
  - D2.1 Report on the benchmarking results, scaling and performance, and optimal runtime parameters

- Effort: 1 months
  - 1<sup>st</sup> February 2010 31<sup>st</sup> March 2010
- Task 1: Identify appropriate dissemination routes
  - HECToR website and User mailings
  - may be via a paper or poster to an appropriate conference
    - AHM2010, Open CFD International, etc
- Task 2: Dissemination
  - Write up benchmarking results
  - Create a OpenFOAM User Guide on HECToR website
- Outputs:
  - D3.1 Paper/poster on the benchmark performance
  - D3.2 Web-based reference on using OpenFOAM on HECToR

### Installation details

- OpenFOAM installation directory must be visible to compute nodes
  - despite best efforts by Cray and EPCC.
  - installation resides in /work/y07/y07/openfoam
    - other 3<sup>rd</sup> party packages are also only available from /work
- OpenFOAM package account created in /usr/local/packages
  - only contains gzipped tarball to recreate installation quickly
    - /work not backed up, whilst /usr/local/packages is not
- gzipped tarball differs from standard release
  - Code changes
  - Additional HECToR-specific dynamic libraries
  - Excludes
    - html documentation
    - malloc
    - openmpi
    - zlib
    - gcc
  - Includes HECToR-specific user files
    - README, example batch scripts for compilation and testing, etc

#### Changes to source code:

- etc/settings.sh
  - Employed Cray MPI rather an release's own OpenMPI
- wmake/rules
  - added cray\_xt directory for setting compiler flags, location of mpi, etc.
    - very similar to linux64Gcc
- src/Pstream/Allwmake
  - Added MPT target for Cray MPI
- Added several shared and dynamic libraries to /mylib
  - currently only found on the front end,
  - now available to compute nodes during compilation and runtime
    - five hour compilation must be done on back-end
  - libalpslli.a, libalpsutil.so, libgcc\_s.so.1, libpthread.so.0, libalpslli.so, libalpsutil.so.0, libm.so.6, librt.so.1, libalpslli.so.0, libalpsutil.so.0.0, libmpich.so.1.1, libstdc++.so.6, libalpslli.so.0.0, libc.so.6, libpmi.so, libz.so.1, libalpsutil.a, libdl.so.2, libportals.so.1

#### **Current status**

- Three versions of OpenFOAM are currently available
  - 1.6 (current), 1.5 (previous) and a 1.5-dev version
  - basic optimization with –O3
- Early Adopters' User Guide emailed to small, select group
  - group includes 3 actual users identified via the HECToR Helpdesk
  - Guide available via HECToR 3<sup>rd</sup> Party Software Wiki by end of Sept., '09.
- All OpenFOAM executables can be run in either serial or parallel
  - hence both dual- and quad-core versions available for all three versions
  - quad-core binaries run in serial queue may fail on the dual-core nodes
- Users can either
  - run OpenFOAM from package account or
  - copy our modified source, augment and install in their own workspace

#!/bin/bash --login **#PBS** -q serial **#PBS -N compile\_OF** #PBS -l cput=05:00:00 **#PBS -A y07** . /opt/modules/3.1.6/init/bash module swap PrgEnv-pgi PrgEnv-gnu #module load xtpe-quadcore module swap gcc gcc/4.3.3 module swap xt-mpt xt-mpt/3.2.0 cd /work/y07/y07/openfoam/dual-core/OpenFOAM/OpenFOAM-1.5 source etc/bashrc export LD\_LIBRARY\_PATH=\$WM\_PROJECT/mylib:\$LD\_LIBRARY\_PATH ./Allwmake

## **Compilation fails**

- Compilation currently fails
  - [../OpenFOAM/OpenFOAM-1.5/lib/crayxtDPOpt/libuserd-foam.so] Error 1
  - This is due to the currently employed Cray XT4 CSE 2. does not ship the necessary dynamic libraries.
    - Fixed in CSE 2.2.
  - The compilation script provided for HECToR users includes a work-around.
- Some portals warnings during compilation
  - only if /mylib not in \$LD\_LIBRARY\_PATH
  - portals are what the MPI is built upon
  - can ignore them as they are not required at runtime as we employ the portals static libraries.
  - number of dummy libraries in /mylib to calm the compilation and the runtime environment

#### Example Batch Script for serial jobs

#!/bin/bash --login **#PBS** -q serial **#PBS -N testInstall** #PBS -I cput=01:00:00 **#PBS -A 701** . /opt/modules/3.1.6/init/bash module swap PrgEnv-pgi PrgEnv-gnu module swap gcc gcc/4.3.3 module swap xt-mpt xt-mpt/3.2.0 source /work/z01/z01/gavin/OpenFOAM/OpenFOAM-1.6/etc/bashrc export LD\_LIBRARY\_PATH=\$WM\_PROJECT\_DIR/mylib:\$LD\_LIBRARY\_PATH cd /work/z01/z01/gavin/OpenFOAM/gavin-1.6/run/tutorials Allclean

Alltest

#### Example Batch Script for a Parallel Job

#!/bin/bash --login **#PBS -I mppwidth=8** #PBS -I mppnppn=4 **#PBS -N dam tutorial** #PBS -I cput=01:00:00 **#PBS -A z01** export NSLOTS=`qstat -f \$PBS\_JOBID | awk '/mppwidth/ {print \$3}'` export NTASK=`qstat -f \$PBS JOBID | awk '/mppnppn/ {print \$3}'` . /opt/modules/3.1.6/init/bash module swap PrgEnv-pgi PrgEnv-gnu module swap gcc gcc/4.3.3 module swap xt-mpt xt-mpt/3.2.0 source /work/z01/z01/gavin/OpenFOAM/OpenFOAM-1.6/etc/bashrc export LD\_LIBRARY\_PATH=\$WM\_PROJECT\_DIR/mylib:\$LD\_LIBRARY\_PATH cd \$TUTORIALS/... aprun -n \$NSLOTS -N \$NTASK interFoam –parallel

#### **Future Work**



- By end of September, 2009
  - Complete WP1 and deliver D1.1 and D1.2 on time
    - On target
  - Release Early Adopters' User Guide on HECToR's 3<sup>rd</sup> Party Package Wiki
  - Contact OpenFOAM code authors re
    - compilation warnings
      - i.e. non-standard C++ usage
    - tutorial test suite errors
- Attending Open CFD International in Barcelona in Nov. '09.
  - speak to users to gauge usage profile and popular modules
  - gain more experience in running 'cases'
  - increase profile of upcoming HECToR installation

#### Fin



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- Any questions?
  - gavin@epcc.ed.ac.uk