Final Report

Project Number: DE-SC0001724
Awardee Institute: Colorado State University

Project Title: *Collaboration Proposal: Transforming How Climate System Models are Used: A Global, Multiresolution Approach*

Principal Investigator: Donald Estep

Project Start: Aug. 15, 2009
Project End: Aug. 14, 2012

Overview

The overarching goal of the project was to investigate the robust, efficient, and accurate global solution of regional ocean models through the use of multi-resolution grids, verifiable refinement strategies, parameterizations that take advantage of enhanced regional resolution, and superior discretization techniques. To achieve this goal, we pursued both theoretical and computational means to resolve several basic modeling and algorithmic issues. Some of the key issues we addressed included:

- The effect of various forms of coupling, including temporal, spatial, and in the system of equations in the model
- A posteriori error analysis for the shallow water equations
- A posteriori error analysis for finite volume schemes
- Development and analysis of efficient adaptive multi-discretization methods for coupled systems
- The analysis of uncertain stochastic parameters input into models

Findings

The numerical solution of a regional climate model is an exceedingly complex undertaking that involves many discretization choices, including spatial and temporal discretization methods, spatial and temporal coupling strategies, choice of iterative solver and the number of iterations, parameter modeling, boundary conditions, and so forth. These choices are made under the pressure of intense computational costs associated with climate model solution. A full analysis and development of the ability to compute accurate estimates of all these effects is a desirable goal both for the purpose of quantifying uncertainty in model predictions and for efficient computation through adaptive adjustment of various discretization choices. After the initial discussions with

project investigator Todd Ringler (LANL), it became clear that a treatment of the entire range of issues could not be undertaken during the span of the project. Thus, we focused on a number of key issues that are core to the entire solution process.

The focus of our part of the project was on development and implementation of a posteriori error estimates for specified quantities of interest computed from a model. These computational estimates provide accurate information about the error in the physically relevant quantities desired from the model. Our approach employs variational analysis, adjoint problems, and computable residuals. Long in use for finite element methods, these estimates are not in widespread use in the climate community, nor have the estimates previously been extended to include the full range of discretization issues encountered in climate model simulations.

The key issues we addressed during the time of the project include:

- Treatment of the effects of employing a finite number of iterations in the coupled solution of systems of equations, including temporal, spatial, and parameter coupling. The key issue here is identifying a suitable adjoint problem, as the adjoint associated with a completely implicit, fully coupled solution is typically not the correct choice. We also have to identify residuals that represent the effects of coupling in terms of state variables.

- Treatment of the effects of multi-discretization involving different meshes, time steps, and even discretization methods for different components of a system of equations. These approaches involve the translation of information computed using one discretization to be accessible to the discretizations used in the other components. This translation may have a significant effect on accuracy.

- A posteriori error analysis for finite volume methods for the shallow water equations. The SWE often forms the core of a number of climate models.

- A posteriori error estimate and stochastic propagation of discretization and representation errors in the geometry of the domain of a PDE, including solution of a PDE on a manifold (the earth) and in the boundary geometry

- Development of a “block” adaptive algorithm, and the supporting a posteriori error estimate, for PDEs that employs as a discrete sequence of nonuniform spatial meshes corresponding to a set of macro-time intervals constructed to be accurate during the time intervals that each mesh is used. This is an alternative to the adaptive approach that involves changing the spatial mesh at each time step. This brings many benefits, including reduced negative effects of mesh changes on accuracy and reduced need to load balance in an HPC platform.

In addition, we produced several other results that are indirectly connected to the project goals.

The overall achievement of the project is establishing rigorously valid computational techniques to accurately estimate the effects of a number of discretization issues used in the solution of climate models, and to efficiently adjust various discretization choices in order to obtain a desired level of accuracy in specified quantities of interest.

During the course of the project, we undertook a number of activities directed towards distributing the results of the project to relevant application communities and the broader research communities. D. Estep also was engaged in a number of activities that are indirectly related to the goals of the project and the DOE.

Publications

Color Coding: Directly related to project goals, indirectly related to project goals, auxiliary results

Publications accepted/appeared

[1] *Nonparametric density estimation for randomly perturbed elliptic problems II: Applications and adaptive modeling*, D. Estep, A. Malqvist, S. Tavener, International Journal for Numerical Methods in Engineering 80 (2009), 846-867

[2] *A posteriori error analysis for a transient conjugate heat transfer problem*, D. Estep, S. Tavener, T. Wildey, Finite Elements in Analysis and Design 45 (2009), 263-271

[3] *Nonparametric density estimation for randomly perturbed elliptic problems I: Computational methods, a posteriori analysis, and adaptive error control*, D. Estep, A. Malqvist, and S. Tavener, SIAM Journal on Scientific Computing 31 (2009), 2935-2959

[4] *A posteriori error analysis of a cell-centered finite volume method for semilinear elliptic problems*, D. Estep, M. Pernice, D. Pham, S. Tavener, H. Wang, Journal of Computational and Applied Mathematics 233 (2009), 459-472

[5] *A posteriori error estimation and adaptive mesh refinement for a multi-discretization operator decomposition approach to fluid-solid heat transfer*, D. Estep, S. Tavener, T. Wildey, Journal of Computational Physics 229 (2010), 4143-4158

[6] *Blockwise adaptivity for time dependent problems based on coarse scale adjoint solutions*, V. Carey, D. Estep, A. Johansson, M. Larson, and S. Tavener, SIAM Journal on Scientific Computing 32 (2010), 2121-2145

[7] *A measure-theoretic computational method for inverse sensitivity problems I: Method and analysis*, J. Breidt, T. Butler and D. Estep, SIAM Journal on Numerical Analysis 49 (2011), 1836-1859

[8] *A posteriori error analysis for a cut cell finite volume method*, D. Estep, S. Tavener, M. Pernice and H. Wang, Computer Methods in Applied Mechanics and Engineering 200 (2011), 2768-2781

[9] *Nonparametric density estimation for randomly perturbed elliptic problems III: Convergence, complexity, and generalizations*, D. Estep, M. Holst, A. Malqvist, Journal of Applied Mathematics and Computing 38 (2012), 367-387

[10] *Parameter estimation and directional leverage with applications in differential equations*, N. Burch, D. Estep, and J. Hoeting, Metrika, DOI: 10.1007/s00184-011-0358-4, 2011

[11] *Continuum Modeling and Control of Large Mobile Networks*, Y. Zhang, E. K. P. Chong, J.

Hannig, and D. Estep, Proceedings of the 49th Annual Allerton Conference on Communication, Control and Computing, Illinois, 2011

[12] *A computational measure theoretic approach to inverse sensitivity problems II: A posteriori error analysis*, T. Butler, D. Estep and J. Sandelin, SIAM Journal on Numerical Analysis, 50 (2012)

[13] *Viscoelastic Effects During Loading Play an Integral Role in Soft Tissue Mechanics*, K. Troyer, D. Estep, and C. Puttlitz, Acta Biomaterialia 8 (2012), 234-244

[14] *A posteriori analysis of multirate numerical method for ordinary differential equations*, D. Estep, V. Ginting, S. Tavener, 2012, Computer Methods in Applied Mechanics and Engineering, 223-224 (2012), 10-27

[15] *Adaptive error control for an elliptic optimization problem*, Applicable Analysis, D. Estep and S. Lee, 2012, DOI:10.1080/00036811.2012.683785, 1-15

[16] *Analysis of routing protocols and interference-limited communication in large networks via continuum modeling*, N. Burch, E. Chong, D. Estep, J. Hannig, Journal of Engineering Mathematics, 2012, (DOI) 10.1007/s10665-012-9566-9

[17] *A numerical method for solving a stochastic inverse problem for parameters*, T. Butler and D. Estep, Annals of Nuclear Energy, 2012, 86-94, 10.1016/j.anucene.2012.05.016

[18] *Multiphysics Simulations: Challenges and Opportunities*, D. E. Keyes, L. C. McInnes, C. Woodward, W. Gropp, E. Myra, M. Pernice, J. Bell, J. Brown, A. Clo, J. Connors, E. Constantinescu, D. Estep, K. Evans, C. Farhat, A. Hakim, G. Hammond, G. Hansen, J. Hill, T. Isaac, X. Jiao, K. Jordan, D. Kaushik, E. Kaxiras, A. Koniges, K. Lee, A. Lott, Q. Lu, J. Magerlein, R. Maxwell, M. McCourt, M. Mehl, R. Pawlowski, A. Peters Randles, D. Reynolds, B. Riviere, U. Ruede, T. Scheibe, J. Shadid, B. Sheehan, M. Shephard, A. Siegel, B. Smith, X. Tang, C. Wilson, and B. Wohlmuth, International Journal of High Performance Computing Applications (27), 2013.

[19] *Continuum Modeling and Control of Large Nonuniform Wireless Networks via Nonlinear Partial Differential Equations*, Y. Zhang, E. Chong, J. Hannig, and D. Estep, Abstract and Applied Analysis, 2013, to appear

Publications submitted

[1] *A posteriori analysis and adaptive error control for multiscale operator decomposition solution of elliptic systems II: Fully coupled systems*, V. Carey, D. Estep, S. Tavener, International Journal of Numerical Methods in Engineering, 2011, in revision

[2] *A-posteriori error estimates for mixed finite element and finite volume methods for problems coupled through a boundary with non-matching grids*, T. Arbogast, D. Estep, B. Sheehan, and S. Tavener, IMA J. Numerical Analysis, 2012, in revision

[3] *A posteriori error estimates for explicit time integration methods*, J. Collins, D. Estep and S. Tavener, BIT Numerical Mathematics, 2012, submitted

[4] *A posteriori analysis of an iterative multi-discretization method for reaction-diffusion systems*, J. Chaudhry, D. Estep. V. Ginting, and S. Tavener, Computer Methods in Applied Mechanics and Engineering, 2012, submitted

[5] *Continuum Limits of Markov Chains with Application to Wireless Network Modeling*, Y. Zhang, E. Chong, J. Hannig, and D. Estep, IEEE Access, 2013, submitted

[6] *The interaction of iteration error and stability for time dependent linear PDE's coupled*

through an interface, B. Sheehan, D. Estep, S. Tavener, J. Cary, S. Kruger, A. Hakim, A. Pletzer, J. Carlsson, Applied Numerical Mathematics, 2013, submitted

[7] *A posteriori error estimation for the Lax-Wendroff finite difference scheme*, J. B. Collins, D. Estep, and S. Tavener, Journal of Computational and Applied Mathematics, 2013, submitted

Book Chapters

[1] *Bridging the Scales in Science and Engineering*, Editor J. Fish, Oxford University Press, Chapter 11: *Error Estimation for Multiscale Operator Decomposition for Multiphysics Problems*, D. Estep, 2010

[2] *Building Confidence in Computational Models: The Science of Verification, Validation, and Uncertainty Quantification*, Committee on Mathematical Foundations of Verification, Validation, and Uncertainty Quantification, The National Academies Press, 2012, *Appendix B: Adjoint Operators*, D. Estep.

Publications in Preparation

[1] *An adaptive time stepping algorithm that allows for cancellation of errors*, J, Chaudhry, D. Estep, J. Sandelin

[2] *An a posteriori analysis of iterative techniques for a system of ordinary differential equations*, J. Chaudry, D. Estep, V. Ginting, and S. Tavener.

[3] *Density estimation for a class of elliptic problems on uncertain domains*, N. Burch and D. Estep

[4] *A posteriori error estimates for the Poisson problem on closed two-dimensional surfaces*, D. Estep, M. Holst, and W. Newton

[5] *A measure-theoretic computational method for inverse sensitivity problems III: Multiple quantities of interest*, T. Butler, D. Estep, S. Tavener, C. Dawson, and J. Westerink

[6] Adaptive finite element solution of coupled PDE-ODE systems, V. Carey, J. Chaudhry, D. Estep, V. Ginting, A. Johansson, M. Larson, and S. Tavener

Invited Presentations at Professional Meetings for D. Estep

11/09 *Adaptive and Multilevel Methods for Partial Differential Equations*, University of California San Diego

3/11 *SIAM Computational Science and Engineering Conference, Minisymposia on Numerical Discretization Error Estimation for Uncertainty Quantification, Progress in Computational Methods and Software for Tightly-coupled Multiphysics Applications, Numerical Methods for Stochastic Computation and Uncertainty Quantification, Numerical Challenges in Microstructure Modeling for Materials Science*, Reno, Nevada

8/11 *ICiS Workshop on Multiphysics Simulations: Challenges and Opportunities*, Park City, Utah, *Plenary Speaker*

5/12 *Uncertainty Quantification for High-Performance Computing Workshop*, Oak Ridge National Laboratory

7/12 *6th International Conference on Automatic Differentiation*, Fort Collins, CO

8/12 *Joint Statistical Meetings*, Invited Papers, Uncertainty Quantification at SAMSI

Invited Colloquia and Seminars for D. Estep

9/09	University of Wyoming
12/09	Lawrence Livermore National Laboratory
1/10	Atmospheric Sciences, CSU
2/10	University of Wisconsin
3/10	Brown University
3/10	University of Chicago
8/10	Sandia National Laboratory
9/10	Lawrence Livermore National Laboratory
9/10	Purdue University
11/10	North Carolina State University
1/11	Lawrence Livermore National Laboratory
3/11	University of Southern California
11/11	University of Chicago
3/12	Florida State University
4/12	Colorado School of Mines
4/12	SAMSI

Ph.D. Students and Postdocs Advised

- W. Newton, Graduate Student, Department of Mathematics, Colorado State University, 2011, *A Posteriori Error Estimates for the Poisson Problem on Closed, Two-Dimensional Surfaces.* Currently, research scientist, Department of Mathematics, Colorado State University
- N. Burch, Graduate Student, Department of Mathematics, Colorado State University, 2011, *Probabilistic Foundation of Nonlocal Diffusion and Formulation and Analysis for Elliptic Problems on Uncertain Domains.* Currently, postdoc, Statistical and Applied Mathematical Sciences Institute (SAMSI)
- R. Mckeown, Graduate Student, Department of Forestry, Rangeland, and Watershed Stewardship, Colorado State University, in progress
- B. Bugbee, (joint with J. Breidt), Graduate Student, Department of Statistics, Colorado State University, in progress
- J. Sandelin, Postdoc, from Colorado State University (my student), 2010. Currently, GeoEye, Inc.
- M. Presho, Postdoc, from University of Wyoming (student of V. Ginting), 2011. Currently, HyperComp, Inc.
- V. Carey, Postdoc, from Cornell University (student of L. Wahlbin), 2012. Currently, ICES, University of Texas at Austin.
- B. Sheehan, Postdoc, from University of Colorado Boulder (student of T. Mantueffel), in progress
- J. Collins, Postdoc, from North Carolina State University (student of P. Gremaud), in progress
- W. Newton, Postdoc, from Colorado State University (my student), in progress
- J. Chaudhry, Postdoc, from University of Illinois (student of L. Olson), in progress

- T. Butler, Postdoc, from University of Texas Austin, in progress

Estep Professional Activities

Awards

2011	University Scholarship Impact Award, Colorado State University
2012	Appointed Editor in Chief (founding), *SIAM/ASA Journal on Uncertainty Quantification*

Editorial Boards

- Editor in Chief (founding), *SIAM/ASA Journal on Uncertainty Quantification,* 2012 -
- Editor in Chief, *SIAM Book Series on Computational Science and Engineering,* 2009 -
- Associate Editor, *SIAM Journal on Numerical Analysis,* 2005-
- Associate Editor, *International Journal for Uncertainty Quantification,* 2010 -
- Advisory Editor, *International Journal of Computer Mathematics,* 2012 -
- Associate Editor, *Multiphysics Modeling Book Series,* A. A. Balkema Publishing, 2009-
- Associate Editor, *Journal of Applied Mathematics and Computing,* 2008 –

Conferences Organized

2011	*SAMSI-Sandia Summer School on Uncertainty Quantification,* 2011, co-organizer with Jim Stewart, Sandia
2011	*Workshop on Working with Uncertainty, IEEE VisWeek 2011,* Program Committee
2011-12	*SIAM/ASA/USACM Conference on Uncertainty Quantification,* Co-chair

Professional Service

- Advisory Board, Center for Advanced Modeling and Simulation, Idaho National Laboratory, 2009 – 2012
- Governing Board, Statistical and Applied Mathematical Sciences Institute (SAMSI), 2009-
- Member, National Science Foundation Office of Cyberinfrastructure Grand Challenges Communities Task Force, 2009-2010, co-author of Task Force report
- Moderator, SAMSI National SIAM and ASA Town Hall Meeting on Uncertainty Quantification, 2010
- Co-Organizer and first Chair, SIAM Activity Group on Uncertainty Quantification, 2010-12
- Program Leader, SAMSI Program on Uncertainty Quantification, 2011-2012
- American Mathematical Society Simmons Travel Grants Committee, 2011-2013
- Moderator, Mathematics in the Geosciences Workshop, Northwestern University, 2011
- Breakout Lead and Report co-author, *Uncertainty Quantification/Stochastic Systems, Department of Energy Cross-Cutting Technologies for Computing at the Exascale,* 2010

- Invited participant, *Fusion Simulation Program Definition Workshop,* 2011
- Co-Author, *Proposal to establish a SIAM/ASA Journal on Uncertainty Quantification,* (with J. Berger and M. Gunzburger). Initially submitted to SIAM in 2010 and ASA in 2011, approved by ASA and SIAM in 2012.
- Co-Author, *Fostering Interactions Between the Geosciences and Mathematics, Statistics, and Computer Science,* Technical Report TR-2012-02, Department of Computer Science, University of Chicago, 2012
- Co-Author, *Multiphysics Simulations: Challenges and Opportunities,* Tech. Report ANL/MCS-TM-321, Argonne National Laboratory, 2011
- *University of California San Diego Interdisciplinary Graduate Program in Computational Science, Mathematics, and Engineering,* 2009. Proposal review
- Mathematics Review Panel, *Norman Hackerman Advanced Research Program,* Texas, 2009
- Reviewer, 2010, Fusion Simulation Prototype Centers, Department of Energy
- Reviewer, 2011, King Abdullah University of Science and Technology (KAUST) Strategic Research Initiative (SRI) program, Center Proposals
- Member, Sandia Computing and Information Sciences Review Panel, 2012
- Reviewer, Advanced Methods for Manufacturing, Department of Energy

<u>Interdisciplinary Interaction with Atmospheric Science</u>

8/10-12/10	Internal Sabbatical, Department of Atmospheric Sciences, Colorado State University

Carey Professional Activities

- Invited seminar, University of Uppsala, 2009
- Poster, DOE Climate Workshop, 2010
- Invited Seminar, Los Alamos National Laboratory, 2010
- Contributed talk, IMUM, 2010
- Organized minisymposium at SIAM CS&E Conference, 2011
- Contributed talk, ANS, 201
- Contributed talk, Society for Experimental Mechanics, 2011
- Contributed talk, ICIAM, 2012
- Invited Seminar, Sandia National Laboratory, 2012
- Invited Seminar, ICES, University of Texas at Austin, 2012
- Participant, SAMSI Workshops on UQ, 2012