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High Performance Computing driven software development for next-generation modelling of the world's oceans

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dCSE ICOM Collaborations

- Applied Modeling and Computation Group, Imperial College, London (AMCG, http://amcg.ese.ic.ac.uk/)
- ARC, The Computational Science & Engineering Department (CSED), STFC (http:// www.cse.clrc.ac.uk/)
- Proudman Oceanographic Laboratory, Liverpool (POL, http://www.pol.ac.uk/)

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INTRODUCTION

- Overview of Imperial College Ocean Model (ICOM) – the next generation ocean model
- Solver Comparison
- Profiling and Performance Analysis
- Summary

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Motivations for the next generation ocean model

- To resolve a wide range of spatial and temporal scales
- Model internal waves, boundary currents, eddies, overflows, convection events, …, accurately and efficiently within a global and coupled context
- Need for accurate and efficient representation of highly complex domains
- Ability to model interaction of flow with small scale topography, shelf seas, coastal regions, islands, estuaries, harbours,…

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A overview of the Computational Characteristic of ICOM

- Unstructured FEM Code
  - Start with Fluidity – an open source control volume finite element solver for 3D compressible multi-phase fluids. Has been developed by AMCG for more than a decade and is the basis for a range of multi-physics multi-scale applications
  - Initial mesh generation to follow complex bathymetry and coastlines -- **terrno**
- Adaptive Mesh, solving from large scales to small scales.
  - Add an adaptivity library which performs topological operations on the mesh, and mesh movement, to optimise the size and shape of elements in response to error measures
  - Dynamic load balance method -- **Zoltan**

- Most time spent solving Ax=b, where A is a Sparse Matrix
  - FEM Matrix assembly
  - Using PETSc's preconditioner and Iterative Solver
  - Most Computing time is spent here
- Fortran, C++/C, Python MPI Based
- Makes use of open source solutions for I/O, Visualisation, etc
  - Advantage – using latest software features

ICOM Software Package Lists

- VTK
- CGNS
- BLAS
- LAPACK
- XML2
- MPI
- PETSc
- ParMetis
- APPACK
- NetCDF
- UDUnits
- Python Development Environments
- Trang
- Spatial-Index
- Fortran 90 Compilers
- C++
- Subvision (SVN)

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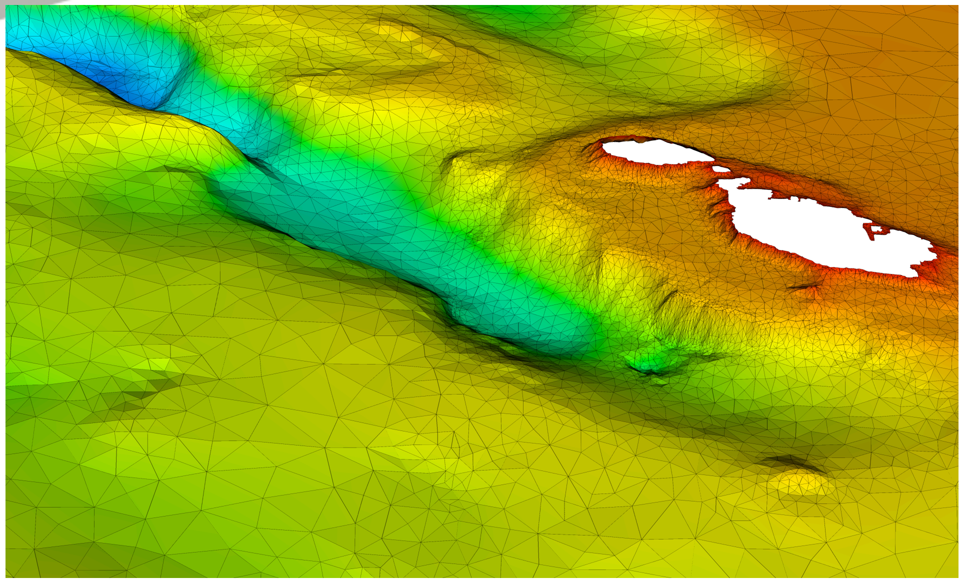

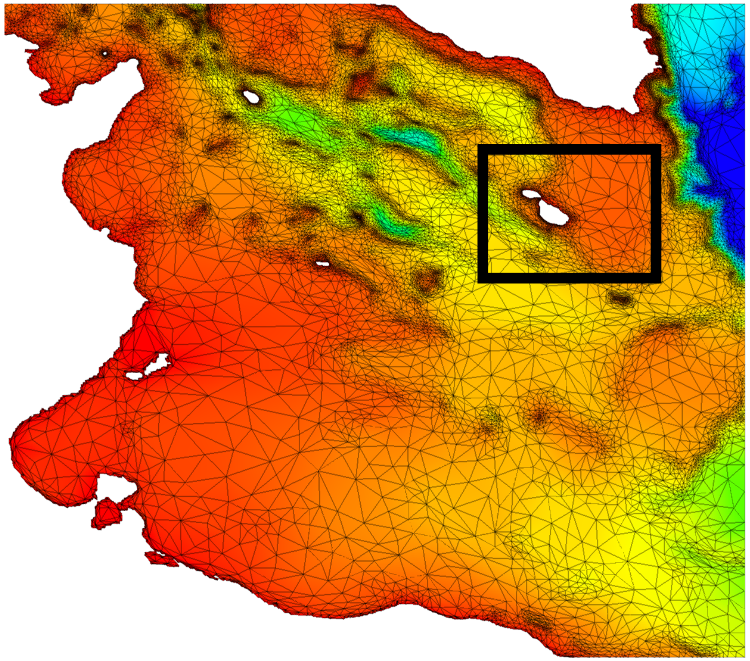

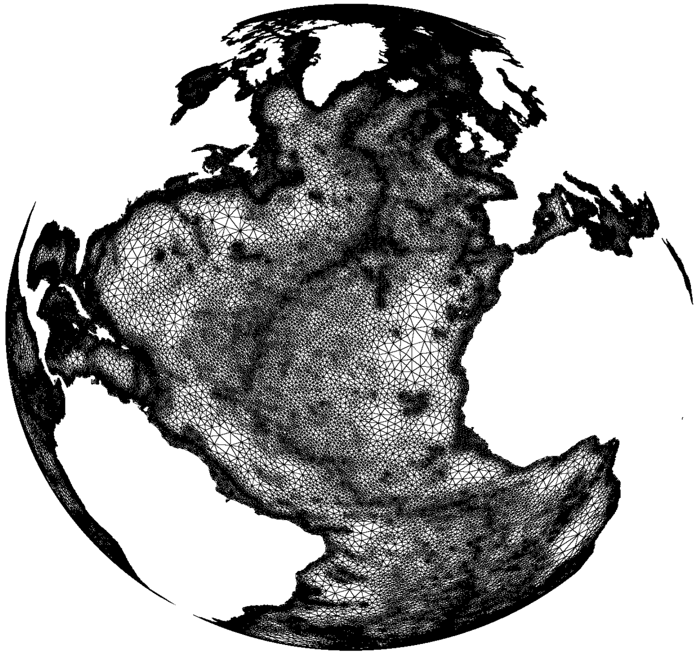

Unstructured meshes are an Ideal choice for representing complex problem domains and a coupled range of scales without the need for grid nesting

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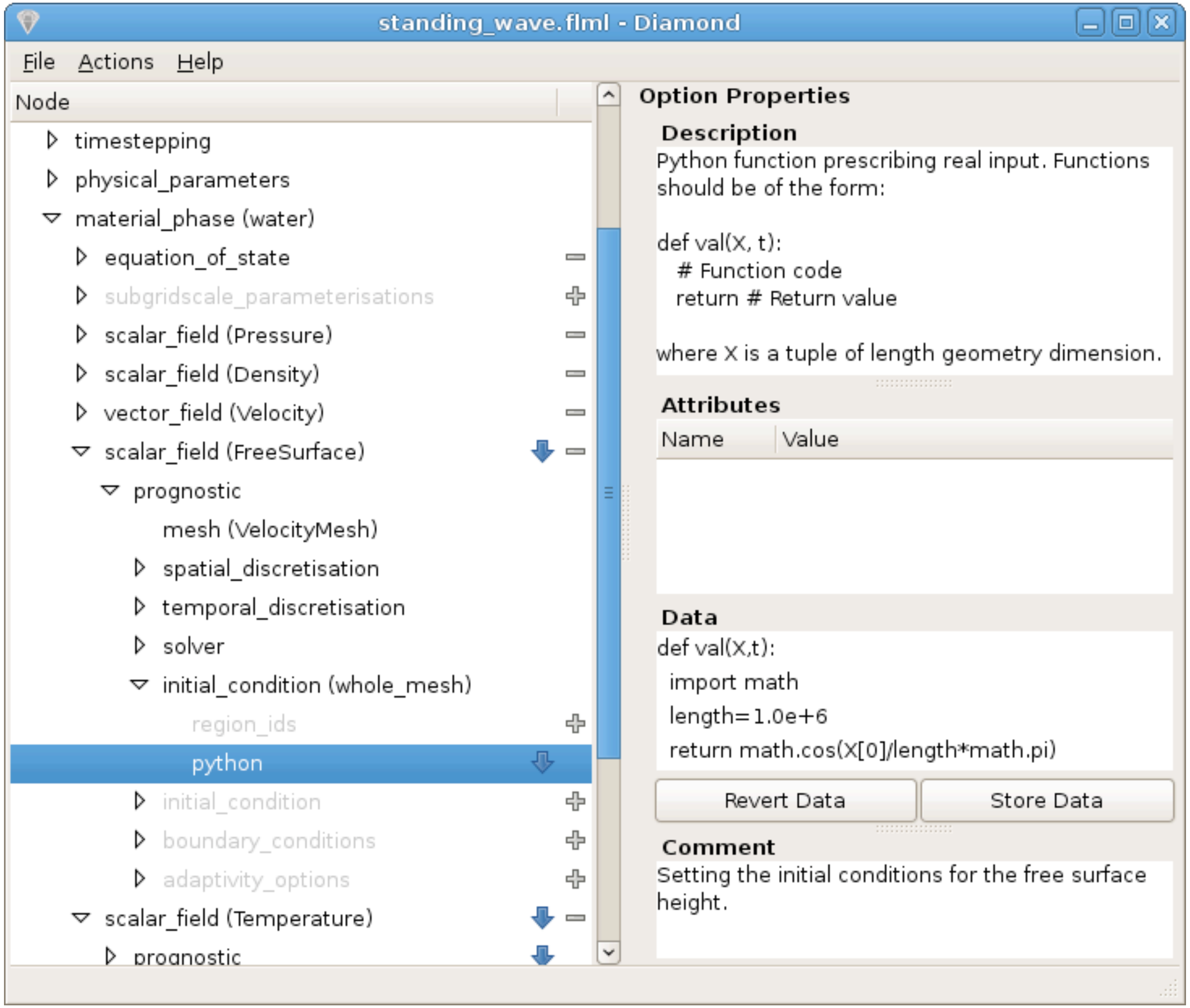
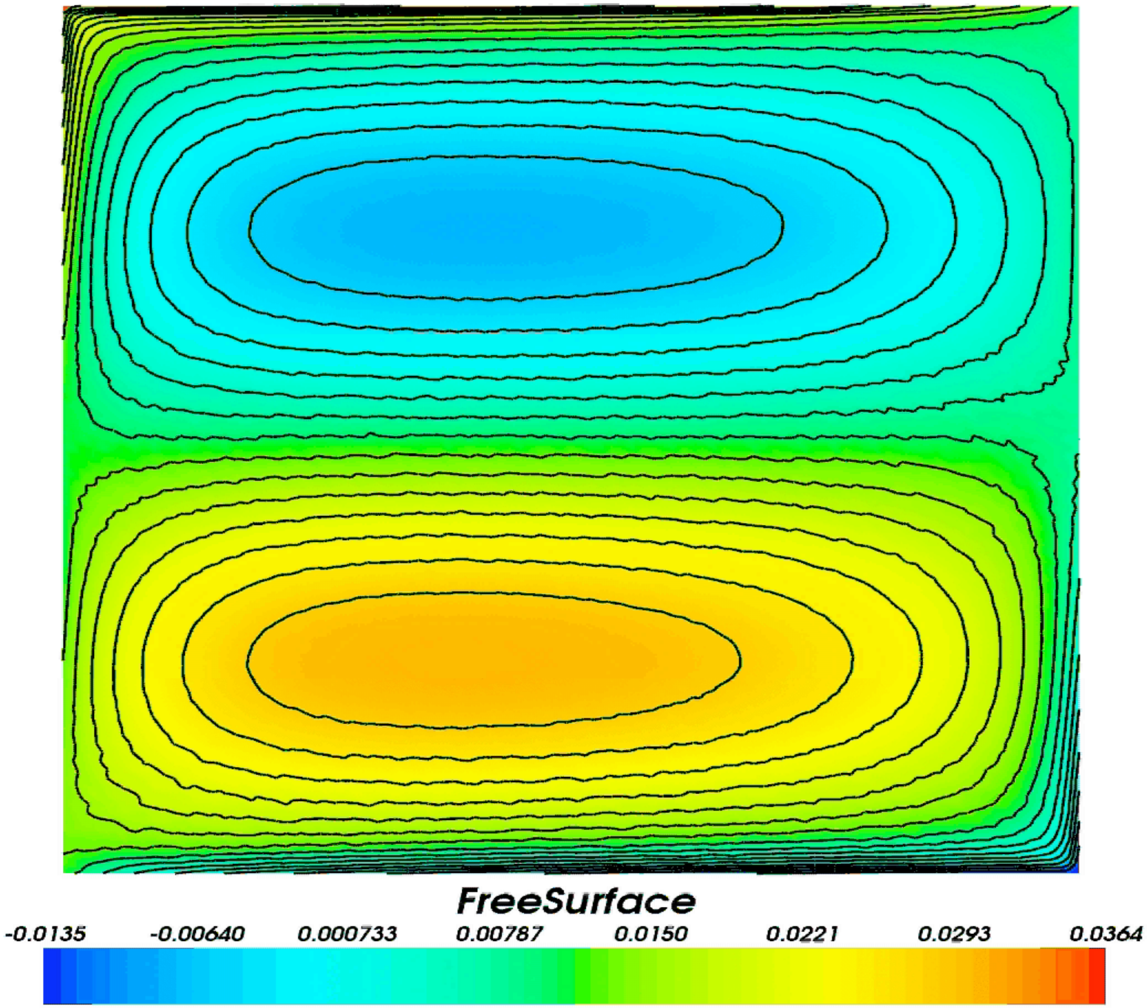
Diamond automatic pre-processing tool

- An xml schema file describes the rules that govern model options
- Diamond uses this to automatically generate a GUI based on the schema
- Options are entered and output as another xml file containing the options values
- This is read into an options library accessible from anywhere in code
- Includes many features, including the ability to define python functions executed at run time



Configuration of test case

- Baroclinic gyre benchmark test case has 10 million vertices; resulting in 200 million degrees of freedom for velocity
- The basic configuration is set-up to run for 4 time steps and not to adapt.
- Considering primarily the matrix assembly and linear solver stages of a model run.



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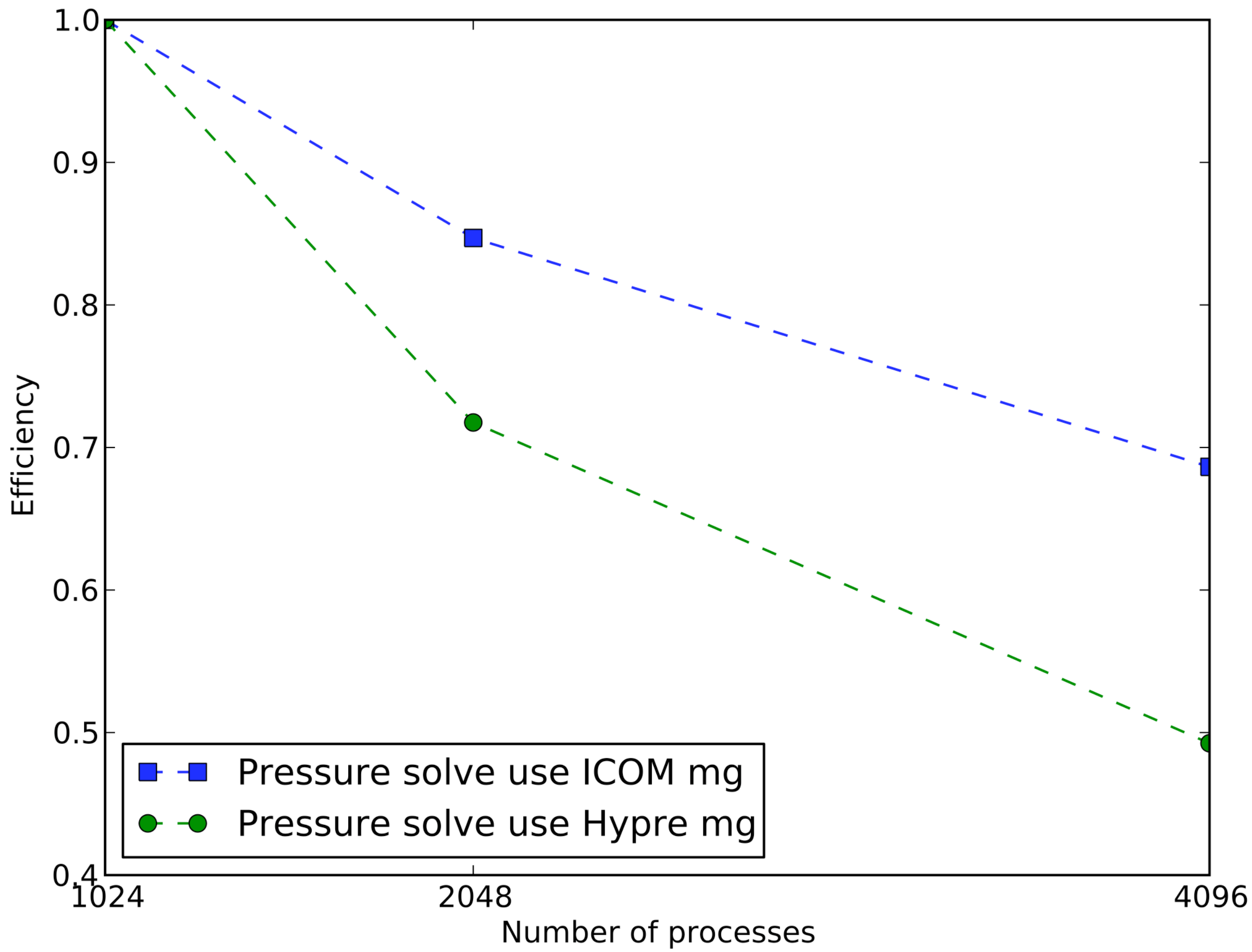
Solver Comparisons

- The pressure matrix has a very high condition number

- ICOM MG targeted specially at large-scale, large aspect ratio ocean problems

- ICOM MG has better scalability than BoomerAMG due to its specialised nature.

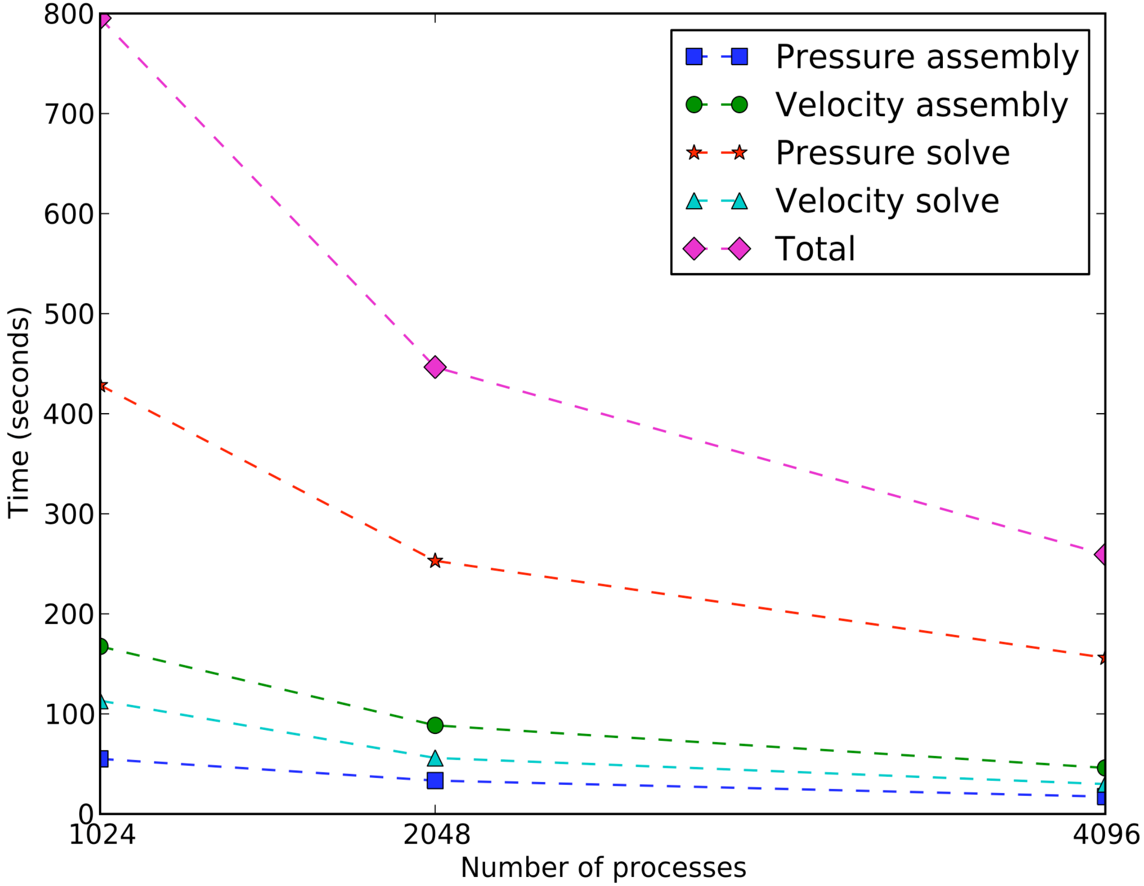


Profiling and Performance Analysis

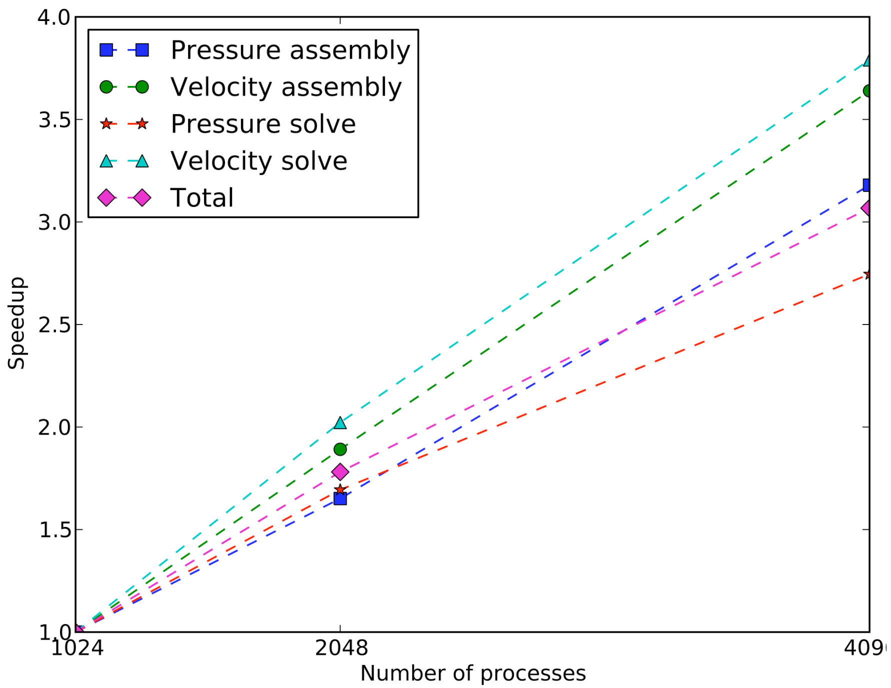
- Users should not spend time optimizing a code until after having determined where it spends the bulk of its time on realistically sized problems.
- Using CrayPAT/Vampir to address the parallel aspects, such as parallel efficiency, load balancing and communications overheads.
- Automatic tools in Profiling tools didn't work for ICOM profiling
- Simple timing hooks in the code to get a coarse grain profile of code performance

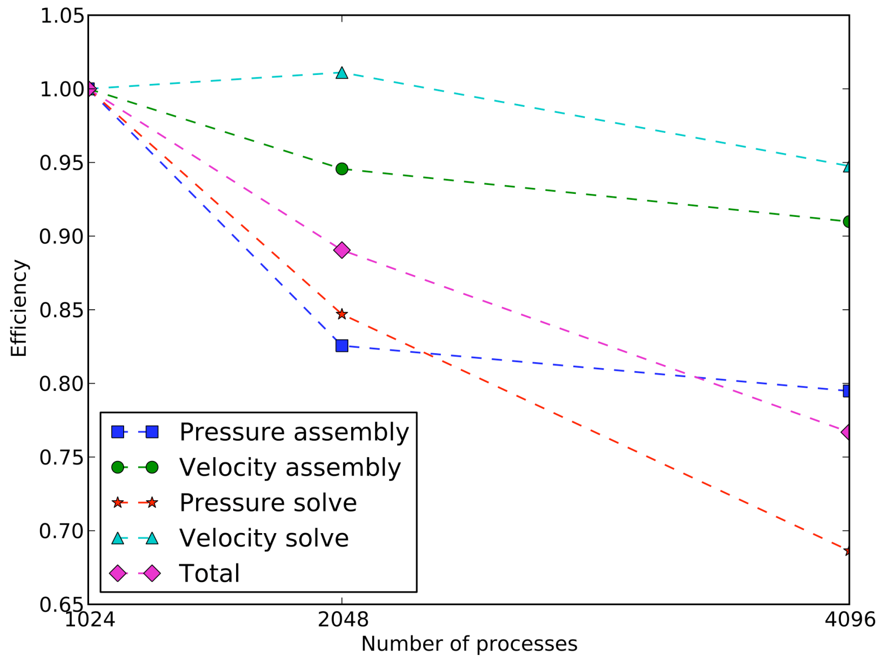
Basic Timings

- The solution process consists of the assembly of the linear systems representing the discretised momentum equation and the pressure equation.
- Matrix assembly for pressure and velocity can take more than 30% of the total simulation time with 1024 cores.
- Pressure solver is the main cost
- Matrix assembly phase is expensive
  - Significant loop nesting, where the innermost loop increases in size with increasing quadrature;
  - Indirect addressing (due to unstructured meshes)
  - Cache re-use.



Speedup and Efficiency





the speedup and efficiency of momentum solver and each of its components

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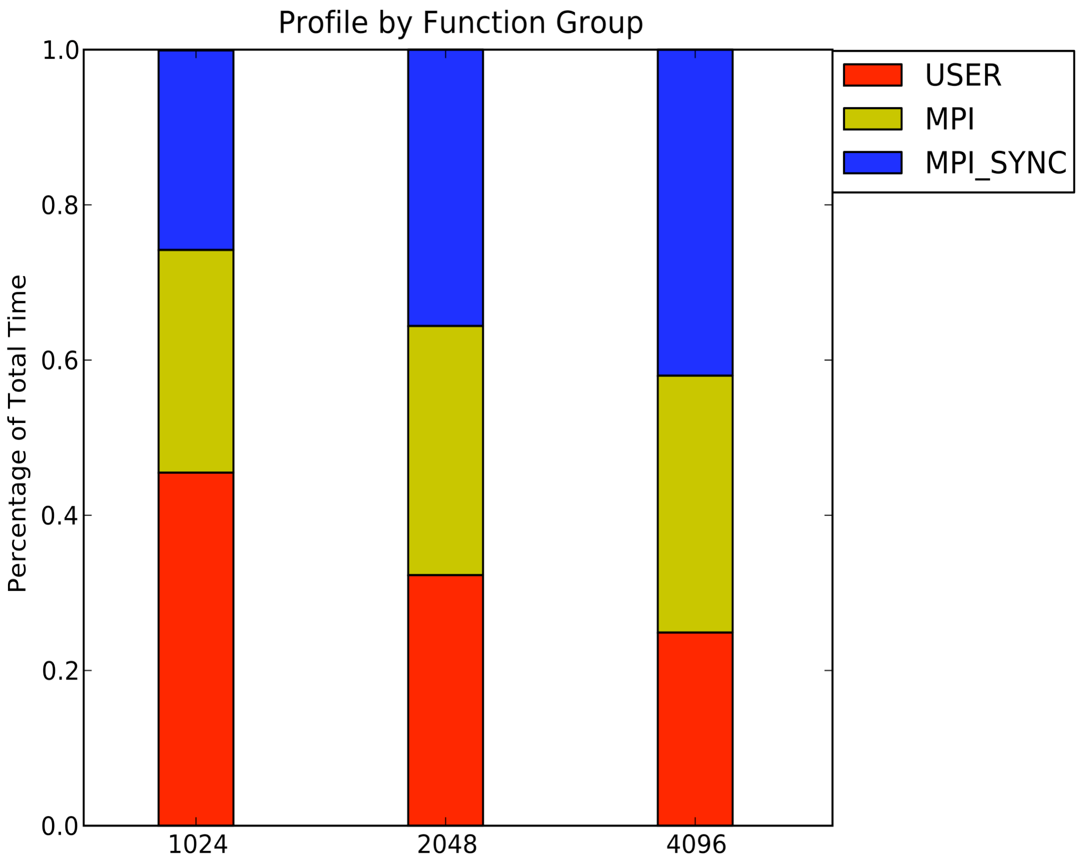
Communication overhead and load balance analysis

- Using **CrayPAT**, we obtained the statistic of three groups of functions, namely **MPI** functions, **USER** functions and **MPI_SYNC** functions.
- **MPI_SYNC** is used in the trace wrapper for each collective subroutine to measure the time spent waiting at the barrier call before entering the subroutine.
- The time percentage of MPI SYNC increases from 25.7% to 42.0%.
- The time percentage spent in MPI increases from 28.7% to 33.1% while USER functions drop from 45.5% to 24.9%

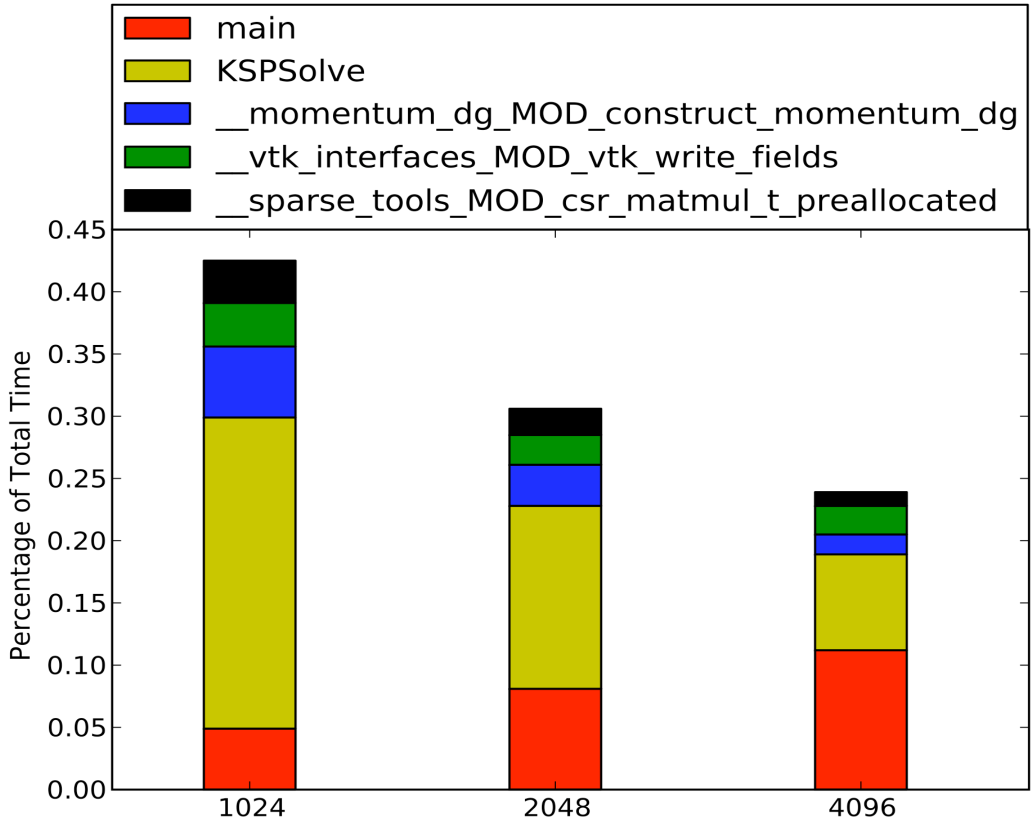


Top time consuming USER functions

- The speed up of the linear solver KSPSolve is about 3.5 with 4096 cores comparing with 1024 cores according to the CrayPAT tracing results.

- The function **main** represents the functions that have not been traced in the code. These functions are outside of momentum solver

- Future work will focus on these functions of poor scaling behaviour.

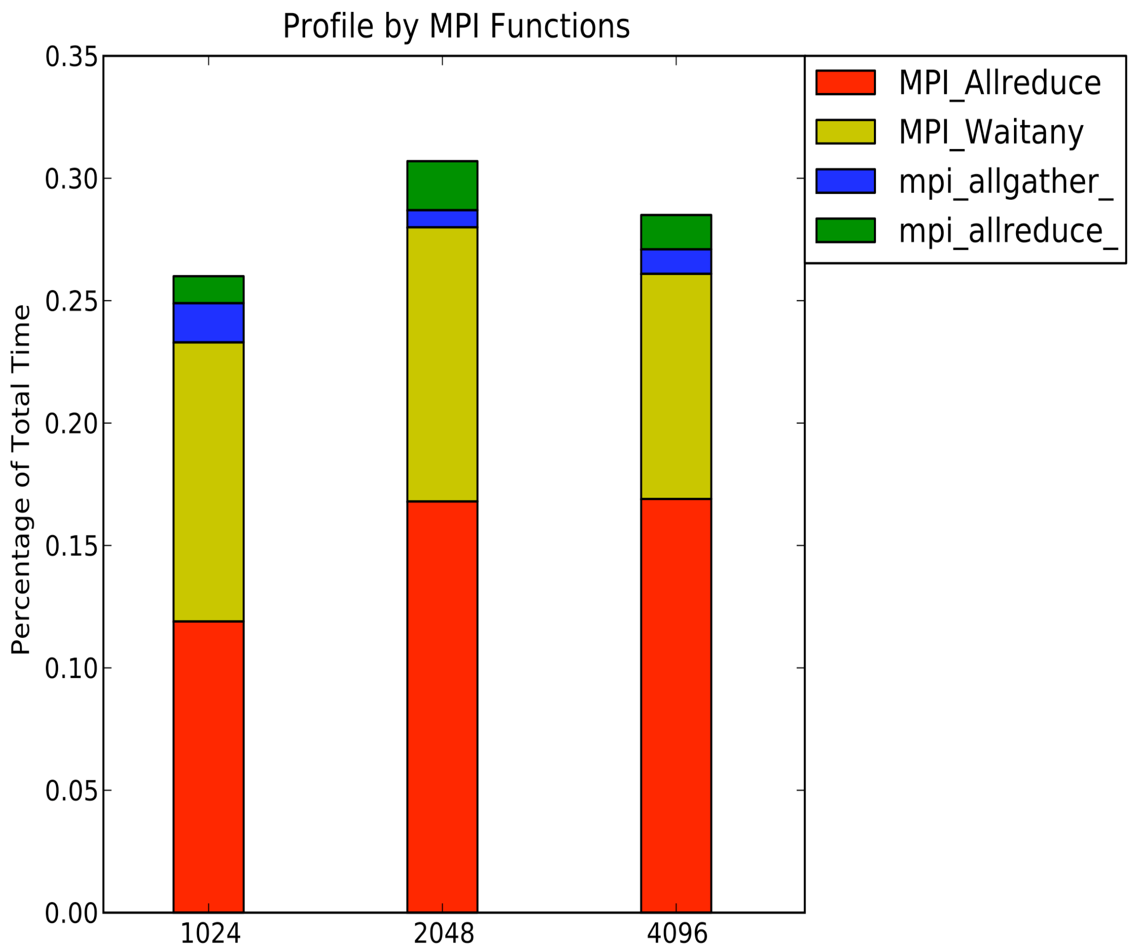


Top time consuming MPI functions

- The most time consuming of the **MPI** groups is **MPI_Allreduce.**

- From the call tree generated by **CrayPAT**, it becomes clear that this function is called from **PetscMaxSum** within **PETSc.**

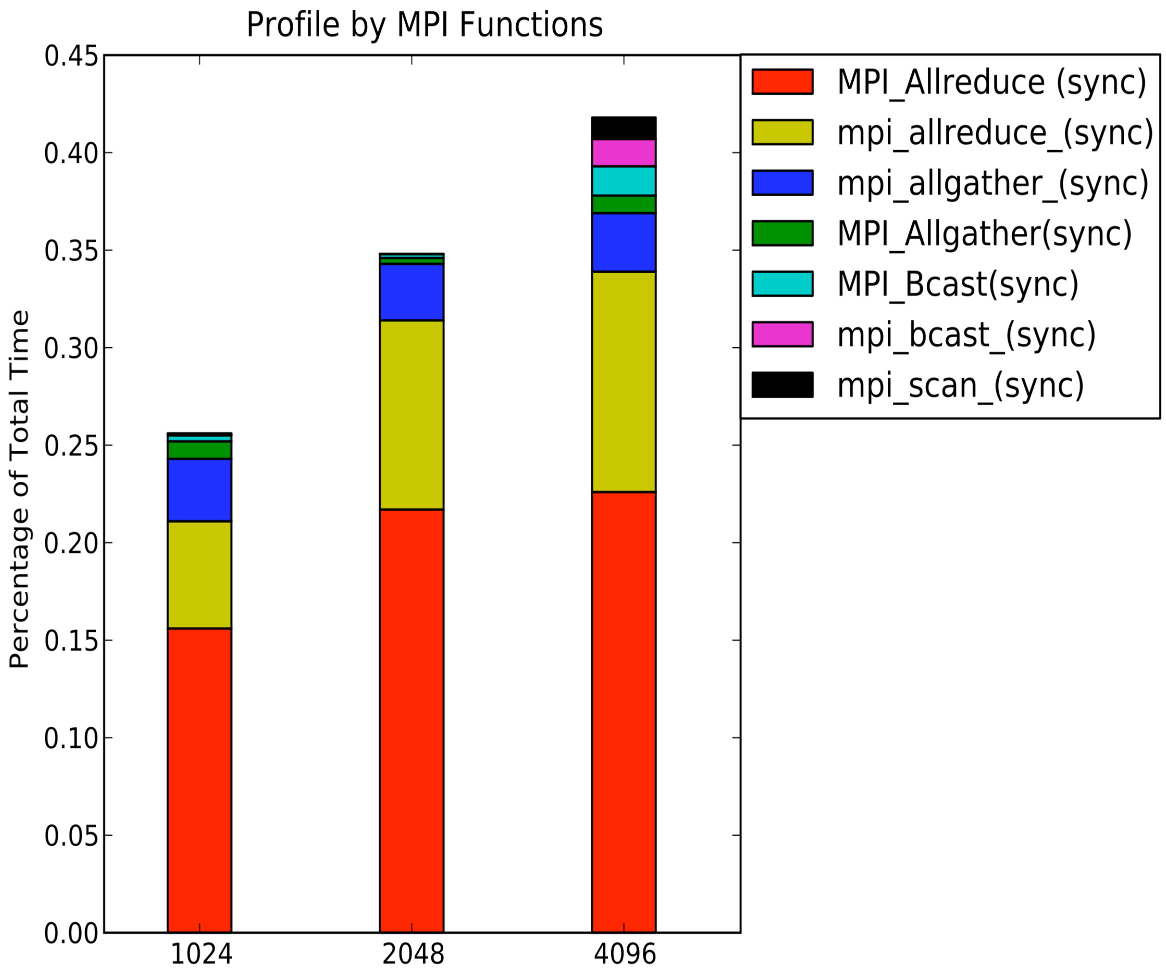
- **MPI_Waitany** is indicative of the quality of the load balancing. Given that this amount does not increase significantly between runs on 1024 to 4096 cores



Top time consuming MPI_SYNC functions

MPI_Allreduce accounts the most part of waiting time spent in the barrier, it is worth to check if there are possibility to combine several **MPI_Allreduces** together.

MPI_Bcast and **MPI_SCAN** are becoming more significant on 4096 cores, compared to runs on 1024 and 2048 cores



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Guidelines for third party library tracing for ICOM

- Requiring direct access to the source file or the object file, which limits the analysis of third party software performance, like **PETSc**.
- Properly reducing the profiling data determines qualities of profiling.
- Coarse time profiling + Fine grain profiling of specific parts of the code with CrayPAT/Vampir has been effective for ICOM

Summary

- From a starting point where the code was only routinely run on 64 cores on a local cluster, the **ICOM dCSE** project has significantly improved the performance of the code to enable efficient usage of large high performance computing systems such as the Hector Cray XT4.
- Presently the code is now scaling well up to at least 4096 cores on **HECToR**.
- Porting the code to **HECToR** has involved several challenges.
  - the code requires a range of third party libraries which need to be maintained on the target platform
  - Some Fortran 95 programming constructs caused compiler issues (stress-tested) for the various compilers. Resolving these required substantial effort from different groups including the developers, STFC ARC group and HECToR Support.
- Profiling the real world applications is a big challenge
  - Need to reduce the profiling data size whilst maintaining a representative dataset
  - Manual instrumentation was required in order to focus on specific sections of the ICOM code.
  - **CrayPAT** and **Vampir** are well suited to fine grain profiling on specific sections of the code

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