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HPC – the Perspective of a CFD Practitioner

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Summary

- Navier-Stokes Equations and CFD
- CFD Challenges
- Two Examples of HPC Applications
  - Modelling of a scramjet engine
  - Massively parallel hybrid CFD solver for ocean applications
- Where Are We?
- Concluding Remarks

Navier-Stokes Equations and CFD

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Navier-Stokes Equations and CFD

History

- Navier-Stokes equations govern motion of a viscous fluid.
- Claude Louis Marie Henri Navier derived the Navier-Stokes equations in 1822. His derivation was based on a molecular theory of attraction and repulsion between neighbouring molecules; Navier did not recognize the physical significance of viscosity and attributed the viscosity coefficient to be a function of molecular spacing.
- Euler had already derived the equations for an ideal fluid in 1755, which did not include the effects of viscosity.
- George Gabriel Stokes, in 1845, published a derivation of the equations as they are understood today.
- One hundred seventy years later the solution of these equations still is a challenge.

Navier-Stokes Equations and CFD

The equations

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}\left[\rho u_i u_j + p\delta_{ij} - \tau_{ji}\right] = 0, \quad i = 1, 2, 3$$

- These equations are valid for a single-phase fluid - liquid or gas, and they result from the application of Newton's second law to a continuum; in fact, these equations are applicable to any non-relativistic continuum.
- For a Newtonian fluid, assuming Stokes Law for mono-atomic gases, the viscous stress is given by

$$\tau_{ij} = 2\mu S^*_{ij}$$

- The viscous strain-rate is defined as

$$S^*_{ij} \equiv \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}$$

Navier-Stokes Equations and CFD

Additional governing equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_j\right] = 0$$

- This equation is the most general form of the continuity equation, which regardless of the flow assumptions, is a statement of the conservation of mass.
- The Navier-Stokes, despite their numerous applications offer a major challenge to mathematicians.
- It remains to be proven for three dimensions the existence and smoothness of their solutions, i.e., solutions always exist (**existence**), or that if they do exist, then they do not contain any singularity (**smoothness**).
- The Clay Mathematics Institute offers a **US$1,000,000** prize for the proof of **existence** and **smoothness** of the Navier-Stokes equations.

Navier-Stokes Equations and CFD

Example of an accompanying equation

$$\frac{\partial}{\partial t}(\rho e_0) + \frac{\partial}{\partial x_j}\left[\rho u_j e_0 + u_j p + q_j - u_i \tau_{ij}\right] = 0$$

- This equation is the governing equation for the energy of a single-phase fluid, and directly derived from a balance of energy (1st law of Thermodynamics).
- The nomenclature - e_0: *total energy;* q_j: *heat-flux.*

$$e_0 \equiv e + \frac{u_k u_k}{2}$$

and

$$q_j = -\lambda \frac{\partial T}{\partial x_j}$$

λ: thermal conductivity

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Navier-Stokes Equations and CFD

CFD

- The Navier-Stokes equations have only a few analytical solutions, even so major assumptions and simplifications are required.

- However, in practice, these equations are too difficult to solve analytically.

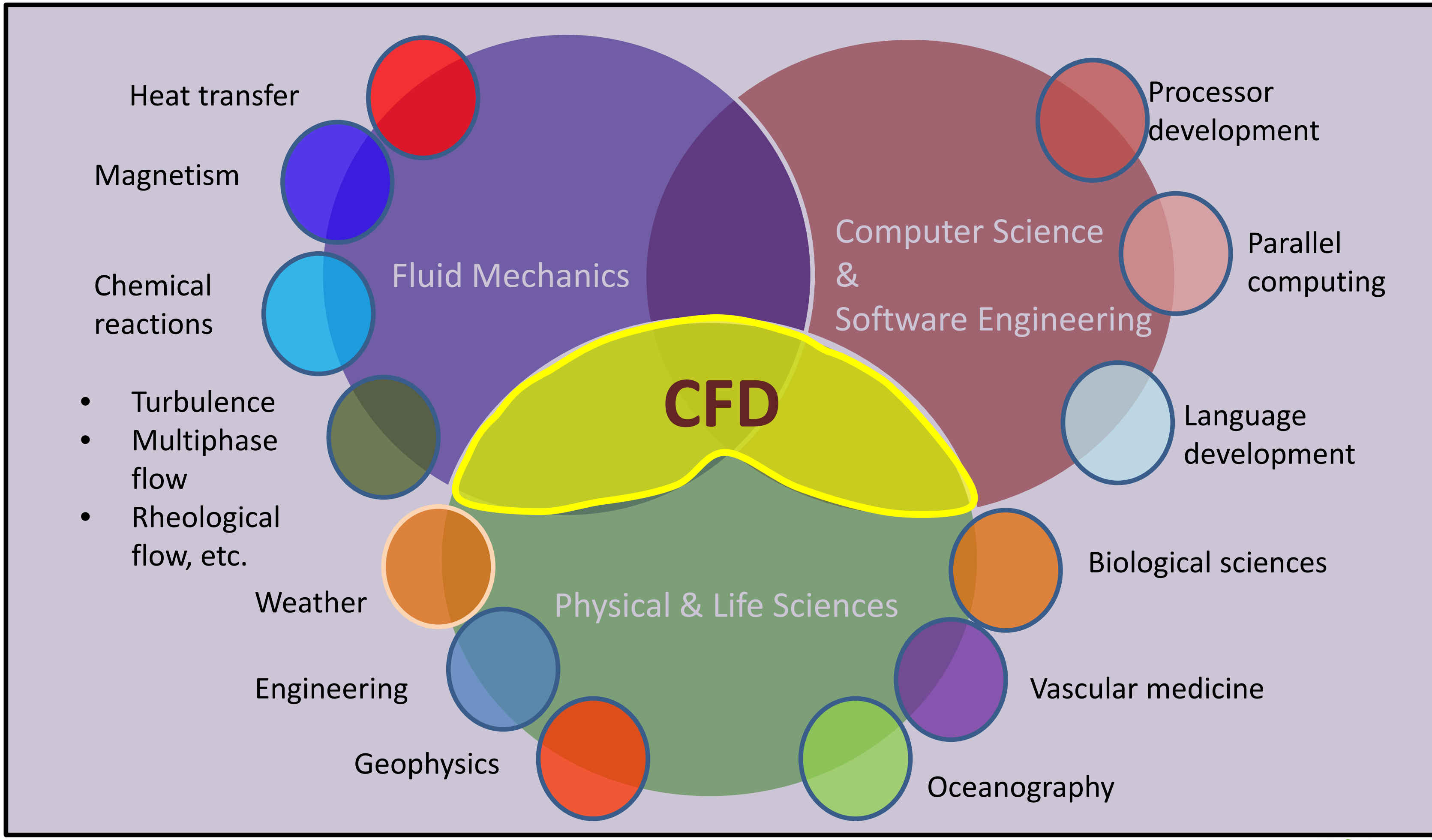
- The major trend is to solve approximations to the equations using a variety of methods like finite difference (FD), finite volume (FV), finite element (FE), and spectral methods (SE). This area of study is traditionally called **Computational Fluid Dynamics (CFD)**.

- The above-mentioned methods have in common the "discretization" (i.e., mapping the region of interest with a finite number of points) of the partial differential equations, and then link the neighbouring points using specified profiles (functions).

CFD Challenges

HPC – the Perspective of a CFD Practitioner

CFD Challenges



HPC – the Perspective of a CFD Practitioner

CFD Challenges

I have no power to foresee the future; however, the current CFD trends indicate the ongoing CFD challenges will remain in place for some time, and they are:

- Physical models
- Computational requirements
  - Faster processors and larger memories,
  - “Intelligent” software algorithms
- Benchmarking and validation
  - Error evaluation of the numerical predictions

CFD Challenges

Realism vs. Accuracy

(The desired accuracy for each predicted quantity depends on the technical issues associated with the analysis)

Pool Fire

- FDS simulation of one-meter methane pool fire (Sandia Test # 17);
- 15 mm resolution and colored by temperature.
- Supporting document: Kevin McGrattan *et al.*, Fire Dynamics Simulator Technical Reference Guide, Volume 3: Validation, NIST Special Publication 1018-5, October 29, 2010.

CFD Challenges

Pool Fire

CFD Challenges

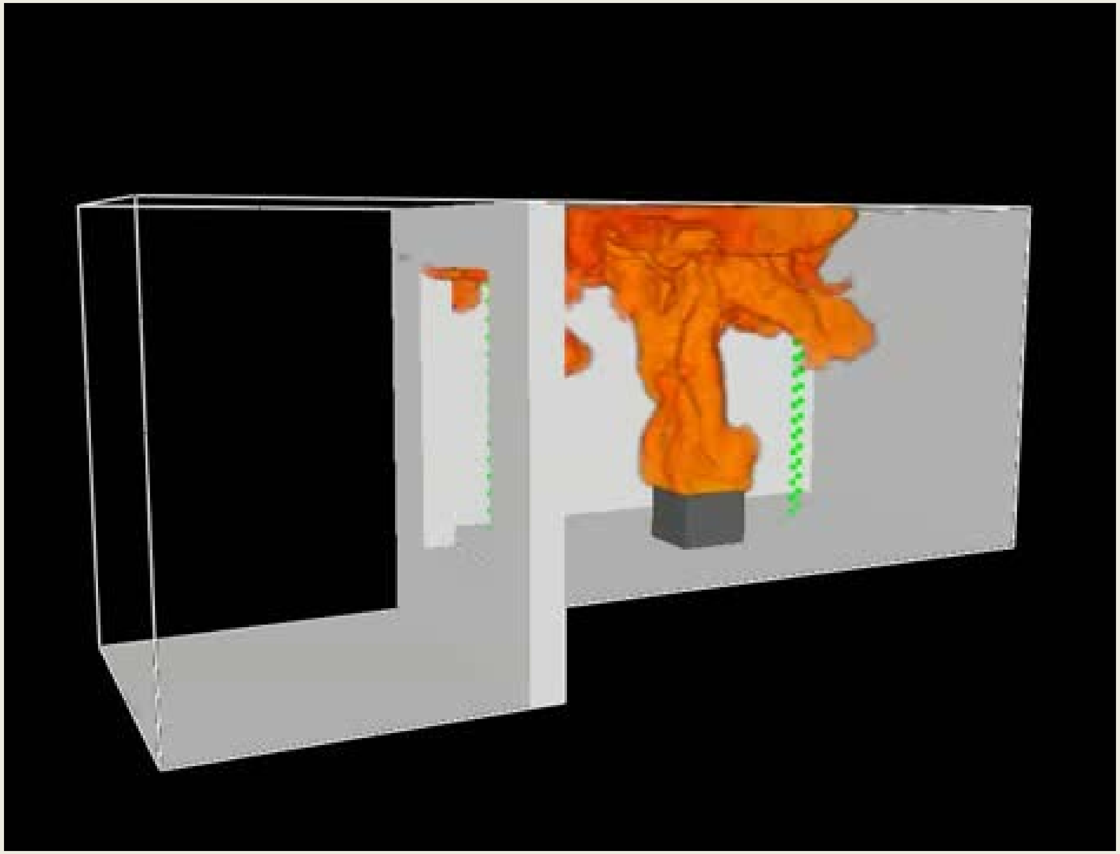
Realism vs. Accuracy

Underventilated Compartment Fire

- FDS simulation of a compartment fire;
- The heat source is a 600 kW methane pool fire;
- Supporting document for the experimental data: NIST_RSE_1994_600.

CFD Challenges

Underventilated Compartment Fire



CFD Challenges

Realism vs. Accuracy

Fire with Soot Deposition

- FDS simulation of a propane fire with deposition of soot;
- The smoke and flame are volume rendered;
- Soot is tracked explicitly and deposited on the walls via turbulent, thermophoretic and gravitational mechanisms;
- The soot surface deposition boundary is colored from gray to black.(http://code.google.com/p/fds-smv/)

CFD Challenges

Fire with Soot Deposition

Two Examples of HPC Applications

1. **Modelling of a scramjet engine**

2. **Massively parallel hybrid CFD solver for ocean applications**

Two Examples of HPC Applications

1. Modelling of a scramjet engine

(Predictive Science Academic Alliance Program - PSAAP)

Project Director: **Professor Parviz Moin** (Stanford University)

Objective

To investigate hypersonic aircraft, which may fly through the atmosphere at six to twelve times the speed of sound, in particular:

- Study the fuel and air flow through a hypersonic aircraft engine (scramjet engine);

- Quantify the uncertainties of the numerical predictions resulting from the supercomputer simulations.

Two Examples of HPC Applications

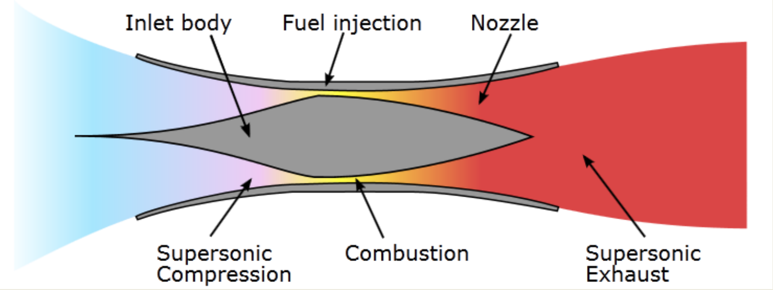
1. Modelling of a scramjet engine

(Predictive Science Academic Alliance Program - PSAAP)

What is a scramjet engine?

A scramjet (Supersonic Combustion Ramjet) engine is a propulsion system in which the oxygen needed by the engine to combust the fuel is taken from the atmosphere passing through the vehicle; this system differs from rockets, which combine a liquid fuel with liquid oxygen to create thrust. The scramjet takes away the need for liquid oxygen, and it can carry more payload.

In the absence of mechanical compressors, scramjets require the high kinetic energy of a hypersonic flow to compress the incoming air to operational conditions.



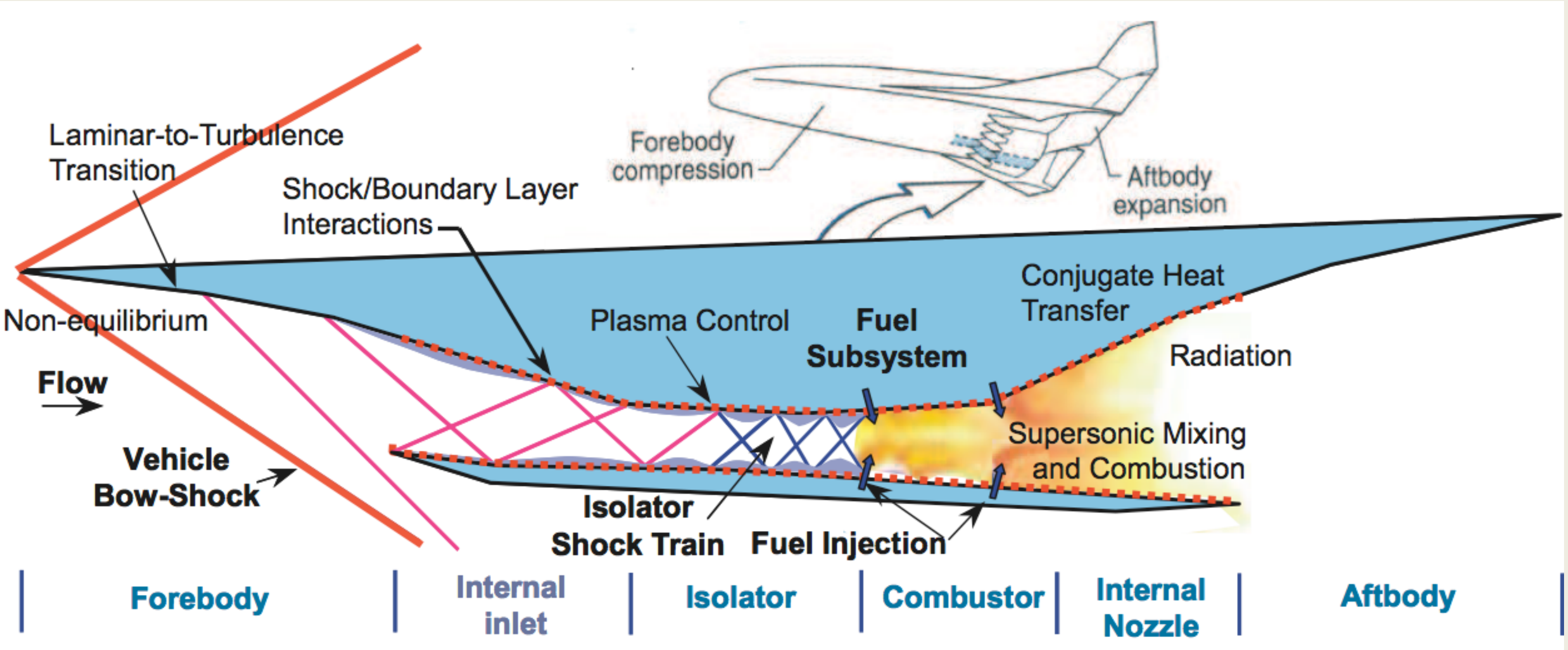
HPC – the Perspective of a CFD Practitioner

Two Examples of HPC Applications

1. Modelling of a scramjet engine

(Predictive Science Academic Alliance Program - PSAAP)

Integrated Physics of a Hypersonic Vehicle

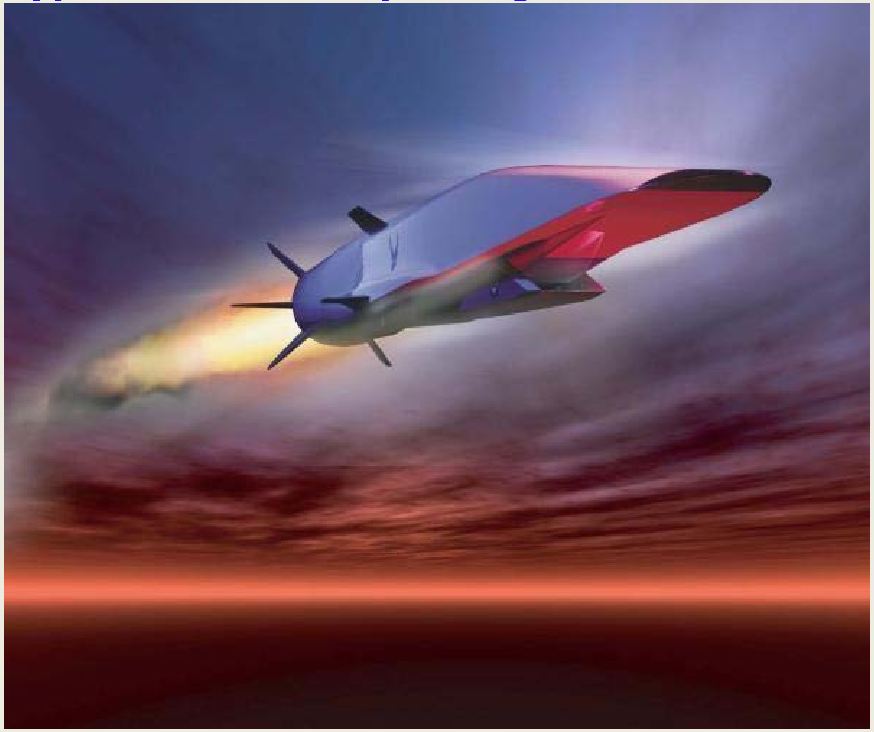


Two Examples of HPC Applications

1. Modelling of a scramjet engine

(Predictive Science Academic Alliance Program - PSAAP)

Hypersonic scramjet engine



*The X-51A Waverider is set to demonstrate hypersonic flight. Powered by a Pratt & Whitney Rocketdyne SJY61 scramjet engine, it is designed to ride on its own shockwave and accelerate to about Mach 6. (Credit: **U.S. Air Force graphic**).*

The aircraft completed successfully an unmanned scramjet-engine hypersonic flight-test in May 26, 2010 off the southern California Pacific coast. It was the longest supersonic combustion ramjet-powered hypersonic flight with more than a 200 s burn.

The aircraft uses a rocket booster

Two Examples of HPC Applications

1. Modelling of a scramjet engine

(Predictive Science Academic Alliance Program - PSAAP)

A few unsolved problems

- Excess fuel when starting the engine mat lead to a phenomenon called thermal choking, where shock waves propagate back through the engine; therefore, the engine does not get enough oxygen and it dies.
- Simulation of temperature fluctuations from a scramjet engine's exhaust run at Stanford University is one of the largest engineering calculations ever undertaken.
- Due to limitation of cost and power available, real world computer simulations have to make trade-offs yielding errors that creep into the computations. Most likely, the full simulations modelling the complete physics may need computers 100 to 1,000 times larger than those available today!
- Physical models are scarce for hypersonic scramjet engines, and there is very limited experimental evidence to benchmark them.

Two Examples of HPC Applications

1. Modelling of a scramjet engine

(Predictive Science Academic Alliance Program - PSAAP)

Modelling and simulations

PSAAP researchers

- run their simulations on supercomputers at Lawrence Livermore National Laboratory in California and Sandia National Laboratories in Albuquerque, N.M.;
- use for their simulations an open-source code called HyShot 2, which was originally developed in the Centre for Hypersonics at the University of Queensland in Brisbane, Australia;
- conduct their calculations on 163,000 processors simultaneously.

Two Examples of HPC Applications

1. Modelling of a scramjet engine

(Predictive Science Academic Alliance Program - PSAAP)

Modelling and simulations

- PSAAP simulations are run in supercomputers with 10 to 20 petaflop range - which are still small when compared to today's simulation and computational power needs.
- Educated predictions indicate a 1,000-fold increase in computational power by 2018; those computers may have millions of processors and independent computational units.
- Future programming is a major unknown. To this end, within PSAAP, it was developed at Stanford University a programming language (**Liszt**), which separates the computation from the coding - Liszt can solve partial differential equations and then it automatically writes low-level code that can target any one of the future machines with no need to rewrite the code.

Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

Project Director: **Professor Andrew G. Gerber** (University of New Brunswick)

Objective

The project aims to develop a CFD program called EXN/Aero specifically designed to exploit performance gains from new hybrid multicore-manycore computer architectures. The hybrid multicore-manycore design is outlined along with performance and validation testing on:

- an underwater vehicle

and

- tidal power applications.

Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

Motivation

-The HPC future will see massive levels of parallelism available at low cost, thereby affecting how device-level CFD is undertaken and who can participate.

-Entry barriers should become much lower for many organizations traditionally not taking advantage of HPC capabilities.

-Performance gains in the new HPC manycore landscape require substantial code re-development; the EXN/Aero* is specifically designed to incorporate manycore processing.

* Gerber, A.G., U.S. Prov. Patent App. (US61/427,888), "Method and System for Cell Based Computer Aided Analysis Using Manycore Processors", filed December 29, 2010.

Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

EXN/Aero software

The software adapts well-established numerical methods to new parallel processing development; it has the following main core features:

- Implicit in time employing the SIMPLE approach for pressure-velocity coupling.
- Collocated primitive variable solution on structured and unstructured (including hybrid) meshes.
- Solution of the Navier-Stokes equation in Reynolds averaged (SST) and filtered LES forms, and if required combined in a DES formulation .
- Upwind biased scheme for second order advection behaviour.
- Multigrid acceleration using the additive correction methodology .
- CGNS standard to organize input and output files.

2. Massively parallel hybrid CFD solver for ocean applications

EXN platform

- ✓ The novelty of the software platform EXN is to isolate architecture (**resource**) evolution from the **application**.
- ✓ A **cell based mapping module** (**cbmm**) detects computer resources available and optimizes the distribution of **application** *tasks* across the available **resources** taking into consideration speed of data transfer (both between host and coprocessor and on a coprocessor), type of coprocessors and host processor topology, and the **application** topology which includes data types with sizes and **application** model settings.
- ✓ The **application** in the present case is the CFD solver Aero. To work in conjunction with the EXN platform, the **application** reduces the problem specified in the input CGNS (CFD General Notation System) file to high level *physics*, *cell* and *interface* objects.

Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

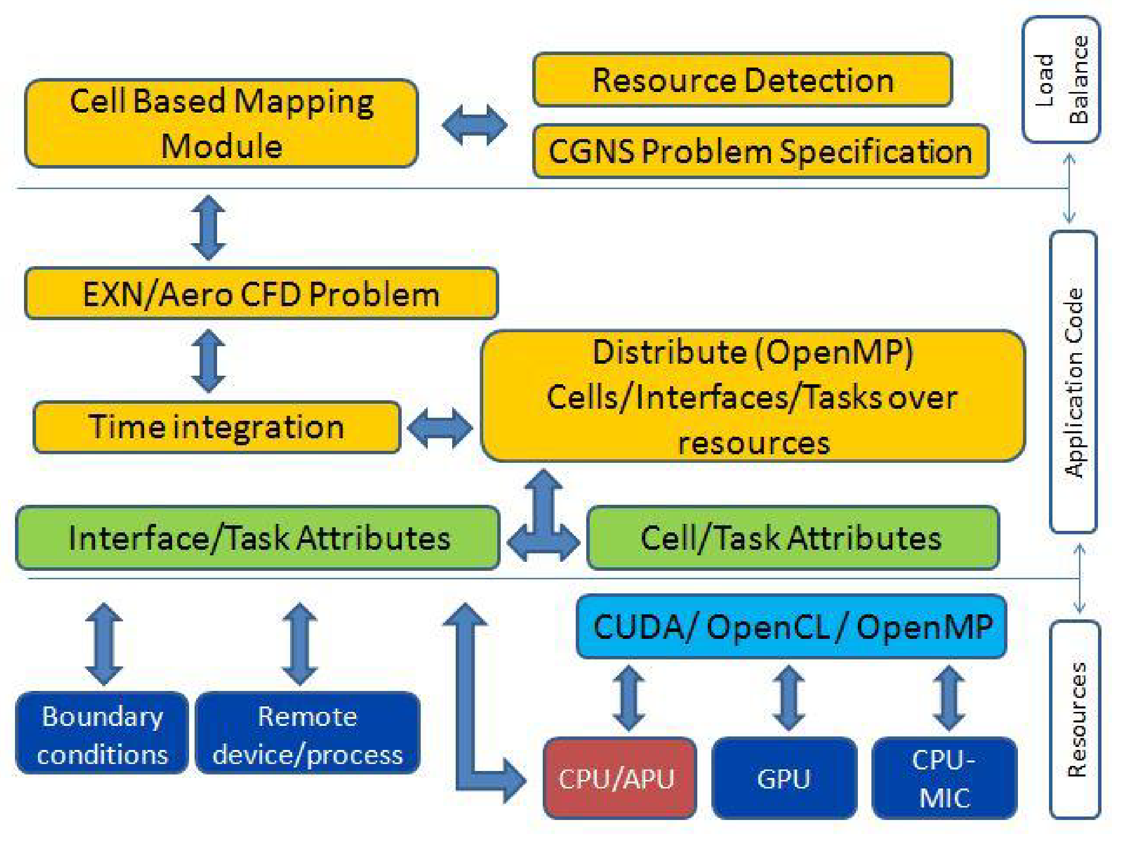
CFD application

- ✓ *Cell* objects encapsulate data for a collection of control-volumes that share similar *attributes*; the *cell attributes* guide **resource** selection for the associated *cell tasks* through the **cbmm**.
- ✓ *Interface* objects encapsulate the data for inter-cell interactions and interactions between a *cell* and an external input, such as a boundary condition or a connection to a remote network service/device.
- ✓ Similar to the *cells*, *interface attributes* guide **resource** selection for *interface tasks* through the **cbmm**.
- ✓ The *physics* object maintains information on the problem as a whole and is common to all *cells* and *interfaces*; it does not have independent *tasks*. (The overall organization is broadly described in the next Figure).

2. Massively parallel hybrid CFD solver for ocean applications

EXN/Aero organization

EXN/Aero organization using the Cell Based Mapping Module (**cbmm**) to deploy a load balanced **application** against available computer **resources**. An **application** is organized of *physics* (not shown), *cell* and *interface* objects with associated *tasks*. Load balancing utilizes *attribute* information associated with **application** objects

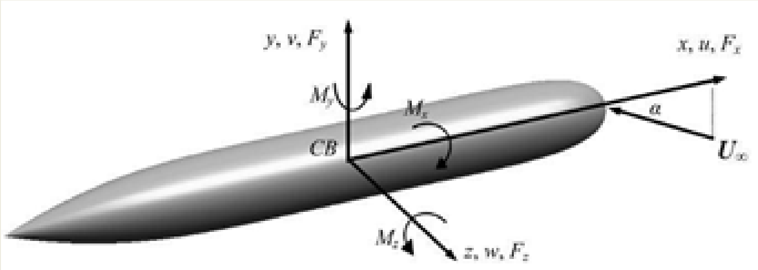


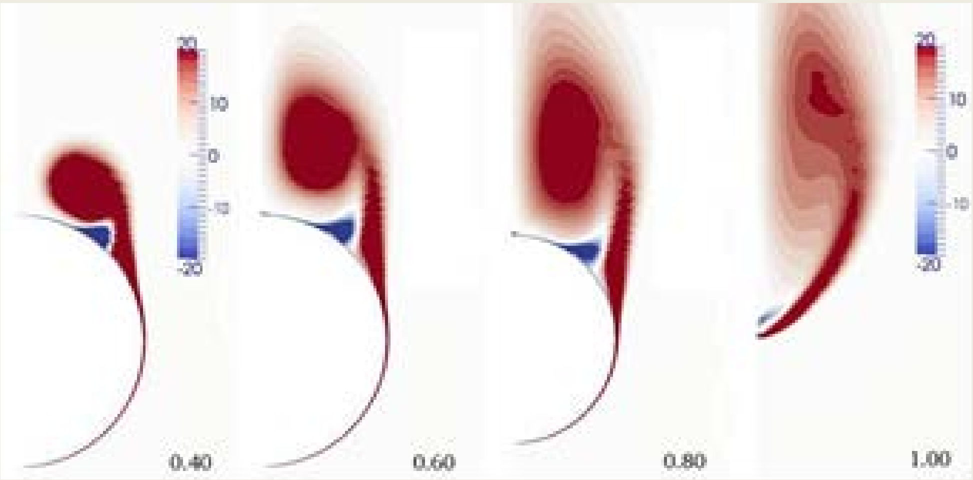
Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

Validation – Flow around an axis-symmetric submarine hull at incidence

(DRDC submarine shape – Defence R&D Canada)



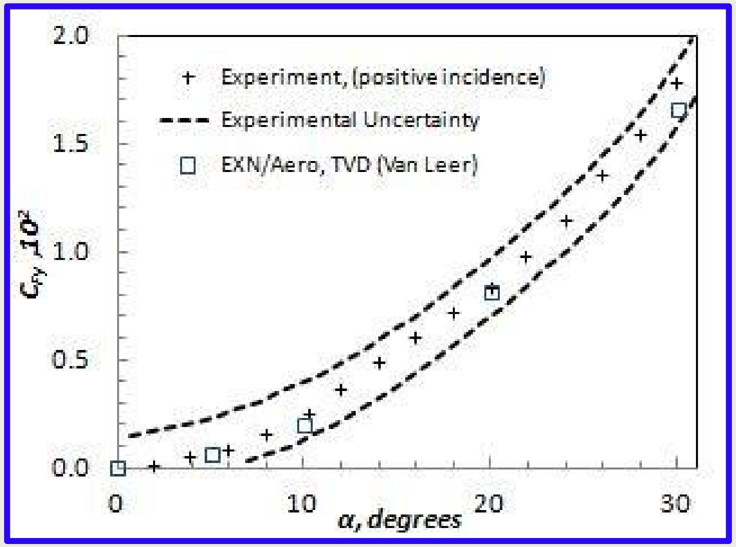


Axis-symmetric DRDC hull shape with typical axial vorticity results at different axial locations (percentage of hull length) for a=30°, U_∞=3.46 m/s and Re=2.3x10^7 (SST turbulence model and 5M mesh elements).

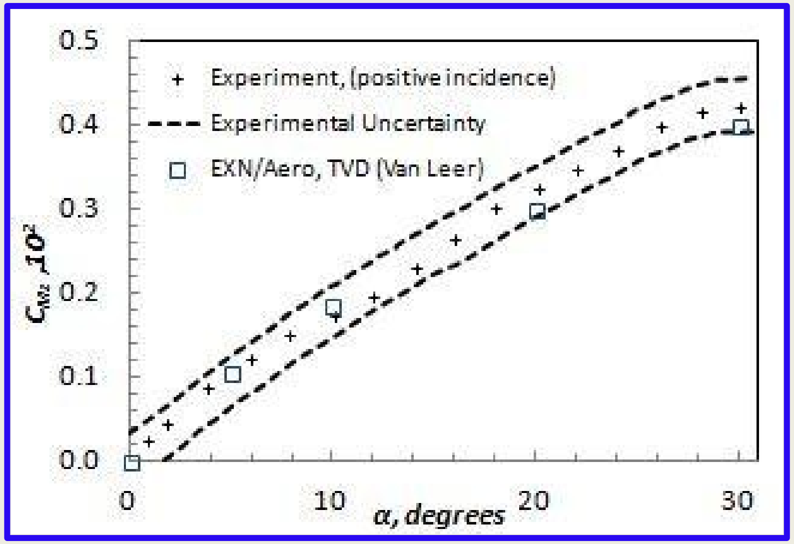
Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

Validation – Flow around an axis-symmetric submarine hull at incidence



a)



b)

Axis-symmetric DRDC hull shape normal force (a) and moment (b) coefficient predictions over a range of incidence angles a (U_∞= 3.46 m/s, Re=2.3x10^7, SST turbulence model, 5M mesh elements).

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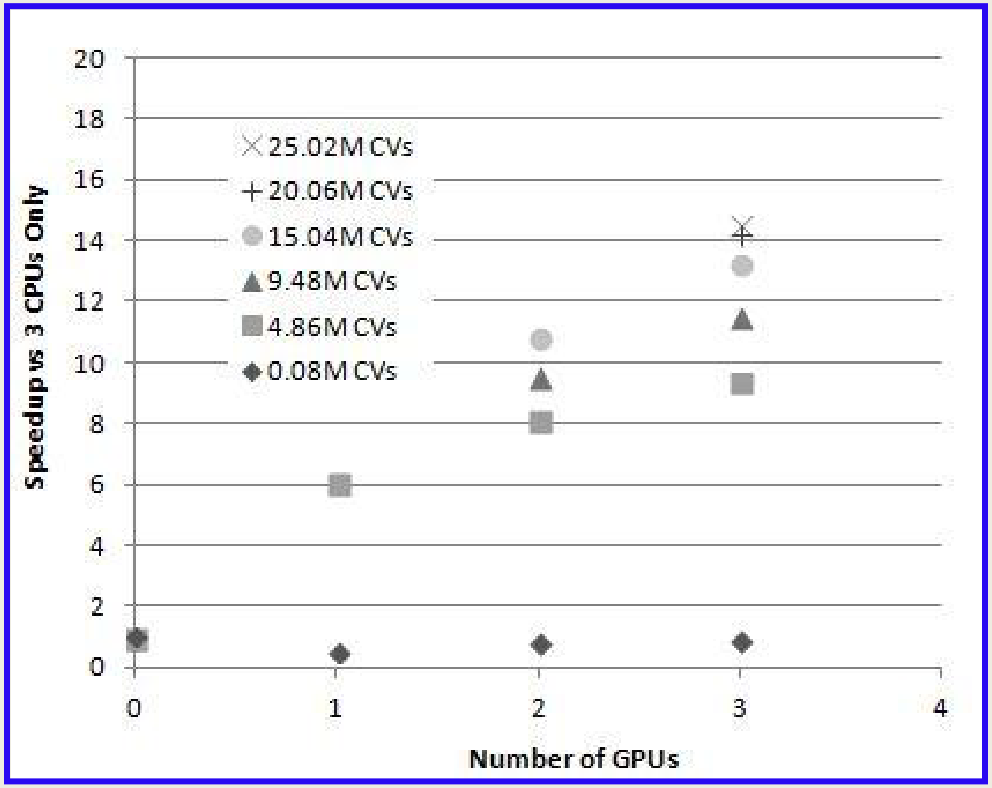
2. Massively parallel hybrid CFD solver for ocean applications

Validation – Flow around an axis-symmetric submarine hull at incidence



For a range of mesh sizes (CVs – control volumes) multi-GPU speedup versus a three CPU solution (all cases using the same 4CPU-Xeon/3GPU-Fermi system).

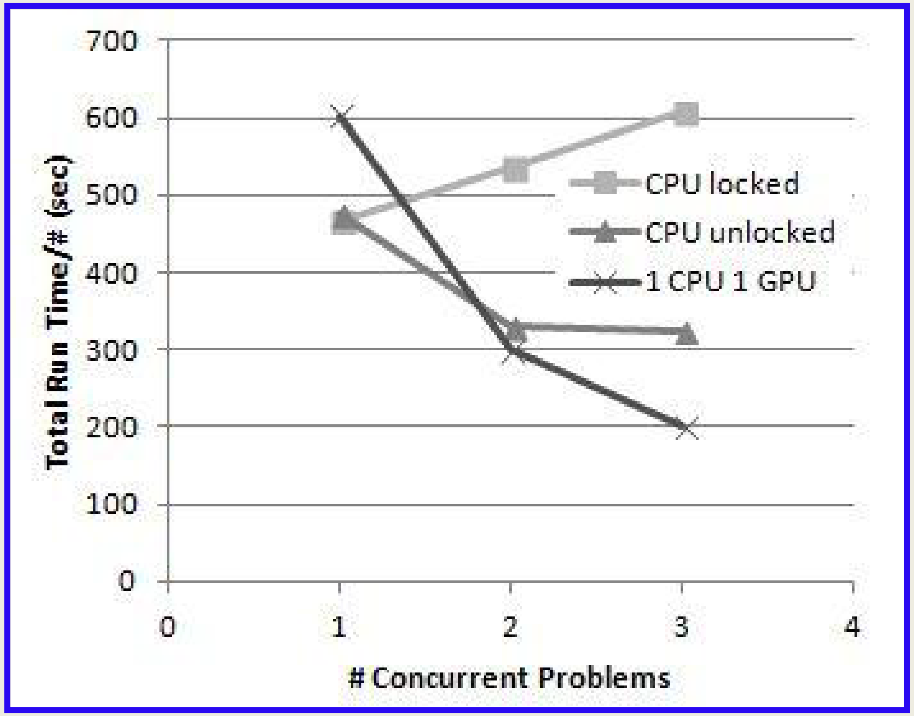
HPC – the Perspective of a CFD Practitioner

Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

Validation – Flow around an axis-symmetric submarine hull at incidence

(DRDC submarine shape – Defence R&D Canada)



Average problem solution time versus number of concurrent problems executed on a 4CPU-Xeon/3GPU-Fermi system. Test case uses a 5M control-volume DRDC model; all cases use three CPUs managing *interfaces* and three GPUs for *cell* execution .

Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

Validation – CFD characterization of a tidal energy site*

(*Minas Passage, Bay of Fundy, Nova Scotia, Canada)

Description

- ✓ Minas Passage, a channel connecting the Bay of Fundy to the Minas Basin, has the world's highest tides, with current speeds reaching 5 m/s.
- ✓ Estimates indicate that 2.5 GW of tidal power can be safely extracted from this region that is approximately 5 km wide at its narrowest point, 15 km long and up to 170 m deep.
- ✓ Prediction of the unsteady turbulent flow field in this region is essential for successful deployment of tidal turbines.
- ✓ CFD predictions must include the effects of local bathymetry and time varying boundary conditions on the turbulent flow field.

Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

Validation – CFD characterization of a tidal energy site

Physical models

The fluid flow is governed by the incompressible Navier-Stokes (NS) equations represented in either Reynolds time averaged or spatially filtered forms to model turbulent motion.

a) the Reynolds Averaged Navier-Stokes (RANS) form employs the SST turbulence model for regions of the flow where turbulence integral length scales are too fine to be resolved directly by more general forms of the NS equations.

b) when the mesh is fine enough to resolve a significant portion of the turbulence energy , it is used a Smagorinsky- Lilly large-eddy simulation (LES) approach using spatial filtering.

c) the current model both the SST and LES methods are co-applied in a Detached Eddy Simulation (DES) model.

2. Massively parallel hybrid CFD solver for ocean applications

Validation – CFD characterization of a tidal energy site

CFD grid design

The CFD grid is based on the bathymetry for the region of interest (red rectangle in the Fig.) - this region (Crown Lease Area) has an approximate area of 1 km x 1.5 km and it is located in the north-western section of Minas Passage. The bathymetry is provided as 400 mm x 400 mm structured data.

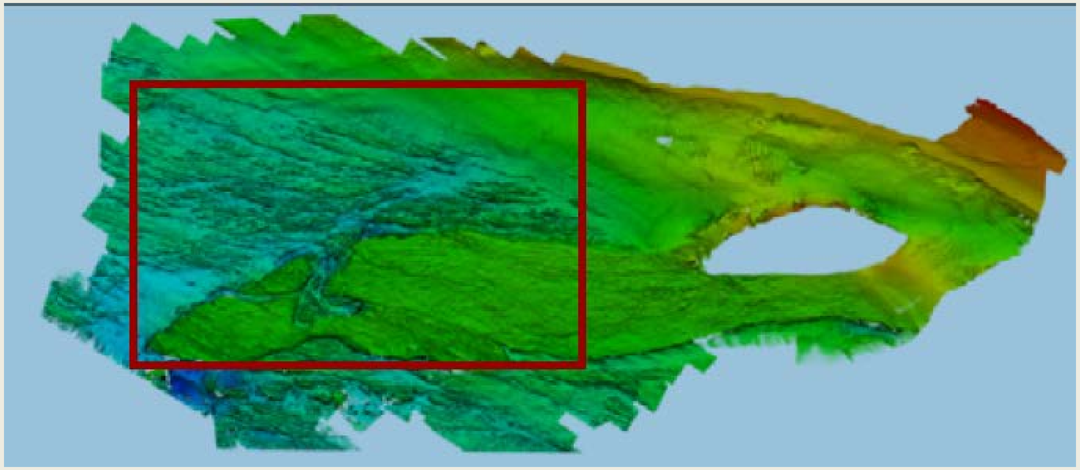
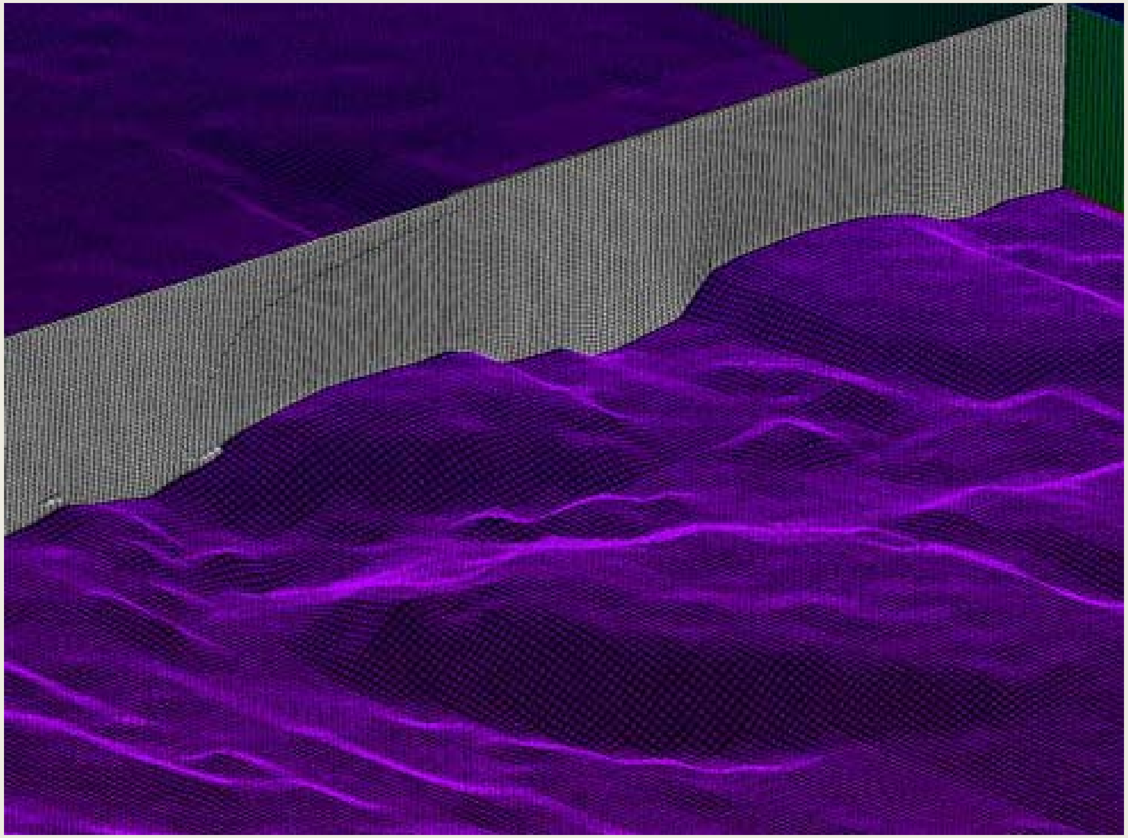


Fig.: Contour of high resolution bathymetry of FORCE region used to generate the CFD grid. (FORCE: The Fundy Ocean Research Center for Energy)

2. Massively parallel hybrid CFD solver for ocean applications

Validation – CFD characterization of a tidal energy site

CFD grid design



The structured grid consists of ~20 million control volumes. A zoomed in view of the surface mesh along with a cross-section of the structured grid through the water column is shown in the Fig.

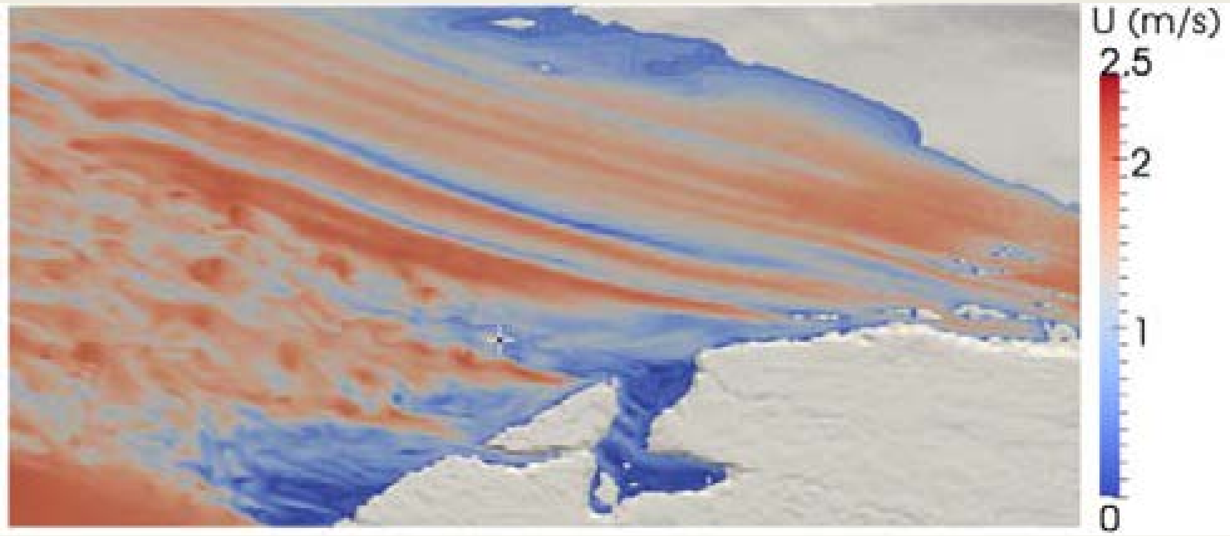
Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

Validation – CFD characterization of a tidal energy site

Results

Snapshots of the unsteady tidal flow are shown for the low-tide case at the final simulation time step.



Velocity field

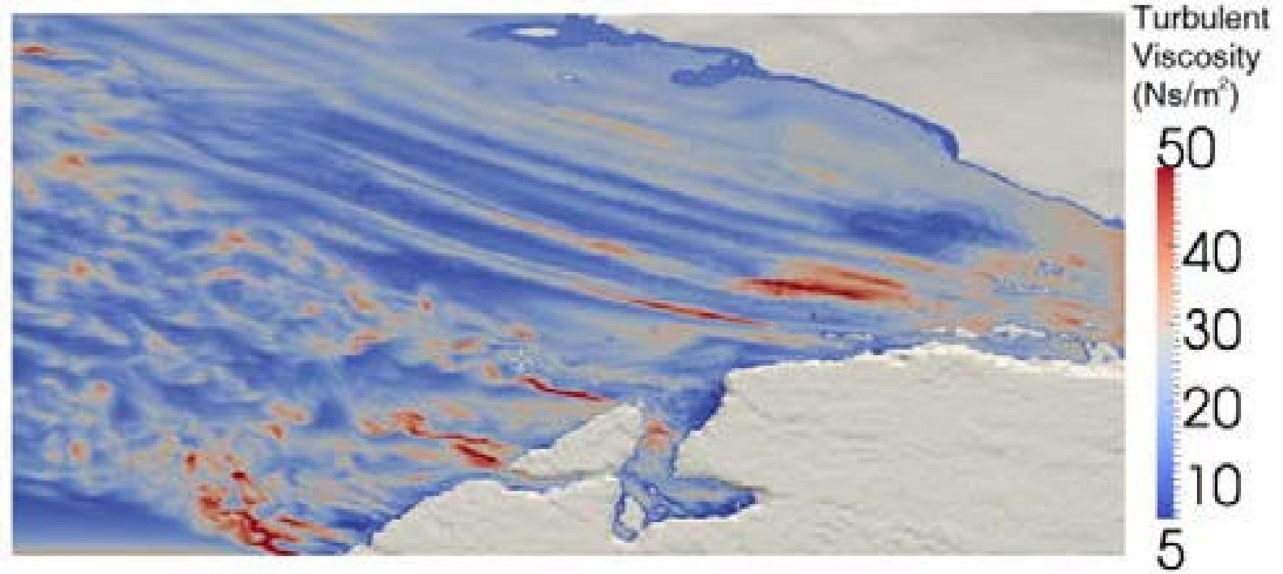
Two Examples of HPC Applications

2. Massively parallel hybrid CFD solver for ocean applications

Validation – CFD characterization of a tidal energy site

Results

Snapshots of the unsteady tidal flow are shown for the low-tide case at the final simulation time step.



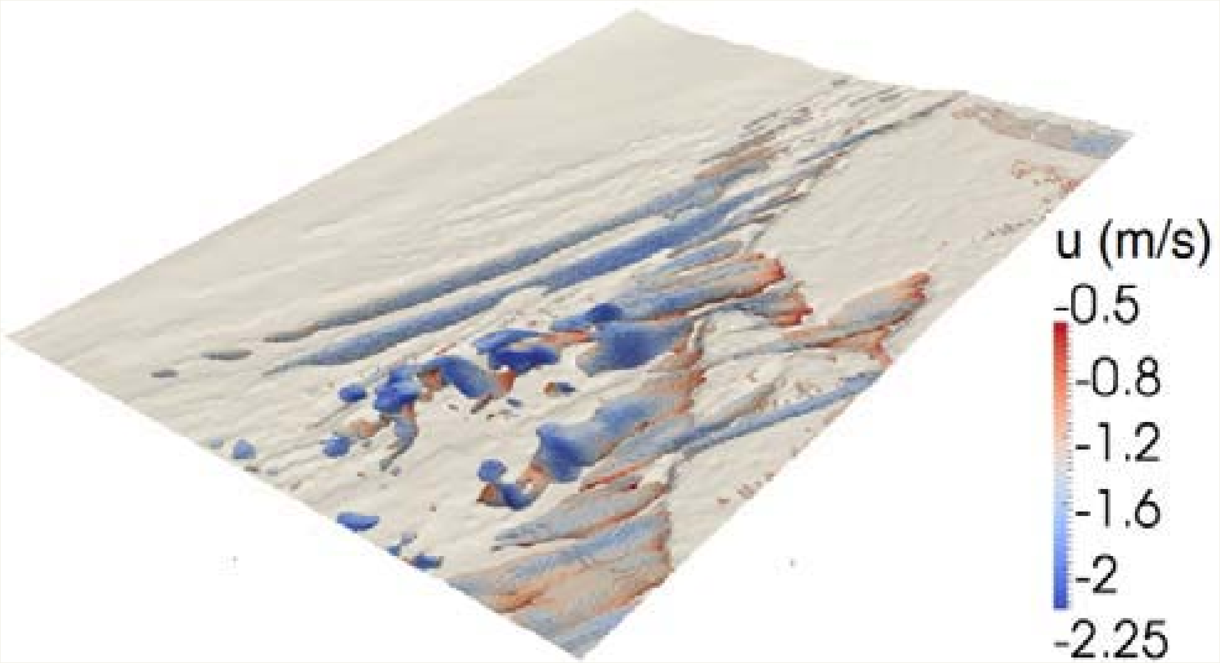
Sub-grid turbulent viscosity

2. Massively parallel hybrid CFD solver for ocean applications

Validation – CFD characterization of a tidal energy site

Results

Snapshots of the unsteady tidal flow are shown for the low-tide case at the final simulation time step.



An isometric view of the turbulent structures downstream of the ridge is highlighted using a threshold plot of sub-grid turbulent viscosity (35-92 Ns/m2) coloured with *x* component of velocity, *u*.

2. Massively parallel hybrid CFD solver for ocean applications

Validation – CFD characterization of a tidal energy site

Speed-up

- The completion for one time step using five CPU cores on average was **3263.4** seconds.
- Adding five GPU co-processors to assist the solution reduced this time to **37.5** seconds, a speedup of 87x.
- Using eight CPU's assisted by eight co-processors reduced the average time to **36** seconds. The speedup relative to the five CPU case improved further to ~91x. (A greater speed-up would have been expected for this latter case).
- Many issues related to the use of multiple co-processors on a desktop workstation environment are to be investigated, in particular when the turbines are also to be modelled.

Where Are We?

Where Are We?

HPC

Facts

- ✓ HPC is a proven game-changing technology.
- ✓ HPC plays a vital role in driving private-sector competitiveness.
- ✓ All businesses – large and small - that adopt HPC consider it indispensable for their ability to compete and survive.

Ref: Advance. Benchmarking Industrial Use of High Performance Computing for Innovation, Council on Competitiveness, 2008. http://www.compete.org/publications/idea/28/high-performance-computing/2/)

Success (an example)

- ✓ Boeing used HPC modelling and simulation in many design areas for its Boeing 787 Dreamline aircraft. The use of HPC made possible that only **11** prototype wing designs were required to be submitted to expensive "live" experimental tests versus **77** wing designs for the prior-generation Boeing 777 plane.

Where Are We?

HPC

Personal view

- HPC has indeed facilitated the solution of many complex CFD simulations and the growth in the usage of CFD;
- However, the application of detailed approaches (such as, DNS) for industrial standard configurations with typical operating conditions are still beyond today's computing capability.
- The CFD practitioner, often, is not technically equipped for the usage of advanced hardware, resulting in lower than expected level of performance;
- There is an information gap, particularly in the private sector, between the CFD practitioner (engineer or scientist), who is typically an expert in his/her technical disciplines/applications, and the hardware specialists who are well-acquainted with the hardware usage;

Direct Numerical Simulation (DNS)

The Kolmogorov microscale (η)

$$\eta = (\nu^3/\varepsilon)^{1/4}$$

where ν is the kinematic viscosity and ε is the rate of kinetic energy dissipation.

- The integral scale, L, depends usually on the spatial scale of the boundary conditions.
- To satisfy the resolution requirements, the number of points (*N)* along a given mesh direction with increments *h*, must be

$$N.h > L$$

  ◦ in this way the integral scale is contained within the computational domain, and

$$h \leq \eta$$

  ◦ so that the Kolmogorov scale can be resolved.

Direct Numerical Simulation (DNS)

The Kolmogorov microscale (η)

- In atmospheric flows , where the length scale for those eddies having the most turbulence energy (and most responsible for the Reynolds stress) can be measured in kilometers, typical values of the Kolmogorov microscale range from 0.1−10 mm.

- For instance, the Kolmogorov microscale for u' = 1 m/s and l = 0.1 m for air is

  $Re_t = 1 \times (0.1)/15 \times 10^{-6} \approx 7 \times 10^3$. Therefore $l/\eta \approx 8 \times 10^2$, so $\eta \approx 1.2 \times 10^{-4}$m or 0.12mm.

Note:

- The number of time steps grows also as a power law of the turbulent Reynolds number.
- An estimate of the number of floating-point operations required to complete the simulation is proportional to Re_t^3 (based on the number of mesh points and the number of time steps).

HPC

Personal view

- There is a growing demand for HPC to solve **multidisciplinary analysis and optimization** problems yielding a need to improve the software performance; however, I am uncertain that it will possible to achieve automated solutions for he best usage of key features of the HPC clusters, including multi-core processor performance, host channel adapters, multi-rail networks, message passing implementations.

Where Are We?

HPC

Personal view (and disappointment!)

- Automatic meshing still seems to be an eluding goal – meshing depends on geometry and physics; however, often, the physics is understood only after solving the problem.
- To manage and to explore large data sets generated by CFD calculations still is a major problem.
- The dominance of Navier-Stokes equations based solvers remains; alternatives, such as, Lattice Boltzmann Method, have made minor impact.

HPC

Personal view - LBM vs. Navier-Stokes solvers

Advantages

- LBM has intrinsic linear scalability in parallel computing, given the fact that collisions are calculated locally.
- LBM is amenable to geometric complexity, including movement of the walls and domain deformation.
- LBM incorporates phase interaction into the particle collisions; therefore, inter-phase interaction for multiphase flows is accomplished in a very efficient manner.

Where Are We?

HPC

Personal view - LBM vs. Navier-Stokes solvers

Past disadvantages

- **Computationally expensive** - GPUs, which make viable single instruction multiple data (SIMD) computation, are well-suited accelerators for LBM solvers.
- **Turbulence**
- Turbulence modeling – there is an already sizeable body of literature reporting on successful applications of LBM along with two-equation models and LES (e.g., an extensive review is presented by Leila Jahanshaloo *et al., Num. Heat Transfer*, Part A, 64: 938–953, 2013).
- DNS – Recent results illustrated that even the simplest LBM, at a similar resolution, would show statistics of the same or better quality than those predicted by pseudo-spectral methods, and at very competitive computational cost.
- **Numerically unstable** – The so-called Entropic LBM (ELBM) allows computations at high Re values and it is capable of circumventing stability difficulties.

Concluding Remarks

HPC – the Perspective of a CFD Practitioner

Concluding Remarks

The advent of more advanced computers and configurations, HPC will allow :

- more realistic CFD simulations not only in terms of the quality of the predictions by including multiphysics phenomena, but also by having an error band for the predictions, and
- further the possibilities of using CFD, along multiphysics software, for real-world optimized design of equipment with major reduction in development time and costs.

However, HPC may face major hurdles, namely:

- the operation and maintenance (O&M) of the most powerful computers involve very large costs, beyond the capital costs. The O&M costs can be as high as ~10 M US dollars – just the power requirement can be of the order of 10 MW, and
- the electronic components in the minimization process are moving at a fast pace from "micro" to "nano" with the full uncertainty about the applicability of the classic laws of the physics.

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THE END