

IMAGE RESEARCH: NEW ALGORITHMS, TOOLS, AND GEOPHYSICAL MODELS

The power of mathematical science is that similar methods and models can be used to solve problems in very different contexts. The Institute of Mathematics Applied to Geosciences (IMAGe) was formed in October 2004 to develop tools, methods, and models that can address some of NCAR's fundamental science problems. IMAGe is also actively introducing the mathematics community to new problems that are posed by geophysical processes and observations. Two important vehicles that support this interdisciplinary activity are the Theme of the Year workshops and publically available software for numerical and statistical methods. IMAGe contributes to the NCAR strategic priorities of "Conducting research in computer science, applied mathematics, statistics, and numerical methods" and "Engaging a broader and more diverse community."

Geophysical-Astrophysical Spectral-Element Adaptive Refinement code has been extended to use adaptive three-dimensional grids and has been tested under an advection/diffusion solver. Turbulence was studied in rotating, neutral fluids, and the interactions between rotation, helicity, and transfer of energy between scales was quantified. A promising MHD simulation exploiting Taylor-Green symmetries has produced features in current sheets observed in the solar wind.

combined with a state-of-the-art mesh database to produce a code with excellent



This image summarizes preliminary results from an aqua-planet simulation using the HOMME global atmospheric model and an approximation of atmospheric physics that includes a new method for representing convection. The Earth's Madden-Julian Oscillation (MJO) is approximated by a traveling wave of convection in the tropical ocean with a period of approximately 30-60 days. Convection processes such as tropical thunderstorms are very important to the Earth's climate because they distribute heat from the surface into the troposphere. Therefore, accurate simulation of the MJO helps us understand this fundamental geophysical process.

The figure is a standard summary of the dynamical properties of the atmosphere where the energy from traveling waves is decomposed into the spatial size of the waves (horizontal axis in wave number) and their speed (vertical axis in period). The color scale indicates the kinetic energy that can be attributed to different combinations of scales and speeds, and the labeling indicates several well-known atmospheric waves. The MJO is more difficult to detect as it has a relatively long period. However, preliminary evidence for its presence appears in this simulation.

The discontinuous Galerkin (DG) method was This experiment is important because the precise mechanisms of the MJO are still unknown, and past numerical models have had difficulty simulating it.

scaling to many processors. A third-order DG transport scheme was implemented within HOMME with a new monotonic limiter and was shown to eliminate spurious oscillations from the numerical solution.

A design study was completed that indicates the value of including an energy balance model as part of past climate proxy reconstructions. The multivariate, spatial lattice model was completed for interpreting in a joint manner the temperture and precipitation from climate model projections.

The Data Assimilation Research Testbed was successful for real-time forecast of CO concentrations in support for the ARCTUS field program. In addition, DART/CAM was able to produce specific reanalysis fields for the Arctic region for diagnosing mechanisms of sea ice formation and also for improving the filtering at high latitudes in the CAM finite volume dynamical core.

Multiscale modeling plans: A Boussinesq capability is being added in GASpAR to work on atmospheric flows. The FFT libraries in GHOST (Geophysical High Order Suite for Turbulence) are being extended to do pencil (1D) decompositions. Results of the Advanced Science and Discovery experiments on rotating flows with helicity will be compared to a subgrid-scale parameterization for the effect of eddys.

Numerics plans: The DG conservative transport will be tested in CAM/HOMME using the aqua-planet simulations. In addition, a multi-tracer transport algorithm based on conservative remapping will be studied for future implementation. Adaptive mesh refinement algorithms will be developed in the context of a two-dimensional solver for compressible fluids. A multi-grid algorithm will be included. Software infrastructure to perform three-dimensional simulations on general curvilinear domains will be built. Finally, algorithms will be developed for node placement in the context of using radial basis functions (RBF) for the adaptive solution of the shallow water equations.

Statistics plans: Bayesian methods for spatial paleoclimate reconstructions will be completed for North America using multiple proxies. Statistical analysis will be completed for a subset of the NARCCAP experiments for extreme precipitation and a multimodel synthesis that includes the skill in reproducing current climate and interactions among GCM/RCM pairings.

Data Assimilation plans: Development will continue on parallel implementations of DART with WRF and CAM interfaces. Adaptive inflation and localization data algorithms will be refined and applied to improve tropical cyclone analysis and prediction, as well as for organized convective systems over the continental U.S. and contiguous coastal oceans.

IMAGe is supported by NSF Core funding.



DATA ASSIMILATION RESEARCH

Data assimilation is the process of merging data from observations with computer models. It can transform diverse and incomplete observations to gridded estimates that can easily be used and interpreted. The assimilation process also produces quantitative information on model error, forecast skill, and observational errors, all of which allows us to improve models.

Data assimilation is providing rapid advances in geophysical studies. The Data Assimilation Research Section (DAReS) of IMAGe performs fundamental research on ensemble data assimilation methodologies for application across a wide range of geophysical problems. DAReS develops and maintains the Data Assimilation Research Testbed (DART), a software facility for doing ensemble data assimilation. DAReS also provides support to a growing community of NCAR, university, and government laboratory partners who are interested in applying ensemble data assimilation methods.



http://www.nar.ucar.edu/2008/CISL/3res/3.1.1.dar.php

use of DART assimilations.

DAReS supports three of NCAR's strategic priorities: "Developing community models," "Developing and providing advanced services and tools," and "Enhancing science education." The DART user community includes members from many NCAR divisions, more than a dozen universities, and many government labs. NCAR projects supported by DART during 2008 included:

- Year-long reanalyses with several versions of CGD's CAM climate model identified and led to the correction of errors in the polar filter.
- The impact of COSMIC GPS radio occultation measurements was evaluated for large scales in CAM and for hurricane predictions in MMM's WRF model.
- Researchers in ACD used DART with the CAM/CHEM model to provide real-time analyses of weather and carbon monoxide for the ARCTAS field campaign.
- Researchers in CGD are using DART/CAM analyses and forecasts to explore mechanisms for the rapid loss of Arctic sea ice observed in 2007.
- Researchers in MMM have developed DART-based forecast sensitivity tools and used them to address questions about the impact of observations on forecasts of hurricane position and strength.

A growing number of university groups are using both DART/WRF and DART/CAM for research and instruction. For instance, a joint DAReS/University of Wisconsin project is investigating the impact of advanced hyperspectral infrared retrievals on hurricane prediction. Research partners at Cal Tech have completed implementing a version of DART/WRF configured for prediction on Mars. At the University of Colorado, DART has been used to explore assimilating velocity observations of the flow exiting a laboratory slit jet.

DAReS has supported the incorporation of two new large geophysical models this year: a version of the MIT ocean GCM in partnership with Scripps Institution of Oceanography and the Navy's COAMPS® model in partnership with NRL Monterey. DART/WRF is also being evaluated for typhoon predictions in non-operational tests by the Central Weather Bureau in Taiwan. DAReS continues to incorporate feedback from all partners to develop more powerful and generic assimilation tools.

Fundamental ensemble data assimilation research has focused on dealing with non-Gaussian distributions of observational error. An algorithm developed last year has been further refined, used to produce year-long assimilations in CAM, and is being tested for assimilation of radar reflectivity in WRF. Research on designing filters that can tolerate both non-gaussianity and nonlinearity will be the key focus during the next year. Such tools would improve analysis and prediction using radar and remote sensing observations in hurricanes and severe convection.

Data assimilation research in IMAGe is supported by NSF Core funding and NASA Grant NNX08A23G.



GEOPHYSICAL STATISTICS PROJECT

From our unique position within CISL and IMAGe, the Geophysical Statistics Project (GSP) has been a leader in training and research emphasizing the synergy between the geosciences and the statistical sciences. In addition to basic methodological and theoretical statistical research, GSP has a strong training component supporting graduate students and postdoctoral visiting scientists. These young researchers are immersed in research activities that not only focus their skills as applied statisticians but also expose them to important applications in the geosciences.



Northern Hemisphere mean temperature reconstructions based on synthetic proxies embedded in noise and forcings. The proxies are generated by the algorithms that approximate the relationship between proxies and temperatures using the synthetic temperatures from global climate model output. The top panel compares the reconstruction using different types of proxies: PF uses 15 local temperatures as proxies; R uses tree ring only; RP uses tree ring and pollen; RB uses tree ring and borehole; and RPB uses tree ring, pollen, and borehole. Among the four reconstructions from different combinations of proxies, RBP has lowest bias and mean squared error. So in the bottom panel, the reconstruction from RBP with its 95% uncertainty band (gray area) is displayed. The reconstruction follows the trend of the target fairly well, and the uncertainty band covers the target most of the time.

In addition to these core activities, GSP also has an active visitor program providing research opportunities for visiting faculty members from across the nation and abroad. Our goal is to foster collaboration between graduate students, postdocs, the permanent and visiting statistical staff, and NCAR scientists. These programs, as well as the research and training aspects of GSP that emphasize the interaction between statistics and the geosciences, embody the tenets of integration, innovation, and community building within the NCAR strategic plan. Specifically, this program supports the NCAR strategic priorities of "Conducting computer science, computational science, applied mathematics, statistics, and numerical methods R&D," "Supporting and enhancing formal science education at all levels," and "Engaging a broader and more diverse community in the atmospheric and geosciences."

During FY2008, GSP researchers have been involved in numerous important projects, including:

- Design and analysis of computer experiments, in particular focusing on regional climate models and models of the upper atmosphere and the magnetosphere
- Developing methodology for analyzing extremes of weather and climate
- Stochastic weather generators
- Modeling uncertainty in climate reconstruction



GSP continues to develop theory and methodology for analyzing spatial data, including nonstationary covariance models, models for spatial lattice data, multivariate spatial observations, spatial-temporal models, as well as general methodology for computational statistics and Bayesian hierarchical models.

In FY2009, the scientific focus on computer models will continue, in particular through GSP scientists being involved in such NCAR programs as the North American Regional Climate Model Assessment Program (NARCCAP) as well as in collaborations with other computer modeling groups across NCAR. Beyond computer models, GSP scientists will continue to assess the impacts of climate and climate change on public health, to develop methodology for analyzing extremes, to develop methodology for modeling daily weather scenarios,



Results of a calibration experiment matching the output of the Lyon-Fedder-Mobary (LFM) computer model of the magnetosphere to observations from the Polar Ultraviolet Image (UVI) during a geomagnetic storm. The blue dots indicate the initial values of calibration parameters (alpha, beta, and R) based on space-filling experimental design. These parameters transform the standard MHD parameters into the average energy and flux of the precipitating electrons. The contours represent approximate 50 (red), 75 (yellow), and 95 (white) percent contour shells of the posterior distribution of the optimal calibration values for alpha, beta, and R based on a novel statistical approach to calibrating computer models with high-dimensional outputs.

to develop methodology for quantifying the uncertainty in climate reconstructions, and to develop statistical methodology for the analysis of complex, spatial and spatial-temporal data.

This project is made possible through NSF Core funding, as well as grants through NSF's Division of Mathematical Sciences and NSF's Collaboration in Mathematical Geosciences.



GEOPHYSICAL TURBULENCE PROGRAM

Research on turbulence has been a significant part of the NCAR scientific program since its beginning in the early 1960s. The original scientific leaders of NCAR recognized that to understand the dynamics of the atmosphere, the oceans, the climate, the sun, and solar-terretrial interactions, understanding relevant turbulent processes would be essential. A number of scientific appointments in the first 10-15 years of NCAR's existence reflected this view and provided an in-house base from which to productively interact and collaborate with the world turbulence community. From these beginnings, a sustained emphasis on geophysical turbulence at NCAR has emerged in research, visitors, seminars, and workshops that continues to this day. Most of this emphasis manifests itself currently in the Geophysical Turbulence Program (GTP).



Structure of thermal convection over a heated plane. Vertical velocities after six hours of simulated time are shown within the boundary layer depth; bright and dark volumes denote updrafts and downdrafts, respectively. The only difference between the solutions in the left and right panels are the values of viscosity in the horizontal entries of the stress tensor, respectively, 2.5 versus 70 meter-squared per second. These results are part of research that addresses numerical effects that influence the structure of simulated convection in the planetary boundary layer, which becomes an increasingly important issue as numerical weather prediction models use increasingly higher resolutions.

By design, GTP is an interdiscplinary group of about 40 members that spans many divisions and laboratories at NCAR with a few external affiliates. It encompasses research at NCAR on multi-scale nonlinear processes with an array of applications in a broad variety of areas. GTP is also the outreach arm of this research, and is complementary to the <u>Turbulence Numerics Team</u>.

In FY2008, GTP sponsored eight seminars and hosted five long-term (greater that 1 week) visitors. Several of these visitors were students, where the research conducted formed part of the students' graduate requirements. The topics covered in collaboration with NCAR staff represent a broad variety of interests:

- Studies of turbulent enhancement of droplet formation
- Numerical thermal convection
- Improved trajectory schemes for Lagrangian methods in fluid dynamics
- Effects of turbulent entrainment and mixing on cloud dynamics
- · Coupled dynamics of boundary layers and evolutionary landforms
- Research on <u>cumulus convection and measurement</u>
- Self-organized criticality-like representation of statistical measurements of turbulent MHD flows
- Studies of differences in turbulence statistics between <u>canopy/roughness sublayers and intertial sublayers</u>
- The statistical mechanics of fully developed turbulence

In FY2009, GTP will continue organizing workshops, holding seminars, and hosting short-term and long-term visitors. It will also provide a small amount of funds for a short (summer) visit by one or two graduate students who support the scientific agenda of research in multi-scale physics for geophysical flows.

GTP activities advance NCAR's strategic priorities of "Conducting computer science, computational science, applied mathematics, statistics, and numerical methods R&D" and "Engaging a broader and more diverse community in the atmospheric and geosciences." GTP activities are sponsored entirely by the NSF cooperative agreement through UCAR.



TURBULENCE SCIENCE: NUMERICAL ALGORITHMS AND CODE DEVELOPMENT

The Turbulence Numerics Team (TNT) is complementary to the <u>Geophysical Turbulence Program</u> (GTP) and is focused on the accurate simulation and understanding of turbulence for fluids such as the atmosphere, and for charged flows in the presence of magnetic fields. TNT research emphasizes simplified physical systems that still reproduce the complexity and multi-scale properties associated with turbulent flow.

TNT staff is composed of Julien Baerenzung (Postdoctoral researcher), Aimé Fournier (Project Scientist), Ed Lee (Graduate Student in Applied Mathematics, Columbia U.), Pablo Mininni (Scientist I, 25% FTE), Annick Pouquet (Senior Scientist and Section Head, 60% FTE) and Duane Rosenberg (Software Engineer). More information on what is reported below can be found in the Research Catalog items linked from the text, and also available under the names of the Team members.

Research on turbulent flows

We have pursued investigations of homogeneous, isotropic and non-isotropic turbulence and turbulent structures at high Reynolds numbers in a broad variety of fundamental contexts and of physical conditions (with or without magnetic fields, with or without rotation, with or without modeling). We have been active this year in studying <u>rotating flows</u> from both the perspective of direct numerical simulation (DNS) and that of modeling. Rotational effects are expected to become important when the Rossby number, Ro, (the ratio of the convective to the Coriolis acceleration) is sufficiently small.





Zoom-in visualization of vorticity magnitude in a low Rossby (strong rotation) three-dimensional simulation showing the top view of the computational domain (top figure), and a side view (bottom figure). Both a direct (to smaller scales) and inverse cascade (to larger scales) of energy appear to occur simultaneously with rapid rotation although some intermittency behavior is similar to homogeneous, non-rotating turbulence. Note the large-scale columns comprised of small-scale structures. Similar features are found in high-resolution hurricane simulations, suggesting that studies of hurricane formation and development may benefit from such detailed analysis of rotating turbulence.

We have explored with DNS rotating non-magnetic flows at high Reynolds number, Re, down to Ro=0.03 (note that Ro~0.1 in the atmosphere). It is found that in the non-helical case (i.e. in the absence of correlation between the velocity field and its curl, the vorticity), energy transfer between wavemodes parallel to the rotation is strongly quenched, so that the direct transfer of energy to small scales is mediated by interactions with eddies whose wave vectors are perpendicular to the rotation direction. For rapid rotation, direct and indirect cascades appear to take place simultaneously. For the helical case, it is found that at small Ro, there is a direct cascade of energy (as expected), but that helicity can dominate the cascade to small scales and alter the dynamics.

We are also beginning to consider rotating flows from the point of view of modeling. This work will be extended in the upcoming year; it stems from efforts carried out with our postdoc on a conceptual framework for modeling non-rotating turbulent flows. This work will be generalized to anisotropic non-magnetohydrodynamic (non-MHD) rotating flows, using as a guide a closure model (the Eddy Damped Quasi Normal Markovian, or EDQNM) written for rotating flows by Cambon and Jacquin (JFM 202, 1989), variants and simplifications.

The group continues to explore facets of turbulent flows with magnetic fields also from the modeling perspective. <u>EDQNM</u> spectral modeling has been developed that uses an eddy viscosity independent of the form of the energy spectrum, and that utilizes an eddy noise that follows the closure instead of being an arbitrary stochastic forcing. In addition, we continue to work on regularization procedures of the primitive equations viewed as models of flows and as discussed in the FY2007 <u>CISL annual</u> report. We have found that for MHD that there is no enhanced bottlneck effect, contrary to fluids, and thus that we can reach a reduction factor of ~200 in the number of required degrees of freedom when compared to a DNS of MHD on a large grid of

1536³ points at the same Reynolds number. These results suggest that the use of this type of subgrid scale (SGS) model may offer significant computational savings for MHD simulations, and yield models that can be used for a better understanding of the Earth core dynamics, the interplanetary medium and space weather or the solar convection zone, all topics of interest within the NCAR community.

Finally in the MHD modeling context, we have shown that <u>Clebsch</u> variables can be used as a diagnostic for reconnection events in neutral fluid and MHD flows in two dimensions (2D), and we have initiated a study in which we investigate the scaling laws of linear size and energy distributions of 3D structures in the manner of self-organized criticality (SOC) models of MHD.

One <u>promising avenue</u> of MHD DNS research has been carried out in which the velocity and magnetic field have spatial symmetries that are preserved by the dynamical equations as the system evolves. We have developed a new code (MAYTAG) and have begun to conduct high-resolution runs of a non-dissipative case up to an equivalent resolution of 2048³ grid points,

and found by considering the logarithmic decrement of the energy spectrum that there is no appearance of a singularity. We do find, however, evolving structures that are similar to those observed in the solar wind. We have also considered the dissipative case with grids up to 2048³, and find that global temporal evolution is accelerated compared to the corresponding neutral fluid case.

Lastly, we have used a variable high-order adaptive mesh refinement DNS scheme to model turbulent flows in 2D-MHD, and have demonstrated the statistical accuracy of the technique (see below) by comparing with a pseudo-spectral simulation of a nearly inviscid initially strongly randomized broad-spectrum state that evolves to a very smooth maximum-entropy state through the process of selective decay.

Algorithms, numerics, and code development

TNT develops both tools and models that enhance our capability to investigate geophysical turbulence, and applies these capabilities to fundamental scientific objectives. TNT members have broad experience in developing a variety of algorithms, numerical schemes, and large development efforts for studying turbulence.

The algorithms, numerics, and code development undertaken by TNT all pertain directly to several NCAR strategic goals. Under the strategic goal to "Improve understanding of the atmosphere, the Earth System, and the Sun," TNT works to: (1) Explore atmospheric, Earth System, and solar processes, variability, and change, and (2) Develop community models. Under the strategic goal to "Provide robust, accessible, and innovative information services and tools," we also work heavily toward the NCAR strategic priority of "conducting computer science, computational science, applied mathematics, statistics, and numerical methods R&D."

The Geophysical High Order Suite for Turbulence (<u>GHOST</u>) code is a highly scalable code used to numerically integrate the hydrodynamic, magnetohydrodynamic, or Hall-magnetohydrodynamic equations in three dimensions with periodic boundary

conditions. GHOST was recently selected for an <u>Accelerated Scientific Discovery</u> award, to make a high-resolution (1536³) study of turbulent rotating flows. We have invested efforts this year into providing support for rotating flows by including a Coriolis force and testing the results of rotating turbulent simulations <u>rigorously</u>.

Currently, GHOST uses a slab domain decomposition method in which the N^3 computational cube is decomposed into $N-N^2$ sized slabs and distributed to the processors. This decomposition will prevent us from running jobs on systems with processor counts greater than N. Thus, we will begin in FY2009 to modify this distribution method to allow for a pencil distribution, in which the cube is decomposed into 1D arrays of length N and distributed. In this way we will be prepared to run on the largeprocessor, small-memory-footprint petascale systems that will be available in the near future. In addition, we will begin the modifications necessary in GHOST to allow the code to be operated in single and double precision so that roundoff errors at extremely small scale do not adversely impact the solution in very high Reynolds computations afforted by this new generation of systems.

TNT continues its long-term commitment to develop high-order adaptive methods for use in problems of relevance to the turbulence phenomenology community. This work is carried out using the Geophysical-Astrophysical Spectral-Element Adaptive Refinement (<u>GASpAR</u>) code, which is a framework for solving PDEs using the spectral element method (SEM).

In FY2008, we completed a detailed comparison between GASpAR and a fixed low-order scheme used often in the literature, and demonstrated explicitly that there are some problems where high-order is simply required for any reasonable number of computational degrees of freedom. In collaboration with the Computational Math Group, we completed the first phase of an optimized restricted additive Schwarz preconditioner, and showed that it confirms the asymptotic theory even for the case of staggered grids used in the MHD and Navier-Stokes solvers. In a significant accomplishment in FY2008, the code was modified to include 3D adaptive elements and connectivity, and preliminary tests have been made using the advection-diffusion solver in 3D (please see the accompanying figure). This entailed substantial modification of the existing connectivity code interfaces as well as some re-architecting of the mesh dynamics code. We were able to progress a good deal further than we had anticipated in the FY2007 program plan and include nonconforming -- as well as conforming --



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We have also developed a low-storage Runge-Kutta scheme that preserves conservation properties for nonlinear problems, and is accurate for the pseudospectral and SEM codes to third and fourth order.

We continue to pursue other aspects of SEMs as well. We have formulated an SEM using globally continuous test & trial functions for arbitrary spatial dimensions, and we have also demonstrated a SEM-based Fourier analysis that includes domain partitioning in



Isosurface rendering of a linearly-advected 3D spherical Gaussian distribution with adaptive refinement of the grid. The sphere starts in the corner (0,0), and is advected along the cube diagonal to coordinates (1,1). This is a preliminary result using the 3D mesh dynamics of the GASpAR (see text) code that demonstrates the ability of the mesh to track isolated distributions properly, and it also highlights the operation of the advection-diffusion solver in three dimensions. The capability encapsulated in this figure is essential for correct adaptively refined solutions to all nonlinear partial differential equations for which the code serves as a framework.

the context of a GASpAR study of vortex interactions characterized by strong nonlinear interactions. Finally, in collaboration with Sandia National Laboratory, we discovered that the SEM can be formulated as a <u>conservative</u> scheme that preserves vector-calculus identities after discretization.

There are a large number of SEM numerical issues we will address and GASpAR developments we anticipate in the upcoming year. Here we provide some details as to our current thinking, but add that scientific, technical, and other influences may alter the feasibility of carrying out any particular item or otherwise limit their scope. In FY2009, we intend to add a coarse-grid solver to precondition the long-wavelength modes in the optimized RAS preconditioner. If there is time, we will effect the modifications required to enable the entire optimized precondioner to operate with non-conforming discretizations, for which there is no direct mathematical theory at present. We will continue a program to optimize the adaptive mesh refinement algorithms, and, time permitting, we will add partitioning (including load balancing) software, some of which involves modification of existing code.

We will, in FY2009, test the Navier-Stokes or MHD solvers (or both) on 3D adaptive grids, and address any problems that arise due to the operator application in our Krylov solvers, such as the lack of symmetric-positive-definiteness, which can be a time-consuming effort. We currently plan to also begin development of a 3D (2D is a subset automatically) Boussinesq solver (which will immediately take advantage of the adaptive grid) to begin a long-term project on atmospheric boundary layer flows.

Finally, we will either implement a multi-resolution based adaptivity criterion (which guarantees a prescribed mean-square accuracy), or implement an exactly mass- and energy-conserving spectral element formulation that will enable more robust long-time-scale simulations; the choice will depend on priorities emerging from both technical and scientific considerations.

Community service and outreach

TNT was heavily involved in community service and outreach activities in FY2008. The IMAGe <u>Theme of the Year</u> (TOY) 2008 was designed to support the geophysical and mathematical communities through a series of workshops exploring turbulence from the perspectives of mathematical and physical modeling, computational science, observation and experiment. The overarching goal of the 2008 TOY was to make manifest and increase the interconnections among theory, computation, and experiment.

TOY 2008, co-directed by Keith Julien (CU), consisted of three workshops and a summer school held at NCAR. The titles and dates were:

- W1 "Turbulent Theory and Modeling," 27-29 February 2008
- W2 "Petascale Computing: Its Impact on Geophysical Modeling and Simulation," 5-7 May 2008
- W3 "Observing the Turbulent Atmosphere: Sampling Strategies, Technology, and Applications," 28-30 May 2008
- S4 "Summer School: Geophysical Turbulence," 14 July 1 August 2008

The workshops accommodated 20-30 people and were a blend of research presentations along with ample time for discussion and more informal interactions. The summer school drew on the material from the preceding workshops and featured prominent researchers in turbulence.

In addition to this extensive effort, TNT was largely responsible for organizing a mini-symposium, the Symposium on Turbulence and Dynamos at Petaspeed in October 2007, hosted jointly by IMAGe and by the Joint Institute for Laboratory Astrophysics at the University of Colorado (JILA). The <u>intent</u> of this effort was to elucidate the challenges of scientific computing at the petascale, and to offer potential solution paths for them. The speakers were notable researchers in the field of high-end scientific and engineering computing, and the symposium was very well received. Partial funding for the symposium was provided by the NSF cooperative agreement and by the NASA Heliophysics Theory Program grant to JILA.

TNT research and service activitues are sponsored by the NSF cooperative agreement through UCAR.

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IMAGE THEME FOR 2008: GEOPHYSICAL TURBULENCE PHENOMENA

The Theme-of-the-Year (TOY) is a program that focuses on specific areas of research that will benefit from intense collaborative effort. The topics are selected by the IMAGe external advisory panel and are coordinated by a visiting co-director. The scientific leaders of NCAR recognized early on that to understand the dynamics of the atmosphere and oceans and the planetary boundary layer, the sun and solar-terrestrial interactions, investigating relevant turbulent processes at a fundamental level would be essential.

Turbulence has remained both a vital and challenging field, taking on added importance as the geosciences tackles the multi-scale interactions that characterize the Earth-Sun system. The difficulty of solving classical problems in turbulence through direct mathematical analysis has engendered a multidisciplinary approach where mathematical and physical models, computational science, observations, and experiments are combined to make advances.

The Theme-of-the-Year (TOY) for 2008 was designed to support the geophysical and mathematical communities in this effort through a series of workshops exploring turbulence from these different perspectives with the goal of increasing the interconnections among theory, computation, and experiments. The final activity of the 2008 TOY was a summer school designed to bring new researchers into this field and give them a multidisciplinary perspective.

The 2008 TOY was led by Keith Julien (Applied Mathematics, University of Colorado at Boulder) and Annick Pouquet (Geophysical Turbulence Program,

NCAR). They convened three workshops and a summer school in Boulder, Colorado:

- W1 "Turbulent Theory and Modeling," 27-29 February 2008
- W2 "Petascale Computing: Its Impact on Geophysical Modeling and Simulation," 5-7 May 2008
- W3 "Observing the Turbulent Atmosphere: Sampling Strategies, Technology, and Applications," 28-30 May 2008
- S4 "Summer School: Geophysical Turbulence," 14 July 1 August 2008

The workshops accommodated 30-50 people and were a blend of research presentations along with ample time for discussion and more informal interactions. The summer school included about 30 Ph.D. students from around the globe, drew on the material from the preceding workshops, and featured prominent researchers in turbulence. There were a total of 150 workshop and summer school participants from outside NCAR, including 53 first-time visitors to NCAR and 54 new researchers.

The main lecturers

The organizing committee of W1 included Jeffrey Weiss (CU) and Elizabeth Wingate (LANL).

The invited speakers at W1 were Peter Bartello (McGill), Raffaele Ferrari (MIT), Uriel Frisch (OCA, Nice), Andrew Majada (Courant), James McWilliams (UCLA), David Nolan (Miami), Alan Norton (NCAR), Antonello Provenzale (Turin), Leslie Smith (Wisconsin), and Geoffrey Vallis (GFDL). The organizing committee of W2 included Bjorn Stevens (UCLA) and Joe Werne (CORA).

The principal lecturers at W2 were Mark Berliner (Ohio), Éric Chassignet (Florida State), John Clyne (NCAR), Bengt Fornberg



Rendering of a 3D Kelvin-Helmholtz instability using the VAPOR visualization and analysis platform. This image was created by Benjamin Jamroz, Ed Lee, and Thorwald Stein, while participating in the IMAGe Theme-of-the-Year 2008 Summer School on Geophysical Turbulence. Students of the summer school received hands-on experience performing the end-to-end processes of numerical simulation, visualization, and analysis using state-of-the-art resources.

(CU), Hassan A. Hassan (North Carolina), Phillip Jones (LANL), Yukio Kaneda (Nagoya), Edward Kansa (U. Davis), Yoshifumi Kimura (Nagoya), Steve Krueger (Utah), Ed Lee (NCAR), Rich Loft (NCAR), Thomas Lund (CORA), Scott McRae (North Carolina), Mark Rast (CU), Damian Rouson (Sandia), Piotr Smolarkiewicz (NCAR), Amik St. Cyr (NCAR), Peter Sullivan (NCAR), Chenning Tong (Clemson U.), Joe Werne (CORA), Grady Wright (Boise State U.), John Wyngaard (Penn State), and David Yuen (Minnesota).

The organizing committee of W3 included Larry Cornman (RAL, NCAR), Don Lenschow (ESSL, NCAR), Tom Horst (EOL, NCAR), and Steven Oncley (EOL, NCAR).

The keynote speakers at W3 were Jakob Mann (Risøo), Harm Jonker (Delft U.), Andreas Muschinski (Amherst), Hans Peter Schmid (U. of Karlsruhe), and Joe Fernando (Arizona).

Finally, the organizing committee of the school included Jeff Weiss (CU) and Beth Wingate (LANL). The principal lecturers at the three-week school were John Clyne (NCAR), Joe Fernando (Arizona), Andrew Majda (Courant), Leslie Smith (Wisconsin) and Joseph Werne (CORA).

FY2008 accomplishments

Each workshop set the stage for the next ones and for the school. A lengthier report is in preparation for NSF. The workshops and school were made successful not only by the quality of the presentations from all the speakers, but also through the intense interactions that took place between students and lecturers and between sessions. The organizers would like to thank all of the participants, IMAGe, CISL, EOL, ESSL, and RAL at NCAR, and the National Science Foundation for their continuing support on research into the nature of geophysical turbulence.

We cite week three of the school as an example of the effort and scale of the summer school and the participation it elicited from students. Week three was an intensive computational lab coorganized by CISL's Data Analysis Services Group (DASG) and NorthWest Research Associates (NWRA). Intermixed with lectures on practical issues in numerical modeling and data analysis, students were provided a hands-on experience with end-to-end computational science: from numerical simulation to presentation of results. Divided into small groups, each was tasked with exploring a problem in atmospheric turbulence modeling (either Kelvin-Helmholtz instability or breaking gravity waves) using one of two numerical methods: Direct Numerical Simulation or Large Eddy Simulation. Students relied on knowledge gained during the previous two weeks of the school to help them parameterize a 3D simulation code provided by NWRA. Tens of thousands of CPU hours on CISL's Blue Gene/L supercomputer, frost, were then brought to bear to run the students' experiments.

After conducting their simulations and archiving results to NCAR's Mass Storage System, the groups focused on analyzing the hundreds of gigabytes of data generated, using CISL's visualization cluster, storm. The centerpiece of the students' data analysis toolkit was the NCAR-developed VAPOR software. Finally, the students presented the results of their efforts to their peers and to the summer school organizers and instructors.

FY2009 plans

The Theme of the Year program is chosen each year by the IMAGe Council together with affiliated members. TOY09 will focus on numerics with scientific leadership from the computational mathematics group in IMAGe. Following our plan of alternating large and small TOYs, the numerics year will be a smaller effort than TOY08, consisting of two or three small workshops focused on adaptive methods in computation. The format will use working groups where a small group of researchers are brought to NCAR to outline specific approaches to solving a particular problem. Adaptive numerics resonates with the need for increasing or decreasing resolution of the numerical computation to adapt to the multiscale structure of a complex geophysical flow. There are also plans for longer-term visitors who will reinforce the adpative numerics theme.

Solicitations will also be made for TOY10 through advertisements in mathematics and geophysical newsletters and also through an e-mailing to potential codirectors. Having cycled through the IMAGe sections, the topic for TOY10 is open and will be selected through outside proposals and discussion with the IMAGe advisory board.

Rationale and sponsorship

By enhancing collaborations with the university community and by performing valuable education and outreach activities at the highest available level, this work supports the NCAR strategic priorities "Engaging a broader and more diverse community in the atmospheric and geosciences" and "Supporting and enhancing formal science education at all levels." TOY workshops and schools are sponsored by the NSF cooperative agreement through UCAR and by NSF funding through the division of mathematical sciences.

CISL Annual Report

NUMERICAL METHODS: APPLICATION OF RADIAL BASIS FUNCTIONS TO MODELING

While computer technology has advanced dramatically in recent years, numerical schemes currently used for climate and solar modeling fall drastically short of scientists' expectations. Spherical harmonics require large grids to resolve small features, and this is computationally impractical. Spectral element methods can resolve small features, but they require higher resolution near artificial boundaries to achieve high accuracy.

Both methods involve high algorithmic complexity and are impossible or awkward to apply to irregular geometries. As a result, geoscientists and computational mathematicians are searching for new options. Radial basis functions (RBFs) offer the geosciences a novel numerical approach for solving time-dependent partial differential equations (PDEs).

Building on the accomplishments of FY2007, the IMAGe Computational Mathematics Group together with Boise State University, University of Colorado-Boulder, Arizona State University, and Uppsala University, Sweden continue research in the developing area of RBFs for climate and solar modeling.

This year saw the completed development of the first-ever RBF shallow-water model on the sphere. The table at right summarizes the results for one of the test cases: a forced translating low-pressure center that is superimposed on a westerly jet stream (see 8 MB movie). The system is modeled by the unsteady nonlinear shallow water equations. RBFs are compared with spherical harmonics (SH), double Fourier series (DF), spectral elements on a cube (SE), and spectral elements with mesh refinement (SE/MR).

The table shows that RBFs easily outperform the other methods as measured by the L2 error both with regard to the number of node points N they use and the large time step they can take.

In 2008, our efforts furthered the topic of applying RBFs to the geosciences by performing the first-ever local node refinement on the sphere. The scheme was tested by following the wrap-up of two vortices on the sphere as they are advected at a 45° angle to the polar axis (see 14 MB movie). The nodes were distributed according to the gradient of the angular velocity, being most concentrated where the gradient was the largest as shown in the figure below.



Left: Final state of vortex wrap-up test case after 12 days (1 revolution around sphere) on an unrolled sphere. Vertical axis is latitude with 0 being the equator. Right: Local node refinement corresponding to vortex wrap-up test case.

Method	N	L2 error	Time step
RBF	1849	3e-3	24 minutes
	3136	8e-6	15 minutes
	4096	3e-7	8 minutes
	5041	4e-8	6 minutes
SH	8192	2e-3	3 minutes
DF	2048	4e-1	6 minutes
	8192	8e-4	3 minutes
	32768	4e-4	90 seconds
SE	6144	6e-3	90 seconds
	24576	4e-5	45 seconds
SE/MR	31104	7e-4	1 minute

In the coming year, we will focus on various areas of RBF mathematical development, from adaptive local node refinement to non-uniform fast Fourier transforms and filtering methods, to hybrid RBFpseudospectral and RBF-finite difference schemes.

This work advances NCAR's strategic priority of "Conducting computer science, computational science, applied mathematics, statistics, and numerical methods R&D" and is supported by NSF grant ATM-0620100.

CISL Annual Report

MULTISCALE SIMULATION TECHNIQUES

To continue its scientific leadership, NCAR needs a unified simulation environment that can dynamically resolve time and space scales on petascale computers. A framework that encompasses such an environment relieves the scientists from becoming fluent in advanced scalable numerical methods and enables them to focus on their research issues. We are progressing toward a unified simulation environment by pursuing novel developments in the areas of adaptive h-p grids, multi-method time-stepping, and Jacobian-free techniques.

Current work toward this goal in IMAGe's Computational Mathematics Group includes the development of a linearly implicit Runge-Kutta time-stepping procedure to accelerate integrations of PDEs common in atmospheric and oceanic models. We are also coupling an h-p discontinuous Galerkin solver to a state-of-the-art library for mesh adaptation. The latter has shown excellent scalability on the IBM Blue Gene/L system, and is currently being coupled with a prototypical time-implicit nonhydrostatic fluid flow solver. Preliminary results with the coupled solver promise unprecedented scalability. Future work includes completion of a 2D AMR compressible solver, inclusion of the multigrid algorithm, and the capacity to perform 3D simulations on general curvilinear domains.

This research intends to develop efficient computational methods for solving multiscale, multidisciplinary physics on petascale systems by using numerical methods that satisfy the following criteria:

- 1. Highly scalable: strong scaling enabling
- 2. A well-defined mathematical background
- 3. Multiphysics capable: generic enough to solve more than a single problem
- 4. Multiscale capable: locally change the resolution for time and space scales

Developing these techniques spawned various subprojects.

Spatial scales project

To develop the capacity for increasing the spatial resolution during a simulation, a flexible method is required for the spatial discretization of equation (1). The approach must efficiently exploit cache-based memory architectures and be highly parallelizable. It is widely accepted that high-order methods are very effective for solving wavepropagation-type problems. When spectral convergence occurs, either in a compute cell or in a part of the simulation domain, no method can provide more resolution for the same given number of grid points. The discontinuous Galerkin method (DGM) is somewhere between a finite element (FE) and a finite volume (FV) method. The technique lay dormant for several years, but it has recently become popular for solving fluid dynamics or electromagnetic problems.

DG was then quickly used to solve a variety of physical problems with great success and is thus our method of choice for an all-scales multiphysics solver. We are currently investigating a high-order, high-performance



This animation depicts the simple convection of a cone using a prescribed flow that deforms the initial cylinder in two spirals. This test can be employed to measure the built-in dissipation of our proposed approach. Compared to non-conforming spectral elements, the DG approach is much simpler and necessitates a single exchange between elements instead of two. (Click image for animation.)

DG method on unstructured meshes combined with non-conforming mesh adaptation. Also, when it is possible to resolve a wider range of scales with new techniques, different equation sets representing more realistic physics need to be employed. Future work will couple the high-performance adaptive techniques to the compressible Euler equations.





The high-order h-p DG solver adaptation is driven by a state-of-the-art mesh database with excellent scalability properties. Left: Number of elements refined/de-refined per second as a function of processor count. Right: Spherical shell used for 3D test in the mesh database.



Advection of a simple cosine bell in an unstructured adaptive mesh using the h-p DG prototype with isoparametric elements.

Temporal scales project

Time-stepping techniques create one of the bottlenecks in numerical simulation today. These techniques inhibit the ability of current climate, weather, and other models to achieve strong parallel scaling. We are investigating various approaches to improve time-stepping methods:

- 1. Linearly implicit methods: Rosenbrock w-methods
- 2. Multirate techniques and spectral deferred corrections
- 3. The Parareal algorithm

The linearly implicit technique seems promising because it has a lower computational cost compared to traditional non-linear solvers. When applied to the fully compressible Euler equations, accelerations are observed with respect to fully explicit techniques.





Scalable elliptic solvers project

The quest for a correct coarse-grid correction for optimized Schwarz techniques started in FY2008. The coarse correction is required to obtain an iterative elliptic solver that yields a number of iterations independent of the number of spectral elements employed or their local polynomial orders. Initial experiments with the GASpAR code exhibited some problems concerning the treatment of corners with the optimized Schwarz algorithm. However, when high-order is employed and the corners are kept in the formulation of the optimized Schwarz, a factor of two reduction of the time to solution is observed.

Recent results for two-dimensional grids with the optimized Schwarz algorithm applied to spectral elements coupled to a coarse solver show that the number of iterations is fixed independently of the resolution of the mesh. The theoretical basis for modifying the penalty terms present in the optimized Schwarz algorithm is not yet fully understood, but a <u>first approach</u> is being explored.



Left: Plot of iteration count vs. polynomial degree for different preconditioners with and without corner communication on an 8x8-element grid. Right: Comparison of CPU time vs. polynomial degree preconditioners with corner communication on a 16x16-element grid (note that the optimized version is twice as fast for high Nv).

Support

This work supports NCAR's strategic priorities of "Conducting research in computer science, applied mathematics, statistics, and numerical methods," "Developing community models," and "Improving prediction of weather, climate, and other atmospheric phenomena." It will yield more efficient and accurate models, help reinforce NCAR's image as a leader in cutting-edge numerical methods, and may set the standard for next-generation climate and weather models. These projects are made possible through NSF Core funding.

NCAR

CISL Annual Report

HOMME-CAM INTEGRATION USING HOMME'S SPECTRAL-ELEMENT DYNAMICAL CORE

Petascale computing facilities are being planned for the near future, and models must be developed to exploit these new architectures. NCAR, IBM, and DOE researchers are addressing this need by integrating the spectral element dynamical core in HOMME (High-Order Method Modeling Environment) with the physics of the Community Atmosphere Model (CAM 3.5.29). HOMME's spectral element dynamical core is well developed and ensures high parallel efficiency when running on computers with very large numbers of processors. CAM is a sophisticated model that realistically simulates the physics of Earth's atmosphere. The goal of the HOMME-CAM integration project is to prepare a highly accurate and efficient model that will provide capabilities such as full carbon cycle representation in climate simulations when petascale computing systems become available.

The spectral element dynamical core in HOMME is continually being revised and further parallelized to run more efficiently on the architectures of the most capable supercomputers available. Software engineers in the Climate and Global Dynamics division of NCAR's Earth and Sun Systems Laboratory modified the structure of CAM to simplify the integration of new dynamical cores. These efforts were facilitated by collaborations with an IBM software engineering consultant. This work made it possible to address the biggest challenge of the project: integrating HOMME with all the physical processes in CAM.

In collaboration with Sandia Laboratories (DOE), CISL, CGD, and IBM researchers produced significant results from the HOMME-CAM prototype using the IBM Blue Gene/L system at Lawrence Livermore National Laboratories. The transition in the kinetic energy spectrum that appears at the mesoscale boundary (see -3 and -5/3 trend lines on figure) has been approximated by the NEC Earth System Simulator in Japan, but the fidelity of the HOMME-CAM simulation is unprecedented.

In FY2008, nearly complete integration of HOMME's spectral-element dynamical core with CAM physics was achieved. An aquaplanet integration at 1/8-degree resolution produced the most realistic simulation to date of a little-understood feature in the kinetic energy spectrum of the Earth's atmosphere.

For FY2009, work will focus on refining surface processes to account for the effects of topography, ice, and oceans. FY2009 work will also improve the mapping of the CAM lat-lon grid to the HOMME cubed-sphere grid. The revised model will then serve as a testbed for new numerical algorithms to increase the simulation rate and produce results more quickly. After FY2009, the production version of CAM may begin using the HOMME dynamical core.

HOMME was developed by CISL to provide a foundation for building a new generation of atmospheric general circulation models for the atmospheric science community. HOMME is a vehicle to investigate using high-order-element-based methods to build conservative and accurate dynamical cores that efficiently scale to hundreds-of-



This plot depicts the kinetic energy spectra near the tropopause. From measurements and experiments conducted by Nastrom and Gage (1985), it is known that this spectrum exhibits a transition from a -3 slope to a shallower -5/3 slope near the 100-km scale. Many competing theories are trying to explain this transition. The -3 slope is well understood and is related to geostrophic turbulence theory (Charney 1971) while the -5/3 slope corresponding to mesoscale (weather scale) is difficult to explain. To understand and validate theories, models need to reproduce this transition.

The plot was obtained using HOMME's spectral element dynamical core coupled with CAM's physics at a global resolution of 12.5 km running an aqua-planet experiment (planet surface is water). The HOMME-CAM model was run using 57,600 processors of the Blue Gene/L system at Lawrence Livermore National Laboratories. This is the first time this transition has been reproduced with such fidelity by an atmospheric general circulation model. It also vindicates HOMME's numerical methods.

thousands of processors, achieve scientifically useful integration rates, and can easily couple to community physics packages. Currently, HOMME employs the <u>Discontinuous Galerkin</u> and spectral element methods on a cubed-sphere tiled with quadrilateral elements.

This effort to accurately simulate observed processes in Earth's atmosphere supports NCAR's mission "to understand the behavior of the atmospheric and related systems and the global environment," NCAR's strategic goal of "Developing community models for weather, climate, atmospheric chemistry, and solar-terrestrial research," and NCAR's strategic priorities of "Developing and providing advanced services and tools" and "Creating an Earth system knowledge environment." This work is supported by NSF Core funds and DOE's Scientific Discovery through Advanced Computing (SciDAC) program.

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HOMME: DISCONTINUOUS GALERKIN METHOD

The future evolution of the Community Climate System Model (CCSM) into an Earth System model will require a highly scalable and accurate flux-form formulation of atmospheric dynamics. Flux form is required to conserve long-lived trace species in the stratosphere. Accurate numerical schemes are essential to ensure high-fidelity simulations capable of capturing the convective dynamics in the atmosphere and their contribution to the global hydrological cycle. Scalable performance is necessary to exploit the massively parallel petascale systems that will dominate high-performance computing (HPC) for the foreseeable future. This activity directly supports NCAR's strategic goal of "Developing community models for weather, climate, atmospheric chemistry, and solar-terrestrial research."

The High-Order Method Modeling Environment (HOMME) is a vehicle to investigate using high-order-element-based methods to build conservative and accurate dynamical cores. Currently, HOMME employs the Discontinuous Galerkin (DG) and <u>spectral</u> <u>element</u> methods on a cubed-sphere tiled with quadrilateral elements. HOMME can be configured to solve the shallow water or the dry/moist primitive equations, and has been shown to efficiently scale to nearly 100,000 processors of an IBM BlueGene/L.

The objective of this project is to extend HOMME to a framework capable of providing the atmospheric science community with a new generation of atmospheric general circulation models (AGCMs) for CCSM based on high-order numerical methods on the cubed-sphere that efficiently scale to hundreds of thousands of processors, achieve scientifically useful integration rates, provide monotonic and mass-conserving transport of multiple species, and easily couple to community physics packages such as Community Atmosphere Model (CAM) physics. Achieving these objectives will allow climate scientists to take full advantage of the extraordinary petascale computing capabilities being deployed by NSF in the next five years, and will lead to dramatic increases in climate science productivity. The development timeline is designed to make the proposed technology freely available to the community for the Intergovernmental Panel on Climate Change (IPCC) fifth assessment science runs, currently scheduled to begin in April 2010. To achieve this requires work in four areas: physics, validation and verification, time integration, and scalability.

A fully fledged climate model is required to transport moisture variables and dozens of chemical tracers. The transport (advection) schemes must have several essential properties such as accuracy, efficiency, mass conservation, and non-oscillatory (monotonic) properties. A monotonic transport scheme avoids the creation of spurious unrealistic oscillations (e.g., negative humidity or pressure, etc.) in the transported solution. For the HOMME transport scheme, all these features except the monotonic property are available by the model design. Since HOMME is based on high-order spectral elements, implementing monotonic limiters is a big challenge.



This figure shows the solid-body rotation test of a non-smooth scalar (tracer) field after one revolution. A third-order discontinuous Galerkin (DG) transport scheme combined with a monotonic limiter was used for testing. The left panel shows the initial field, the central panel shows the monotonic (non-oscillatory) solution, and the right panel shows the oscillatory solution (without limiter). The monotonic limiter conserves mass and preserves the positivity of the advecting scalar field, and it completely eliminates spurious oscillations.

To address this issue, a new monotonic transport scheme based on a third-order DG method was developed in FY2008. This scheme can also preserve the positivity of the solution while being mass conservative. The first figure shows the solid-body rotation test results with the new scheme that eliminates spurious overshoots and undershoots from the numerical solution. The monotonic DG transport in a more realistic (divergent flow) simulation is shown in the second figure.

Initial Tracer Fields (Concentration)







This figure shows an example of monotonic tracer transport in a non-linear divergent flow as in the case of real atmosphere. The left panel shows the initial tracer field which is an idealized "Gaussian plume" with concentration ranging from 0 to 100%, and the right panel shows the simulated tracer field transported to the east direction after 5 days. A 2D version of the HOMME-DG model (shallow water model) with horizontal resolution of approximately 1 degree is used for this simulation.

For FY2009, more comprehensive tests are being developed, such as aqua-planet simulation with the new transport scheme in the HOMME-DG version. This scheme will be tested further in HOMME/CAM simulations during FY2009.

This research and development effort supports NCAR's strategic priorities of "Developing and providing advanced services and tools" and "Creating an Earth system knowledge environment." In addition to NSF Core funding support, two Department of Energy programs sponsor this research: the Climate Change Prediction Program (CCPP) and the Scientific Discovery through Advanced Computing (SciDAC) program.