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Next-Generation Global and Mesoscale Atmospheric Models

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LONG-TERM GOALS

The long-term goal of this research is to construct a unified global and mesoscale nonhydrostatic numerical weather prediction (NWP) models for the U.S. Navy using new numerical methods specifically designed for modern computer architectures; this unified model is called the Non-hydrostatic Unified Model of the Atmosphere or NUMA. To take full advantage of distributed-memory computers, the global domains of NUMA is partitioned into local sub-domains, or elements, that can then be solved independently on multiple processors and graphical processing units or GPUs. The numerical methods used on these sub-domains are local, high-order accurate, fully conservative, highly efficient, and geometrically flexible. Using these ideas we are developing global and mesoscale nonhydrostatic atmospheric models that will improve the operational models currently used by all U.S. agencies including the U.S. Navy.

OBJECTIVES

The objective of this project is to construct new high-order local methods for the Navy's next-generation global and mesoscale nonhydrostatic NWP models. The high-order accuracy of these methods will improve the accuracy of the dynamics for the current global spherical harmonics model (NOGAPS) and the finite difference local-area model (COAMPS). It is conjectured that improving the accuracy of the dynamics (including tracers) will increase the overall accuracy of the forecast; however, such improvements will also have to be made to both the physics and the data assimilation systems but these two topics are currently beyond the scope of this project. The objective of this project is to improve the accuracy of the dynamics while increasing the geometric flexibility in order to use any grid as well as to increase the efficiency of these models on large processor-count distributed-memory computers. Higher efficiency means that the new models will require less computing time that then allows for increasing the number of ensemble members and/or increasing the resolution of the NWP models. The methods that we propose to use for these models are state-of-the-art and are not being used by either current or newly emerging NWP models.

APPROACH

To meet our objectives we explore: 1) Unified high-order continuous Galerkin (CG) and discontinuous Galerkin (DG) spatial discretization methods; 2) Unified high-order implicit-explicit (IMEX) time-integrators with adaptive time-stepping for improved efficiency; 3) unified global and mesoscale models based on the nonhydrostatic equations; 4) fully unstructured and adaptive grids; and 5) scalable parallel implementations. The power of CG and DG methods is that they are high-order accurate yet are completely local in nature – meaning that the equations are solved independently within each individual element and, on parallel computers, may reside on separate processors. Furthermore, high-order methods have minimal dispersion error – this is an important property for capturing fine-scale atmospheric phenomena (e.g., tropical cyclones, Kelvin and Rossby waves). All numerical methods exhibit dispersion errors but the main point is to filter those high-frequency waves which cannot be resolved. Fortunately, CG and DG methods admit additional mechanisms for curtailing the dispersion errors of these high frequency waves. Minimizing dispersion errors is particularly important when, e.g., nonconforming adaptive mesh refinement is used. If dispersion errors are present, then such fine to coarse regions in the grid will produce unphysical reflections. The theoretical development of CG and DG methods are now well established and these methods are arguably the two most successful methods found in the literature for fluid flow problems.

Semi-implicit (SI) and fully-implicit (FI) time-integrators offer vast improvements in efficiency due to the longer time steps that they permit; semi-implicit methods can be classified under the heading of implicit-explicit (IMEX) methods that has garnered much attention in the computational mathematics literature. Furthermore, in order to reap the full benefits of high-order spatial discretization methods requires increasing the order of accuracy of the time-integration methods as well; this is a topic that too often has been ignored by most scientific computing communities, including the NWP community, but has been at the forefront of research efforts in this project. For example, split-explicit methods (ubiquitous in nonhydrostatic models) are mainly used because they offer efficient time-to-solution. However, the large splitting errors inherent to these methods are not usually scrutinized. It is conjectured that similar methods to split-explicit methods can be designed that minimize the splitting errors that they currently exhibit.

Before committing resources towards the development of new NWP models, it is important to identify the form of the governing equations that is most capable of conserving all quantities deemed important. We have been performing studies on this topic for the past few years – that is, to identify the form of the governing equations capable of representing conservation of either mass, energy, or both. In addition, we have analyzed various forms of the governing equations with respect to robustness, flexibility, and efficiency in the context of implicit-explicit (IMEX) time-integration methods. Two of the papers developed within this project are now becoming the standard papers for identifying the proper equation sets and test cases for nonhydrostatic atmospheric modeling (Giraldo-Restelli JCP 2008 and Giraldo et al. SISC 2010). According to Google Scholar, Giraldo-Restelli JCP 2008 already has 99 citations (16 citations per year).

One final area that needs to be explored is the use of adaptive mesh refinement (AMR). We have now developed the necessary machinery (data structures) to allow NUMA to use nonconforming AMR both within the CG and DG formulations. One advantage of AMR is that it may be possible to run simulations not previously feasible with AMR. Another advantage of AMR is that one, in principle,

could achieve the same level of accuracy as a uniform resolution simulation at a fraction of the computational cost. We explore such questions in this project.

WORK COMPLETED

In this section, we describe the work completed this fiscal year. It consists of: analysis of non-conforming adaptive mesh refinement (AMR), stabilization methods for including subgrid-scale parameterizations, the inclusion of moist processes to verify that NUMA will have no issues with subgrid-scale parameterization, and visualization of cloud simulations.

Adaptive Mesh Refinement. We have been arguing in the course of this project that the best next-generation models will be those based on element-based Galerkin (EBG) methods such as the spectral element (SE/CG) and discontinuous Galerkin (DG) methods. However, we have only partly showed the benefits of this approach such as: high parallel efficiency and high-order accuracy. Two years ago, we began a study of adaptive non-conforming quadrilateral grids (we published our results for non-conforming AMR for DG in Ref. [3] and AMR with CG and DG in Ref. [6]). One of the attractions of NUMA is that it uses either CG or DG methods. In other words, the CG and DG spatial discretizations have been written in a unified way which allows the model to use either method and both methods can now be run with AMR. Our AMR algorithm only takes 1% of the total runtime and works well in unison with our IMEX methods, iterative solvers, and preconditioners. Although non-conforming AMR for both CG and DG has been presented before, the contribution of our work is in showing how to extend this approach to nonhydrostatic atmospheric models. Moreover, to our knowledge, the results published in Refs. [3] and [6] are the only known results showing the conservation of mass up to machine precision for non-conforming AMR.

Stabilization Methods. CG and DG methods are both high-order methods. This means that when strong gradients are encountered in a simulation, it is possible to produce numerical oscillations due to the high-order representation of non-smooth flow regions. This situation is exacerbated when tracers that need to remain positive experience Gibbs phenomena because their values may become negative – this is clearly unphysical and must be avoided. To ameliorate this situation, stabilization methods need to be introduced. Low order methods have inherent dissipation so they may not require too much additional stabilization but the CG method is a completely non-dissipative method and thereby requires special treatment. DG, on the other hand, can use built-in dissipation and thereby is more straightforward to stabilize. We have conducted a series of studies on stabilizing CG methods. For example, we have explored the typical hyper-viscosity operators (4th order) used in most atmospheric models whereby the viscosity coefficient is constant although can be defined anisotropically. In addition, we have explored adaptive viscosity approaches typical of Smagorinsky-like methods (e.g., Moeng, etc.). This work can be found in Refs. [4] and [7]. The value of adaptive viscosity methods is that when no stabilization is required, the viscosity coefficient goes to zero, which means that the solutions will not be overly damped. In this project, we have also extended two new types of stabilization methods based on adaptive viscosity approaches: these are the Variational Multi-scale method (VMS) and the Nazarov turbulence model. The idea in these methods is that the stabilization term is only non-zero when the residual of the governing equations is non-zero. As this residual goes to zero (implies convergence) the stabilization term vanishes. This class of stabilization methods is preferable to methods that apply stabilization always because adaptive viscosity methods can be proved to be consistent, which is a necessary (but insufficient) condition for proving convergence.

Moist Processes. In this portion of the project, we analyzed the capability of NUMA to handle subgrid scale parameterizations such as condensation and precipitation. For this purpose we use the Kessler warm rain moisture. The question that we aim to answer in this study is whether or not the non-uniform spacing along the vertical direction in NUMA will cause problems with using pre-existing subgrid-scale physical parameterizations. Although there exist operational CG codes (such as the spectral element core in CAM-SE), NUMA is the only model currently in existence that uses SE and/or DG in all three directions. As an example, CAM-SE uses SE in the horizontal but with 2nd order finite differences in the vertical. It has been conjectured by some that the non-uniform spacing in the vertical direction will be problematic. The aim of this work is to show that that conjecture is false. To do so, we have run NUMA on standard 3D storm simulations (e.g., supercells and squall lines) from the literature and have confirmed that NUMA can handle moist processes well. In addition, we used these storm simulations to compare the various stabilization methods available within the NUMA model.

Visualization. An often-ignored aspect of the scientific computing pipeline is the value of visualization. All scientists are aware that visualization is important but far too often standard visualization software is not sufficiently sophisticated to help the scientist visualize the data and the most realistic way possible. We have begun looking at using visualization packages previously used by the movie industry to visualize the data with high fidelity.

RESULTS

The main results for this year can be divided into the following sections: 1) analysis of adaptive mesh refinement for both CG and DG; 2) stabilization methods for CG and DG methods; 3) the inclusion of 3D moist processes within NUMA; and 4) the visualization of this data.

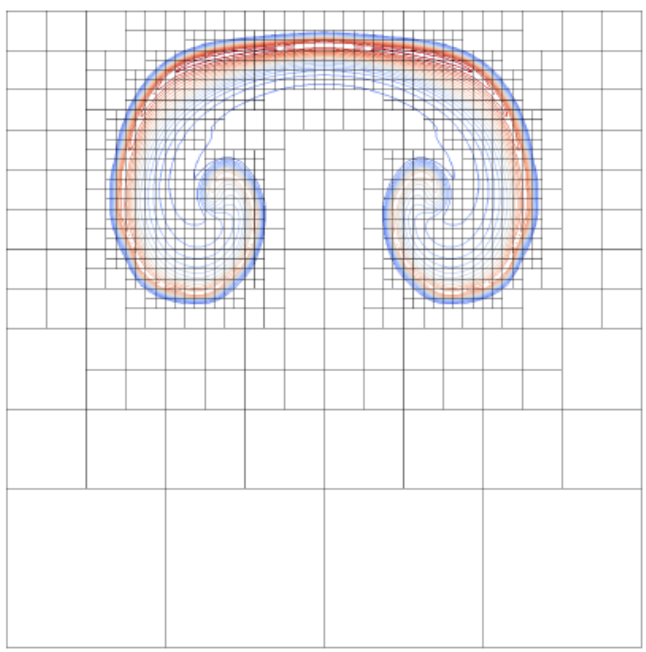

Figure 1: Adaptive mesh refinement for the rising thermal bubble case. The black lines are the elements where each element is comprised of 8th order polynomials.

Adaptive Mesh Refinement. One of the distinguishing features of NUMA is that it is the only model from all the ESPC-considered models that has the capacity for adaptive mesh refinement (AMR). Currently, AMR is only available in the 2D versions of NUMA but the extension to 3D-NUMA is underway. Although it is not clear if AMR can be used for all types of simulations, it is certainly a good candidate for high-resolution hurricane simulations. To explain AMR let's consider Fig. 3 where a density current simulation is illustrated.

Figure 1 shows the potential temperature contours plotted with the grid. Note that some grid boxes are smaller than others. The AMR algorithm automatically figures out which grid box needs to be small (where something is happening) and which boxes can be large (where nothing is happening). This way one can follow an interesting feature with high precision yet use far fewer degrees of freedom compared to a uniform high-resolution simulation where all the grid boxes are small. The question that one might ask is: is AMR faster than using a uniform simulation? In other words, what is the overhead in using the AMR algorithm?

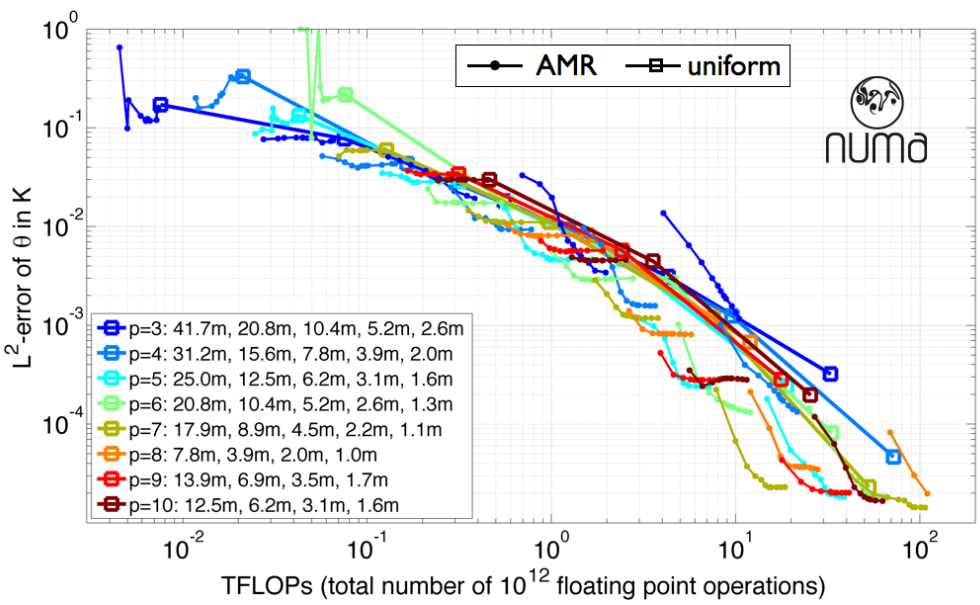

Figure 2: The L2 error versus total floating point operations for various simulations. Lines with a square denote the uniform grid simulations whereas lines with a circle denote the adaptive simulations.

Figure 2 shows the L2 error (where a high-order simulation is used as the exact solution) as a function of the total number of floating point operations (TFLOPs); we use TFLOPs as a proxy for the computational cost. Figure 2 shows the entire parameter space of simulations used to measure the effectiveness of AMR in bringing down the computational cost. For example, polynomial orders 3 through 10 are analyzed where for each polynomial order the number of elements is varied to achieve the grid resolution given in the legend of Fig. 2. For example, for p=3 polynomials, we use grids with resolutions of 31.2 m, 15.6m, 7.8m, 3.9m and 2.0m. We vary the resolution for polynomial orders p=3 through p=10. In addition, we show the results for uniform grid simulations (lines with a square) and also for adaptive grid simulations (lines with circles). To our knowledge, such a detailed study of the cost of AMR has never been conducted.

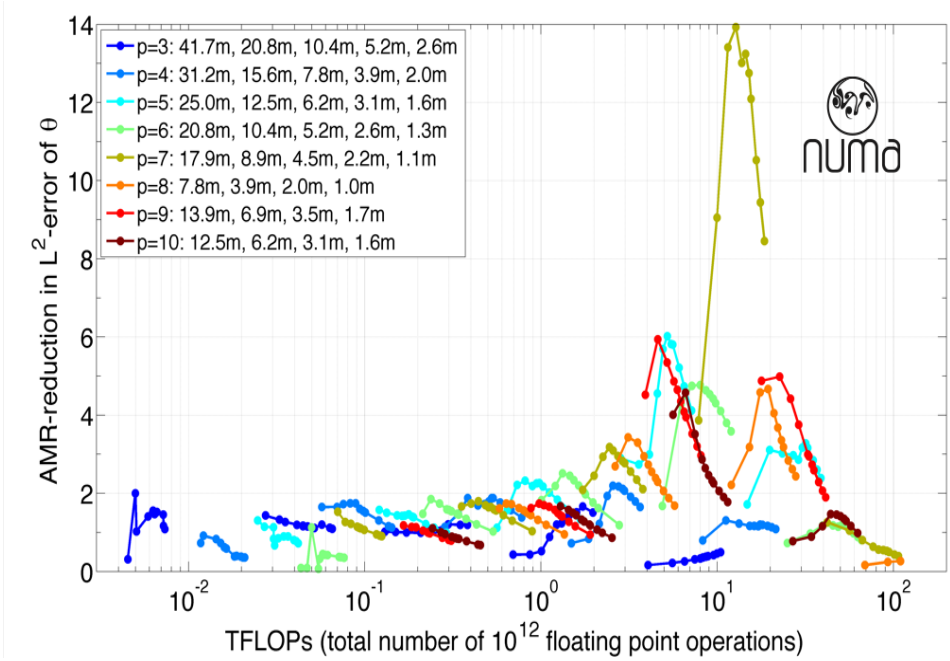

Figure 3: The reduction in L2 error by using AMR.

The data in Fig. 2 can be processed differently to reveal the benefit of AMR. Figure 3 shows the reduction in error by using AMR as compared to a high-resolution uniform simulation of the same polynomial order. For p=7 (gold curve), we can achieve almost a factor of 14 reduction in error for the same number TFLOPs. Processing the data in Fig. 2 a different way produces Fig. 4 that shows the reduction in floating point operations by the use of AMR. We achieve the largest speedups for p=3 (under-resolved regime) and p=7 (at the better resolved regime) which is close to a factor of 4.

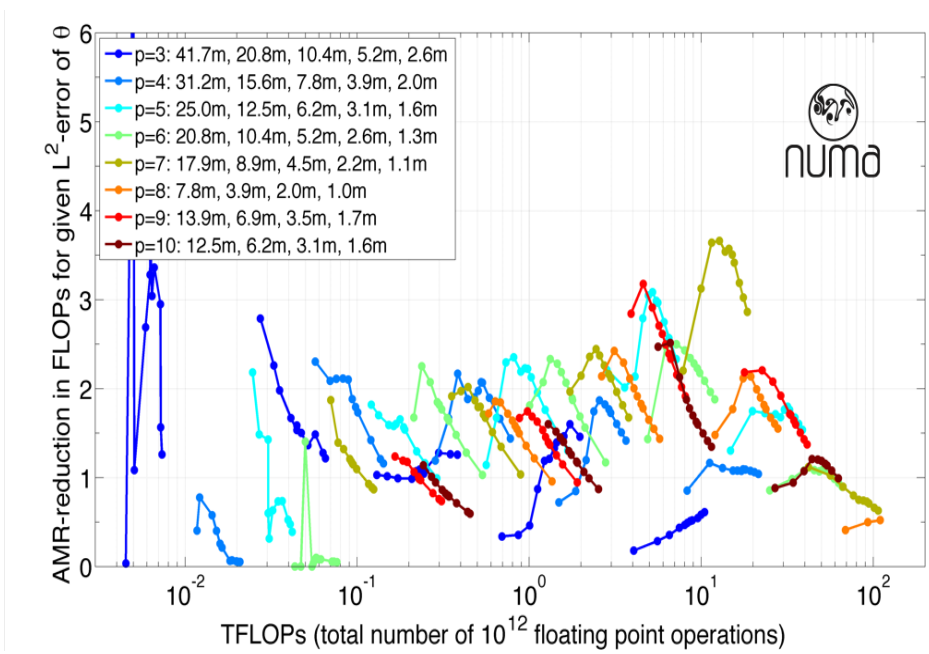

Figure 4: The reduction in FLOPs by using AMR.

To show that our AMR algorithm is not dependent on the actual geometry of the problem (Fig. 1 only shows results in the x-z plane) we have also verified the accuracy of the AMR algorithm on spherical geometries. In Fig. 5, we show results for the Galewsky barotropic unstable jet after the waves have broken. The results of Fig. 5 have been published in Ref. [5] where a detailed study of AMR on spherical geometries was conducted. Looking at Fig. 5, one can see that it does not matter the type of grid that NUMA with AMR can use as long as it is comprised of quadrilaterals (hexahedra in 3D). Figure 5 shows results on cubed-sphere (left panel), latitude-longitude (center panel), and icosahedral (right panel) grids. In other words, NUMA can run on a latitude-longitude grid if this is so desired or on any other type of grid. This type of grid flexibility is unprecedented in any current NWP model; currently, all models are built on a specific grid. NUMA does not care what the grid is. In fact, NUMA has been retrofitted to use off-the-shelf grid generators, which gives NUMA a huge advantage since it is able to use specifically optimized grids.

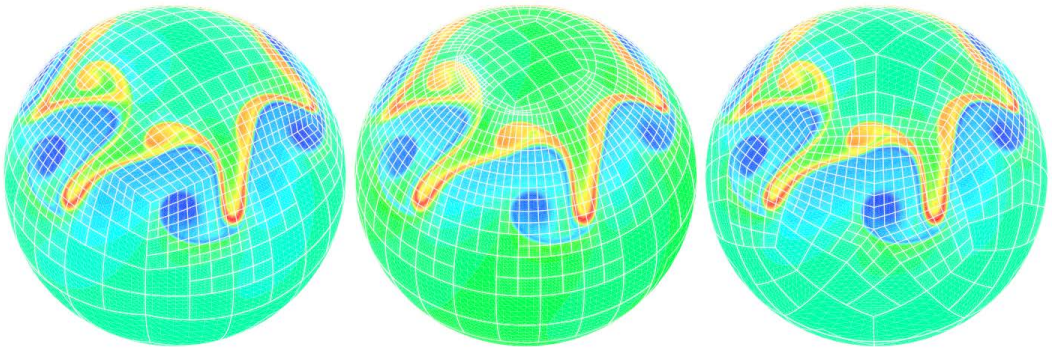

Figure 5: The adaptive grid (white lines) and the vorticity contours (red and blue contours) of the Galewsky barotropic unstable jet using a cubed-sphere (left panel), latitude-longitude (center panel), and icosahedral (right panel) adaptive mesh.

<u>*Stabilization Methods*</u>. All NWP models require some form of dissipation to execute a complete simulation stably especially when moist processes are included. Typical stabilization methods include artificial viscosity in one form or another. Be they constant viscosity coefficients or adaptive ones by way of Smagorinsky-type diffusion that are more akin to Large-Eddy Simulation (LES) mechanisms. In this part of our work, we have sought to develop turbulence models within NUMA that may be used towards a number of ends: 1) as stabilization methods to be able to simulate complex flows robustly even with the inclusion of subgrid-scale parameterizations and 2) towards developing turbulence models for studying (and improving) subgrid-scale parameterizations especially for NUMA. This year we have included three LES schemes to the dynamics: 1) Nazarov-Hoffman (2013), 2) Lilly (1962)-Smagorinsky (1963), and 3) Deardoff (1980)–Moeng (1984). In addition, we have added the following stabilization schemes to the moist variables: 1) constant, yet anisotropic artificial viscosity and 2) Variational Multi-scale methods (VMS) with discontinuity capturing (DC).

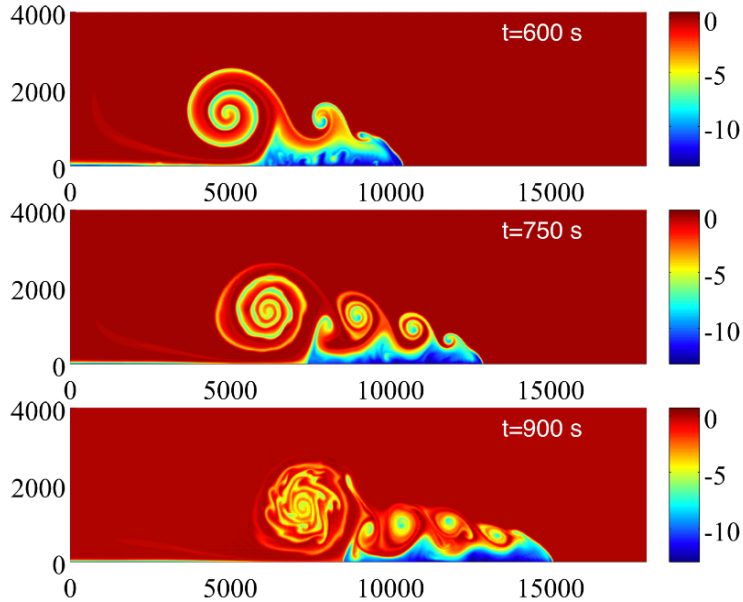

Figure 7: Density current: perturbation of potential temperature at during 900 seconds. Simulation on a 25 m grid resolution (256 x 1 x64 elements)

As an example of what these methods are able to do, we show in Fig. 7 the simulation of the well-known density current test case of Straka et al. (1993) that requires some form of viscosity to run stably; typically, a constant coefficient is used. In Fig. 7, we use the Nazarov-Hoffman stabilization, which uses and adaptive viscosity based on the required viscosity of the compressible Navier-Stokes equations. The snapshots of the simulation at the three different times (600, 750, and 900 seconds) show that the solution is stable yet exhibiting far more fine-detailed structure than other density current simulations. The reason for this is that the Navarov-Hoffman LES scheme uses only the minimal amount of viscosity required to maintain stability and therefore does not damp other structures. Since NUMA is a high-order model, more resolution means that finer scale structures are captured, which is evident in Fig. 7. This is an exciting result because it means that using such LES schemes with NUMA will perhaps allow us to achieve better-resolved vortex-structures in atmospheric flows, which then translates to better resolution of tropical cyclones (both with regards to intensity and trajectory).

<u>*Moist Simulations*</u>. In order to verify that the vertical grid structure of NUMA poses no difficulties to the inclusion of subgrid-scale parameterizations, we have added simple moist physics to NUMA and have analyzed the production of clouds. To this end, we chose well-known works from the literature including Weisman-Klemp (1982), Weisman et al. (1988), and Kurowski and Grabowski (2013).

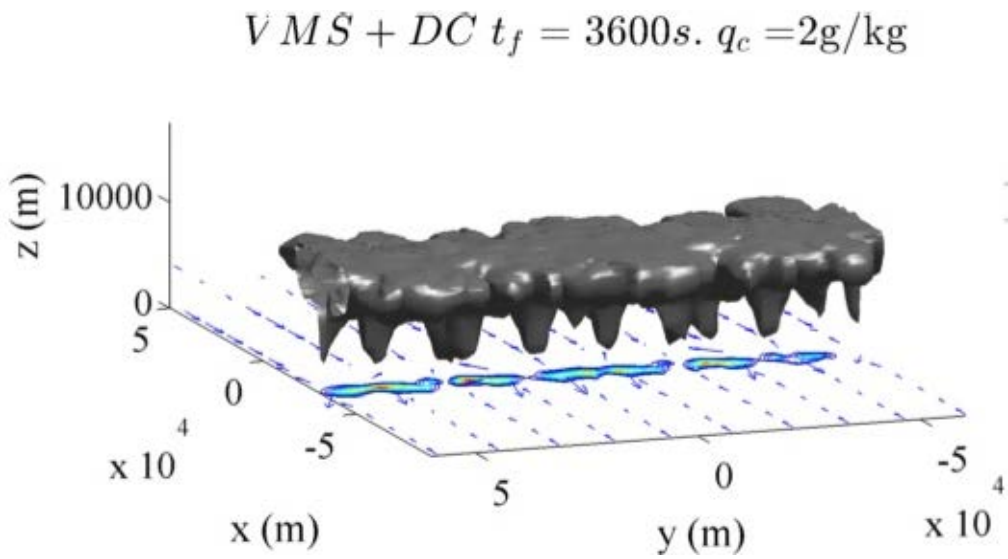

Figure 8: A squall line simulation with NUMA. Two cloud trains are present although only the one in the far end is shown. The one nearest the xyz axis is not shown in order to plot velocity vectors. The bottom panel shows the cold pools formed by the density current triggered by the evaporating rain.

In Fig. 8, we show the squall line simulation with the test setup from Weisman-Klemp (MWR 1982). We ran the squall line test case with a large parameter space of stabilization methods. For example, we used various constant hyper-viscosity values as well as anistropic values (different viscosities in the vertical and horizontal directions). In addition, we compare the results of these classical stabilization methods with the new VMS method that we have incorporated within NUMA.

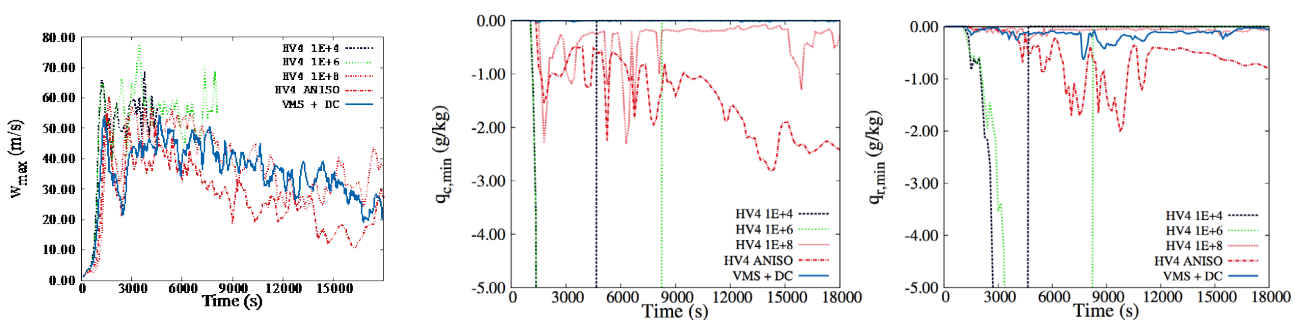

Figure 9: A squall line simulation with NUMA using various stabilization methods: 4th order hyper-viscosity (HV4), 4th order anisotropic hyper-viscosity (HV4 ANISO), and variational multi-scale methods with discontinuity capturing (VMS+DC). The left panel shows the maximum vertical velocities, the center panel shows the minimum cloud concentrations and the right panel shows the minimum rain concentrations.

Figure 9 shows the vertical velocities (left panel), minimum cloud content (center panel), and minimum rain content (right panel) for all the stabilization methods studied. The results with VMS+DC are clearly the best for the following reasons: on the left panel, we see that the VMS+DC (blue curves) yield similar vertical velocities to HV4=1x10^8 and to the HV4 with anisotropic viscosity.

When we then look at the center and right panels, we see that VMS+DC yields almost perfect positivity for cloud content (center panel) and, although not as good as HV4=$1x10^8$for positivity preserving for rain (right panel), still does quite well. Furthermore, these results are completely parameter-free meaning that the VMS+DC automatically adjusts the amount of diffusion required to stabilize the flow while yielding very good positivity-preservation. VMS+DC is not perfect, but the results are at least as good as a finally tuned HV4 coefficient, yet no tuning is required by VMS+DC.

Visualization. Through collaboration with the MOVES (Modeling of Virtual Environments and Simulations) at the Naval Postgraduate School, we have begun using the Maya (by Autodesk) visualization package to render real-looking simulations of our moist convection simulations. Let us briefly explain the process.

Figure 10: Isosurface of q_c=3.5gr/kg plotted with Paraview (on the left) and with Maya (on the right). A photograph of the Pacific Grove golf links is superimposed on the Maya output.

Figure 10 shows the output of cloud water (condensation) using the scientific visualization software Paraview (left panel) and the same data using the movie industry software Maya (right panel), with some artistic freedom taken on the right panel via the superposition of a photograph. What the Maya software is able to do that Paraview cannot is to give the clouds realistic texture. Moreover, since clouds are translucent, Maya is able to represent this which allows one to see through the clouds to see what is behind this object. This gives the cloud an entirely different look that is far more realistic. Based on this idea, we have used the Maya software to create an animation of a moist convection simulation. Figure 11 shows one frame of this animation. One can see not only the realistic-looking clouds but also real rain (i.e., rain produced by NUMA). The only artistic freedom taken in this animation is: 1) the moonlight and 2) the camera lens spots. To see the simulation please go to the link: http://www.vimeo.com/108201080.

IMPACT/APPLICATIONS

This work targets the next-generation NWP systems for massively parallel computer architectures. NUMA has been designed specifically for these types of computer architectures while offering more flexibility, robustness, and accuracy than the current operational systems. Additionally, the new models are expected to conserve many important quantities such as mass and use state-of-the-art time-integration methods that will greatly improve the capabilities of the Navy's forecast systems.

Figure 11: single frame of a movie rendered with computer graphics software Maya. Postprocessing is done with Adobe Photoshop and Adobe Lightroom software.

TRANSITIONS

Improved algorithms for model processes will be transitioned to 6.4 as they are ready, and will ultimately be transitioned to FNMOC.

RELATED PROJECTS

Some of the technology developed for this project could be used to improve NOGAPS in other NRL projects. The work on the mesoscale models will help improve COAMPS. An example is the time-integration methods that we are exploring for the new models may well be incorporated into the current operational version of COAMPS. In a separate Department of Energy (DoE) project, the Mathematics and Computational Science group at Argonne National Laboratory is working on interfacing NUMA with their highly scalable software PETSc (Portable Extensive Toolkit for Scientific Computing). This union will vastly increase the capability of NUMA through the access to the large suite of time-integrators, preconditioners, and solvers contained in PETSc. Furthermore, having NUMA being scrutinized by software and parallel computing scientists will allow us to improve NUMA.

PUBLICATIONS

Journals

1. Giraldo, F.X., Kelly, J.F., and Constantinescu, E.M., 2013: Implicit-Explicit Formulations for a 3D Nonhydrostatic Unified Model of the Atmosphere (NUMA). *SIAM Sci. Comp.* 35 (5), B1162-B1194 (2013).
2. L. Yelash, A. Mueller, M. Lukacova-Medvidova, F.X. Giraldo, V. Wirth, Adaptive Discontinuous Evolution Galerkin Method for Dry Atmospheric Flow, Journal of Computational Physics Vol. 268, 106-133 (2014).
3. Kopera MA, Giraldo FX. Analysis of adaptive mesh refinement for IMEX discontinuous Galerkin solutions of the compressible Euler equations with application to atmospheric simulations. *J. Comput. Phys.* 2014 (275):92-117.

4. S. Marras, A. Mueller, F. X. Giraldo, Physics-based stabilization of spectral elements for the 3D Euler equations of moist atmospheric convection**,** in Proceedings of ICOSAHOM, Salt Lake City, UT, U.S.A. 2014.
5. Marras S, Kopera A, Giraldo FX. Simulation of shallow water jets with a unified element-based continuous/discontinuous Galerkin model with grid flexibility on the sphere. *Quarterly Journal of the Royal Meteorological Society*. 2014 (in press).
6. Kopera MA, Giraldo FX. Mass conservation of the unified continuous and discontinuous element-based Galerkin methods on dynamically adaptive grids with application to atmospheric simulations. *J. Comput. Phys.* 2014 (in review).
7. S. Marras, F. X. Giraldo (A parameter-free and anisotropic alternative to hyper-viscosity in the simulation of moist convection, J. Comput. Phys. (in review 2014).
8. M. Yu, F.X. Giraldo, M. Peng, and Z.J. Wang, Localized artificial viscosity stabilization of discontinuous Galerkin methods for nonhydrostatic atmospheric modeling, Journal of Computational Physics (in review 2014).
9. S.-J. Choi, F.X. Giraldo, J. Kim, and S. Shin, Verification of a non-hydrostatic dynamical core using horizontally spectral element vertically finite difference methods: 2D aspects, Geoscientific Model Development (in review 2014).
10. S.-J. Choi, F.X. Giraldo, Development and Evaluation of a Hydrostatic dynamical core using the spectral element/discontinuous Galerkin methods, Geoscientific Model Development (in review 2014).

Plenary Talks

1. Giraldo, F.X.: Continuous and Discontinuous Galerkin Methods for Atmospheric Modeling, European Center for Medium-Range Weather Forecasting, Reading UK (September 2013).
2. Giraldo, F.X.: Development of NUMA: a Next-Generation Global Cloud Resolving Dynamical Core, 6th International Conference on Global Cloud Resolving Modeling and 3rd International Workshop on Nonhydrostatic Numerical Models, Kobe, Japan (September 2014).

Invited Talks

1. Giraldo, F.X.: Unified Element-based Galerkin Methods for Atmospheric Modeling, Institute for Computational Engineering and Science, University of Texas at Austin (October 28, 2014).

Conference Abstracts

1. Kopera, M.A., Giraldo, F.X.: Non-conforming Adaptive Mesh Refinement for Discontinuous Galerkin Atmospheric Model. *PDES on the Sphere 2014,* Boulder, CO (September 2014).
2. Giraldo, F.X: IMEX Formulations for CG and DG Methods. ICOSAHOM, Salt Lake City, UT (June 2014).
3. Müller, A., M.A. Kopera, S. Marras, and F.X. Giraldo: Do high order and dynamic adaptive mesh refinement improve the efficiency of atmospheric simulations?, World Weather Open Science Conference, Montreal, Canada (August 2014).

4. Müller, A., M.A. Kopera, S. Marras, and F.X. Giraldo: Comparison of adaptive and uniform 2D Galerkin simulations, Workshop on the Solution of Partial Differential Equations on the Sphere, National Center for Atmospheric Research, Boulder, Colorado, USA (April 2014).
5. S. Marras, A. Mueller, F. X. Giraldo (June 2014), Physics-based stabilization of spectral elements for the 3D Euler equations of moist atmospheric convection**,** in Proceedings of ICOSAHOM, Salt Lake City, UT, U.S.A.