Parallel IO in Code_Saturne

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Acknowledgements to:

Yvan Fournier from EDF R&D, FR

CCP12, UKTC and The Hartree Centre

Webminar – ARCHER – 30/04/14

Motivation (1)

High-End Machines offer hope for more multi-physics & multi-scale for engineering in ever more detailed configurations.

Huge effort has been dedicated to improve/optimise solvers (in our case Navier-Stokes equation solvers) for them to scale on the current existing petaflop machines, but arguably less time is dedicated by CFD developers to IOs.

Several types of IOs and some way around loading/writing huge data files have been identified:-

-INPUT: mesh, domain partition (if already known), restart file (if needed), input data

-OUTPUT: mesh (if changed, with added periodicity for instance), domain partition (if computed by the code), listing file, post-processing file, checkpoint, probes

Motivation (2)

Ways around exist to avoid loading full data set for:-

-INPUT:-

-mesh (mesh joining and mesh multiplication)

-domain partition (partition re-computed by the code)

-OUTPUT:-

-pre-processed mesh (not needed, because computed by the code)

-domain partition (not needed because computed by the code)

-post-processing (co-processing, for instance using Catalyst)

But not for:-

-INPUT:-

-restart file, as/if the whole flow field is needed

-OUTPUT:-

-checkpoint file, as/if the whole flow field is needed

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Contents

Code_Saturne's Features

Technology

-Co-located finite volume, arbitrary unstructured meshes, predictor-corrector
-350 000 lines of code, 37% Fortran, 50% C, 13% Python
-MPI for distributed-memory and some openMP for shared-memory machines

Physical modeling

-Laminar and turbulent flows: k-eps, k-omega, SST, v2f, RSM, LES models
-Radiative transfer (DOM, P-1)
-Coal, heavy-fuel and gas combustion
-Electric arcs and Joule effect
-Lagrangian module for particles tracking
-Atmospheric modeling (merging Mercure_Saturne)
-ALE method for deformable meshes
-Rotor / stator interaction for pump modeling, for marine turbines

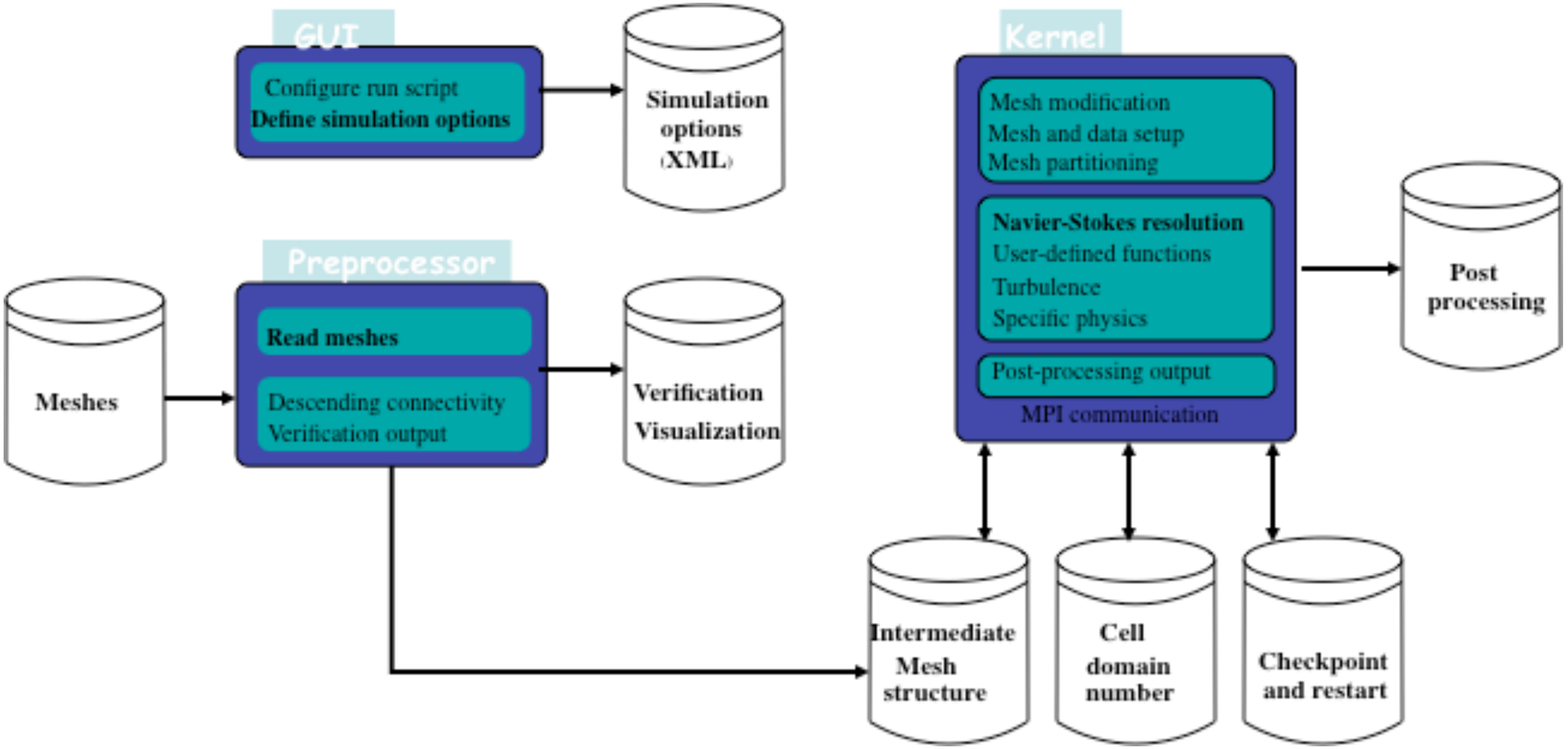
Flexibility

-Portability (Unix, Linux and MacOS X)
-Graphical User Interface with possible integration within the SALOME platform

Toolchain

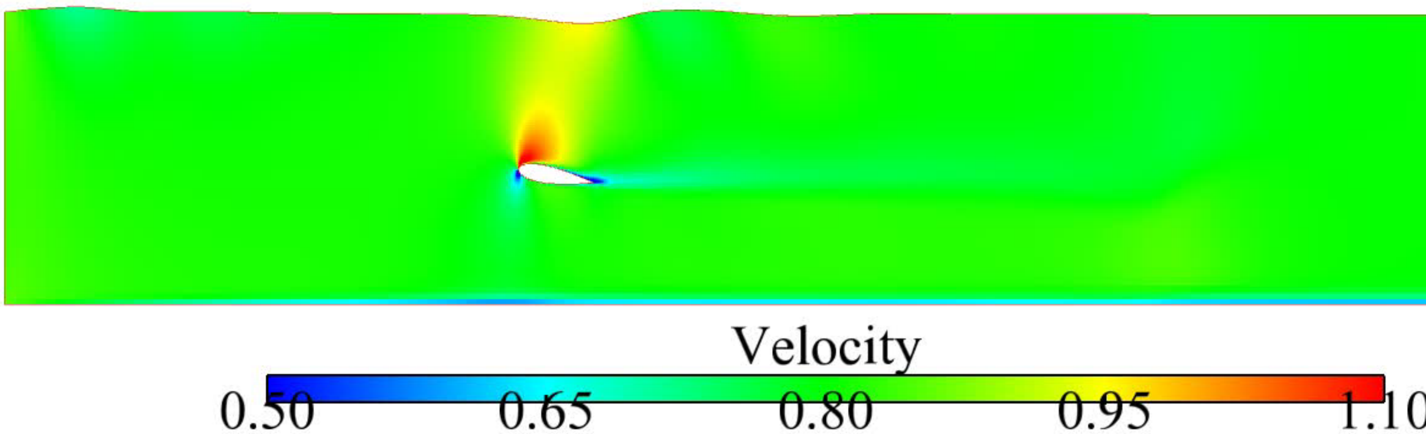
Reduced number of tools

- Each with rich functionality
- Natural separation between interactive and potentially long-running parts
- In-line (pdf) documentation



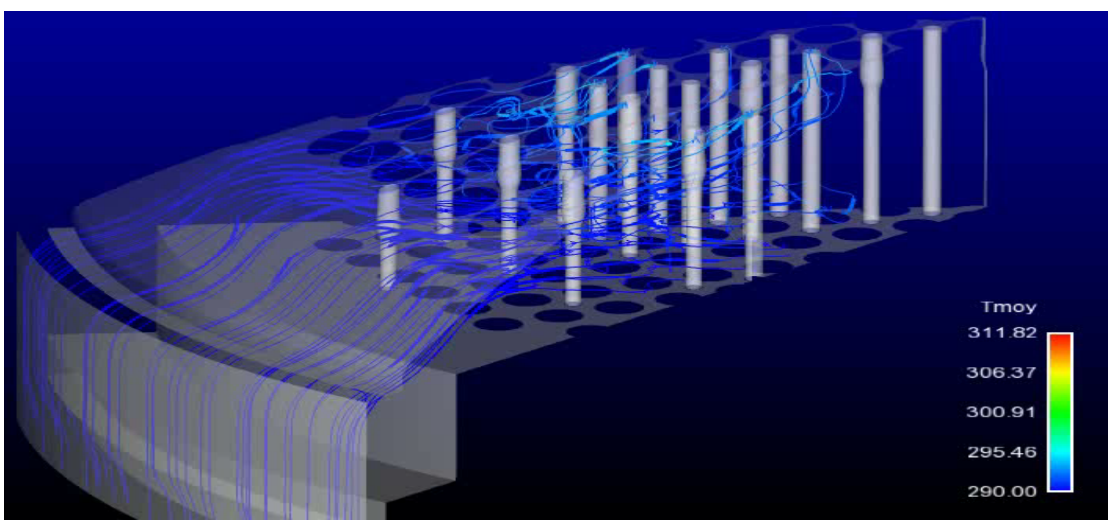
Example of Applications

Free surface modelling (ALE)



Hydrofoil

Thermofluids study of the hot box dome AGR (EDF Energy)



- Complex flow due through the forest of tubes
- Calculation shows little mixing in the centre of the dome
- Temperatures at the dome highest where thermocouples are located

Architectures

ARCHER – XC30 / Lustre

3008 Compute nodes: two 2.7 GHz, 12-core E5-2697 v2 (Ivy Bridge) series processors. Within the node, QuickPath Interconnect (QPI) links to connect the 2 processors

The Cray Aries interconnect links all compute nodes in a Dragonfly topology.

Compute nodes access the file system via IO nodes running the Cray Data Virtualization Service (DVS)

Blue Joule – BGQ / GPFS

6 racks, each rack containing 1,024 16-core, 64 bit, 1.60 GHz A2 PowerPC processors.

All the racks have 8 IO nodes which connect the BGQ racks to the shared GPFS storage over Infiniband.

The minimum block size which can be booted for a job is therefore 1,024/8 nodes, or 128 nodes.

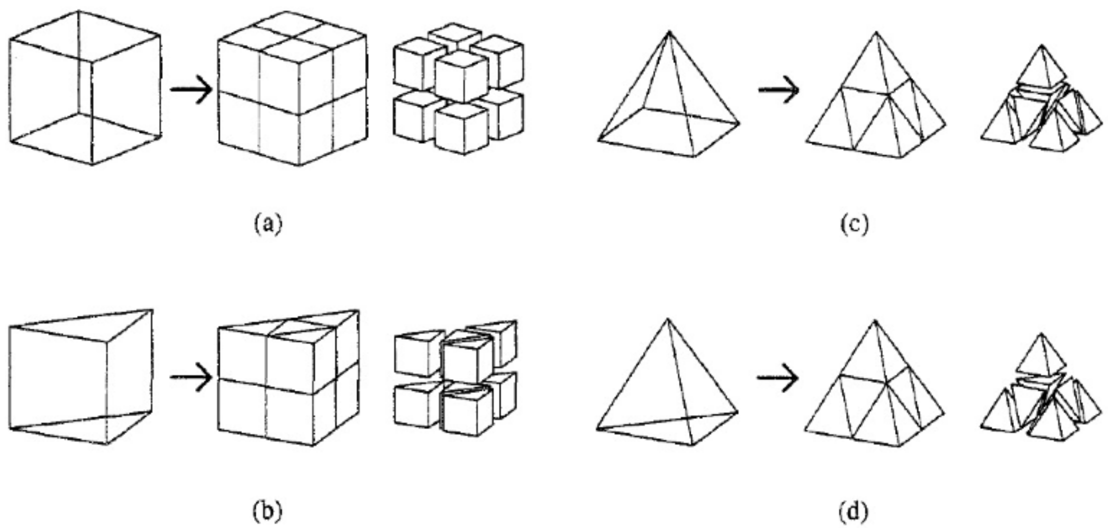
Mesh Multiplication

Most mesh generators are serial and thus memory-limited

A way around to generate extremely large meshes is to build meshes from existing coarse ones and globally refine each cell

This process might be repeated several times

Developed by Ales Ronovsky (VSB, PRACE)



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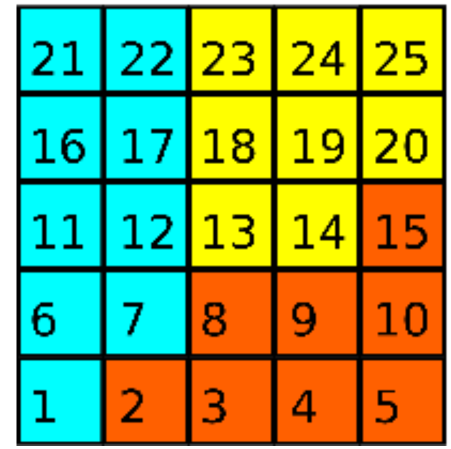
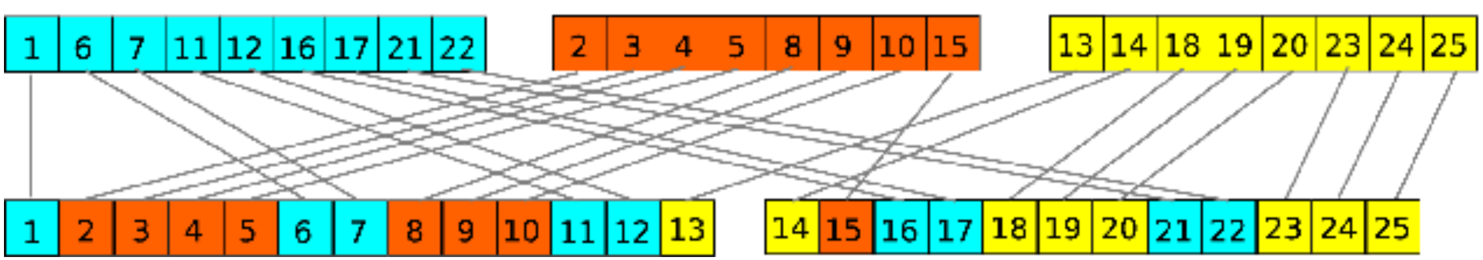
Block-Based IO

Use global numbering

Redistribution on n blocks

- n blocks ≤ n cores
- Minimum block size may be set to avoid many small blocks (for some communication or usage schemes), or to force 1 block (for I/O with non-parallel libraries)
- Rank 0 is collecting info from the blocks



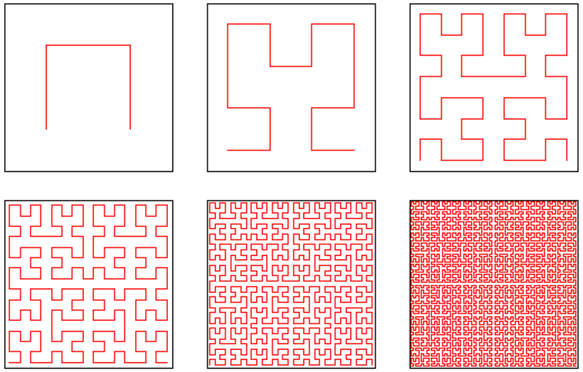


Test Case - Configuration

3D lid-driven cavity - fully unstructured mesh (tetras)

Size of the meshes:
MM Level 0 (13 million cells – Current production runs)
MM Level 1 (111 million cells – Current production runs)
MM Level 2 (890 million cells – Production runs in 2015)
MM Level 3 (7.2 billion cells – Production runs in 2016/2017)

Geometric partitioning using a Space-Filling Curve approach (Hilbert)



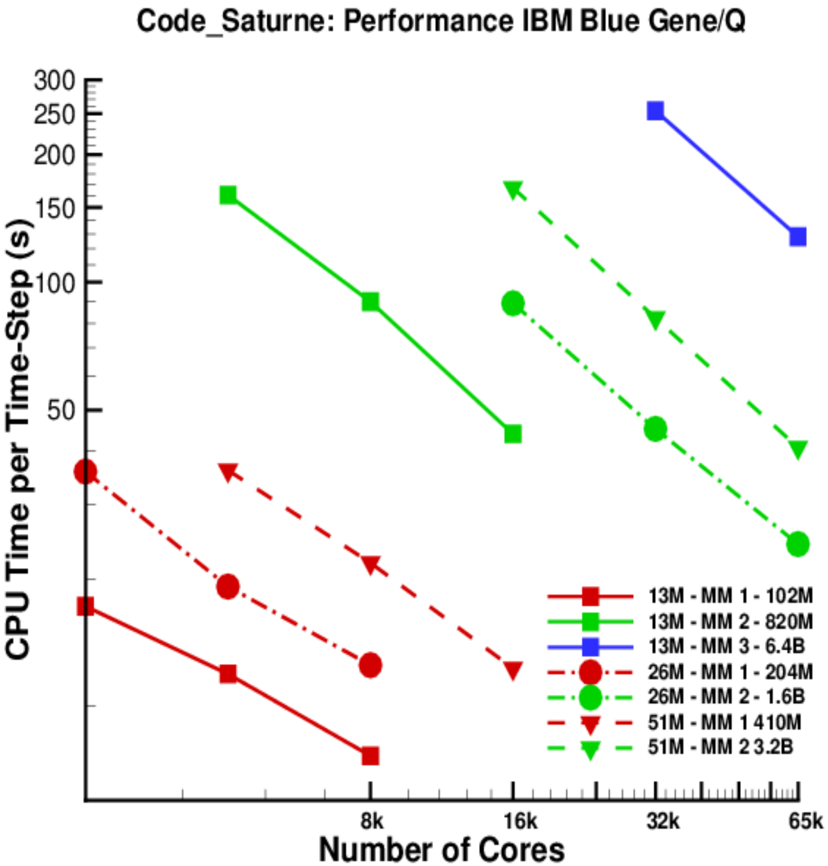
Note

IO tests are performed when the solver performance is still acceptable

If not stated, **machine default settings**. No striping for Lustre, for instance

Scalability at Scale (1)

Mesh generated by Mesh Multiplication



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105B Cell Mesh (MIRA, BGQ)

Cores	Time in Solver
262,144	652.59s
524,288	354.89s

13B Cell Mesh (MIRA, BGQ)

Nodes/Ranks	Time in Solver
16384/32	70.124s
32768/32	50.207s
49152/32	43.465s

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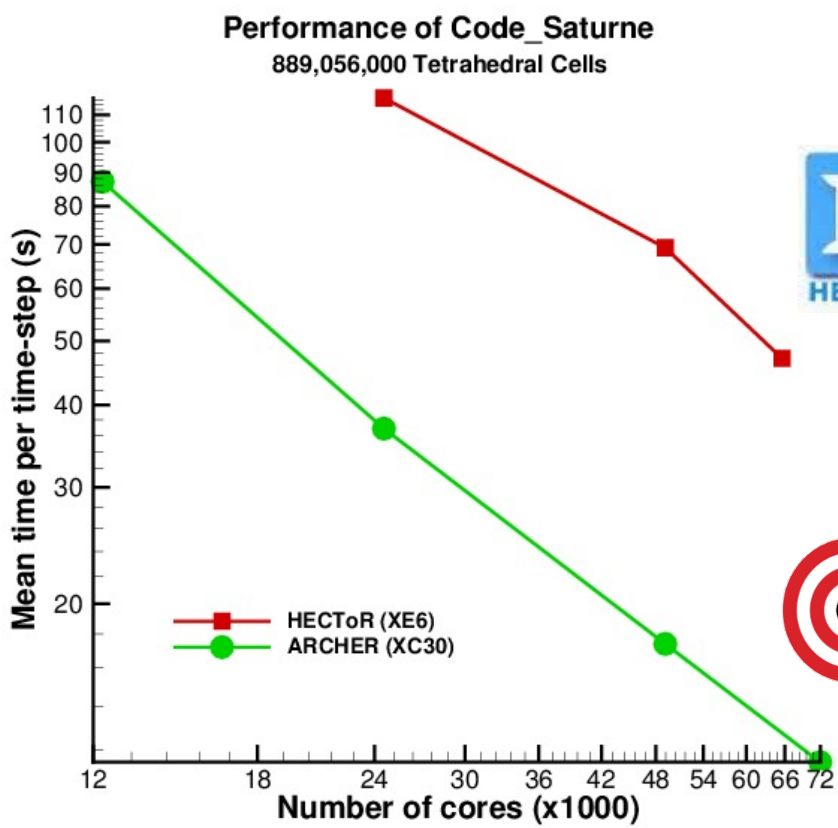
Scalability at Scale (2)

Comparison HECToR – ARCHER

Mesh generated by Mesh Multiplication
Cube meshed with tetra cells



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IO HECToR (Lustre)

Comparison IO per Blocks (Ser-IO) and MPI-IO
Comparison Lustre (Cray) / GPFS (IBM BlueGene/Q)

	HECToR		Blue Joule	
Cores	MPI-IO	Ser-IO	MPI-IO	Ser-IO
2048	633	1203	-	-
4096	608	640	85	1279
8192	859	1147	86	1300
16384	732	747	67	1330
32768	-	-	59	1360

Tube Bundle

812M cells

HECToR

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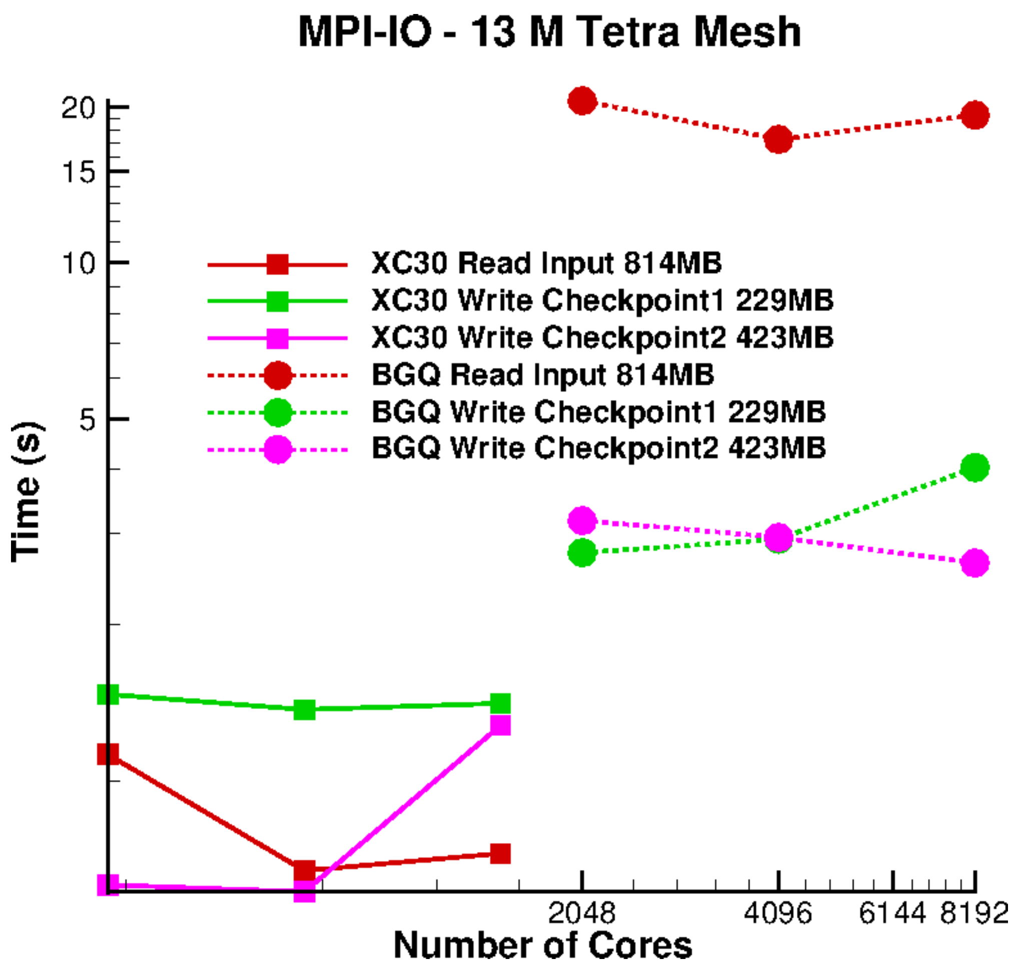
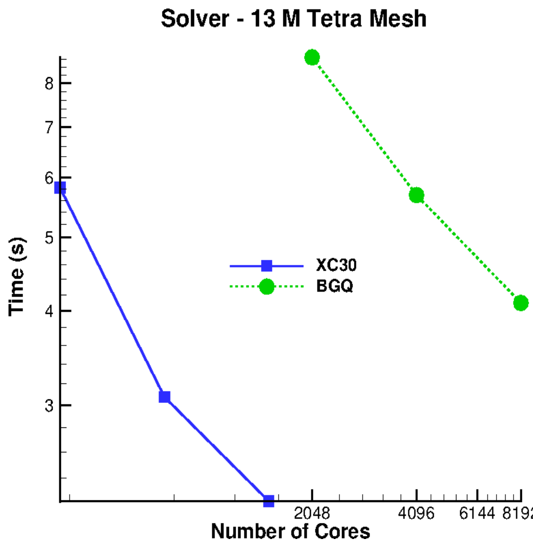
Block IO: ~same performance on Lustre and GPFS

MPI-IO: 8 to 10 times faster with GPFS

MM – Level 0

Writing Checkpoint Files

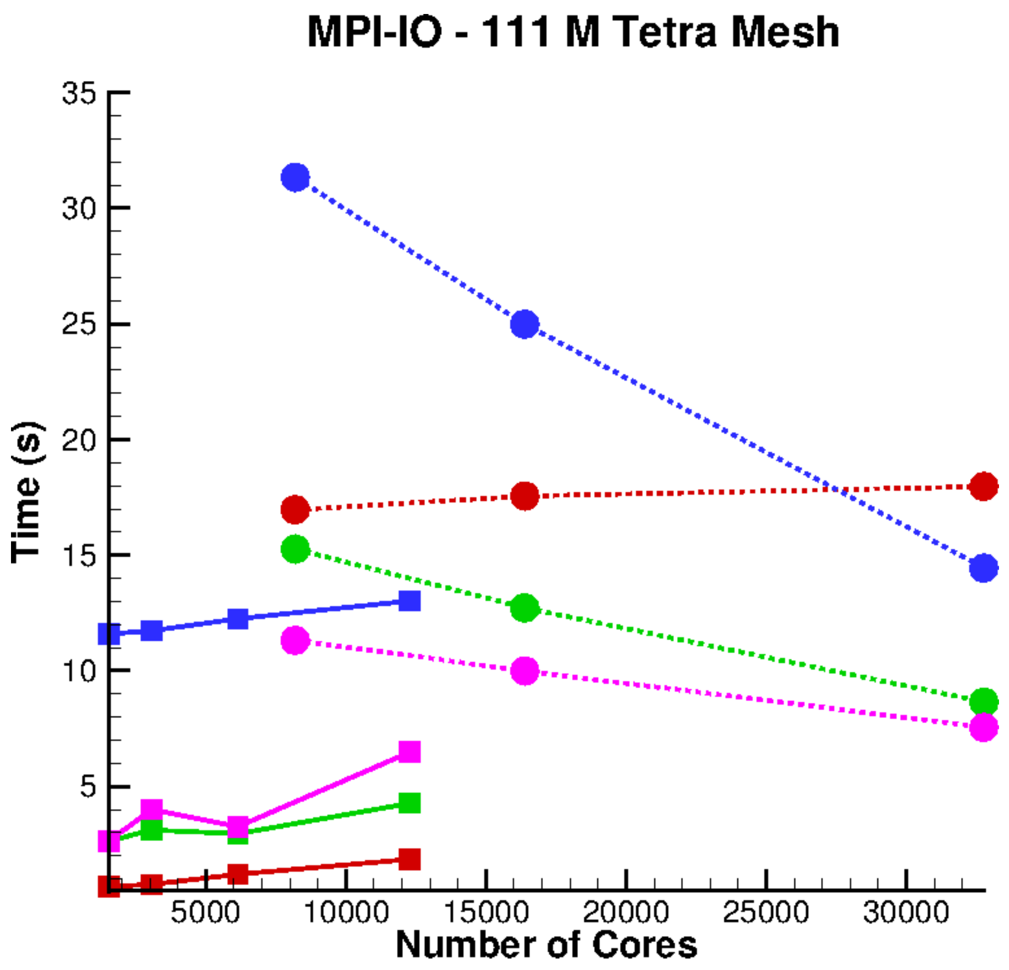


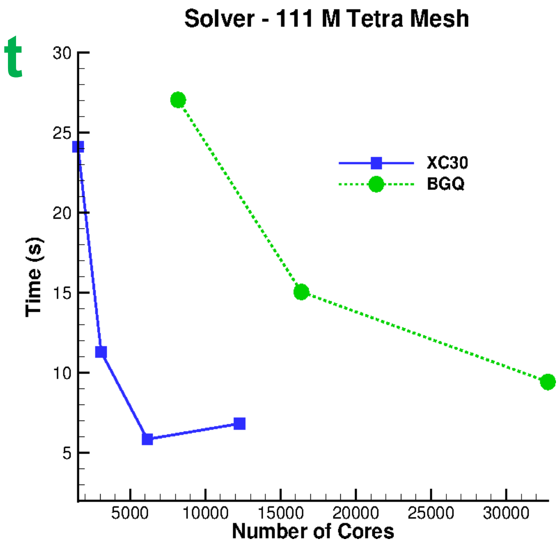


There is no mesh multiplication here

MM – Level 1

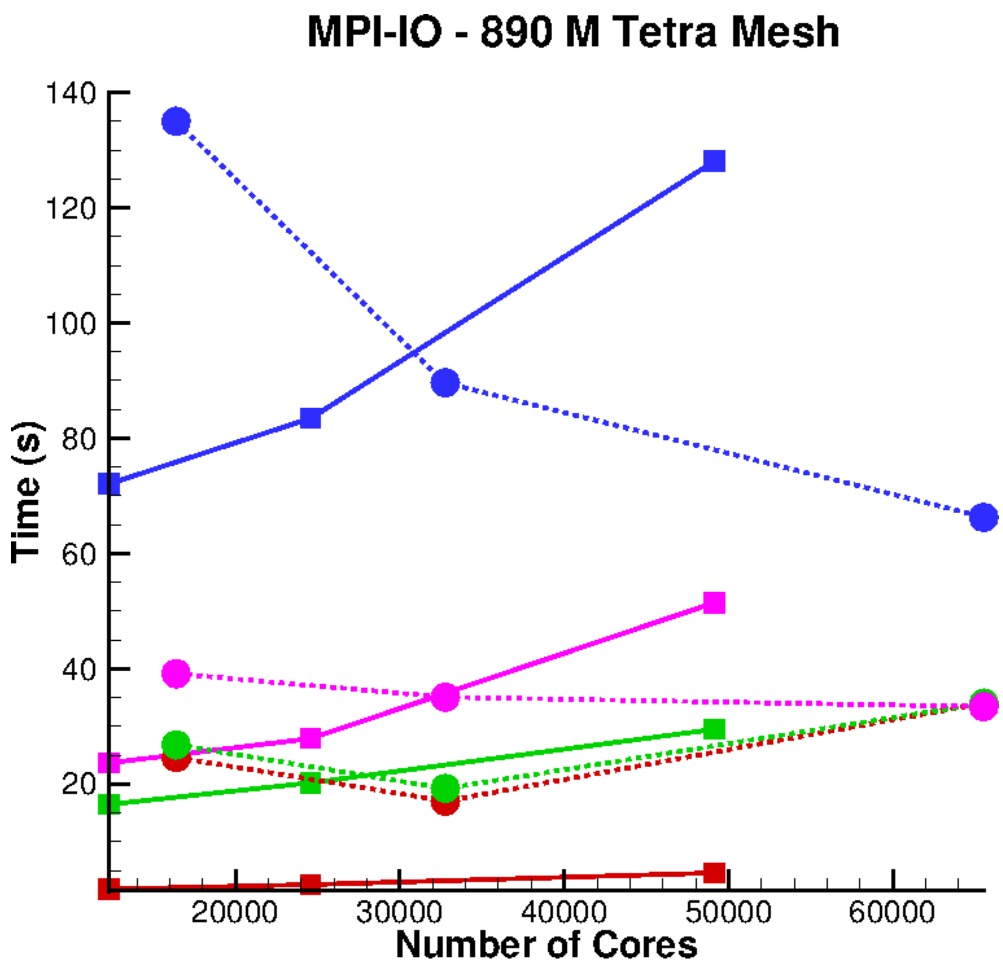
Writing Checkpoint Files – Mesh_Output

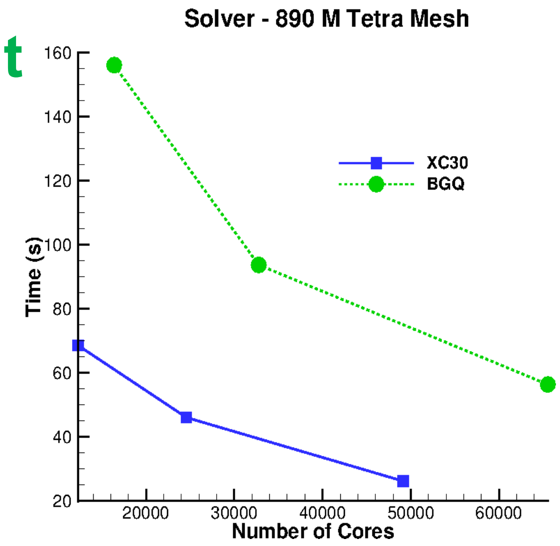




MM – Level 2

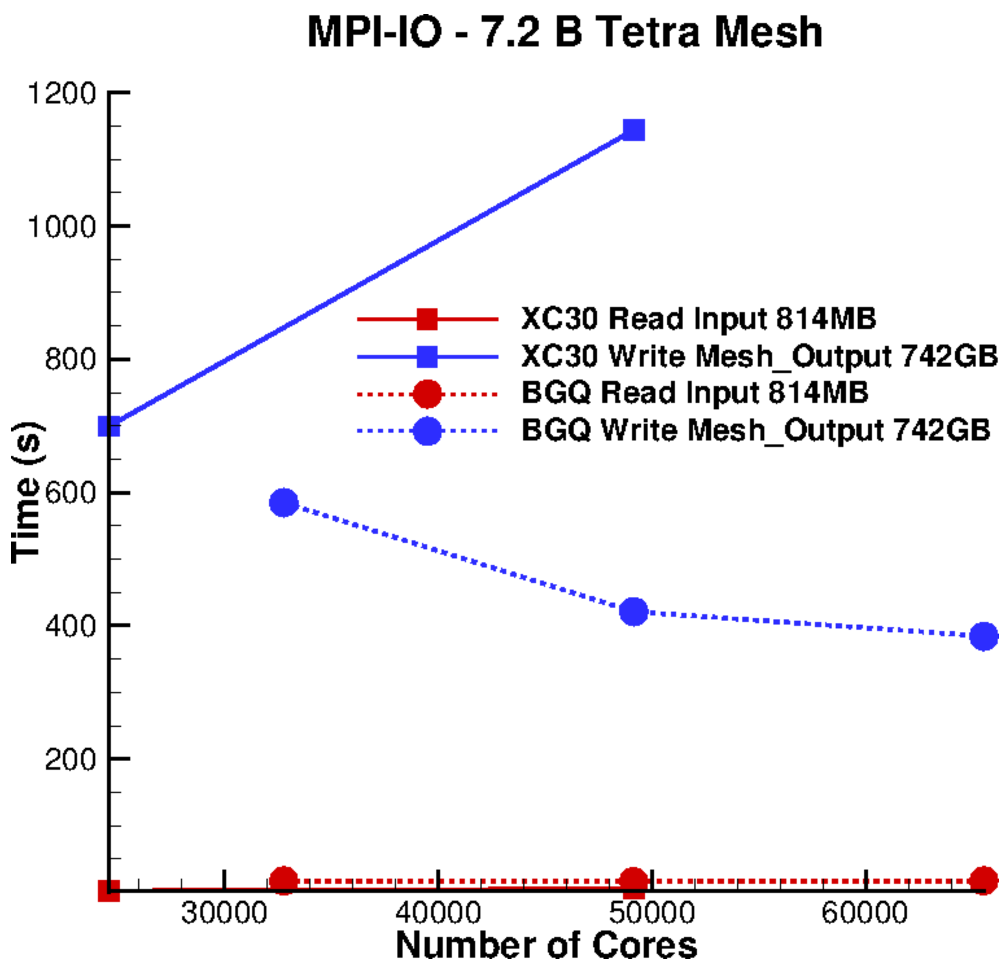
Writing Checkpoint Files – Mesh_Output

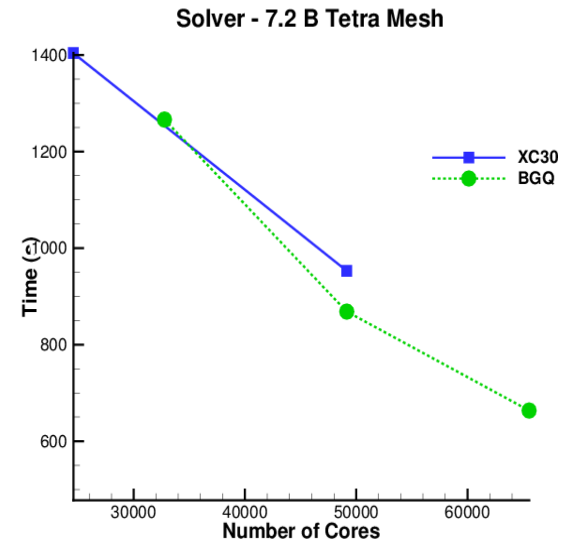




MM – Level 3

Writing Mesh_Output



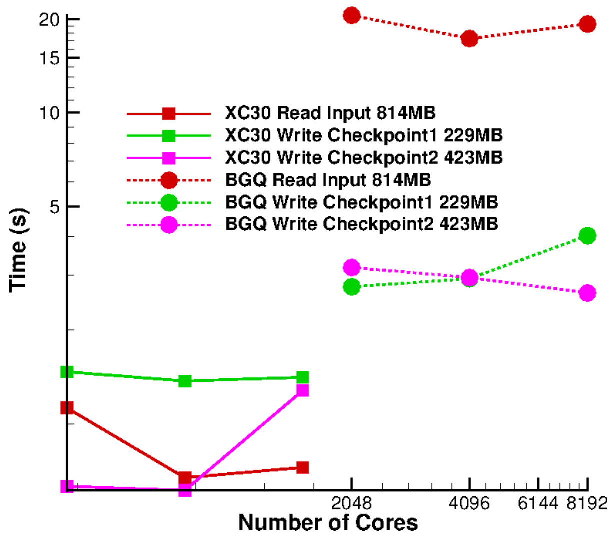


One time step only for the solver.

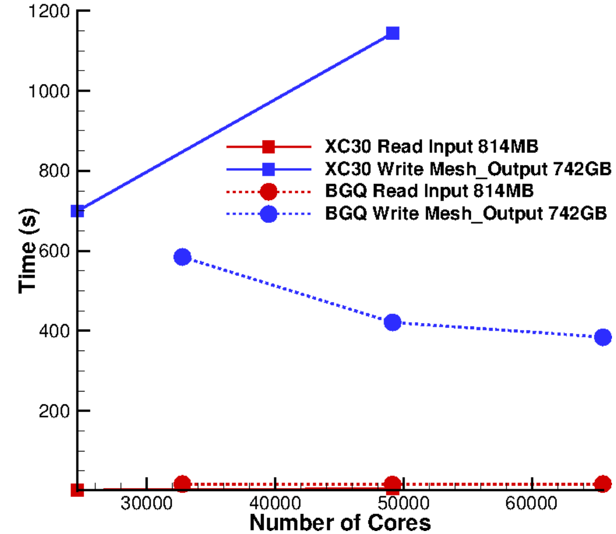
Timing also involves IOs

Quick Summary

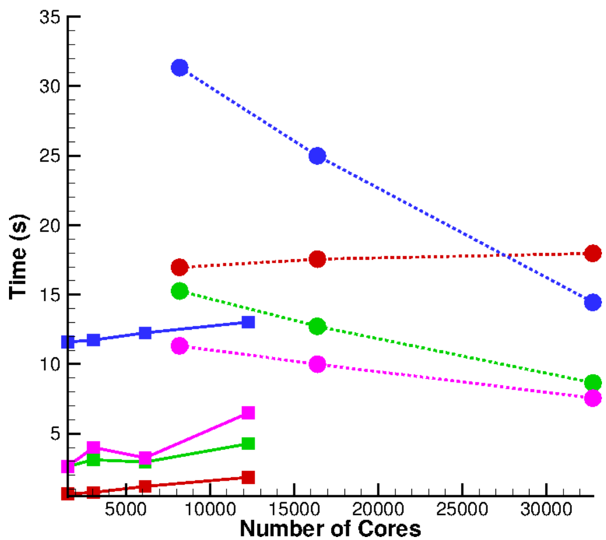
MPI-IO - 13 M Tetra Mesh



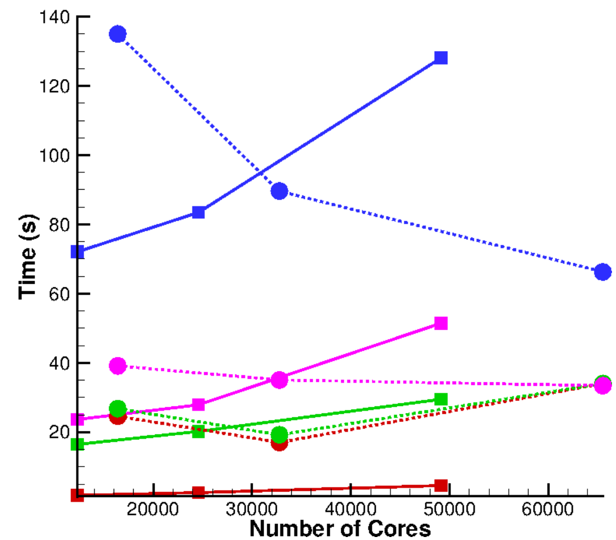
MPI-IO - 7.2 B Tetra Mesh



MPI-IO - 111 M Tetra Mesh

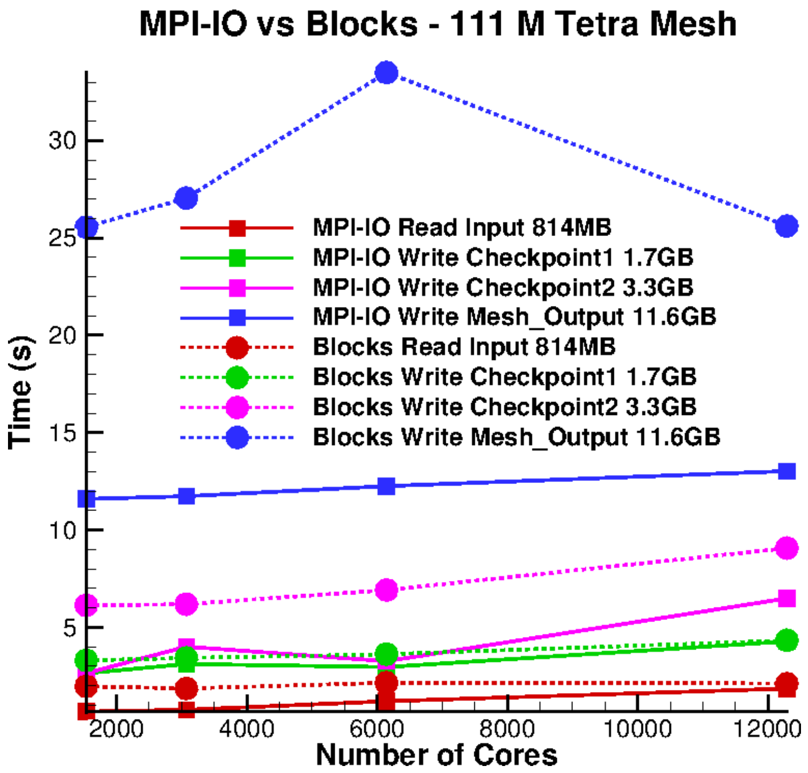


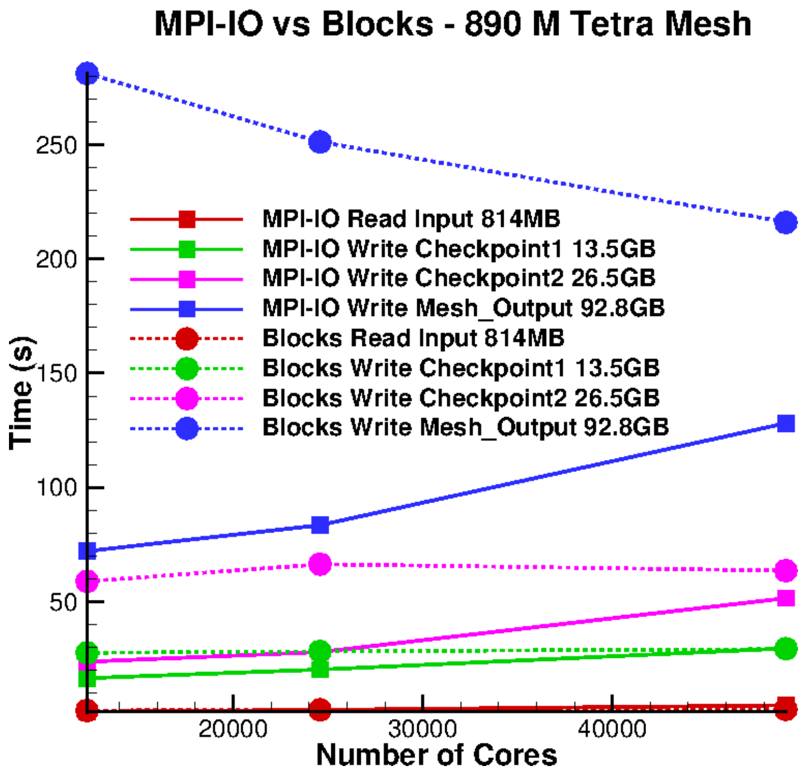
MPI-IO - 890 M Tetra Mesh



MPI – IO vs Block IO

Writing Checkpoint Files – Mesh_Output





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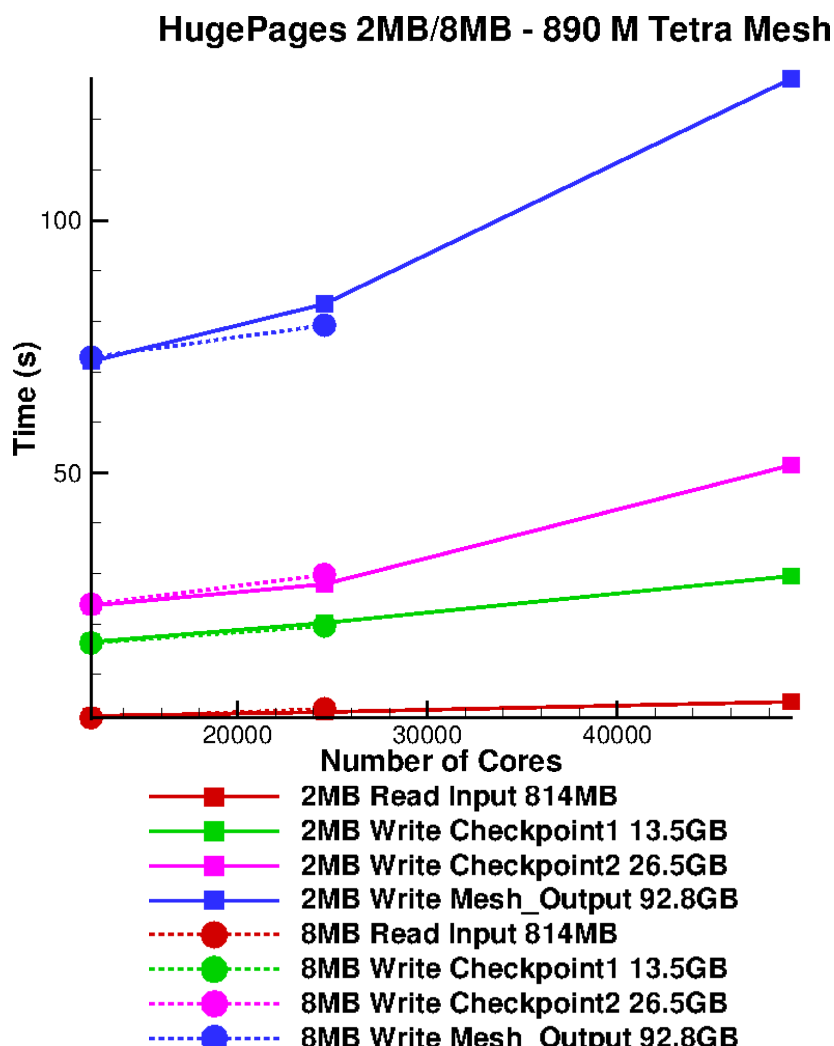
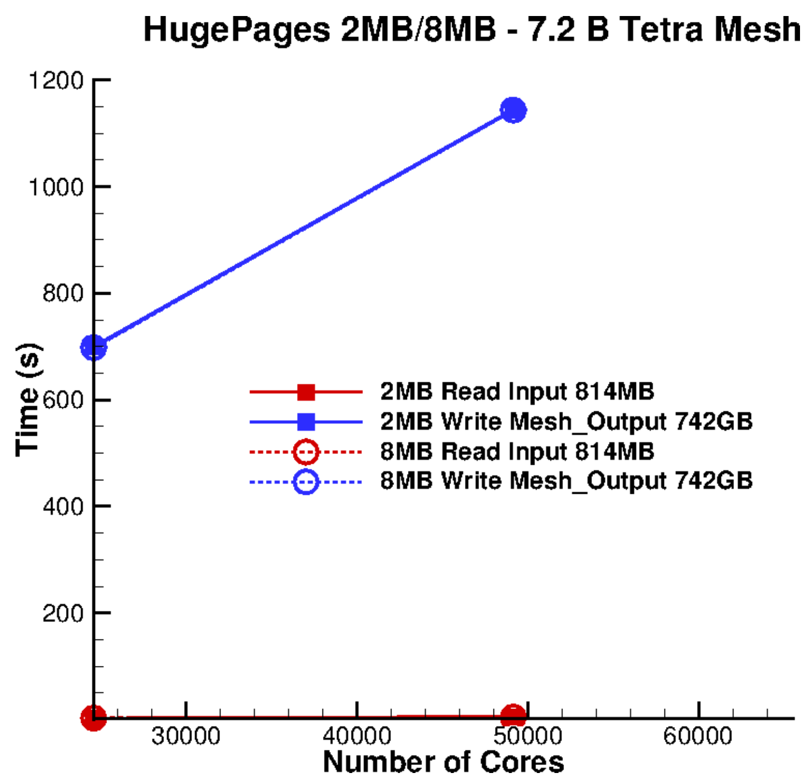
Cray Huge Pages

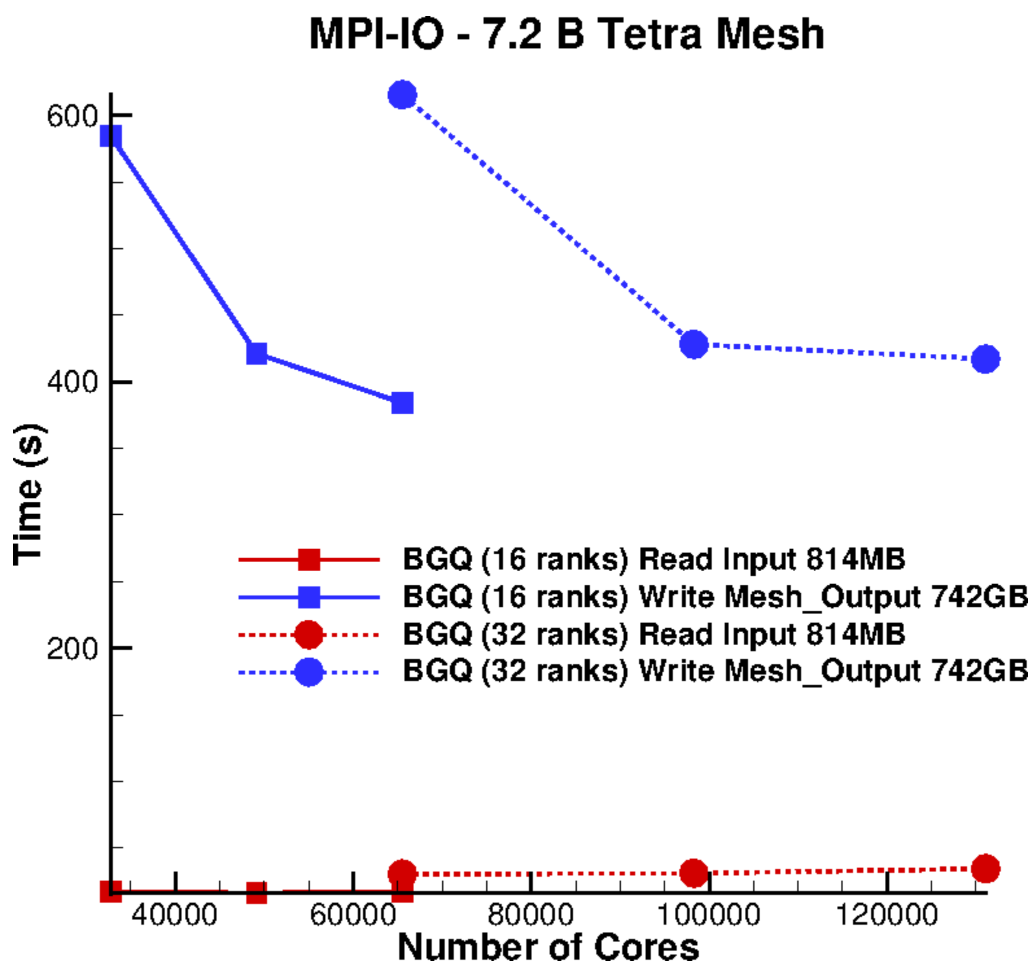
Virtual Memory Pages. They can sometimes provide better performance by reducing the number of TLB misses and by enforcing larger sequential physical memory inside each page

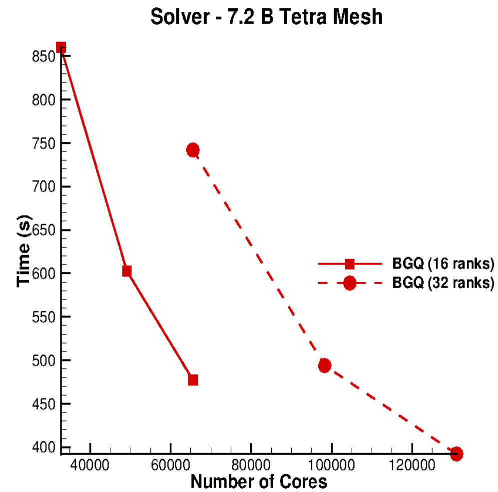




Effect of Hyperthreading?

Writing Mesh_Output





- Tests are performed on the BGQ
- More MPI tasks are used for the same number of compute nodes and IO nodes

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Conclusions

With the current machine/filesystem settings

MPI-IO

ARCHER (Lustre) better for small meshes than larger ones
BlueJoule (GPFS) better for large meshes than smaller ones

MPI-IO vs Block IO

If results on HECToR were comparable, much better obtained with MPI-IO on ARCHER

Cray HugePages (Lustre)

No clear improvement when using 8MB

Hyperthreading (GPFS)

IO time not affected when using hyperthreading

Perspectives

Lustre System

Using "striping" for better performance for large meshes?

BGAS (Blue Gene Active Storage) System

The Active Storage Project is aimed at:-

-enabling close integration of emerging solid-state storage technologies with high performance networks and integrated processing capability

-exploring the application and middleware opportunities presented by such systems

-anticipating future scalable systems comprised of very dense Storage Class Memories (SCM) with fully integrated processing and network capability

Project to test Code_Saturne on the BGAS System

(Collaboration between STFC (the Hartree Centre) and IBM)

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THANK YOU FOR YOUR ATTENTION