Final Report

Project Number: DE -FC02-07ER54909

Awardee Institute: Colorado State University

Project Title: Framework Application for Core-Edge Transport Simulations (FACETS)

Principal Investigator: Donald Estep

Project Start: 02-15-2007

Project End: 08-14-2013

PROJECT DESCRIPTION

FACETS was focused on the development of a multiphysics, parallel framework application that could provide the capability to enable whole-device fusion reactor modeling and, in the process, the development of the modeling infrastructure and computational understanding needed for ITER. It was intended that FACETS be highly flexible, through the use of modern computational methods, including component technology and object oriented design, to facilitate switching from one model to another for a given aspect of the physics, and making it possible to use simplified models for rapid turnaround or high-fidelity models that will take advantage of the largest supercomputer hardware. FACETS was designed in a heterogeneous parallel context, where different parts of the application can take advantage through parallelism based on task farming, domain decomposition, and/or pipelining as needed and applicable.

As with all fusion simulations, an integral part of the FACETS project was treatment of the coupling of different physical processes at different scales interacting closely. A primary example for the FACETS project is the coupling of existing core and edge simulations, with the transport and wall interactions described by reduced models. However, core and edge simulations themselves involve significant coupling of different processes with large scale differences. Numerical treatment of coupling is impacted by a number of factors including, scale differences, form of information transferred between processes, implementation of solvers for different codes, and high performance computing concerns.

Operator decomposition involving the computation of the individual processes individually using appropriate simulation codes and then linking/synchronizing the component simulations at regular points in space and time, is the defacto approach to high performance simulation of multiphysics, multiscale systems. Various forms of operator decomposition are used in nearly all fusion simulations. However, operator decomposition generally has a complex effect on accuracy and stability of numerical simulations. Yet, these effects can be difficult to detect.

The Colorado State University component of the FACETS team led by P. I. D. Estep was focused on analyzing the effects of operator decomposition on fusion simulations. The approach was based on a posteriori error analysis employing adjoint problems, computable residuals, and variational analysis to produce accurate computational error estimates for quantities of interest. Computable residuals are used to quantify the effects of various discretization choices. The generalized Greens function satisfying the adjoint problem quantities the effects of stability.

Technical issues to be addressed included: (1) defining appropriate adjoint operators for operator decomposition discretizations; (2) determining the appropriate residuals for the multifaceted aspects involved with multiphysics discretizations; (3) producing the estimates within the computational framework of existing fusion codes; (4) carrying out the analysis for discretizations used in fusion simulations; and (5) devising efficient approaches to mitigating the effects of discretization.

OVERVIEW OF PERFORMANCE AND OUTCOMES

In a concrete sense, the support of this project contributed substantially to a revolutionary extension of the capabilities for a posteriori error estimation for operator decomposition solutions of multiscale, multiphysics problems that resulted from the activities of Estep's research group over the last six years. The work on this project was undertaken with close collaboration of personnel at TechX Corporation (which was the FACETS project lead). Postdocs Pham and Sheehan worked directly with TechX personnel, with Sheehan in particular spending most of his time at TechX during the project. Consequently, we directed the theoretical aspects of this project to deal with the specific technical issues that arise in the context of fusion reactor simulations. Estep was also generally involved with research in the fusion community, including proposal and panel reviews and participation in fusion research meetings.

In papers [2], [3], [6], and [20], we undertook a systematic extension of a posteriori error analysis to systems of parabolic problems in neighboring domains with coupling of state and normal flux through a common boundary, where the solution is obtained by finite element solution involving iterative operator decomposition. The analysis considered standard finite element discretizations because the variational a posteriori error analysis is well suited to treating finite elements. With quadrature, we can obtain some standard finite difference schemes. We treated both stationary and evolutionary problems, and also extended the work to fluid-solid interaction. The chief accomplishments were determining the appropriate adjoints for the iterative solution operator and identifying residuals associated specifically with errors in the coupling quantities. The adjoint operators associated with such schemes are different than the adjoint operators associated with the original differential equation, and these differences account for the effects of iterative solution on stability of the simulations. We also demonstrate the efficient gain in adaptive computation that is possible when based on the extended error estimates.

Since the physics fusion community largely employs cell-centered finite volume schemes, in [7] we extended a posteriori error estimates to such schemes. To do this, we used old work of M. Wheeler to write the finite volume scheme as an equivalent mixed finite element method with a specialized quadrature. The estimates include specific terms that quantify the effects of the quadrature, hence are very specific for finite volume schemes.

In [12] and [15], we extended the previous work in [2], [3], [6], and [20] to coupled systems discretized with finite volume schemes in which we allow radically different mesh resolutions on the two domains, including one large cell coupled to many smaller cells (as in edge-core coupling). We study various "geometric" coupling schemes that are employed in fusion simulations, which are based largely on heuristic arguments. We also adapted the well studied "mortar element methods" used in porous media flow for coupling such discretizations through an interface with large scale differences in mesh resolution. We show that the mortar element

methods yield much greater accuracy and yet can be implemented in a standard fusion simulation coupling framework with mild implementation work. We also derive a mathematically correct analysis for the typical heuristic stability argument used to justify various coupling schemes and explore the consequences in a systematic fashion.

In [9] and [11], we derive a posteriori error estimates for so-called multirate time integration schemes for ODEs and PDEs that employ different time steps for different components of the system. Using the estimates, we study the effects on accuracy and stability.

In [16], we derive a posteriori error estimates for classical operator splitting methods, again adapting the analysis by deriving appropriate adjoint problems and residuals.

In [24], we derive a posteriori error estimates for explicit time integration methods. Most fusion simulations use implicit methods for the component solves, but we encountered the use of explicit solvers in situations in which fast transient behavior required small time steps.

In [21], we derived a posteriori error estimates for finite volume schemes for problems with discontinuous coefficients across a complex interface. This is related to fusion simulations indirectly in that core-edge system is derived using scale arguments applied to a set of equations that hold for the entire system. If the original complete system were discretized, the large scale differences in the core and edge regions would result in an effective discontinuity across a complex interface between the core and edge.

In [17] and [23], we derive a posteriori error estimates for coupled systems with coupling in coefficients and righthand sides. The goal was to understand the effects of passing errors between components. This kind of coupling arises in the complex models used in separately in the core and edge regions.

In [18], [19], and [23], we develop and analyze error estimates for probability distributions computed from PDES with random coefficients, and develop a new generalized adaptive algorithm. Eventually, fusion simulations will have to include stochastic effects.

In [8], we analyze a blockwise approach to adaptive mesh refinement that is particularly well suited to the regular grid structures used in finite volume schemes.

In [5], [14], and [10], we wrote general overviews and surveys of a posteriori error analysis for operator decomposition solution of multiscale, multiphysics systems in order to make our work accessible to the broad engineering and scientific communities.

Finally, we note that Estep maintained a broad range of research activities during the time of the project, which resulted in a number of papers, students, and postdocs.

LIST OF OUTCOMES AND ACCOMPLISHMENTS

Below we summarize research activities of D. Estep and his group during the FACETS project, including work directly and indirectly related to FACETS as well as his other activities. We also present D. Estep's research activities such as talks, awards, and service during this period.

To summarize some of the highlights, during the period of FACETS, Estep co-authored 40 manuscripts, of which 24 are directly or indirectly related to FACETS. He mentored 8 Ph.D. students and 13 postdocs, with 4 of these postdocs supported by FACETS. One of the FACETS

postdocs is now a technical member of staff at Sandia National Laboratory, while two are still in progress. Two of the FACETS postdocs interacted closely with TechX Corporation. D. Estep gave one short course and over 20 invited talks at conferences and workshops, including a number of plenary and keynote lectures. D. Estep gave over 25 invited seminars and colloquia. D. Estep won a number of professional awards, served as editor on a number of journals (including being a co-founding Editor in Chief of the SIAM/ASA Journal on Uncertainty Quantification), co-organized a number of workshops and conferences, and undertook a number of significant service activities, including many related to the mission of the DOE.

I. PERSONNEL

Faculty Involved with the Project

- Don Estep, Department of Statistics, CSU, Project PI
- Simon Tavener, Department of Mathematics, CSU, co-advisor of postdocs

Personnel Supported by Salary on the Project

- Tim Wildey, research associate, July 2007. Currently, member of technical staff, Sandia National Laboratory
- Du Pham, postdoc, Sep. 2007 to Aug. 2010. Subsequent job: lecturer, Butler University.
- Jehanzeb Chaudhry, postdoc May 2013 to Aug. 2013. Currently, postdoc supported by a DOE UQ grant joint with Sandia National Laboratory.
- Brendan Sheehan, Research Associate, Aug. 2010 to Aug. 2013. Currently, research associate supported by DOE DiaMonD grant.

II. PROJECT OUTCOMES

Peer Reviewed Publications Related to the Primary Project Goals

[1] *Introducing FACETS, the Framework Application for Core-Edge Transport Simulations,* J. R. Cary, J. Candy, R. H. Cohen, S. Krasheninnikov, D. C. McCune, D. J. Estep, J. Larson, A. D. Malony, P. H. Worley, J. A. Carlsson, A. H. Hakim, P. Hamill, S. Kruger, S. Muzsala, A. Pletzer, S. Shasharina, D. Wade-Stein, N. Wang, L. McInnes, T. Wildey, T. Casper, L. Diachin, T. Epperly, T. D. Rognlien, M. R. Fahey, J. A. Kuehn, A. Morris, S. Shende, E. Feibush, G. W. Hammett, K. Indireshkumar, C. Ludescher, L. Randerson, D. Stotler, A. Yu Pigarov, .P Bonoli, C. S. Chang, D. A. D'Ippolito, P. Colella, D. E. Keyes, R. Bramley, J. R. Myra, Journal of Physics: Conference Series 78 (2007), 1-6

[2] *A posteriori error estimation of approximate boundary fluxes*, T. Wildey, S. Tavener, and D. Estep, Communications in Numerical Methods in Engineering, 24 (2008), 421-434

[3] *A posteriori analysis and improved accuracy for an operator decomposition solution of a conjugate heat transfer problem*, D. Estep, S. Tavener, T. Wildey, SIAM Journal on Numerical Analysis, 46 (2008), 2068-2089

[4] *First results from core-edge parallel composition in the FACETS project*, J. R. Cary, J. Candy, R. H. Cohen, S. Krasheninnikov, D. C. McCune, D. J. Estep, J. Larson, A. D. Malony, P. H. Worley, J. A. Carlsson, A. H. Hakim, P. Hamill, S. Kruger, M. Mia, S. Muzsala, A. Pletzer, S. Shasharina, D. Wade-Stein, N. Wang, S. Balay, L. McInnes, H. Zhang, T. Casper, L. Diachin, T. Epperly, T. D. Rognlien, M. R. Fahey, J. Cobb, A. Morris, S. Shende, G. W. Hammett, K. Indireshkumar, D. Stotler, A. Yu Pigarovd, Journal of Physics: Conference Series 125 (2008), 1-5

[5] *A posteriori error analysis of multiscale operator decomposition methods for multiphysics models*, D. Estep, V. Carey, V. Ginting, S. Tavener, T. Wildey, Journal of Physics: Conference Series 125 (2008), 1-16

[6] *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

[7] *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

[8] *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

[9] *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

[10] *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.

[11] *A posteriori analysis of an iterative multi-discretization method for reaction-diffusion systems*, D. Estep. V. Ginting, J. Hameed, and S. Tavener, Computer Methods in Applied Mechanics and Engineering, 2013, to appear

[12] *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, 2013, doi: 10.1093/imanum/drt049

[13] *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

[14] *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.

[15] *The interaction of iteration error and stability for time dependent linear partial differential equations coupled through an interface*, B. Sheehan, D. Estep, S. Tavener, J. Cary, S. Kruger, A. Hakim, A. Pletzer, J. Carlsson, Numerical Algorithms, 2013, submitted

Peer Reviewed Publications Related to Secondary Project Goals

[16] *A posteriori – a priori analysis of multiscale operator splitting*, D. Estep, V. Ginting, D. Ropp, J. Shadid, and S. Tavener, SIAM Journal on Numerical Analysis 46 (2008), 1116-1146

[17] *A posteriori analysis and adaptive error control for multiscale operator decomposition*

methods for coupled elliptic systems I: One way coupled systems, V. Carey, D. Estep, and S. Tavener, SIAM Journal on Numerical Analysis 47 (2009), 740-761

[18] *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

[19] *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

[20] *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

[21] *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

[22] *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

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

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

Research Articles Co-Authored by P.I. Estep Not Related to the Project

[25] *The nonlinear power method*, S. Eastman and D. Estep, Applicable Analysis 86 (2007), 1303 – 1314

[26] *Fast methods for determining the evolution of uncertain parameters in reaction-diffusion equations*, D. Estep and D. Neckels, Computer Methods in Applied Mechanics and Engineering 196 (2007), 3967 – 3979

[27] *Analysis, simulation, and optimal design of large wireless networks using continuum models*, E. Chong, D. Estep, and J. Hannig, International Journal of Numerical Modeling: Electronic Networks, Devices, and Fields, 21 (2008), 169-186

[28] *Analysis of the sensitivity properties of a model of vector-borne bubonic plague*, M. Buzby, D. Neckels, M. Antolin, and D. Estep, Royal Society Journal Interface, 5 (2008), 1099-1107

[29] *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

[30] *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

[31] *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

[32] *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)

[33] *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

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

[35] *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

[36] *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

[37] *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 (16), 2013, doi:10.1155/2013/262581, 1-16.

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

[39] *A measure-theoretic computational method for inverse sensitivity problems III: Multiple quantities of interest*, T. Butler, D. Estep, S. Tavener, C. Dawson, J. Westerink, SIAM Journal on Uncertainty Quantification, 2013, submitted

[40] *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

Doctoral Students Advised by P. I. Estep during the Project

1. T. Wildey, Department of Mathematics, Colorado State University, 2007. Thesis: *A posteriori analysis of operator decomposition on interface problems.* Currently, Research Staff Member, Sandia National Laboratories, Albuquerque.
2. S. Lee, Department of Mathematics, Colorado State University, 2008. Thesis: *An Adaptive Algorithm for an Elliptic Optimization Problem, and Stochastic-Deterministic Coupling: A Mathematical Framework,* Currently, Department of Mathematics, Viterbo University.
3. T. Butler, Department of Mathematics, Colorado State University, 2009. Thesis: *Computational Measure Theoretic Approach to Inverse Sensitivity Analysis: Methods and Analysis*. Currently, Research Scientist, Colorado State University.
4. M. Buzby, Department of Mathematics, Colorado State University 2009. Thesis: *Short time analysis of deterministic ODE solutions and the expected value of a corresponding birth-death process.* Currently, Department of Mathematics, University of Alaska Southeast.
5. W. Newton, 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
6. N. Burch, 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)
7. R. Mckeown, Department of Forestry, Rangeland, and Watershed Stewardship, Colorado State University, in progress

8. B. Bugbee, (joint with J. Breidt), Department of Statistics, Colorado State University, in progress

Postdocs and Research Scientists Advised by P.I. Estep during Project

1. A. Malqvist, from Chalmers University (student of M. Larson), 2007. Currently, associate professor, University of Uppsala, Sweden.
2. V. Ginting, from Texas A&M (student of R. Lazarov and Y. Efendiev), 2007. Currently, Assistant Professor, University of Wyoming.
3. D. Lockwood, from University of California, Davis (student of L. Botsford), 2007. Currently, Postdoc, Department of Biology, Colorado State University.
4. D. Pham, from Indiana University (student of R. Temam), 2009.
5. H. Wang, from University of Minnesota (student of B. Cockburn), 2009.
6. J. Sandelin, from Colorado State University (my student), 2010. Currently, GeoEye, Inc.
7. M. Presho, from University of Wyoming (student of V. Ginting), 2011. Currently, HyperComp, Inc.
8. V. Carey, from Cornell University (student of L. Wahlbin), 2012. Currently, ICES, University of Texas at Austin.
9. T. Butler from University of Texas Austin (my student), 2013. Currently, assistant professor, University of Colorado at Denver
10. J. Collins from North Carolina State University (student of P. Gremaud), in progress
11. W. Newton from Colorado State University (my student), in progress
12. J. Hameed from University of Illinois (student of L. Olson), in progress
13. B. Sheehan, from University of Colorado Boulder (student of T. Mantueffel), in progress

Invited Short Courses Presented by P.I. Estep

4/07 *Duality, Adjoint Operators, and Uncertainty in a Complex World,* 4th Montreal Scientific Computing Days, University of Montreal, Montreal, Canada

Invited Talks at Conferences and Workshops Presented by P.I. Estep

9/06 *International Conference on Computational and Mathematical Methods in Science and Engineering,* Madrid, Spain, *Plenary Lecture*

2/07 *SIAM Conference on Computational Science and Engineering, Minisymposium on A Posteriori Error Estimation and Adaptivity in Computational Science and Engineering*

3/07 *14th International Finite Elements in Flow Problems Conference,* Santa Fe, New Mexico

8/07 *Sandia CSRI Workshop on Mathematical Methods for Verification and Validation,* Albuquerque, New Mexico

9/07 *Management of Numerical Errors In Nuclear Systems Modeling,* Idaho National Laboratory and North Carolina State University, North Carolina

7/08 *SIAM Annual Meeting, Minisymposium on Recent Advances on A Posteriori Error Estimation and Adaptive Error Control* and *Minisymposium on Advances in Uncertainty Quantification*

7/08 *SCIDAC 2008,* Seattle, Washington, *Plenary Address*

7/08 *Uncertainty Analysis in Complex, Multiphysics Applications, PSAAP University Alliance Center,* Stanford University

9/08 *Workshop on Mathematical and Computational Issues in the Solid Earth Geosciences,* Computational Infrastructure for Geosciences, Santa Fe

1/09 *Finite Element Methods in Engineering and Science,* Lake Tahoe, *Plenary Speaker*

2/09 *Pikes Peak Regional Undergraduate Mathematics Conference (PPRUMC), Keynote Speaker*

4/09 *Computational Science and Engineering (CSE) Annual Research Symposium,* University of Illinois, Urbana-Champaign, *Keynote Speaker*

7/09 *SIAM Annual Meeting, Minisymposium on Predictive Computational of Multiscale-Multiphysics Applications,* Denver

8/09 *Workshop on Simulating the Spatial-Temporal Patterns of Anthropogenic Climate Change,* Los Alamos Institute for Advanced Studies, Santa Fe, New Mexico

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

5/13 *Workshop on Reduced Order Modeling in General Relativity,* Caltech, *Plenary Talk*

Seminars and Colloquia Presented by P.I. Estep

11/06 North Carolina State University
11/06 University of North Carolina
4/07 University of Texas at Austin
8/07 Idaho National Laboratory
10/07 Lawrence Livermore National Laboratory
12/07 Columbia University
2/08 Natural Resource Ecology Laboratory
2/08 Rensselaer Polytechnic Institute
9/08 University of Colorado at Boulder
12/08 Idaho National Laboratory
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

III. PROFESSIONAL ACTIVITIES AND ACCOMPLISHMENT OF PROJECT PI

Awards

2007	Excellence in Teaching Award for Graduate Education and Mentoring, College of Natural Sciences, Colorado State University
2009-	University Interdisciplinary Research Scholar, Colorado State University
2009	Oliver P. Pennock Distinguished Service Award, Colorado State University
2011	University Scholarship Impact Award, Colorado State University

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 –

Principal Professional Appointments

- Member, *SIAM Education Committee,* 2006-2011
- Member, Department of Energy, *Applied Mathematics Strategic Plan Recommendation Panel*, 2008, report *Applied Mathematics at the U.S. Department of Energy: Past, Present, and Future* published by DOE and SIAM
- 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

- SIAM Book Committee, 2013-2016

Conferences Organized

2007	*SIAM Conference on Computational Science and Engineering,* invited minisymposium on *Graduate Education in Computational Science and Engineering*.
2007	*CSU Workshop on Small Angle X-ray Scattering in Biological Sciences,* with K. Luger and M. van der Woerd, Colorado State University
2008	*CSU Symposium on Imaging,* with O. Emanouilov, M. Kirby, and J. Mueller, Colorado State University
2008	*SIAM Annual Meeting,* invited minisymposium on *Computational Solution of Multiphysics Problems*, 6 sessions
2009	*SIAM Conference on Computational Science and Engineering,* invited minisymposium on *Graduate Education in Computational Science and Engineering – Needs, Trends, Risks, and Chances*
2009	*SIAM Annual Meeting, Organizing Committee*
2009	*Emerging Methods in Inverse Problems,* with J. Mueller, Colorado State University
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

Other Professional Service

- Panel Co-Leader, *Panel on Validation, Verification, Uncertainty Analysis and Decision Optimization, Department of Energy Computational Subsurface Sciences Workshop,* 2007. Coordinator for Priority Research Direction report "Uncertainty Representation, Uncertainty Propagation, and Sensitivity Analysis for Subsurface System". Contributor on two other Priority Research Direction reports. Final report: *http://subsurface2007.labworks.org/report/*
- 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