Final Technical Report

DOE Award #: DE-FG02-10ER26029; SC0004982

Recipient: University of Wyoming
Office of Research
Old Main, 1000 East University Avenue, Department 33
Laramie, WY 82071-2000

Project Title: Enabling Predictive Simulation and UQ of Complex Multiphysics PDE Systems by the Development of Goal-Oriented Variational Sensitivity Analysis and a-Posteriori Error Estimation Methods

Principal Investigator: Victor Ginting

Project Start: 09/01/2010

Project End: 08/31/2013

Date of Report: 03/15/2014

Period Covered: 09/01/2010-08/31/2013

Accomplishments:
Scientific discovery and technological design often focus on specific critical quantities of interest (QoIs) that are often expressed as functionals of the approximate solutions. Uncertainties in the approximate solutions (and hence in OoIs) arise from discretization errors, boundary and initial conditions, model and physical parameters. It is imperative to carefully quantify the uncertainties because the stability, error, uncertainty propagation and sensitivity characteristics for QoIs can be significantly different from the PDE solution itself. In the project, it was demonstrated that a posteriori analyses in general and in particular one that uses adjoint methods can accurately and efficiently compute numerical error estimates and sensitivity for critical QoIs that depend on a large number of parameters.

Many applications that are of interest to DOE are modeled by complex and coupled multiphysics multiscale nonlinear system of PDEs. It is highly improbable to calculate closed form solutions to this system. This enforces the use of numerical simulation techniques as a viable alternative to understand the prediction governed by these equations. To design accurate numerical simulations for solving the system, reliable quantification of errors associated with the approximation has to be developed appropriately.

Typical approximate solutions are obtained from careful combination of explicit and implicit methods. For reason of practicality and efficiency, it is often imperative to take into account the inherent time scales to inform how the governing system is to be discretized. The term “multirate” refers to the practice of using different time discretization in different component of the system in accordance with the scale exhibited in that component. Some of the components may be solved implicitly while others explicitly. It is not difficult to see the intricacy that one has to face and the need for quantifying the errors.

We have carried out several activities related to the proposed goals in the project:

1. The PIs, postdoc, and personnel involved in the project held a meeting at Colorado State University on September 26-27, 2011 and at Sandia National Laboratories on December 10-11, 2012. We have come up with an agreement on the various tasks assigned to each of the three institutions (SNL, CSU, UW). In particular, the UW has a close collaboration with CSU on the analysis and implementation of several time integration techniques for solving system of ODEs as typically obtained from spatial discretization of PDE systems.

2. Victor Ginting and Donald Estep (along with Simon Tavener) have published a paper on multirate integration methods for ordinary differential equations "*A Posteriori Analysis of a Multirate Numerical Method for Ordinary Differential Equations*", in CMAME. In this paper, we analyze a multirate time integration method for systems of ordinary differential equations that present significantly different scales within the components of the model. We interpret the multirate method as a multiscale operator decomposition method and use this formulation to conduct both an a priori error analysis and a hybrid a priori – a posteriori error analysis. The hybrid analysis has the form of a computable a posteriori leading order expression and a provably-higher order a priori expression. Both analyses distinguish the effects of the discretization of each component from the effects of multirate solution. The effects on stability arising from the multirate solution are reflected in perturbations to certain associated adjoint operators.

3. Victor Ginting, Donald Estep, Simon Tavener, and Jehanzeb Hameed have published a paper on the formulation and analysis of an iterative multi-discretization Galerkin finite element method for multi-scale reaction-diffusion equations: "*A Posteriori Analysis of an Iterative Multi-Discretization Method for Reaction-Diffusion Systems*" in CMAME. Subsystems in such reaction-diffusion equations may exhibit significantly different spatial and temporal scales, motivating a multi-discretization numerical method. We employed adjoint operators and variational analysis to form computable error estimates for a quantity of interest calculated from the multi-discretization finite element method. A key insight in analyzing the multi-discretization method is the realization that the adjoint operator associated with the iterative multi-discretization approximation is different from that of the original problem. Hence, our analysis utilizes two adjoint operators. One of the operators utilizes a different linearization than the one commonly used for nonlinear problems. The other adjoint is based on the property that our iterative multi-discretization Galerkin finite element method is a consistent discretization of the analytic iterative method. We derived a posteriori error estimates to quantify various sources of error in a quantity of interest computed from our iterative finite element method. We first derive estimates for the case when the different components of the system are solved on the same spatial mesh, and then extend the analysis to include distinct meshes. The error estimator has terms indicating errors arising from discretization of each component, finite iteration, differences between the two different adjoints and projection. We demonstrate how refining one or both meshes, or increasing the number of iterations can decrease the specific error components arising from a specific source. Hence our error estimates are useful not only for computing the total error in a quantity of interest, but also applicable in guiding an adaptive refinement strategy.

4. Victor Ginting and Chunjia Bi investigated an inexpensive postprocessing technique to estimate the error of finite element solution of the second-order quasi-linear elliptic problems measured in some global metrics. The proposed technique serves as an accuracy check of the approximation. The findings have been reported in "*Global Superconvergence and A Posteriori Error Estimates of Finite Element Method for Second-order Quasi-linear Elliptic Problems*" published in Journal of Computational and Applied Mathematics.

5. Victor Ginting and Chunjia Bi investigated an application of the residual-based a posteriori error estimates to symmetric interior penalty discontinuous Galerkin method for solving a class of second order quasi-linear elliptic problems. The reliability of the error estimator is established by deriving computable upper and lower bounds on the error measured in terms of a natural mesh-dependent energy norm. The findings have been reported in "*A Posteriori Error Estimates of Discontinuous Galerkin Method for Nonmonotone Quasi-linear Elliptic Problems*" published in Journal of Scientific Computing.

6. Victor Ginting, Donald Estep, Jehanzeb Hameed, and Simon Tavener have completed a posteriori analysis of explicit time integrations for system of linear ordinary differential equations. A class of these integrations can be expressed as fixed-point type iteration. To proceed with the analysis, our strategy is to cast the fixed-point iteration into an expression that is implicit and derive the associated adjoint using standard technique. The capability to write the fixed-point scheme as an implicit equation is made possible through the derivation of a solution operator relating the current iterate to the previous one, and by repeated application to the initial guess, which is usually is the approximate value from the previous time level. The implicit equation that is equivalent to the fixed-point iteration is then written as a composition of the solution operator. Upon comparing with the representation of the exact solution, we get an error equation that is expressed in terms of the difference between two adjoints, one associated with the true solution and the other associated with the fixed-point iteration approximate solution. The findings have been reported in "*A Posteriori Analysis for Iterative Solvers for Non-Autonomous Evolution Problems*" submitted to SIAM Journal of Uncertainty Quantification.

7. Implicit Explicit (IMEX) schemes are an important and widely used class of time integration methods for both parabolic and hyperbolic partial differential equations. The whole multi-institution team has derived accurate a posteriori goal oriented error estimates for a user-defined quantity of interest for two classes of first and second order IMEX schemes for advection-diffusion-reaction problems. We analyzed these by recasting the IMEX schemes into a variational form suitable for a posteriori error analysis employing adjoint problems and computable residuals. The a posteriori estimates quantify distinct contributions from various aspects of discretization, which can be used to evaluate discretization choices. The results have been reported in "*Adjoint Based A Posteriori Analysis of IMEX Time Integration Schemes for Partial Differential Equations*" submitted to SIAM Journal of Scientific Computing.

8. Other research activities:
   a) *Postprocessing finite element solution*: The standard finite element method in

the form of continuous Galerkin formulation using Lagrange basis has been widely used both in commercial applications and in research oriented simulators in the national laboratories. While versatile and robust, a major drawback in the standard finite element solutions is in its inability to satisfy the local conservation law. This is because the finite element solution is derived to satisfy a global property. Since many mathematical governing equations are directly derived from a local conservation principle, obtaining an approximate solution that honors this principle is crucial. It is then desirable to invent an efficient and accurate procedure that allows for the finite element solutions to satisfy local conservation property.

We have constructed of a numerical technique that *postprocesses* existing finite element solution and transform it into a quantity that satisfies a local conservation property pertaining to the original governing equations. The chief innovative trait of the approach is on its simplicity and parallelizability. It is simple because it only requires solving a very low dimensional linear system, for which in several important problems, its closed form solution can be readily obtained. It is the case that this linear system has to be solved for every geometrical object discretizing the domain on which the equation is defined. However, each of these low dimensional linear systems is independent of each other, making them readily suitable for parallel computing environment. Three research papers (two published and one under review) have resulted from this activity.

b) *A Bayesian Framework for Uncertain Quantification of Porous Media Flows*: Uncertainties about the detailed description of aquifer's characteristics are large contributors to the overall uncertainty in the predictive simulations. Reducing this uncertainty can be achieved by integrating additional data in the mathematical models. Integration of data from different sources is a nontrivial task because different data sources scan different length scales of heterogeneity and can have different degrees of precision. In particular, integration of dynamic data leads to an inverse problem. Such inverse problems are computationally intensive and typically require orders of magnitude more computation time compared to the forward simulation of flow and transport.

The nonlinearity of flow and transport thwarts direct computation of the probability distribution of aquifer characteristics. Instead, we infer the characteristics from a large number of realizations from the distribution consistent with flow predictions that, roughly speaking, agree with flow measurements. As expected with such inverse problems, the variability of the aquifer characteristics that are consistent with measured flow can be large. Hence, it is important to incorporate as much data as possible, and where data is lacking, to use our knowledge of the processes at hand to structure prior distributions for unmeasured quantities. For such complex situations, a Bayesian approach has proved to be the only practical solution for integrating data, models, and prior knowledge for a full accounting of uncertainty of all unknown quantities, including critical aquifer characteristics. Several publications have resulted from this activity.

V. Ginting carried out several activities, including

a. Supervised one postdoc and four Ph.D students. One of the students has completed his study and has been nomitated for the University of Wyoming Outstanding Dissertation Award.

b. Published the following papers in refereed journals:

   i. L. Bush, V. Ginting, M. Presho, Application of a Conservative, Generalized Multiscale Finite Element Method to Flow Models, *Journal of Computational and Applied Mathematics*, **260** (2014), pp. 395-409
   ii. C. Bi, V. Ginting, Global Superconvergence and A Posteriori Error Estimates of Finite Element Method for Second-order Quasi-linear Elliptic Problems, *Journal of Computational and Applied Mathematics*, **260** (2014), pp. 78-90
   iii. A. Francisco, V. Ginting, F. Pereira, J. Rigelo, Design and Implementation of a Multiscale Mixed Method Based on a Nonoverlapping Domain Decomposition Procedure, *Mathematics and Computers in Simulation*, **99** (2014), pp. 125-138
   iv. V. Ginting, F. Pereira, A. Rahunanthan, Rapid Quantification of Uncertainty in Permeability and Porosity of Oil Reservoirs for Enabling Predictive Simulation, *Mathematics and Computers in Simulation*, **99** (2014), pp. 139-152
   v. L. Bush, V. Ginting, On the Application of the Continuous Galerkin Finite Element Method for Conservation Problems, *SIAM Journal of Scientific Computing*, **35-6** (2013), pp. A2953-A2975
   vi. J. Chaudhry, D. Estep, V. Ginting, S. Tavener, A Posteriori Analysis of an Iterative Multi-Discretization Method for Reaction-Diffusion Systems, *Computer Methods in Applied Mechanics and Engineering*, **267** (2013), pp. 1-22
   vii. D. Estep, V. Ginting, S. Tavener, A Posteriori Analysis of a Multirate Numerical Method for Ordinary Differential Equations, *Computer Methods in Applied Mechanics and Engineering*, **223** (2012), pp. 10-27
   viii. V. Ginting, F. Pereira, A. Rahunanthan, A Multi-Stage Bayesian Prediction Framework for Subsurface Flows, *International Journal for Uncertainty Quantification*, **3** (2013) no. 6, pp. 499-522
   ix. C. Bi, V. Ginting, A Posteriori Error Estimates of Discontinuous Galerkin Method for Nonmonotone Quasi-Linear Elliptic Problems, *Journal of Scientific Computing*, **55** (2013), no. 3, pp. 659-687
   x. V. Ginting, F. Pereira, M. Presho, S. Wo, Application of the Two-stage Markov Chain Monte Carlo Method for Characterization of Fractured Reservoirs using a Surrogate Flow Model, *Computational Geosciences*, **15** (2011), no. 4, pp. 691-707
   xi. M. Presho, S. Wo, V. Ginting, Calibrated Dual Porosity, Dual Permeability Modeling of Fractured Reservoirs, *Journal of Petroleum Science and Engineering*, **77** (2011), no. 3-4, pp. 326-337

c. Published the following papers in refereed proceedings:

   i. P. Chatzipantelidis, V. Ginting, A Finite Volume Element Method for A Nonlinear Parabolic Problem, *Numerical Solution of Partial Differential Equations: Theory, Algorithms, and Their Applications, Springer Proceedings in Mathematics and Statistics*, **45** (2013), pp 121-136
   ii. V. Ginting, F. Pereira, A. Rahunanthan, Multiple Markov Chains Monte Carlo Approach for Flow Forecasting in Porous Media, *Procedia Computer Science*, **5** (2012), pp. 707-716

iii. V. Ginting, Time Integration Techniques for Richards Equation, *Procedia Computer Science*, **9** (2012), pp. 670-678
iv. V. Ginting, F. Pereira, A. Rahunanthan, Forecasting Production in an Oil Reservoir Simulation and Its Challenges, *Proceedings of ENUMATH 2012, the 9th European Conference on Numerical Mathematics and Advanced Applications*, Leicester - United Kingdom, September 2011 (A. Cangiani et al., eds.), Springer (2013), pp. 693-701

d. Gave the following presentations:
i. 2013, *A Multiscale Method Based on a Nonoverlapping Domain Decomposition Procedure, Minisymposium on Efficient Solvers for Heterogeneous Nonlinear Problems*, International Conference on Domain Decomposition Methods, Lugano, Switzerland
ii. 2013, *Application of Generalized Multiscale Finite Element Method in Multiphase Flow Model*, Minisymposium on Advanced Numerical Methods for PDEs and Applications, International Conference on Applied Mathematics, Modeling Computational Sciences, Waterloo, Ontario, Canada
iii. 2013, *Higher Order Multiscale Finite Element for Solving Problems With Heterogeneous Coefficients*, 4th International Congress on Computational Engineering and Sciences, Las Vegas, Nevada
iv. 2013, *An Adaptive Finite Element for Quasilinear Elliptic Problems*, Analysis and Applied Mathematics Seminar, University of Wyoming
v. 2013, *On the Application of Adjoint Methods in Subsurface Flow Simulations*, Minisymposium on Adjoint Methods for Computational PDEs, SIAM Conference on Computational Science and Engineering Boston, Massachusetts
vi. 2013, *A Multiscale Mixed Method Based on a Nonoverlapping Domain Decomposition Procedure*, Minisymposium on Numerical Analysis and Computation on Multiscale Problems, SIAM Conference on Computational Science and Engineering Boston, Massachusetts
vii. 2013, *On the Application of the Continuous Galerkin Finite Element Method for Solving Multiphase Flow*, invited speaker in Workshop on Numerical Methods for PDEs: In Occasion of Raytcho Lazarov's 70th Birthday, TAMU, College Station, Texas
viii. 2012, *An A Posteriori Analysis of Multirate and Multiscale Evolution Systems*, plenary speaker in the 5th LNCC Meeting on Computational Modeling, Petropolis, Brazil
ix. 2012, *Predictive Simulations for Porous Media Flows on GPUs*, Minisymposium on Recent Developments In Uncertainty Quantification For Multiphase Flows In Heterogeneous Subsurface Formations, 10th World Congress on Computational Mechanics, Sao Paolo, Brazil
x. 2012, *Operator Splitting Multiscale Finite Volume Element Method for Two-Phase Flow with Capillary Pressure*, Minisymposium on Recent Developments In Uncertainty Quantification For Multiphase Flows In Heterogeneous Subsurface Formations, 10th World Congress on Computational Mechanics, Sao Paolo, Brazil
xi. 2012, *Time Integration Techniques for Richards Equation*, International Conference on Computational Science (ICCS)
xii. 2012, *A Multiscale Mixed Method for Porous Media Flows*, 4th International Conference on Porous Media & Annual Meeting of the International Society for Porous Media (INTERPORE), Purdue University, West Lafayette, Indiana
xiii. 2012, *A Comparative Study on Reservoir Characterization using Two Phase Flow Model*, SIAM Conference on Uncertainty Quantification, Raleigh, North Carolina

xiv. 2011, *A Bayesian MCMC for Efficient Uncertainty Quantification in Permeability and Porosity of Reservoir Models*, International Conference on Mathematical Modeling in Industry, University of Sao Paulo, Sao Paulo, Brazil

xv. 2011, *A Posteriori Analysis of Operator Splitting*, Computational Mathematics and Multidisciplinary Science Seminar, Dept. of Mathematics, University of Wyoming

xvi. 2011, *A Bayesian Framework for Efficient Uncertainty Quantification in Permeability and Porosity of Reservoir Models*, The ninth European Conference on Numerical Mathematics and Advanced Applications (ENUMATH), Leicester University, United Kingdom

xvii. 2011, *An A Posteriori Analysis of Fixed Point Iteration for System of ODEs*, The seventh International Congress on Industrial and Applied Mathematics, Vancouver, British Columbia, Canada

xviii. 2011, *A Multiscale Modeling and Uncertainty Quantification in Porous Media Simulation*, Colloquium at the Department of Mathematics, Universitas Sumatera Utara, Medan, Indonesia

e. Serves as an advisory editor for Journal of Computational and Applied Mathematics (CAM)

f. Served in the NSF Panel, Arlington, VA