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Status Report #3 for the joint project: Manycore Computational Fluid Dynamics (CFD) Solver Development (CONTRACT #:W7707-145678/001/HAL)

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PSPC Contract Number: W7707-145678/001/HAL
Technical Authority: Mark Bettle, Defence Scientist
Contractor's date of publication: November, 2014

Defence Research and Development Canada

Contract Report
DRDC-RDDC-2017-C267
November 2017

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Canada

IMPORTANT INFORMATIVE STATEMENTS

STATUS REPORT #3 FOR THE JOINT PROJECT: MANYCORE CFD SOLVER DEVELOPMENT (CONTRACT #:W7707-145678/001/HAL)

A REPORT COMPLETED FOR:

DEFENSE RESEARCH AND DEVELOPMENT CANADA – ATLANTIC

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2014-11-04

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Introduction:

Envenio is now just past the mid-point of year two in a four year development effort with DRDC on implementing ocean vessel models including 6-DOF motions and free surface waves in the EXN/Aero manycore fluid flow solver. The purpose of this report is to provide summary information on the Fiscal Year 2014/15 activities to date.

Since the last report significant effort has been directed towards completion of two important features in EXN/Aero. These are i) hybrid mesh structured/unstructured simulations and ii) mixed precision (single/double) simulations. These two features promote fast simulations by minimizing the use of unstructured and double precision data. Progress on these fronts is considered quite important due to the planned use of EXN/Aero with Pointwise scripts to generate flow solutions for a wide variety of appended submarine configurations. These submarine configurations employ structured/unstructured hybrid meshes and require double precision in regions where flow separation is difficult to predict.

A third feature is that EXN/Aero continues to execute efficiently on mixed architectures (multi-CPU and multi-GPU). Time was spent revisiting solver performance to ensure that recent improvements did not break previous developments.

The remaining activities toward the end of this fiscal year is continuing 6-DOF overset motion development and beginning free-surface modelling.

<u>Progress on hybrid mesh structured and unstructured simulations using Pointwise submarine scripts</u>

The implementation of the hybrid mesh capability is now largely complete with on-going rigorous testing. The first focus of our testing has been on successfully obtaining solutions for fully configured submarines. An example of a hybrid mesh simulation using Pointwise to create the mesh is shown in Figure 1. The simulation results shown are for the standard DRDC hull configured with deck and sail appendages and ~8 million control-volumes. Figure 2 provides a top and side view of the hybrid mesh.

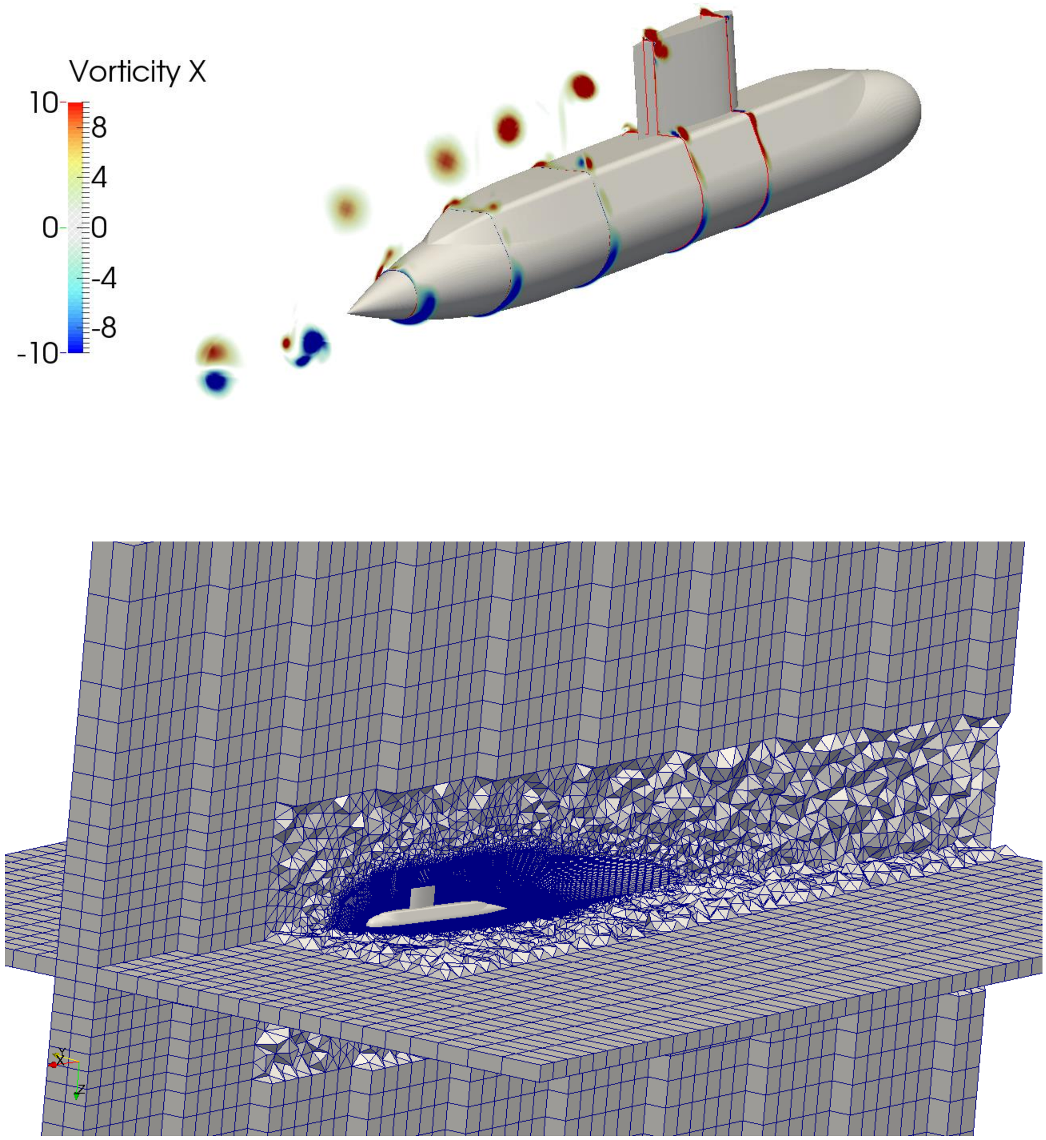


Figure 1 (top) Example EXN/Aero hybrid mesh flow solution with cross flow and resulting x-component of vorticity, (bottom) demonstration of structured/unstructured mesh system involving outer structured, intermediate unstructured, and inner structured regions.

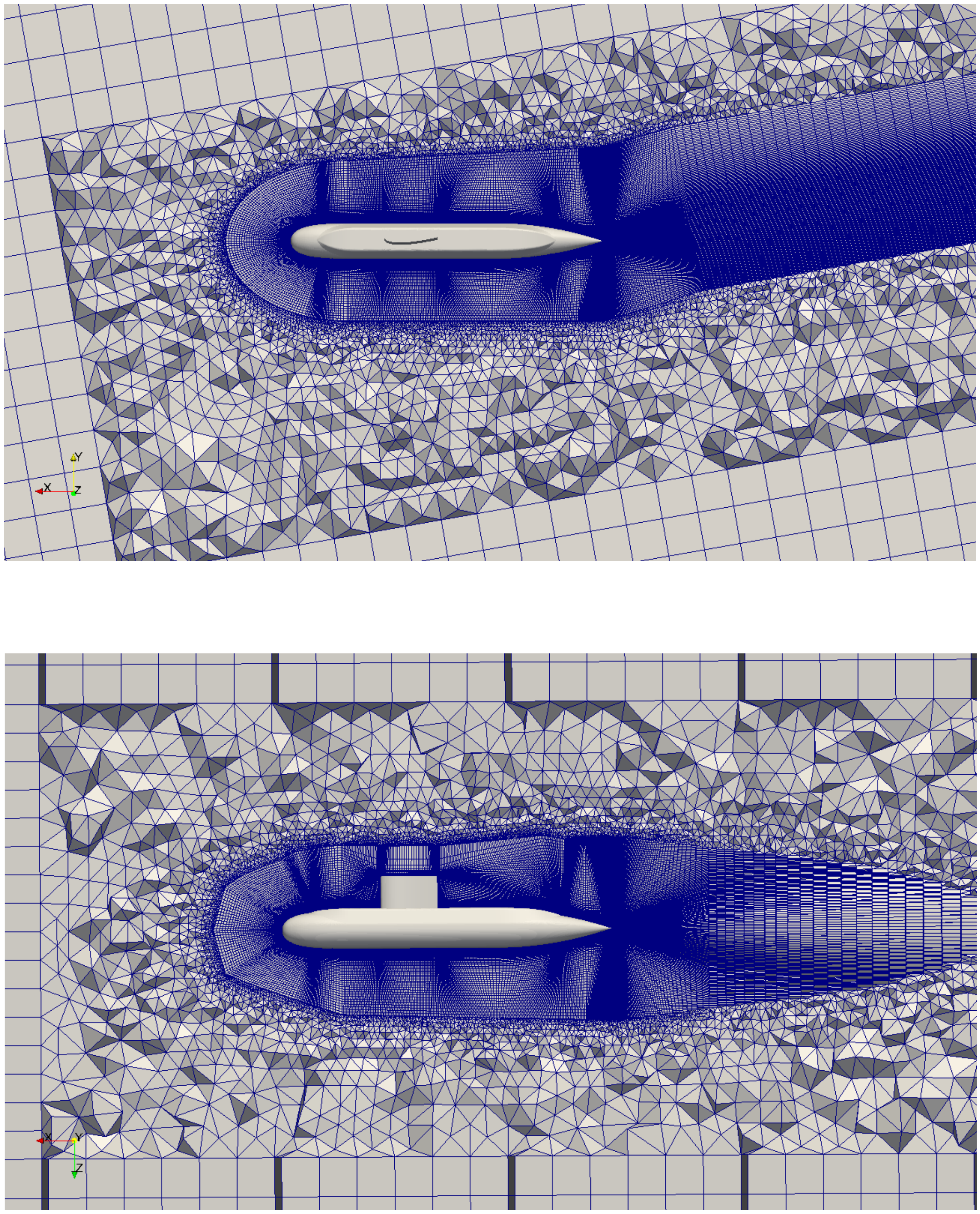


Figure 2 (top) Detailed top view of DRDC hybrid mesh with deck and sail appendages, and (bottom) side view.

We revisited previous EXN/Aero validation efforts (then obtained using only structured data) but now employing a hybrid mesh. The EXN/Aero results are compared to experimental data and ANSYS CFX results. Also tested were different advection schemes. Thehybrid mesh results employed the Van Leer TVD advection scheme.   The EXN/Aero flow solution and associated DRDC axisymmetric hybrid mesh are shown in Figure 3.   In Figure 4 are shown predicted normal forces and moments at different angles of incidence. The hybrid mesh results continue to exhibit similar validation comparisons as earlier tests.

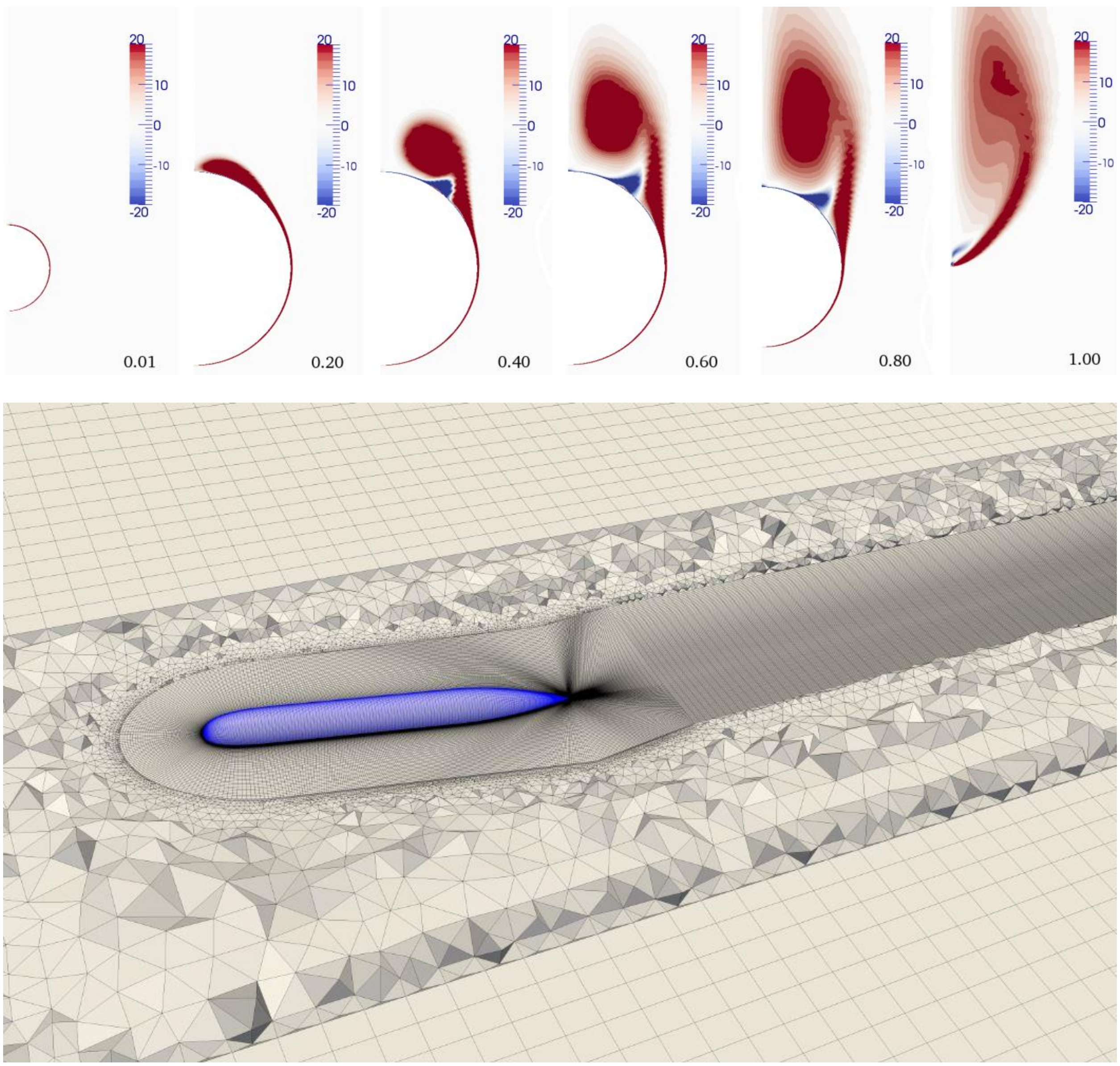
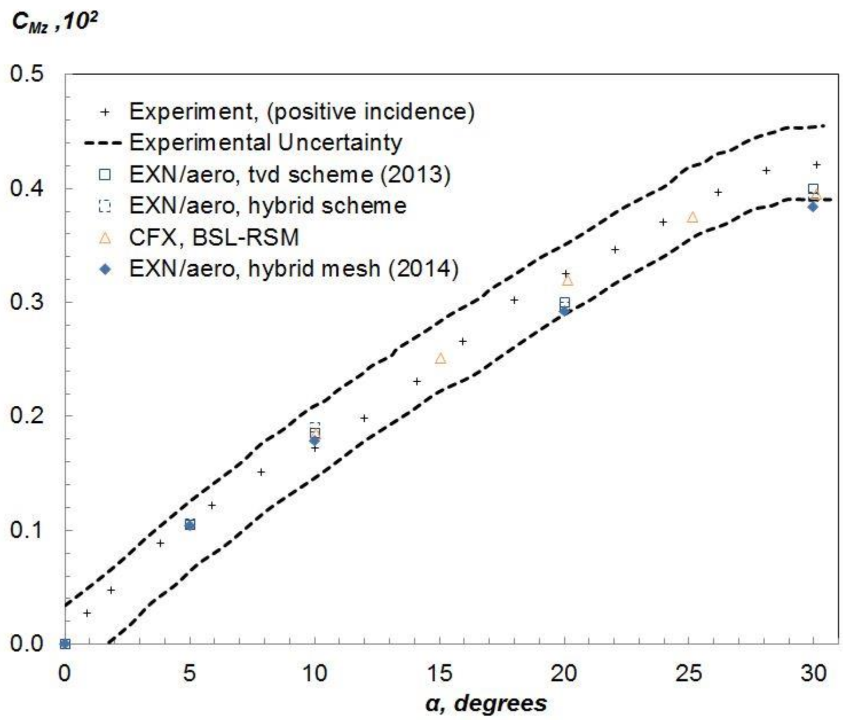


Figure 3 (top) Developing vorticity field at different stations (locations normalized by body length) along the length of the DRDC axisymmetric hull, and (bottom) view of hybrid mesh system employed.



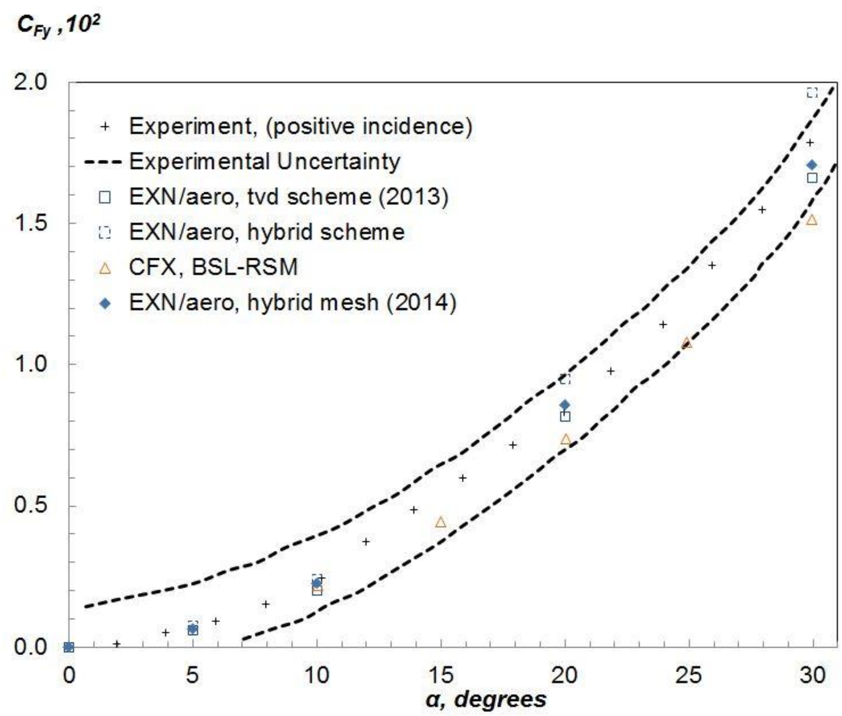


Figure 4 (top) Y-force coefficient at different incidence angles for the DRDC axisymmetric hull, and (bottom) Z-moment coefficient. The hybrid mesh simulations were compared against previous studies.

Testing of the DRDC configured submarine cases using EXN/Aero is proceeding. In Figure 5 is shown a case with deck, sail and tail plane appendages. Simulations on this case are presently on-going.

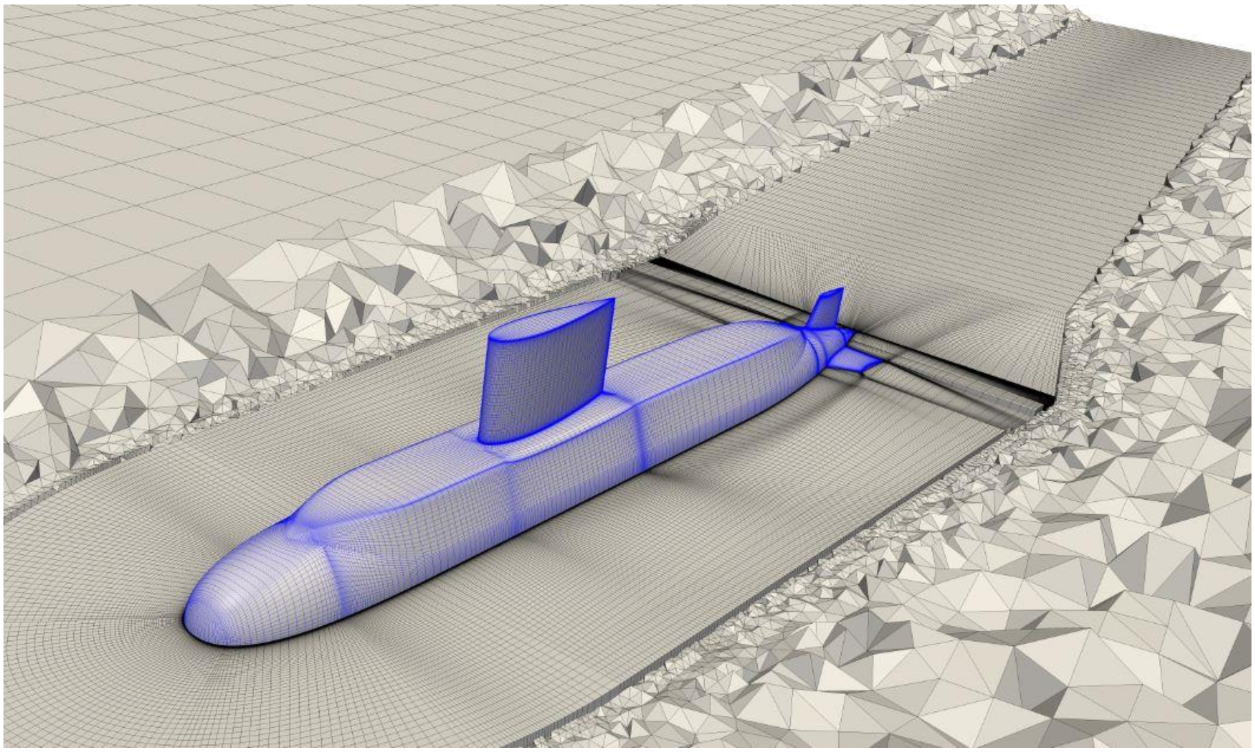


Figure 5 A DRDC hybrid mesh which includes deck, sail and tail plane appendages.

In order to develop a robust hybrid mesh capability, a range of applications are being tested and improved beyond the submarine cases shown above. These cases are based on specific research projects and relate to the various collaboration/leveraging projects described subsequently. Here they are mentioned briefly to show the scope of our testing:

- Low speed aircraft (project 5)
- Industrial mixer (project 6)
- Spiral corrugated pipes (project 7)
- Fullerene manufacturing (project 13)
- Vortex shedding from bluff bodies (project 4 and 10)

Each of the above flow cases is quite different and is allowing us to test and implement interventions in the code based on mesh quality metrics (i.e. element skewness and aspect ratio). These interventions limit the impact of poor unstructured mesh quality on the CFD solution. With good mesh quality the specific interventions are not activated. As should be in any CFD project a high quality mesh is an important input, but in cases where rapid intermediate results are desired by the end user the solver should not fail to provide a solution because of poor quality mesh elements.

Implementation of mixed precision capability

For a CFD solver to be able to concurrently execute both single and double precision regions of the mesh is very new, and is important for solution efficiency particularly when very large unsteady applications are considered. A single precision simulation when run in double precision mode occupies twice the memory and in general runs at about 2/3 of the speed. For simulations that may take many days to run this slowdown is quite wasteful particularly when only narrow regions of the mesh require double precision resolution. In addition GPU device memory is much less than the host system memory and therefore efficient use of that memory is important. The mixed precision capability will allow EXN/Aero to execute problems primarily in single precision mode (thus preserving speed and memory) while employing smaller double precision regions as needed.

The mixed precision capability has required a significant amount of up-front software design and for this purpose a computer science student has been employed since April to work on this task. By the end of August testing on reduced problems led to a workable software design and since then changes have been systematically implemented. The changes are now about 80% complete and we expect by the end of December 2014 to have undertaken mixed-precision simulations.

Mixed multi-cpu and multi-gpu computations

The ability to efficiently use multiple CPU’s and multiple GPU’s concurrently is an important feature of EXN/Aero and to do this in a way that is scalable as problems become larger. This involves a combination of OpenMP course grained parallel directives working with fine-grained CUDA kernels launched using asynchronous streaming. As new features are added making sure that the parallelism remains intact is important. Bug issues with some Portland PGI OpenMP task directives required effort to develop alternate approaches using simpler directives which were successfully completed. Presently this capability is fully activated in EXN/Aero.

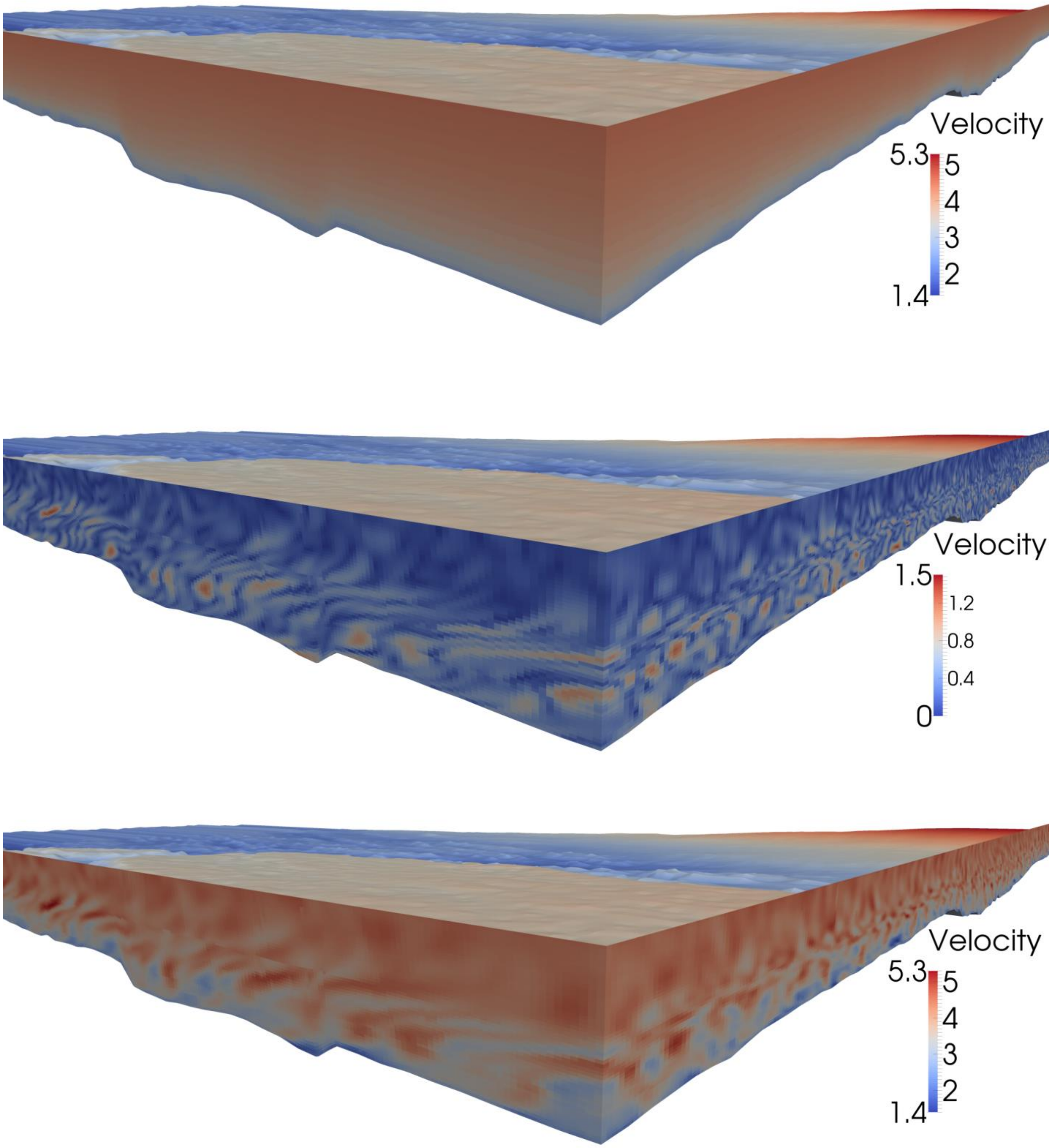


Figure 6 Bay of Fundy Minas Passage (1 km x 1.5 km shelf) simulation with (top) inlet mean velocity field, (middle) the velocity perturbation field and (bottom) the combined velocity field at an instant in time. The perturbation field changes continuously in time over the length of the simulation.

Synthetic Turbulence Model Development

Due to the potential to assist a number of DRDC unsteady simulations (and other non-DRDC application areas as well) a Synthetic Turbulence Model was development and tested. Reference [1] provides one example of its use in the context of tidal energy simulations. The method is general and can be used for DRDC applications. A journal paper is being developed presently to describe the capability in detail.

As an additional example of the utility of the Synthetic Turbulence Model Figure 6 shows the application of unsteadiness to the inlet of a Bay of Fundy Minas Passage simulation (simulation covers a 1 km x 1.5 km shelf region). The unsteadiness can be applied in an isotropic or anisotropic manner and filtered so that the unsteadiness overlaid on the mean flow is relevant to the flow environment.

The Synthetic Turbulence Model when applied is computationally intensive and therefore is being developed to run on GPU's.

Overset Mesh Development Activity

The overset mesh capability described in the last report was expanded to work in conjunction with immersed boundaries. This additional functionality allows for including complex littoral boundaries in simulations that also employ multiple overset meshes. Reference [1] provides an example where complex shorelines have been included using immersed boundary techniques. The simulations in reference [1] also employ LES unsteady flow with 25M node resolution.

In tandem with the immersed boundary work development activities were undertaken to couple all of the overset regions at the multigrid solver level in EXN/Aero. This was to help establish stronger coupling between mesh systems and more rapid convergence. This has been implemented but requires more testing which will occur as work resumes on prescribed 6-DOF motion with overset.

Initial test were undertaken on using gradient based interpolation for updating information between overset mesh systems. This shows promise in speeding up communication of information between mesh systems which will be important in dynamic overset cases.

Properties, Energy Equation and General Source Term Additions

In order to handle a wider range of modeling needs EXN/Aero now has as a general source term facility that allows for easier in implementation of specialized source terms for all equations. In addition, the energy equation capability is being extended to include new models, including a facility to include a wider range of thermodynamic (for example ideal and real gases) and thermophysical properties.

Summary of Collaboration/Leveraging Activities Related to EXN/Aero Development Over Fiscal Year 2014/15

Fiscal Year 2014/15 continues to be an active one for development of the EXN/Aero software. Areas of development are progressing on several fronts with a brief outline following.

1) BCIP (Build in Canada Innovation Program) application has been submitted with a response expected in the next few months. A successful BCIP application will support a year-long testing stage of EXN/Aero at DRDC.
2) UNB Mechanical Engineering was successful in a Canada Foundation for Innovation (CFI) Grant titled "Manycore Infrastructure for High Performance Time Dependent Simulation". The total value of the grant is $368,000 with Envenio acting as the industrial participant. Presently the UNB RFP is open for vendors to submit bids and will close by mid-November. With the RFP stage complete and a successful bidder the next stage will be purchasing and assembling the system.
3) A Mitacs Accelerate+NRCAN IRAP project (Envenio is the industrial sponsor) is underway titled "Visualizing the Performance of Scientific Applications Executing with Space-Time Domain Decomposition " where the primary outcome is a new approach to monitoring (via an advanced GUI) EXN/aero solution output and system performance. The work involves a computer science student with input from a UNB computer science faculty member Eric Aubanel.
4) An NSERC Discovery Grant (by A.Gerber) is used to support EXN/Aero solver development in areas such as manycore parallel processing, unstructured discretization and solution and engineering software design.
5) An NSERC Collaborative Research and Development Grant with industrial partner Forest Protection Limited is in its fourth year of a five year program. Areas of EXN/Aero development are Synthetic Turbulence Modeling coupled with LES and DES modeling, multi-fluid modeling using Direct Quadrature Method of Moments (DQMOM) and overset meshing (primarily stationary and translating).
6) An NSERC Collaborative Research and Development Grant with Nova Chemicals is beginning its first year of a three year project. EXN/Aero is intended to be used in overset prescribed motion mode along with LES turbulence modeling (combined with physical experiments). The project provides an opportunity for testing and improvements combined with experimental validation.
7) Hatch (a large multinational consulting company) completed an Engage grant with UNB Mechanical Engineering to investigate the use of manycore solvers for solving unsteady flows. Subsequently Hatch has contacted Envenio to explore further development of EXN/Aero for their specific needs.
8) Clean Current Power Systems (a tidal/river turbine manufacturer based in Vancouver) has completed an Engage Grant with UNB Mechanical Engineering that involves the testing and validation of the Blade Element Momentum (BEM) turbine models in

EXN/Aero. The same models can be employed for propellers which will be of interest to DRDC.

9) UNB Mechanical Engineering participates in a Government of Canada ecoENERGY Innovation Initiative (ecoEII) with a project titled "*Reducing the cost of in-stream tidal energy generation through comprehensive hydrodynamic site assessment*", through this project work is undertaken on overset mesh technology, turbine design level simulations, and DES simulations in natural environments. This project is in the midst of the second year of a three year program.
10) Department of Mechanical Engineer and Computer Science (faculty member Eric Aubanel) project looking at adding time to the spatial parallelization of CFD problems on manycore computers. EXN/Aero is the code being used for this investigation. Support is funded by the NSERC Discovery Grants of Gerber and Aubanel.
11) Department of Mechanical Engineer and Computer Science (faculty member Eric Aubanel) project looking at optimizing how an EXN/Aero problem is broken up (domain decomposition) and spread across heterogeneous manycore computing devices. This is important to ensuring scalable solution performance is attained and that EXN/Aero is adaptable to future changes to computer architectures. Support is funded by the NSERC Discovery Grants of Gerber and Aubanel.
12) To support the validation of EXN/Aero for unsteady turbulent flows in the vicinity of moving bodies, a Mitacs project with Joe Hall at UNB has been initiated with Envenio as the industrial sponsor along with IRAP. This is an experimental program and uses a dynamic test rig developed by Envenio and loaned to UNB for the research.
13) Atlantic Innovation Fund sponsored project that is subcontracting work to simulate flow in a fullerene (nanoparticle) manufacturing process. EXN/Aero is being developed to simulate this process and provides an opportunity to expand its thermal and property modeling capabilities.

The above R&D, fundamental and applied projects, demonstrate an effort to build a state of the art CFD solver that can operate in a wide range of application areas alongside DRDC's primary interests. This is considered necessary for the long term success of EXN/Aero. In addition Envenio has completed negotiations with UNB on acquiring commercial rights to EXN and related software and all documents have been signed. The software design behind EXN/Aero is now patented in Canda with the US application still in review.

Some of the projects above have direct involvement of Envenio while in other cases its involvement is indirect (for example the NSERC CRD projects described above). The indirect involvement arises from Envenio's role in expanding the capabilities of the computational platform (called EXN and is the main component of the patent) that feeds into all of the projects on-going at UNB. Envenio also provides support as needed in the execution of the university projects which in all cases are focused on research and development. Also, it should be pointed out that efforts are being made to incorporate more input from the computer science domain (as shown by the number of projects involving Eric Aubanel as collaborator). The goal is to maintain a proper balance between engineering oriented software development and good software design and practice.

Development Challenges

Over the period since our last report the major technical challenge that needed to be overcome was improving the robustness of EXN/Aero in handling unstructured regions of a CFD solution. Unstructured meshes provide the benefit of greater flexibility in meshing complex geometry but also introduce problems with poor mesh aspect ratio and skewness (and as a result more numerical diffiusion). All CFD solvers require special interventions to improve robustness in the case of unstructured meshes including EXN/Aero.

There were numerous issues with PGI (the compiler employed with EXN/Aero) OpenMP parallel regions, in particular those involving task directives. Because of numerous bug issues we were required to rewrite several parts of the code to employ alternative approaches so as to reduce our dependence on task directives in key areas. The reason for using PGI is that it is the leading Fortran compiler that also includes CUDA programming features. PGI was also recently acquired by NVIDIA to further develop their Fortran CUDA interface.

Immediate Steps Going Forward

The immediate next steps going forward are related to extending the overset mesh capability to a prescribed 6-DOF motion mode (up to this point only linearly accelerating motion has been considered). This follows on preliminary work last year that included testing overset for stationary and accelerating cylinders.

Particular development steps will include using the Hosder & Simpson prescribed motion test case and cylinders based on the experiments to be conducted under project 12 above (under Collaboration/Leveraging activities). An important addition in this phase is to implement gradient based second-order interpolation between overset mesh systems. This approach is expected to improve performance significantly particularly as the project moves toward dynamic 6-DOF overset problems.

The other important area that will be started is a code design and early testing for free-surface modelling. It is now expected that a volume-of-fluid based approach will be employed.

References

[1] K. Wilcox, J.T. Zhang, S. John, A.G. Gerber and T. Jeans, *Development of a High-Resolution Simulation Methodology for In-Situ Tidal Turbine Performance*, International Conference on Ocean Energy, ICOE 2014 conference poster, Halifax Nov. 4-6, 2014.

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3. TITLE (The complete document title as indicated on the title page. Its classification should be indicated by the appropriate abbreviation (S, C or U) in parentheses after the title.)

Status Report #3 for the joint project: Manycore Computational Fluid Dynamics (CFD) Solver Development (CONTRACT #:W7707-145678/001/HAL)

4. AUTHORS (last name, followed by initials – ranks, titles, etc., not to be used)

Gerber, A. G.

5. DATE OF PUBLICATION (Month and year of publication of document.)	6a. NO. OF PAGES (Total containing information, including Annexes, Appendices, etc.)	6b. NO. OF REFS (Total cited in document.)
November 2014	14	1

7. DESCRIPTIVE NOTES (The category of the document, e.g., technical report, technical note or memorandum. If appropriate, enter the type of report, e.g., interim, progress, summary, annual or final. Give the inclusive dates when a specific reporting period is covered.)

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8. SPONSORING ACTIVITY (The name of the department project office or laboratory sponsoring the research and development – include address.)

DRDC – Atlantic Research Centre
Defence Research and Development Canada
9 Grove Street
P.O. Box 1012
Dartmouth, Nova Scotia B2Y 3Z7
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9a. PROJECT OR GRANT NO. (If appropriate, the applicable research and development project or grant number under which the document was written. Please specify whether project or grant.)	9b. CONTRACT NO. (If appropriate, the applicable number under which the document was written.)
01EB - RCN - Ship Systems Readiness	W7707-145678/001/HAL

10a. ORIGINATOR'S DOCUMENT NUMBER (The official document number by which the document is identified by the originating activity. This number must be unique to this document.)	10b. OTHER DOCUMENT NO(s). (Any other numbers which may be assigned this document either by the originator or by the sponsor.)
DRDC-RDDC-2017-C267	

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