### White Paper from Forward Looking Workshop on Mathematical Geosciences

## **November 13, 2011**

Editors: Frank Giraldo, Michel Kern, Malgorzata Peszynska, Ivan Yotov

Key Contributors: Todd Arbogast, Alistair Adcroft, Clint Dawson, Lou Durlofsky, Ken Golden, Olivier Pauluis, Jeroen Tromp, Martin Truffer, Amik St-Cyr, Junping Wang

**Contributors: Participants of the Workshop at large (see Appendix 2)** 

#### **OVERVIEW**

The consensus of the workshop participants is that a program similar to CMG (Collaborations in Mathematical Geosciences) needs to be supported. CMG-like programs facilitate collaborations between mathematicians and geoscientists to successfully tackle societally relevant scientific challenges; a number of such scientific challenges are enumerated in Sections 2 (Research Challenges and Outstanding Problems) and 3 (Methodological Challenges). In fact, at the very least a program similar to CMG should continue and in the best case scenario a CMG-like program should expand to incorporate other directorates/disciplines because many of the problems outlined in the sections below require expertise not only from mathematicians and geoscientists but also from computer scientists, engineers and biological scientists. Computer scientists and/or computational scientists have much to contribute to new science problems considering the rapid changes occurring in computer architectures and the new algorithmic and computing paradigms that need to be developed in order to fully exploit these new architectures.

The participants further observed that the existence of CMG-like programs creates a mathematics-geosciences community that would not exist otherwise. The existence of such a "community" is critical for fostering the training of interdisciplinary faculty capable of tackling the sorts of problems outlined in this document. The existence of such a community (defined through research funding, conferences, workshops, and summer schools) creates an environment that allows interdisciplinary faculty to succeed within their home institutions (e.g., via promotion and tenure). The importance of CMG-like training for graduate students and postdoctoral fellows cannot be over-stated. The opportunity afforded by CMG programs to train these young researchers produces the next generation of interdisciplinary faculty who are then in a position to repeat the cycle and thereby extend the "academic memory" of these interdisciplinary fields.

Section 1 describes the organizational information of the workshop, including how the participants were selected and how the workshop was organized in terms of lectures, working groups, and discussions. Section 2 contains the research challenges and outstanding problems that the participants identified as the most important problems that need to be tackled in the near-term future. Section 3 focuses on the methodological challenges that the mathematics-geosciences community will need to tackle in order to advance the substantive agenda described in Section 2. Finally, Section 4 contains some key recommendations highlighted by the participants.

#### 1. ORGANIZATION OF THE WORKSHOP

The Forward Looking Workshop convened in Crystal City, Washington, D.C. on Sept. 16-17, 2011, and was devoted to presentations and discussions of research and methodological challenges arising at the frontier of geosciences and mathematical and computational research. Participants discussed models and opportunities for successful collaborations that could be supported by interdisciplinary National Science

Foundation (NSF) programs such as the past program on Collaboration in Mathematical Geosciences (CMG). The organizing committee (see Appendix 1) and the participants (see Appendix 2) interacted with NSF officers present at the workshop and discussed current initiatives concerning the mathematical geosciences as well as the many scientific, organizational, and educational challenges facing mathematical geosciences.

The participants of the workshop were selected in the following manner: one group was invited by the organizing committee (to be both speakers and discussion leaders). A second group represented researchers involved to date in CMG-funded projects. Finally, a third group came from an open call issued to the Society for Industrial and Applied Mathematics (SIAM) Activity Group on Geosciences. The workshop was run by the SIAM Conference services which facilitated obtaining funding for the workshop from NSF based on a proposal formulated by the workshop committee. The program of the workshop (see Appendix 3 for the schedule) included break-out sessions in six areas. On the first day, the participants were divided into the following application areas: Earth modeling (subsurface and geophysics), Ocean and Ice modeling, and Atmosphere/Climate modeling. On the second day, the sessions were organized based on the following research tools: Mathematical modeling and analysis, Statistics and uncertainty quantification, and Computing tools.

The participants recalled many success stories of research that resulted from CMG funded projects and discussed current research and methodological challenges. These were identified by the individual panels and are described in Sections 2 and 3. The participants proposed a path forward to meet these challenges and formulated specific recommendations on how to get there; these recommendations are summarized in Section 4. This document provides the summary of the findings; it was prepared by the committee and several panel leaders with input provided by the participants at large.

### 2. RESEARCH CHALLENGES AND OUTSTANDING PROBLEMS.

**2.1 Climate.** The multiscale challenge in climate modeling is that the dynamics (governing equations) and the sub-grid scale parameterization (e.g., solar radiation, clouds, entrainment, etc.) must be developed in tandem in order to develop more sophisticated next-generation models. Consistency between treatment of time-dependence and derivation of the models is needed, and mathematicians working closely with geoscientists can construct consistent sub-grid scale parameterizations (currently such processes are computed based on empirical laws and the numerical methods used in one process may not be consistent with the numerics used in other processes). Furthermore, as computing power increases, computer models are able to use far more degrees of freedom, which adds to the complexity of data that must be analyzed. An emerging challenge in climate modeling involves the modification of existing algorithms for use on new computer architectures. Slight changes in the order of mathematical operations can affect the accuracy of the results to the smallest decimal place which in turn can trigger the microphysics in adverse ways. Clearly, maintaining reproducibility of previous results is important in all fields but especially in climate change studies. Climate scientists are not expected to become experts in both the hardware and software of emerging computer technologies. Here is where computational mathematicians can make a significant contribution to climate change modeling by developing algorithms that are reproducible across different computer platforms.

One of the main challenges in climate modeling is the proper representation of clouds; an accurate representation is absolutely critical for the accurate prediction of climate change. Work on understanding clouds is already ongoing in the meteorology community and pursued by some mathematicians but a concerted effort is necessary to make greater strides.

Another significant challenge in climate modeling is that there are a number of sub-grid scale processes that play a major role in the fate of the polar ice packs, yet they are not realistically incorporated into large scale models. Examples of such processes include melt pond evolution, which controls sea ice

albedo or reflectance, snow-ice formation, the evolution of salinity profiles, air-ocean gas exchanges through the ice, etc. The mathematical and computational challenges presented in studying these processes themselves are significant and the multiscale issues are quite similar to other climate-related geosciences problems.

Yet another challenge in climate modeling concerns the deterministic versus stochastic treatment of these models. Global Circulation Models (GCMs) are deterministic in the sense that they are governed by differential equations. This has meant that uncertainty quantification of GCM output has not had a stochastic element to it. Only recently has there been an effort to incorporate stochastic elements into the evolution of GCMs and it continues to be a big challenge to incorporate these in global climate models.

**2.2 Atmosphere, Ocean and Ice**. Adaptive mesh refinement (AMR) is gaining both interest and importance across various fields of the geosciences. However, the challenge is to ensure that this technology is sufficiently mature to be used in current (and future) operational-type atmosphere, ocean and ice models, since new tools introduced must not slow down the computer codes significantly while offering new capabilities. Computational mathematicians need to evaluate the cost-benefits of the AMR technologies for atmosphere-ocean-ice models. Simultaneously, new computer architectures present opportunities but also challenges since the scientists must continue to rewrite computer applications (whose lifespan may be tens of years) in order to take full advantage of the new computer resources (whose rate of change is much faster). A related challenge comes from the large volumes of output data produced by computational simulations on ever larger computers; these vast amounts of data represent a significant challenge to domain scientists in that meaningful information needs to be extracted from this sea of model output.

Atmosphere-ocean models use grids that are far too coarse to properly capture some important processes such as air-sea interactions, hurricane deintensification, precipitation and condensation. Further complications are introduced by other species of water, e.g., snow and ice, and the complex boundaries below ice shelves and ice sheets. Rigorous mathematical analysis of the boundary conditions, e.g., coupling shallow ice, shallow shelf, and the full Stokes equations, could lead to a significant improvement of the coupled models or to the formulation of one closed system. The disparate time-scales found in the atmosphere, ocean, and ice sheets, pose a significant challenge to domain scientists interested in developing better tools for predicting climate change, and they need the assistance of mathematicians in tackling it through the development of cutting-edge algorithms (e.g., AMR with multi-rate time-stepping).

Some of the biggest challenges in atmosphere-ocean-ice modeling come from the data assimilation used routinely to improve the underlying physical models with inverse and forward models, and to quantify uncertainty. In particular, the data, e.g., satellite data, relevant for coastal and ocean simulations, has enormous volume for which new paradigms of analysis are needed including those of quantifying data error. In addition, in order to detect long-term feedback loops, such as between atmosphere/ocean and ice shelf-ocean models, one has to recognize, detect, and handle efficiently the multiple time scales present. New models are needed to account for friction and roughness at interfaces, boundary layer phenomena and sea-ice-wave interactions. Rainfall processes are currently poorly represented in weather models and their understanding and inclusion in other coupled models is a fundamental issue. It is also recognized that ocean models should include elements of Ocean Biology and Ecology which calls for expanding the scope of collaborative work beyond the current Mathematics and Geosciences communities.

Verification and validation of high-resolution ocean/atmosphere models are difficult due to the fact that these models have a million degrees of freedom and multiple scales, reproduce complex dynamical regimes and transitions between them, and require huge computer resources. Validation of the models is also difficult due to the sparseness of observations.

Ensemble techniques are the basic tool for verification, validation and predictability analysis of atmosphere/ocean models. The fundamental issue of ensemble modeling is how to reconstruct an appropriate distribution function for model output for small size ensembles because a model run is very expensive and therefore, the number of model runs is limited. Gaussian ensembles seem to be a good approximation in some situations but do not allow for predicting extreme events.

Since mathematical analysis of outputs from high-resolution models is required to find the best process to incorporate new modeling elements and to quantify the numerical error, other important questions arise: how to develop inter-model comparisons and how to compare different runs for the same model.

**2.3 Earth**. The challenges in subsurface modeling arise in multiphysics couplings, multiscale and quasicontinuum modeling, and dealing with ill-posedness and uncertainty in the models. Geosystems span a vast array of scales, for example some 10 to 20 orders of magnitude from molecular scales of reactive processes to those of regional watersheds. Extreme scale variation is seen in space and time, and arises both from medium properties (e.g., porous medium heterogeneity) and from dynamic developments within the fluid itself (e.g., mantle viscosity, temperature variation). While multiscale modeling and homogenization have seen some success, primarily for linear problems, much work is needed to develop general nonlinear multiscale theories. In fact, there is very limited theory on upscaling and downscaling even for linear systems across a wide range of scales. Much of the current work on constitutive laws on the coarse scale is ad hoc and fails to capture the effects of fine scale processes.

Many problems exhibit behaviors associated to a moderate number of discrete entities that are neither small enough to model individually nor large enough to approximate as a homogenized macro-system. We may understand in principle how to model these systems discretely, but we do not have the computational resources to solve these problems. Progress on modeling such problems tends to be slow and very problem dependent. Geoscience examples are typical, and include models of discrete fractures and faults, ocean ice sheets, volcano structure, and even such related systems as partially molten (i.e., magma) or melted (i.e., glacier) materials. Collaboration is critical to design realistic models that respect the physical demands of the modeling effort while overcoming computational limitations.

As in atmosphere-ocean-ice modeling, the availability of an unprecedented quantity of newly collected data will present both an opportunity and a challenge. Space-borne and earth-borne data will enable researchers to address a multitude of problems that were unthinkable in the past (one example: a combination of geodetic measurements and high-quality relocated catalogs enables the study of post-seismic deformations and how it relates to the geometric, physical and ambient properties of fault networks). These problems are tightly related to the hazard assessment and forecast studies and may lead to developing a new paradigm in earthquake forecasting. At the same time, to address such problems, one has to develop novel mathematical, computational, and statistical approaches related to the newly available data. A close collaboration between mathematicians, statisticians, and geoscientists is crucial in this research.

Almost by definition, the proper handling of ill-posed problems is application dependent and therefore requires close collaboration between mathematicians, statisticians, and, in our case, geoscientists. Topics that can only be addressed through such close collaborations are techniques to estimate: (1) spatially dependent, highly heterogeneous parameter fields such as permeability and porosity from data collected on various scales from well-bore core analysis to global seismic surveys; (2) real-time incorporation of large data sets into simulations; and (3) complex data assimilation of transient and sparse data as it pertains to, e.g., earthquake modeling. Current techniques are often based on assumptions of statistical stationarity and Gaussian distribution, and often take into account only two-point statistical measures. This is insufficient for realistic subsurface data.

#### 3. METHODOLOGICAL CHALLENGES

The mathematical geoscience community faces a number of methodological challenges that cut across multiple geoscience domains. For the sake of brevity, we mention only a few select challenges that arose in the three panels during the second day of the meeting.

**3.1 Mathematics.** One of the most powerful tools in the mathematics arsenal is the reduction of large complex nonlinear models to simpler models that remain relevant yet are amenable to rigorous analytical techniques. These classes of conceptual models allow for much insight to be extracted from the more complex physical systems that the domain scientists are interested in solving. Therefore it becomes necessary to develop a hierarchy of models from the conceptual (i.e., simpler) models to the more complex physical models that include, e.g., the comprehensive description of the multi-physics processes. The conceptual models are the subject of pure mathematical research while the physical models are the focus of the geoscientists. The challenge that remains is to bridge this gap and cross-coordinate efforts in these two areas in order to ensure that the rigorously derived results of the conceptual problems can be used to shed insight into the more complex physical problems.

Modeling methodology is well developed in certain relatively simple situations; progress is needed on developing a general theory that is applicable to a much wider range of problems. Mathematical analysis can clarify whether the equations reflect the desired physical properties, where they fall short, and what intrinsic mathematical difficulties are present. Many of the simpler equations modeling geoscience applications have been analyzed, but most, especially those that form systems of equations, have not yet been fully analyzed. These systems usually model a range of multiphase, multicomponent wave, reaction, advection, and degenerate diffusion processes, which often alternate as to which process is dominant. The equations generally exhibit degenerate behavior (as, e.g., when a phase is lost), long and short wave phenomena (in, e.g., near-shore shallow water environments, open ocean, the atmosphere, and even the mantle), and singular behavior (such as near wells, fractures, and in phase transitions and geochemistry).

Advances in numerical methods for solving Partial Differential Equations (PDEs) continue to be needed in several geosciences applications and these include but are not limited to: parallel/adaptive/localized in space and time solution methods; physics-based preconditioners; fast direct solvers; development of new concepts on the accuracy of approximations for solutions which capture physical quantities of interest; a posteriori error estimation for complex nonlinear systems; discretizations for discontinuous solutions in complex geometries; new methods and solvers for highly heterogeneous and highly multiscale problems and multiphysics couplings; and development of new algorithms for exascale computers and hybrid architectures. Further development of fractional calculus and nonlocal models is necessary in transport models with multiple scales (time heterogeneity) such as in chemical reactions in Atmosphere and/or Subsurface. Numerical methods and analysis are needed for non-standard PDEs with higher order spatial and temporal derivatives, e.g., Boussinesq and Green-Naghdi models of wave run-up (in coastal ocean applications) require high-order spatial derivatives that need to be treated properly by the numerical models; more rigorous analysis needs to be conducted to ascertain whether these models are better equipped to reproduce the correct physical phenomena. Implementation of transport models on new parallel machines does not allow greater time resolution, since time-stepping, in which information flows sequentially forward, is essentially a serial process. There has been some progress in developing Discontinuous Galerkin (DG) methods and Eulerian-Lagrangian methods; the former (DG) is a powerful method for solving PDEs and the latter is a space-time method that allows for relatively long time steps although more work is needed in order to bring both methods to full maturity for large-scale applications.

Mathematics of inversion is crucial for handling inverse problems arising in all the geosciences. The main contributions of the mathematics of inversion are the following: it provides the right setting, function spaces, and operator kernels for inverse problems; facilitates the studies of lower regularity of coefficients and its effect on regularity of solutions; and allows the study of time reversal in inverse problems. All of

these topics are extremely problem dependent which stresses the need for strong collaborations if we are to make progress in this entire class of problems.

Analysis of systems changing regime or transitioning between states, and of dynamical systems with bifurcations, is crucial for understanding *tipping points*, e.g., in climate and weather models. Coupling of continuum and discrete models and in particular mathematics of networks and hierarchical systems, and development of hierarchies of models and reduction of complexity to capture dominant effects represent the frontiers of mathematical research with significant impact on forward and inverse modeling in subsurface and other areas of the geosciences.

Mathematical foundations and techniques for data analysis need to be further developed. These include: topological data analysis, extracting information from data; data quality, uncertainty, and visualization of data. Inverse-based methods for interpreting high resolution/high bandwidth data are needed. New technologies such as remote sensing, multiscale and multisensor imaging, as well as the availability of observations from satellite imagery and sensors require continued advances in the mathematics of natural images and data analysis. Other concepts such as data fusion and data downscaling need rigorous mathematical treatment.

**3.2 Statistics and Uncertainty Quantification**. Our ability to quantify uncertainties in large, complex, and coupled natural systems is very limited. For example, predictions of earthquakes and tsunamis often underestimate the probability of extreme rare events, while quantification of the uncertainties inherent in climate change predictions is a central issue for risk assessment, and decision-making. The recent controversy in the use of tree ring data as a climate proxy illustrates the need for estimating measurement errors, particularly when observations involve multiple instrument platforms, long time-scales, or complex inverse modeling. The statistical methods currently in use in the geosciences are rarely adequate for this task, given the underlying complexity.

Developments in stochastic processes are needed and in particular further studies of stochastic PDEs for capturing uncertainty, stochastic transport, stochastic time processes, understanding nonlinearities as a function of scale, and predictability as a function of perturbations and scale. Stochastic models in the geosciences have the potential to address some of the known deficiency in physical parameterization in geophysical models (e.g., stochastic representation of convection in atmospheric models that allows backscattering of energy from the convective scale to larger scales and the stochastic description of the permeability field in subsurface flow).

Data assimilation and parameter estimation through Bayesian and non-Bayesian statistics offer a powerful tool to improve physical parameterization in geophysical models. Specific challenges in this area include systems with large numbers of degrees of freedom, non-linear behavior (which are inadequately captured by traditional Kalman Filters), and integrating physical constraints. Statistical methods are needed for model evaluation, selection/rejection and successive improvement. Model selection is frequently a difficult problem in itself, distinct from that of the parameter estimation problem. This is the case, in particular, for the question of finding a parsimonious model in some sparse representation that adequately describes the data generating mechanism.

New statistical methods need to be developed to address specific limitations of geophysical data and models, particularly to address issues such as over-fitting of a statistical model over too short a period of time, small size of forecast ensembles, handling of missing data, or assessing non-stationary data. Statistical methods to compare large datasets and to evaluate the spatio-temporal fluctuations are critical to assess complex numerical models and to combine them with observational data.

One approach to facilitate the knowledge transfer between statistics and geosciences would be to develop "statistical toolboxes" tailored for specific problems. These toolboxes would be used as the basis for diagnostics and intermodel comparisons, (e.g. systematic diagnostic of internal variability in climate models). Such toolboxes require (1) the assessment of the proper statistical method, (2) software implementation, and (3) training of geoscientists in the methodology (for example through joint postdoctoral appointments with climate research centers).

**3.3** Computing. Computing architectures continue to evolve, providing opportunities and posing challenges to geoscientists and mathematicians tasked to develop numerical algorithms. The issues of scalability of algorithms, and of reproducibility of results on new hardware such as General Purpose Graphical Processing Units (GPGPU or GPU for short) and GPU-CPU hybrid parallelization strategies need to be addressed before these new architectures can be used in production codes. Furthermore, efficient software for modern multi-core architectures must minimize data movement and communication. It is not practical to expect that existing algorithms will be rewritten for the new architectures by the geoscientists; rather, there is a need for a paradigm shift in the way algorithms are constructed, which may include custom compilers, tools and/or development of new standards. This issue affects other fields beyond the geosciences. In fact, all scientific disciplines rely on high performance computing and therefore encounter similar difficulties. Mathematicians and computer scientists, working with application scientists, are in a position to make pivotal contributions to this problem.

Critical challenges in computational algorithms include: data mining, pattern recognition, and visualization for extracting information from enormous volumes of data and from simulations while they are executing. Application scientists need to identify the quantities of interest while mathematicians and computational scientists provide appropriate algorithms and software. More robust algorithms and software are needed for successful incorporation of AMR, novel numerical PDE solvers, multiscale and multiphysics couplings into geosciences applications.

The bottom line is that while some of the issues are endemic to many scientific disciplines, most of the challenges identified are specific to the geosciences. However, many geoscience applications require the construction of large complex codes that are now deemed to be either legacy code (targeted for specific computer architectures that have since changed) or have utilized generic algorithms that need to be fine-tuned in order to tackle new types of problems (either due to mathematical and/or computational breakthroughs).

### 4. THE WAY FORWARD AND RECOMMENDATIONS

- **4.1 Summary of Research and Methodological Challenges.** The geosciences contain a wealth of interesting, challenging, and societally relevant problems while our ability to model and quantify key phenomena in large, complex and coupled natural systems is limited. The limitations in mathematical modeling methodologies are readily apparent in the geosciences. In many cases, there is no guiding general theory available to overcome the limitations. Among the scientific issues that continue to present challenges to mathematical geosciences are
  - i) multiple scales and their interplay in coupled physical models, which are difficult to detect and poorly predicted;
  - ii) complexity and enormous volumes of data that need to be analyzed and assimilated in the models;
  - iii) new computational paradigms for which application scientists need external expertise new accurate, robust, and efficient numerical algorithms and improved scalable software;

- iv) quantifying uncertainty in multi-scale systems displaying chaotic behavior;
- v) dealing with ill-posed and inverse problems.

Geoscience applications that contain many of the challenges listed above include (but are not limited to) climate modeling, subsurface applications, data assimilation, and uncertainty quantification. Below is a short summary of such challenges for each of these sub-disciplines.

- **4.1.1** The problem of climate modeling poses severe challenges since accurate simulation of the behavior of the planetary environment requires a "tight" coupling of atmosphere, ocean, and ice models, which is quite difficult to achieve due to the disparate time-scales associated with each component. In addition, the state of both modeling and understanding of important processes is quite different in these three fields particularly due to the varying ability to collect observational data (satellite data is ubiquitous for atmospheric processes, whereas data for both the ocean and ice is far more sparse, with ice data being only available at the surface of the ice sheet/shelf).
- **4.1.2** Many subsurface applications exhibit complex multiphysics couplings, e.g., carbon sequestration involves multiphase multicomponent flow and transport coupled with geomechanics; contaminant remediation in hydrologic systems require coupling of subsurface and surface flow and transport. In addition, fine-scale spatial effects can have large impacts on subsurface flow models (e.g., aquifers, oil and gas reservoirs).
- **4.1.3** Data assimilation in large models, where the data is of different types and at different scales, poses a difficult challenge. The models must be used for decision making or for optimization under uncertainty, and this leads to great computational demands. Furthermore, existing approaches do not adequately capture uncertainty, and as a result we cannot predict, even statistically, rare but important events such as large earthquakes and tsunamis. In addition, current modeling strategies do not adequately quantify the uncertainties inherent in climate change predictions, which is a central issue for risk assessment and decision making. Geoscience applications are especially challenging due to the very low signal to noise ratio inherent in the data, especially as it pertains to the modeling of climate and its change over time.
- **4.2 Need for Funding in Mathematical Geosciences.** There needs to be a mechanism (i.e., a research program) that will allow geoscientists to communicate their needs to the mathematical community. The mathematical community, in turn, develops general tools for solving certain classes of problems, but only through a mutual understanding of the issues at hand and the existing tools available can both communities move towards solving problems critical to the well-being of society. The National Science Foundation is in the best position to promote such discussions between these two communities; in fact, programs such as CMG will enable the healthy continuation of the mathematical geosciences community.

The workshop identified a large number of challenges that arise in the Geosciences. Collaboration is critical in order to focus the research into areas in which the correct equations, and corresponding physical principles such as mass balance and maximum principles, are preserved under (spatial and temporal) discretization. Collaboration is essential to correct ill-formed mathematical models, and to guide the mathematical analysis based on physical insight. As for advances in mathematical sciences, a disciplinary view of mathematical modeling misses the surprisingly complex interactions between the (1) mathematical structure of the governing principles and equations, (2) the behavior of numerical approximation algorithms, (3) constraints imposed by high performance, scientific computers, and (4) the complexity of the natural system under consideration. It is probably an unrealistic expectation that a general theory would be developed in isolation. Instead, it is more reasonable to expect progress in certain problem domains. The geosciences are particularly likely to provide a good application within which to make progress in mathematics toward general theories, due to the complexity and large size of these natural systems.

Next, communication between geoscientists and statisticians is necessary to improve the use of modern statistical tools in the geosciences and to improve existing methods to address the specific need of geophysical models. Specific efforts to demonstrate how physical insight can be gained from the use of a new statistical method can have a multiplier effect on the scientific community.

**4.3 Interdisciplinary Research, Careers, and Training.** One of the most important aspects, and a contributing factor to the successful CMG projects, was extensive and serious collaborative interactions. In fact, the most interesting challenge arises frequently already in the problem/model formulation. The advances in mathematics stemming from new application areas are frequently unexpected because problems are not completely formulated prior to the collaboration. Therefore, the collaborations in the mathematical geosciences need to be supported in a robust and stable manner to inspire and foster research that otherwise would not take place. The transfer of technology and theory from apparently unrelated areas can provide powerful mathematical ideas and methods to the geosciences, and facilitates cross-pollination of ideas across the various fields.

There is a continued strong societal need for scientists well trained in interdisciplinary work. Multidisciplinary programs such as CMG make a strong impact by establishing active collaboration and by training postdoctoral scientists that are uniquely qualified in both mathematics and geosciences. The existence of an interdisciplinary mathematics-geosciences program supports the interdisciplinary faculty not only financially but also by creating a community that understands and appreciates what they do (e.g., by supporting prizes in CMG topics); this has positive repercussions in the tenure and promotion of interdisciplinary faculty and is critical for the continuation of this type of expertise (i.e., interdisciplinary faculty will promote interdisciplinary education that then prolongs the lifespan of their knowledge).

NSF needs to continue to support and encourage interdisciplinary activities through special programs. Such programs both reassure researchers that it is worth the effort required to establish interdisciplinary collaborations, and provide evidence to their institution of the value of their interdisciplinary activities. Programs like CMG have been very successful at connecting the geosciences and mathematical communities in solving many challenging problems in the geosciences while developing new mathematics. They also support successful interdisciplinary collaborations, and training across disciplines. While many new NSF programs and initiatives that can support further interdisciplinary work already exist, the investments made by mathematicians in the geosciences are best communicated and assessed within a combined mathematical-geosciences community; having such a combined community is particularly important when considering that many of the challenges faced by geoscientists are quite unique to this field yet many of these challenges are shared across the various sub-disciplines of the geosciences (e.g., multiscale modeling in the Ocean, Ice, Atmosphere, and Earth communities).

**4.4 Extending the CMG Model for Support of Research and Training Collaborations in Mathematical Geosciences.** CMG has provided a successful platform for interdisciplinary research and training and these activities should continue to be supported. The model that has been successful in previous CMG projects such as mathematicians helping geoscientists or vice-versa should be continued and expanded. For example, a new paradigm of the Frontiers projects in which cutting edge technologies are used to advance the field sciences involved should be available. In addition, many participants would like to see an opportunity for funding for longer periods and larger projects, while many emphasized the importance of scientific, outreach, and educational projects of smaller and shorter scope. The latter could include projects involving scientists from one discipline mentoring postdocs or junior faculty from other fields via exchange visits, sabbaticals, conferences, summer schools, workshops, and support for development of interdisciplinary courses and degree programs.

The participants believe that while CMG primarily supported mathematics + geosciences collaborations, it would be useful to have a program in which even a larger scope of collaborative work involving

scientists from another field or directorate such as life sciences, computer science, engineering, or social sciences, could be included. An important connection to be explored is the involvement of industrial partners: oil and gas exploration companies, insurance companies, and others that are interested in partnerships with academia to support cutting edge research in mathematical geosciences.

**4.5 Summary Statement.** The participants of the workshop agreed that the community needs programs extending and expanding the successful CMG program in order to continue working towards solving the challenging problems of importance to society and to the United States in particular. While various interdisciplinary programs and initiatives exist and opportunities for funding are available, our community needs long-term support to overcome the scientific, educational, and organizational challenges, many of which are unique to the mathematical geosciences. The participants voiced enthusiastic support for funding programs for mathematical geosciences.

# Appendix 1: Organizing Committee of the Forward Looking Workshop in Mathematical Geosciences, Crystal City, Sept.16-17, 2011

Malgorzata Peszynska (Oregon State University), Chair, SIAM Activity Group on Geosciences

Junping Wang (National Science Foundation), Program Director, Department of Mathematical Sciences Frank Giraldo (Naval Postgraduate School)

Michel Kern (INRIA), Program Director, SIAM Activity Group on Geosciences

Ivan Yotov (University of Pittsburgh), Vice-chair, SIAM Activity Group on Geosciences

# Appendix 2: List of participants in the Forward Looking Workshop for Mathematical Geosciences, Crystal City, Sept.16-17, 2011

Alistair Adcroft, Princeton University Kayo Ide, University of Maryland

Todd Arbogast, University of Texas at Austin Leonid Ivanov, Naval Postgraduate School

John Boyd, University of Michigan Michel Kern, INRIA Rocquencourt

Bruce Buffet, University of California Berkeley Charles Lawrence, Brown University

Prabir Daripa, Texas A&M University Xiao-Li Meng, Harvard University

Clint Dawson, University of Texas at Austin Olivier Pauluis, New York University

Maarten de Hoop, Purdue University Malgorzata Peszynska, Oregon State University

Lou Durlofsky, Stanford University Bala Rajaratnam, Stanford University

Efi Foufoula-Georgiou, University of Minnesota Rosemary Renaut, Arizona State University

Frank Giraldo, Naval Postgraduate School Tom Russell, NSF

Kenneth Golden, University of Utah Gabor Szekely, NSF

Patrick Heimbach, MIT Ed Saff, Vanderbilt University

Traian Iliescu, Virginia Tech Piotr Smolarkiewicz, NCAR

Bill Spotz, Sandia National Laboratory

Amik StCyr, Shell Research

Seth Stein, Northwestern University

Deborah Sulsky, University of New Mexico

Hansong Tang, City University of New York

Liz Tennant, SRI

Jeroen Tromp, Princeton University

Martin Truffer, University of Alaska

Ka-Kit Tung, University of Washington

Benjamin Weiss, MIT

Johannes Westerink, University of Notre Dame

Ivan Yotov, University of Pittsburgh

Bill Young, Scripps Institution of Oceanography

llia Zaliapin, University of Nevada

Eric DeWeaver, NSF MPS/DMS

Jia Li, NSF

Baris Mete Uz, NSF GEO/OCE

Michael Morgan, NSF GEO/AGS

Sastry Pantula, NSF MPS/DMS

Andrew Pollington, NSF MPS/DMS

Junping Wang, NSF MPS/DMS

Henry Warchall, NSF MPS/DMS

William Wiseman, NSF

# <u>Appendix 3: Schedule of the Forward Looking Workshop in Mathematical Geosciences, Crystal City, Sept.16-17, 2011</u>

Note: the materials from some talks are available at

http://wiki.siam.org/siag-gs/index.php/Forward Looking Workshop

### **FRIDAY 9/16**

7:00-8:00 <b>Registration</b> a	Registration and breakfast		
8:00-8:30 <b>Overview J. Wang</b>	(Chair. M. Peszynska)	Wilson/Harrison	
8:30-9:10 OCEAN	(Chair F. X .Giraldo)	Wilson/Harrison	
C. Dawson	Mathematical and computational issues in coastal modeling		
A. Adcroft	High order remapping, the spurious mixing problem, and heat uptake in ocean models		
9:10-9:50 ICE	(Chair I. Yotov)	Wilson/Harrison	
M. Truffer	<b>M. Truffer</b> The role of mathematics in glaciology: Ice sheet modeling and invers modeling		
K. Golden	Sea ice, climate, and multiscale composites		
9:50-10:30 ATM/CLI	(Chair F. X. Giraldo)	Wilson/Harrison	
O. Pauluis	Reconstructing the global circulation using the Statistica Eulerian Mean	l Transformed	
10:30-10:50 Industry <b>A. St-Cyr</b>	(Chair F. X. Giraldo)  Geosciences and Computing in the Industry	Wilson/Harrison	
10:50-11:10 <b>Coffee break</b>			
11:10-11:50 GEOPH	(Chair <b>M. Kern</b> )	Wilson/Harrison	
M. De Hoop	Imaging and nonlinear inverse problems in seismology with large data sets		
J. Tromp	Seismic Imaging based on Spectral-element and Adjoint	Methods	

11:50-12:30 SUBS (Chair **I. Yotov**) Wilson/Harrison **T. Arbogast** Some Issues in the Mathematical and Computational Modeling of the

### Earth's Subsurface

# **L. Durlofsky**Computational Challenges for Subsurface Flow Modeling and Optimization

12:30-12:45 Wrap-up, overview of afternoon sessions Commitee Wilson/Harrison

12:45-2:00 **Lunch** 

### 2:00-6:00 Breakout sessions

Session		Leaders	Room
EARTH=SUB	S+GEOPH	T. Arbogast	Madison
OCEAN+ICE		J. Westerink, M. Truffer	Monroe
ATMO+CLIM	ATE	O. Pauluis, Amik St-Cyr	VanBuren
6:00-7:00	<b>Dinner</b> Opportunity to me	eet Division Directors of NSF-DMS and NSF-I	Earth Sciences
7:00-8:30	Report from sess	sions	Wilson/Harrison

# SATURDAY, 9/17

7:00-7:30 **Breakfast** Wilson/Harrison

7:30-10:00 **Breakout sessions** 

Session		Leaders		Room
MATH+MODELING		C. Dawson, M. De Hoop		Madison
STAT+UNCERTAINTY		L. Durlofsky, O. Pauluis		Monroe
COMPUTING+CROSSCUTTING		J. Tromp, K. Golden		VanBuren
10:00-10:30	Coffee			
10:30-12:00	Report from sessions, wrap-up		LEADERS / COMMITTEE Wilson/	Harrison
12:00-3:00	Boxed lunch and report draft		LEADERS / COMMITTEE	VanBuren