Defense Threat Reduction Agency
8725 John J. Kingman Road, MS 6201
Fort Belvoir, VA 22060-6201

DTRA-TR-14-33

TECHNICAL REPORT

A Posteriori Error Analysis and Uncertainty Quantification for Adaptive Multiscale Operator Decomposition Methods for Multiphysics Problems

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April 2014

HDTRA1-09-1-0036

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	**2. REPORT TYPE**	**3. DATES COVERED** *(From - To)*
	Technical	March 27, 2009 - April 5, 2013

4. TITLE AND SUBTITLE

A Posteriori Error Analysis and Uncertainty Quantification for Adaptive Multiscale Operator Decomposition Methods for Multiphysics Problems

5a. CONTRACT NUMBER
HDTRA1-09-1-0036

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

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5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

, Fort Collins, CO 80523

Department of Mathmatics, University of California San Diego 92103

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Defense Threat Reduction Agency
8725 John J. Kingman Road STOP 6201
Fort Belvoir, VA 22060
PM/James Reed

10. SPONSOR/MONITOR'S ACRONYM(S)
DTRA

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
DTRA-TR-14-33

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

This project was concerned with numerical solution and quantification of accuracy of numerical solution of multiphysics systems that couple together different physical processes acting across a long range of scales are encountered in virtually all areas of interest to Defense Threat Reduction Agency. The overall goal of this project was to develop a mathematically sound yet computationally practical methodology for estimating and mitigating the effects of error and uncertainty in information computed from numerical solutions of multiphysics problems. In addition, the proposed work provided computational tools for modern prediction, uncertainty quantification, parameter optimization, and verification and validation. A primary goal of this project was to construct a posteriori analysis framework for a number of multiphysics problems important to the DTRA mission. They used the results to devise innovative adaptive discretization algorithms. They also used the methods to develop and analyze fast methods for foward and inverse sensitivity analysis of multiphysics problems.

15. SUBJECT TERMS

multiphysics systems posterior error analysis adaptive error control stochastic sensitivity analysis

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			James Reed
Unclassified	Unclassified	Unclassified	UU	54	**19b. TELEPHONE NUMBER** *(include area code)* 703-767-8793

CONVERSION TABLE

Conversion Factors for U.S. Customary to metric (SI) units of measurement.

MULTIPLY →	BY →	TO GET
TO GET ←	BY ←	DIVIDE

angstrom	1.000 000 x E -10	meters (m)
atmosphere (normal)	1.013 25 x E +2	kilo pascal (kPa)
bar	1.000 000 x E +2	kilo pascal (kPa)
barn	1.000 000 x E -28	meter^2 (m^2)
British thermal unit (thermochemical)	1.054 350 x E +3	joule (J)
calorie (thermochemical)	4.184 000	joule (J)
cal (thermochemical/cm^2)	4.184 000 x E -2	mega joule/m^2 (MJ/m^2)
curie	3.700 000 x E +1	*giga bacquerel (GBq)
degree (angle)	1.745 329 x E -2	radian (rad)
degree Fahrenheit	$t_k = (t^\circ f + 459.67)/1.8$	degree kelvin (K)
electron volt	1.602 19 x E -19	joule (J)
erg	1.000 000 x E -7	joule (J)
erg/second	1.000 000 x E -7	watt (W)
foot	3.048 000 x E -1	meter (m)
foot-pound-force	1.355 818	joule (J)
gallon (U.S. liquid)	3.785 412 x E -3	meter^3 (m^3)
inch	2.540 000 x E -2	meter (m)
jerk	1.000 000 x E +9	joule (J)
joule/kilogram (J/kg) radiation dose absorbed	1.000 000	Gray (Gy)
kilotons	4.183	terajoules
kip (1000 lbf)	4.448 222 x E +3	newton (N)
kip/inch^2 (ksi)	6.894 757 x E +3	kilo pascal (kPa)
ktap	1.000 000 x E +2	newton-second/m^2 ($N-s/m^2$)
micron	1.000 000 x E -6	meter (m)
mil	2.540 000 x E -5	meter (m)
mile (international)	1.609 344 x E +3	meter (m)
ounce	2.834 952 x E -2	kilogram (kg)
pound-force (lbs avoirdupois)	4.448 222	newton (N)
pound-force inch	1.129 848 x E -1	newton-meter (N-m)
pound-force/inch	1.751 268 x E +2	newton/meter (N/m)
pound-force/foot^2	4.788 026 x E -2	kilo pascal (kPa)
pound-force/inch^2 (psi)	6.894 757	kilo pascal (kPa)
pound-mass (lbm avoirdupois)	4.535 924 x E -1	kilogram (kg)
pound-mass-foot^2 (moment of inertia)	4.214 011 x E -2	kilogram-meter^2 ($kg-m^2$)
pound-mass/foot^3	1.601 846 x E +1	kilogram-meter^3 (kg/m^3)
rad (radiation dose absorbed)	1.000 000 x E -2	**Gray (Gy)
roentgen	2.579 760 x E -4	coulomb/kilogram (C/kg)
shake	1.000 000 x E -8	second (s)
slug	1.459 390 x E +1	kilogram (kg)
torr (mm Hg, 0^0 C)	1.333 22 x E -1	kilo pascal (kPa)

*The bacquerel (Bq) is the SI unit of radioactivity; 1 Bq = 1 event/s.

**The Gray (GY) is the SI unit of absorbed radiation.

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Defense Threat Reduction Agency
Final Report

DTRA Grant: HDTRA1-09-0036

Title: *A Posteriori Error Analysis and Uncertainty Quantification for Adaptive Multiscale Operator Decomposition Methods for Multiphysics Problems*

Project Start Date: March 27, 2009
Project End Date: April 5, 2013

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1. Accomplishments

1.1. Summary of accomplishments

The mission of the Defense Threat Reduction Agency requires the quantitative study and accurate prediction for complex multiphysics systems that couple together physical processes spanning wide range of scales in behavior. Treatment of such systems depends on accurate numerical simulation of mathematical models expressed as systems of partial differential equations posed on domains with complicated geometry. Prediction of the behavior involves treating the propagation of stochastic uncertainty through the mathematical models and solving inverse problems for determining parameters based on observations on model output. Quantifying the accuracy of such computations requires accurate estimation of the numerical error in quantities of interest computed from numerical solutions that take into account all sources of error, e.g. from discretization, representation of geometry, finite sampling.

This project focuses on development of mathematical tools for dealing with these problems in the context of multiphysics models of interest using relevant numerical methods to the mission of the DTRA. The main approach is a posteriori error analysis based on computable residuals, solution of adjoint problems, and variational analysis. This approach estimates the error in specified quantities of interest. Computable residuals involving the approximate solution are used to quantify the size of various discretization errors while the solution of adjoint equations (generalized Green's functions) are used to quantify the effects of stability in producing errors. Much of the project dealt with dealing the significant mathematical issues that arise when numerically solving complex multiphysics models. Practical computational constraints requires the use of a wide variety of discretization approaches, e.g. operator decomposition and splitting, explicit time integration, iterative solution methods with few iterations, finite volume and specialized finite difference methods. The introduction of such techniques complicates both the identification of suitable residuals and definition of suitable adjoint problems. The project also dealt with issues arising in "multi-discretization" approaches, when various components of a coupled system are solved with different numerical methods and numerical grids. Another focus was the treatment of problems posed on complex domains, e.g. on manifold surfaces in space and/or on domains with complex boundaries. In this case, the goal was to treat the effects of inaccuracies and/or uncertainty in the representation of the domain geometry. Finally, we also establshed several rigorous convergence results for a class of goal-oriented adaptive methods that are designed to drivdriving the error in a specific quantity of interest below a given tolerance.

Along with theoretical development, the project studied the practical implementation of a posteriori error estimates for complex physics, including high performance issues. The project also addressed the question of efficient computation. The availability of accurate error estimates raises the ability to develop efficient adaptive error control algorithms in which various discretization parameters are adjusted based on relative contributions to the overall error in order to achieve a desired accuracy with minimal computational work. In another direct, the project expanded a posteriori error estimates for computed distributions and probabilities arising in computational sensitivity analysis and developed generalized adaptive algorithms that allow for balancing all sources of error and uncertainty affecting the analysis.

The project P.I.s' undertook a significant degree of interdisciplinary interaction during the projects in order to insure that project accomplishments would have impact in science and engineering.

1.2. Detailed descriptions of specific accomplishments

In this section, we describe specific technical accomplishments of the project.

A posteriori error analysis for a transient conjugate heat transfer

We analyzed the accuracy of an operator decomposition finite element method for a transient conjugate heat transfer problem consisting of two materials coupled through a common boundary. We derive accurate a posteriori error estimates that account for the transfer of error between compo-

nents of the operator decomposition method as well as the errors in solving the iterative system. We address a loss of order of convergence that results from the decomposition, and show that the order of convergence is limited by the accuracy of the transferred gradient information. We extend a boundary flux recovery method to transient problems and use it to regain the expected order of accuracy in an efficient manner. In addition, we use the a posteriori error estimates to adaptively compute the recovered boundary flux only within the domain of dependence for a quantity of interest.

A posteriori error estimation and adaptive mesh refinement for a multiscale operator decomposition approach to fluid-solid heat transfer

We analyze a multiscale operator decomposition finite element method for a conjugate heat transfer problem consisting of a fluid and a solid coupled through a common boundary. We derive accurate a posteriori error estimates that account for all sources of error, and in particular the transfer of error between fluid and solid domains. We use these estimates to guide adaptive mesh refinement. In addition, we provide compelling numerical evidence that the order of convergence of the operator decomposition method is limited by the accuracy of the transferred gradient information, and adapt a so-called boundary flux recovery method developed for elliptic problems in order to regain the optimal order of accuracy in an efficient manner. In an appendix, we provide an argument that explains the numerical results provided sufficient smoothness is assumed.

Nonparametric density estimation for randomly perturbed elliptic problems

We study the nonparametric density estimation problem for a quantity of interest computed from solutions of an elliptic partial differential equation with randomly perturbed coefficients and data. We derive an efficient method for computing samples and generating an approximate probability distribution based on Lion's domain decomposition method and the Neumann series. We then derive an a posteriori error estimate for the computed probability distribution reflecting all sources of deterministic and statistical errors. Finally, we develop an adaptive error control algorithm based on the a posteriori estimate. we extend the analysis to include a "modeling error" term that accounts for the effects of the resolution of the statistical description of the random variation and modify the adaptive algorithm to adapt the resolution of the statistical description. We also prove some related convergence results.

A posteriori error analysis for cell-centered finite volume methods for semilinear elliptic problems

We conduct a goal-oriented a posteriori analysis for the error in a quantity of interest computed from a cell-centered finite volume scheme for a semilinear elliptic problem. To carry out the analysis, we use an equivalence between the cell-centered finite volume scheme and a mixed finite element method with special choice of quadrature.

Blockwise adaptivity for time dependent problems based on coarse scale adjoint solutions

We describe and test an adaptive algorithm for evolution problems that employs a sequence of "blocks" consisting of fixed, though non-uniform, space meshes. This approach offers the advantages of adaptive mesh refinement but with reduced overhead costs associated with load balancing, re-meshing, matrix reassembly, and the solution of adjoint problems used to estimate discretization error and the effects of mesh changes. We describe several strategies to determine appropriate block discretizations from coarse scale solution information using adjoint-based a posteriori error estimates and demonstrate the behavior of the algorithms in a set of examples.

Conservative discretization and a posteriori error analysis for a cut cell diffusion problems with complex geometry

We study the solution of a diffusive process in a domain where the diffusion coefficient changes discontinuously across a curved interface. We consider discretizations that use regularly-shaped meshes, so that the interface "cuts" through the cells (elements or volumes) without respecting the regular geometry of the mesh. Consequently, the discontinuity in the diffusion coefficients has a strong impact on the accuracy and convergence of the numerical method. This motivates the

derivation of computational error estimates that yield accurate estimates for specified quantities of interest. For this purpose, we adapt the well-known adjoint based *a posteriori* error analysis technique used for finite element methods. In order to employ this method, we describe a systematic approach to discretizing a cut-cell problem that handles complex geometry in the interface in a natural fashion yet reduces to the well-known Ghost Fluid Method in simple cases. We test the accuracy of the estimates in a series of examples.

A measure-theoretic computational method for inverse sensitivity problems

We consider the inverse sensitivity analysis problem of quantifying the uncertainty of inputs to a deterministic map given specified uncertainty in a linear functional of the output of the map. This is a version of the model calibration or parameter estimation problem for a deterministic map. We assume that the uncertainty in the quantity of interest is represented by a random variable with a given distribution and we use the Law of Total Probability to express the inverse problem for the corresponding probability measure on the input space. Assuming that the map from the input space to the quantity of interest is smooth, we solve the generally ill-posed inverse problem by using the Implicit Function Theorem to derive a method for approximating the set-valued inverse that provides an approximate quotient space representation of the input space. We then derive an efficient computational approach to compute a measure theoretic approximation of the probability measure on the input space imparted by the approximate set-valued inverse that solves the inverse problem. We also treat the situation in which the output of the map is determined implicitly and is difficult and/or expensive to evaluate, e.g requiring the solution of a differential equation, and hence the output of the map is approximated numerically. The main goal is an a posteriori error estimate that can be used to evaluate the accuracy of the computed distribution solving the inverse problem taking into account all sources of statistical and numerical deterministic errors. We present a general analysis for the method and then apply the analysis to the case of a map determined by the solution of an initial value problem.

A posteriori analysis of multirate numerical methods for multiscale ordinary differential equations

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.

Convergence theory for goal-oriented adaptive methods

In the first of the convergence theory subprojects of the DTRA project, We developed a new convergence theory for a general class of adaptive approximation algorithms for nonlinear operator equations, and then used the theory to obtain convergence, contraction, and optimality results for practical adaptive finite element methods (AFEM) applied to several classes of nonlinear elliptic equations and systems of elliptic equations. The results can be viewed as extending the recent convergence results for linear problems of Morin, Siebert and Veeser, and of Nochetto et. al to more general nonlinear problems (with G. Tsogtgerel and Y. Zhu). We also develop new mathematical results for hierarchical error indicators to drive AFEM algorithms, and establish condition number estimates for appropriate preconditioners (with J. Ovall and R. Szypowski). We have further extended these results to the class of adaptive methods that were the target of this DTRA research probejct: goal-oriented adaptive methods that are designed to drive the error in a quantity of interest below a given tolerance. In 2009, Mommer and Stevenson developed a goal-oriented adaptive method for the Poisson equation, together with rigorous convergence and complexity results for their method, establishing what was apparently the first convergence result for a goal-oriented adaptive method. We have now extended the results of Mommer and Stevenson to goal-oriented

adaptive methods for general linear convection-diffusion elliptic problems (with S. Pollock). In a second manuscript, these results were further extended to a large class of scalar nonlinear problems (with S. Pollock and Y. Zhu). All three articles have now been posted on arXiv, submitted for publication, and are currently in review. All of the techniques are demonstrated for practical problems of interest using the FETK software (see below).

Analysis of multiphysics problems with complex domains

We analyzed a large class of regularized Navier-Stokes and Magnetohydrodynamics (MHD) models in three-dimensional spatial domains, a class which includes the Navier-Stokes equations, the Navier-Stokes-alpha model, the Leray-alpha model, the Modified Leray-alpha model, the Simplified Bardina model, the Navier-Stokes-Voight model, the Navier-Stokes-alpha-like models, and certain MHD models, in addition to representing a larger 3-parameter family of models not previously analyzed. We recovered a number of known results for established models, but also obtained new results for all models in this general family, including existence, regularity, uniqueness, stability, attractor existence and dimension, and existence of determining operators. (J. Nonlinear Science 2009, with E. Lunasin and G. Tsogtgerel.)

We then develop and analyze numerical methods for approximation of stationary and evolution problems on surfaces, including coupled elliptic-parabolic systems. A major theoretical breaktrough was showing how the recent finite element error estimates of Demlow and Dziuk can be recovered from a more general approach involving the analysis of variational crimes in Hilbert complexes, generalizing their results for surface finite elements to arbitrary spatial dimension and to applications involving higher-dimensional differential forms and both linear and nonlinear equations. This generalization was made possible through the use and extension of *finite element exterior calculus (FEEC)*. (Found. Comput. Math. 2012, with A. Stern.) We have now extended this work in FEEC in the direction of time-dependent problems; we completed and submitted a new manuscript in 2012 that extends these results on surface finite element methods to scalar parabolic and hyperbolic problems, including again nonlinear problems (with A. Gillette). We also give an analysis of the singularities in a fundamentally important model in biochemistry, and develop a number of AFEM-based numerical techniques for treating these degenerate features in a provably high-fidelity way (Comm. Comput. Phys. 2012, with J. McCammon, Y. Zhou, Y. Zhu, Z. Yu).

In addition, we have developed and implemented goal-oriented, adjoint-based, a posteriori error estimates for elliptic problems on smooth manifolds. In particular, the estimates take into account the effects of domain curvature on accuracy. We also considered the problem of small random perturbations to the manifold, pointing the way to treat problems in which the domain is determined experimentally or by measurement. This work is nearing completion and will be submitted in Summer 2012 (with W. Newton)

Analysis of elliptic problems on domains with randomly perturbed boundaries

We developed a systematic approach to solve elliptic problems on domains that have randomly perturbed boundaries, after first classifying such problems into several different classes. The results are particularly relevant to situations in which the boundaries are obtained through measurement or are subject to error. The approach avoids the need to remesh each new domain in a random sampling Monte Carlo solution. Moreover, we derive a posteriori error estimates that indicate how random perturbations in the boundary affect the accuracy of computed solutions.

A posteriori error analysis of explicit, IMEX, and truncated Picard iteration time integration methods

Explicit, Implicit/Explicit (IMEX), and truncated Picard iteration time integration methods are widely employed to solve multiphysics applications in defense and department of energy enterprises, e.g. such as reacting flows. Such methods requires significant alterations for a posteriori error analysis in order to describe the effects of these approaches on both stability and accuracy. Therefore, last year we undertook the systematic study of a posteriori error analysis for explicit, truncated Picard iteration, and implicit/explicit (IMEX) time integration methods. For explicit

methods, we introduce special projection operators into the standard finite element formulation for evolution problems. These projection operators are (1) a truncated Taylor expansion computed at a past time node and (2) extrapolation from a interpolatory polynomial using values at a collection of previous nodes. We then alter the a posteriori error analysis to include terms that measure the effects of these projections, yielding distinct "explicit" time integration terms in the a posteriori error analysis. We recently have extended this approach to treat IMEX methods. To analyze truncated Picard iteration methods, we exploit an old result of H. Keller and J. Keller for the "matricant", which is the exponential form of the solution operator of a linear ***non-autonomous*** evolution problem. This provides a way to define the adjoint for a solution obtained by truncated Picard iteration, which we then use in the a posteriori error analysis. We have also extended this analysis to implicit methods that employ Jacobi iteration to solve the systems at each step.

Coupled parabolic-elliptic systems

Estep and Holst collaborated on the development methods and a posteriori error analysis for coupled parabolic-elliptic systems of equations. The main application is on modeling of black holes. A new development in the Holst group has been the extension of their recent work on finite element exterior calculus to parabolic and hyperbolic problems (completed and submitted in 2012), which will provide a very strong mathematical framework for the development of methods and a posteriori analysis for coupled parabolic-elliptic problems. This extension to FEEC is now being combined with our recent work on goal-oriented adaptive methods using a variational framework, by which the elliptic component of the system is combined with implicit time-stepping schemes to provide "constraints" in a Lagrange multiplier formulation. We are able to show convergence for the adaptive scheme, generalizing our recent work on convergence theory for goal-oriented adaptive methods (with S. Pollock, Y. Zhu).

Coupled ordinary differential equation - parabolic differential equation

Estep and Hameed (along with collaborators) derived and implemented a posteriori error estimates for systems of evolution equations consisting of a reaction-diffusion problem posed on a global domain coupled to systems of ordinary differential equations in a collection of small cells partitioning the global domain. The local cell problems model chemical reactions that determine the local physical conditions driving the parabolic problem. The analysis takes into account the iteration error in solving the coupled systems.

New approaches to adaptive error control for evolution problems

Estep and Hameed (along with collaborators) developed new adaptive error control algorithms that take into account cancellation of errors to improve efficiency. The approach identifies periods of time over which there is significant cancellation. Inside the regions, uniform refinements are used to preserve the favorable cancellation, while the time step sizes in the various regions are adjusted according to the contribution to the overall error from the regions.

Implementation of theoretical results

The last major goal in this project is implementation of the theoretical results into the FETK code. For this purpose, we recruited a full time postdoc, Ryan Szypowski, working at UCSD under the supervision of co-PI Michael Holst with responsibility to carry out the implementation and testing. He is being jointly supervised by the PI D. Estep. This FETK deveopment has focused on providing a robust, theory-based convergent adaptive finite element implementation for nonlinear problems which retains linear complexity. This has included work on the following specific components, which have been implemented in both the MATLAB subset FETKLab of the 2D code in FETK as well as in the full 2D/3D code in FETK:

1. The element marking strategy was updated to be based on "Dorfler Marking". Special care was taken to use a linear-time complexity binning approach as opposed to an actual sort. Only this type of marking strategy, which is not often used in practice due to its potential costs unless carefully implemented, allows for establishing both convergence and linear overall computational complexity of the adaptive algorithms.

2. A number of new error estimators were added. They include:

   (a) A hierarchical error estimator based on face-bump functions which was proven in our recent publications to be efficient, reliable, and robust. This work included the addition of a new cubic bump finite element space, which led to a better understanding of how we can improve the finite element space implementation to allow for future additions.

   (b) An error estimator based on the solution of a dual problem, which we refer to as dual-weighted residual (DWR). This implementation involved leveraging the work on the bump-function library above, as well as the development of high-order quadrature rules, and the ability to maintain two distinct and unrelated adaptive meshes during a computation, with quantities being projected back and forth between the meshes as needed.

   (c) An error estimator based on smoothed gradients. This is based on recent work of R. Bank and J. Xu, collaborators of the PIs.

3. W. Newton, co-advised by Estep and Holst, implemented the a posteriori error estimates that account for error in the description of the manifold on which the problem is posed developed in his thesis.

4. A driver application for solving nonlinear problems using inexact Newton solvers based on a multilevel approach was written. This has been used for most of the problems described above.

5. Prior to 2013, FETK and the FETKLab MATLAB subset of FETK were primarily based on linear finite element discretizations, with enough partial support for higher-order elements to allow for the use of e.g. bump functions in error indicators and formulation of dual problems. A general element class was developed in early 2013 to allow for use of any type of Lagrange-type element for either the primarl or dual problem. Both linear and quadratic elements were then implemented and are provided with the FETK code base as element examples. Our recent manuscripts with new convergence results for goal-oriented methods contain a large collection of numerical examples that now exploit this infrastructure to carefully compare a number of adaptive methods based on goal functions (with S. Pollock and Y. Zhu).

2. Training and Professional Development

The support of this project has partially contributed to the training and professional development for three graduate students and three postdocs. This includes specialized research-level instruction and individual mentoring as well as participation in large research group activities directed by the PIs. Students and postdocs were encouraged to participate in professional meetings and to interact with researchers in other universities and in national DOE laboratories as appropriate. Students and postdocs were trained to write and prepare and deliver professional presentations.

Details for the trainees:

- Will Newton received his Ph.D. from CSU in 2011, and then was hired as a Research Scientist Class I in PI Estep's group. His primary focus is a project on multiscale models of new nuclear fuels supported by a contract from Idaho National Laboratory. He has continued to work on research related to this project following up on the work in his thesis. Thesis is "A Posteriori Error Estimates for the Poisson Problem on Closed, Two-Dimensional Surfaces", available from Colorado State University Library.

- Nate Burch received his Ph.D. from CSU in 2011, and then took a two year postdoc position at SAMSI (Statistical and Mathematical Sciences Institute) as part of the Program on Uncertainty Quantification. Thesis is "Probabilistic Foundation of Nonlocal Diffusion

and Formulation and Analysis for Elliptic Problems on Uncertain Domains", available from Colorado State University Library.

- The CSU postdoc Jehanzeb Hameed is in the second year of his position in PI Estep's group. His primary focus is a project on a Department of Energy Uncertainty Quantification project that is jointly conducted with Sandia National Laboratory. Part of his research is related to the activities supported in this project.

- Jonny Serencsa received his Ph.D. from UCSD in 2012, and has been doing pre- and post-doctoral work at UC Davis. His doctoral work was jointly supervised by PI Holst and S. Shkoller at UC Davis, and he is currently working for a startup company in the Bay Area.

- Ryan Szypowski received his Ph.D. from UCSD in 2008, and remained at UCSD working with Holst as a postdoc and then research scientist until 2012. He moved to a tenure-track position in the Mathematics Department at Cal Poly Pomona in Fall 2012.

- Andrew Gillette received his Ph.D. from UT Austin in 2011, and joined Holst's group at UCSD as a postdoctoral fellow in Fall 2011. He helped push forward both the the project involving Ryan Szypowski, and the development of an FEEC-based error analysis framework for parabolic and hyperbolic problems. In Fall 2013, Andrew is starting a tenure-track faculty position in the mathematics department at the University of Arizona.

- Sara Pollock received her Ph.D. from UCSD 2012, and remained at UCSD working with Holst as a postdoc during the 2012-2012 academic year. In Fall 2013, Sara is starting a 3-year named postdoctoral position in the mathematics department at Texas A&M.

3. Dissemination

We have disseminated the research in this project through submission of peer-reviewed research articles, presenting many invited talks at universities and conferences, and publishing software developed in this project for public access. A summary of this activity during this project:

- 53 research articles related to the project research have appeared or are accepted

- 19 research articles related to the project research are currently under review

- 5 book and/or book chapters have appeared or are being written

- 60 invited lectures at universities and professional meetings

Applications to multiscale/multiphysics physical and engineering systems

In conjunction with collaborators in engineering, chemistry and biophysics, we have applied many of the algorithms and techniques for multiphysics and multiscale problems developed in this DTRA-supported research program. Our focus continues to be on applications in material, chemical and biological physics of relevance to DOD, DTRA, and DOE missions. In addition to our publications placed in the mathematics literature, we have placed joint publications from these research collaborations with physical scientists and engineers in a broad spectrum of leading scientific journals to maximize the impact of our results, including: *Physical Review Letters*, *Physical Review D*, *Journal of Nonlinear Science*, *Classical and Quantum Gravity*, *Journal of Chemical Theory and Computation*, *Journal of Cell Science*, *Journal of Structural Biology*, *Biophysical Journal*, *PLoS Computational Biology*, *IMA Journal on Applied Mathematics*, *Computer Aided Geometric Design*, *BIT*, *Applied Numerical Mathematics*, *IEEE Journal on Engineering in Medicine and Biology*, *IEEE Transactions on Biomedical Computing*, *Frontiers in Computational Physiology and Medicine*, *Investigative Ophthalmology and Visual Science*, *Journal of Scientific Computing*, *Journal of Applied Mathematics and Computation*, *Communications in Computational Physics*,

Journal of Molecular Graphics and Modeling, *Journal of Physical Chemistry B*, *Journal of Chemical Physics*, *Communications in Mathematical Physics*, *Annals of Nuclear Engineering*, *Journal of Computational Physics*, *Acta Biomaterialia*, *Computer Methods in Applied Mechanics and Engineering*, *Journal of Engineering Mathematics*, and *Foundations of Computational Mathematics*.

4. Products

4.1. Publications, conference papers, and presentations

The following papers were accepted or appeared during March 27, 2009 - September 1, 2009

- *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

- *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

- *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

- *Solving the Einstein constraints on multi-block triangulations using finite elements*, O. Korobkin, B. Aksoylu, M. Holst, E. Pazos, and M. Tiglio, Class. Quant. Grav. 26 (2009), No. 14, 145007 (28 pp). (arXiv:gr-qc/0801.1823)

- *An adaptive finite element method for solving the exact Kohn-Sham equation of density functional theory*, E. Bylaska, M. Holst, and J. Weare, Journal of Chemical Theory and Computation, 5 (2009), pp. 937–948.

- *Finite Element Analysis of Drug Electrostatic Diffusion: Inhibition Rate Studies in N1 Neuraminidase*, Y. Cheng, M. Holst, and J.A. McCammon, Biocomputing 2009: Proceedings of the Pacific Symposium, R.B. Altman, A.K. Dunker, L. Hunter, T. Murray, and T.E. Klein, eds., 2009, pp. 281-292.

- *Three-dimensional reconstruction reveals new details of membrane systems for calcium signaling in the heart*, T. Hayashi, M.E. Martone, Z. Yu, A. Thor, M. Doi, M. Holst, M.H. Ellisman, and M. Hoshijima, J. Cell Sci., Vol. 122 (April, 2009), No. 7, pp. 1005-1013.

- *Rough Solutions of the Einstein Constraints on closed manifolds without near-CMC conditions*, M. Holst, G. Nagy, and G. Tsogtgerel, Comm. Math. Phys., Vol. 288 (June 2009), No. 2, pp. 547-613. (arXiv:gr-qc/0712.0798)

- *Multi-Scale Modeling of Ventricular Myocytes: Contributions of structural and functional heterogeneities to excitation-contraction coupling in the normal and failing rodent heart*, S. Lu, A. Michailova, J. Saucerman, Y. Cheng Z. Yu, T. Kaiser, W. Li, R. Bank, M. Holst, A. McCammon, T. Hayashi, M. Hoshijima, P. Arzberger, and A. McCulloch, IEEE Journal on Engineering in Medicine and Biology, Vol. 28 (March-April 2009), No. 2, pp. 46-57.

- *Convergence and Optimality of Adaptive Mixed Finite Element Methods*, L. Chen, M. Holst, and J. Xu, Math. Comp., Vol. 78 (2009), No. 265, pp. 33-53.

The following papers were accepted or appeared during September 2, 2009 - September 1, 2010

- *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

- *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

- *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

- *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

- *Numerical analysis of Ca2+ signaling in rat ventricular myocytes with realistic transverse-axial tubular geometry and inhibited sarcoplasmic reticulum*, Y. Cheng, Z. Yu, M. Hoshijima, M. Holst, A. McCulloch, and J. M. ad A.P. Michailova, PLoS Computational Biology, 6 (2010), pp. e1000972:1–16.

- *Poisson-Nernst-Planck equations for simulation biomolecular diffusion-reaction processes I: Finite element solutions*, B. Lu, M. Holst, J. McCammon, and Y. Zhou, J. of Comput. Phys. 229 (2010), 6679-7794 (16 pp).

- *Analysis of a general family of regularized Navier-Stokes and MHD models*, M. Holst, E. Lunasin, and G. Tsogtgerel, J. Nonlin. Sci., 20 (2010), pp. 523–567.

The following book chapter appeared during September 2, 2009 - September 1, 2010

- *Error estimation for multiscale operator decomposition for multiphysics problems*, D. Estep, Chapter 11, in *Bridging the Scales in Science and Engineering*, J. Fish, editor, Oxford University Press, 2010

The following books were under contract or appeared during September 2, 2009 - April 5, 2013

- *Practical Analysis in Many Variables*, D. Estep, SIAM, 2010.

- *Green's Functions and Boundary Value Problems, Third Edition*, I. Stakgold and M. Holst, John-Wiley, 888 pages, February 2011.

The following nonrefereed papers appeared during September 2, 2009 - September 1, 2010

- *CSE 2009: Graduate Education in CSE - Structure for the Zoo?*, H.-J. Bungartz and D. Estep, SIAM News 42, 2009

- *Computational Science and Engineering Education: SIAM's Perspective*, H.-J. Bungartz, D. Estep, U. Rude, and P. Turner, IEEE Computing in Science and Engineering 11 (2009), 5-11

- *Interview with Chief Editor of the SIAM CSE Book Series*, D. Estep, SIAM News 43 (2010)

The following papers were accepted or appeared during September 2, 2010 - September 1, 2011

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

- *A posteriori error analysis for a cut cell finite volume method*, D. Estep, S. Tavener, M. Pernice, H. Wang, Computer Methods in Applied Mechanics and Engineering, 2010, 233 (2009), 459-472

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

- *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

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

- *An efficient, reliable and robust error estimator for elliptic problems in* $\mathbb{R}^3$, M. Holst, J. Ovall, and R. Szypowski, Applied Numerical Mathematics, 61 (2011), 675695

- *Efficient mesh optimization schemes based on optimal delaunay triangulations*, L. Chen and M. Holst, Computer Methods in Applied Mechanics and Engineering 200 (2011), 967984

- *Adaptive finite element modeling techniques for the Poisson-Boltzmann equation*, M. Holst, J. McCammon, Z. Yu, Y. Zhou, and Y. Zhu, Communications in Computational Physics, 11 (2012), pp. 179–214.

- *Convergence analysis of finite element approximations of the Joule heating problem in three spatial dimensions*, M. Holst, M. Larson, A. Malqvist, and R. Soderlund, BIT, 50 (2010), pp. 781–795.

- *Semilinear mixed problems on Hilbert complexes and their numerical approximation*, M. Holst AND A. Stern, Foundations of Computational Mathematics, 2010, 12 (2012), pp. 363–387

- *Adaptive solution of the Poisson-Boltzmann equation using goal-oriented error indicators*, B. Aksoylu, S. Bond, E. Cyr, AND M. Holst, J. Sci. Comput. 52 (2012), 202-225 (23 pp).

The following papers were accepted or appeared during September 2, 2011 - September 1, 2012

- *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)

- *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

- *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

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

- *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

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

- *Geometric variational crimes: Hilbert complexes, finite element exterior calculus, and problems on hypersurfaces*, M. Holst and A. Stern, Foundations of Computational Mathematics, 12 (2012), pp. 263–293.

- *Multi-scale modeling of calcium dynamics in ventricular myocytes with realistic transverse tubules*, Z. Yu, G. Yao, M. Hoshijima, A. Michailova, and M. Holst, IEEE TBME Letters, Special Issue on Multi-Scale Modeling and Analysis for Computational Biology and Medicine, 58 (2011), No. 10, 2947-2951 (4 pp).

- *Multiscale continuum modeling and simulation of biological processes: From molecular electro-diffusion to sub-cellular signaling transduction*, Y. Cheng, M. Holst, J. McCammon, and A. Michailova, Comput. Sci. Disc., 5 (2012), 015002-015015 (13 pp).

- *The Navier-Stokes-Voight model for image inpainting*, M. Ebrahimi, M. Holst, and E. Lunasin, IMA J. Appl. Math., doi:10.1093/imamat/hxr069 (2012), 1-26 (26 pp).

- *Numerical bifurcation analysis of conformal formulations of the Einstein constraints*, M. Holst and V. Kungurtsev, Phys. Rev. D, 84 (2011), pp. 124038(1)–124038(8).

- *Modeling cardiac calcium sparks in a three-dimensional reconstruction of a calcium release unit*, J. Hake, A. Edwards, Z. Yu, P. Kekenes-Huskey, A. Michailova, A. McCammon, M. Holst, M. Hoshijima, and A. McCulloch, J. Physiol., 590 (2012), No. 18, 4403-4422 (18 pp).

- *Localized glaucomatous change detection within the proper orthogonal decomposition framework*, M. Balasubramanian, D. Kriegman, C. Bowd, M. Holst, R. Winreb, P. Sample, and L. Zangwill, Invest. Ophthalmol. Vis. Sci., 53 (2012), No. 7, 3615-3628 (14 pp).

- *Quality tetrahedral mesh smoothing via boundary-optimized Delaunay triangulation*, Z. Gao, Z. Yu, and M. Holst, Computer Aided Geometric Design, 29(9):707-721, 2012.

- *Modeling effects of L-type Ca2+ current and Na+-Ca2+ exchanger on Ca2+ trigger flux in rabbit myocytes with realistic T-tubule geometries*, P. Kekenes-Huskey, Y. Cheng, J. Hake, F. Sachse, J. Bridge, M. Holst, J. McCammon, A. McCulloch, and A. Michailova, Frontiers in Physiology, 3 (2012), pp. 1–14.

The following papers were accepted, appeared or were submitted and still pending review during September 2, 2011 - September 1, 2012

- *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

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

- *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

- *Multilevel preconditioners for discontinuous Galerkin approximations of elliptic problems with jump coefficients*, B. Ayuso de Dios, M. Holst, Y. Zhu, and L. Zikatanov, in Proceedings of the Twentieth International Conference on Domain Decomposition Methods, San Diego, USA, San Diego, CA, USA, February 2011.

- *Local multilevel preconditioners for elliptic equations with jump coefficients on bisection grids*, L. Chen, M. Holst, J. Xu, and Y. Zhu, Submitted for publication.

- *Local convergence of adaptive methods for nonlinear partial differential equations*, M. Holst, G. Tsogtgerel, and Y. Zhu, Submitted for publication.

- *The Lichnerowicz equation on compact manifolds with boundary*, M. Holst and G. Tsogtgerel, Submitted for publication.

- *Adaptive finite element methods with inexact solvers for the nonlinear Poisson-Boltzmann equation*, M. Holst, R. Szypowski, and Y. Zhu, in Proceedings of the Twentieth International Conference on Domain Decomposition Methods, San Diego, USA, San Diego, CA, USA, February 2011.

- *Barrier methods for critical exponent problems in geometric analysis and mathematical physics*, J. Erway and M. Holst, Submitted for publication.

- *Finite element error estimates for critical exponent semilinear problems without angle conditions*, R. Bank, M. Holst, R. Szypowski, and Y. Zhu, Submitted for publication.

- *Convergence and optimality of goal-orientied adaptive finite element methods for nonsymmetric problems*, M. Holst and S. Pollock, Submitted for publication.

- *Generalized solutions to semilinear elliptic PDE with applications to the Lichnerowicz equation*, M. Holst and C. Meier, Submitted for publication.

- *Finite element exterior calculus for evolution problems*, A. Gillette and M. Holst, Submitted for publication.

- *Two-grid methods for semilinear interface problems*, M. Holst, R. Szypowski, and Y. Zhu, Accepted for publication in Numer. Methods Partial Differtial Equations.

- *Convergence of goal-oriented adaptive finite element methods for semilinear problems*, M. Holst, S. Pollock, and Y. Zhu, Submitted for publication.

- *Feature-preserving surface mesh smoothing via suboptional Delaunay triangulation*, Z. Gao, Z. Yu, and M. Holst, Graphical Models, 75 (2013), pp. 23–38.

The following papers were accepted, appeared or were submitted and still pending review during September 2, 2012 - April 5, 2012

- *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.

- *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

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

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

- *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

- *Convergence and optimality of adaptive methods in the Finite Element Exterior Calculus framework*, M. Holst, A. Mihalik, and R. Szypowski, Submitted for publication.

- *An alternative between non-unique and negative yamabe solutions to the conformal formulation of the einstein constraint equations*, M. Holst and C. Meier, Submitted for publication.

- *Non-uniqueness of solutions to the conformal formulation*, M. Holst and C. Meier, Submitted for publication.

- *Efficient computational in multiscale geometric modeling for biomolecular complexes*, T. Liao, Y. Zhang, P. Kekenes-Huskey, A. Michailova, M. Holst, and J. A. McCammon, Submitted for publication.

- *Multilevel preconditioners for discontinuous Galerkin approximations of elliptic problems with jump coefficients*, B. Ayuso de Dios, M. Holst, Y. Zhu, and L. Zikatanov, Accepted for publication in Math. Comp.

4.2. *Presentations at meetings, conferences, seminars*

The following presentations were made during March 27, 2009 - September 1, 2009

Burch: Research Seminar, Sandia National Laboratory, Albuquerque, New Mexico, 8/09

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

Estep: SIAM Annual Meeting, Minisymposium on Predictive Computational of Multiscale-Multiphysics Applications, invited speaker, 7/09

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

Estep: Colloquium, Department of Mathematics, University of Wyoming, 9/09

Holst 25th Pacific Coast Gravity Meeting (PCGM25), Eugene, Oregon, 4/09

Holst: 5th Annual Structured Integrators Workshop, Caltech, Pasadena, California, Plenary Speaker, 5/09

Holst: FEniCS 2009 Workshop, Oslo, Norway, Plenary Speaker, 6/09

Holst: Numerische Mathematik 50, Munich, Germany, Plenary Speaker, 6/09

Holst: Mathematical and Numerical Geometric Analysis Workshop, Frieburg, Germany, Plenary Speaker, 9/09

Holst: ICNAAM Conference, Crete, Greece, Minisymposium Speaker, 9/09

Serencsa: CSME Seminar Series, UC San Diego, San Diego, California, 6/09

The following presentations were made during September 2, 2009 - September 1, 2010

Burch: *ICMS Workshop on Uncertainty Quantification*, Edinburgh, UK, 05/10

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

Estep: Seminar, Lawrence Livermore National Laboratory, 12/09

Estep: Colloquium, Department of Atmospheric Science, Colorado State University, 1/10

Estep: Seminar, University of Wisconsin, 2/10

Estep: Seminar, Brown University, 3/10

Estep: Seminar, University of Chicago, 3/10

Serencsa: CCoM Seminar Series, UC San Diego, San Diego, California, 11/09

Holst: Plenary Lecture, Symposium on Mathematical Systems Biology, UCI, Irvine, California, 1/10

Holst: Lecture, 26th Pacific Coast Gravity Meeting (PCGM26), San Diego, CA, 3/10

Holst: Plenary Lecture, Workshop on Unstructured Mesh Methods in Mathematical Physics, Jena, Germany, 8/10

Holst: Invited Lecture, Department of Mathematics, Free University of Berlin, Berlin, Germany, 8/10

Holst: Invited Lecture, Department of Mathematics, Technical University of Berlin, Berlin, Germany, 8/10

Holst: Invited Lecture, Department of Mathematics, Jacobs University, Brehmen, Germany, 9/10

The following presentations were made during September 2, 2010 - September 1, 2011

Estep: *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, 2011

Estep: Seminar, Lawrence Livermore National Laboratory, 9/10

Estep: Seminar, Purdue University, 9/10

Estep: Seminar, North Carolina State University, 11/10

Estep: Seminar, Lawrence Livermore National Laboratory, 1/11

Estep: Seminar, University of Southern California, 3/11

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

Holst: Invited Lecture, Department of Mathematics, Jacobs University, Bremen, Germany, 9/10

Holst: Invited Lecture, Workshop on Latest Trends and Developments in Computational Technology and Methods for Solids, Structures, Fluids and Fluid-Structure Interaction, La Jolla, CA, 9/10

Holst: Invited ICES Lecture, University of Texas, Austin, TX, 2/11

Holst: Invited CVS Lecture, University of Texas, Austin, TX, 2/11

Holst: Colloquium, Department of Mathematics, University of Wisconsin, Madison, WI, 4/11

Holst: Colloquium, Department of Mathematics, The Penn State University, State College, PA, 4/11

Holst: Colloquium, Department of Applied Mathematics, University of Washington, Seattle, WA, 5/11

Holst: Seminar, Pacific Northwest National Laboratory, Richland, WA, 5/11

Holst: Plenary Lecture, Workshop on Advances and Challenges in Computational General Relativity, Brown University, Providence, RI, 5/11

Holst: Invited Lecture, Schnelle Löser für partielle Differentialgleichungen, Mathematisches Forschungsinstitut Oberwolfach, Oberwolfach, Germany, 5/11

The following presentations were made during September 2, 2011 - September 1, 2012

Estep: Invited Lecture, Uncertainty Quantification for High-Performance Computing Workshop, Oak Ridge National Laboratory, 5/12

Estep: Invited Lecture, 6th International Conference on Automatic Differentiation, Fort Collins, CO, 7/12

Estep: Invited Paper, Joint Statistical Meetings, 8/12

Estep: Invited Seminar, University of Chicago, 9/11

Estep: Invited Seminar, Florida State University, 4/12

Estep: Invited Seminar, Colorado School of Mines, 4/12

Estep: Invited Colloquium, Statistical and Applied Mathematical Sciences Institute (SAMSI), 4/12

Holst: Invited Lecture, Workshop on Geometric Partial Differential Equations: Theory, Numerics and Appli- cations, Mathematisches Forschungsinstitut Oberwolfach, Oberwolfach, Germany, 11/11

Holst: Invited Lecture, JTO Faculty Fellowship Lecture (1 of 2), Institute for Computational Engineering and Science (ICES), University of Texas, Austin, TX, 11/11

Holst: Invited Lecture, JTO Faculty Fellowship Lecture (2 of 2), Institute for Computational Engineering and Science (ICES), University of Texas, Austin, TX, 1/12

Holst: Plenary Lecture, CSU Research Colloquium, Physics at CSU: Neutrinos to Nano Science, Colorado State University, Fort Collins, CO, 3/12

Holst: Plenary Lecture, 21st International Conference on Domain Decomposition Methods, Rennes, Frances, 6/12

The following presentations were made during September 2, 2012 - April 5, 2013

Pollock: Center for Computational Mathematics Seminar, UCSD, San Diego, CA, 1/13.

Pollock: Joint MAA-AMS Mathematics Meetings, San Diego, CA, 1/13.

Pollock: Numerical analysis seminar, Texas A&M University, College Station, TX, 4/13.

Pollock: CSME Seminar, UCSD, San Diego, CA, 4/13.

Pollock: Minisymposium Lecture, SIAM Annual Meeting, San Diego, CA, 7/13.

4.3. Websites

Research results and software are presented at

- http://www.stat.colostate.edu/~estep/
- http://ccom.ucsd.edu/~mholst/

4.4. Technologies and techniques

Over the last several years, our DTRA-supported research team has led the development of the Finite Element ToolKit, which is an opensource finite element modeling toolkit designed for the simulation of coupled multiphysics problems with multiscale phenomena. The software has been designed and developed collaboratively by both Holst and Estep, and consists of a collection of object-oriented class libraries written in C, C++, Objective C, and Python. There is also a MATLAB/Octave-based prototyping tool (FETKLab), the development of which has been done by both Estep and Holst, as well as several of their graduate students. FETK (and FETKLab) are designed to adaptive discretize and solve coupled reaction-diffusion systems, and is based around state-of-the-art algorithms for simplex mesh generation, error estimation, mesh refinement, finite element discretization, iterative nonlinear and optimization techniques, and fast multilevel and domain decomposition-based linear solvers and preconditions. Many of the algorithms developed in our research articles as described in this report have been prototyped, implemented, and applied to applications in conjunction with physical scientists using FETK. The entire FETK source tree was released in June 2010 on the FETK.org website, as a major milestone of this DTRA project. A substantial extention to both FETK and FETKLab was completed in Spring 2013 that added general Lagrange-type elements for either primal or dual problems, and this new capability has been exploited in a number of our recent articles.

In addition, we continue development on GAASP (Globally Accurate, Adaptive Sensitivity analysis Package) to extend its capabilities for both forward and inverse stochastic sensitivity analysis of differential equations.

5. Impact

5.1. Impact on the principal disciplines of the project

The numerical solution of multiscale, multiphysics models on complex domains along with the development of tools for predictive science and uncertainty quantification is one of the grand challenges facing the mathematical sciences at present. Such problems present a very complex picture in terms of stability and important behaviors interacting across a wide range of scales, which makes the straightforward use of classical numerical methods and analyses extremely problematic, if not impossible. Classic approaches were developed in the context of models involving single physics phenomena operating at a narrow range of scales. While building on classic approaches, the research in this project contributes at a fundamental theoretical level by laying the foundation for reliably accurate and efficient numerical solution based on a posteriori error analysis that accounts for the numerical complexities involved with simulating such systems. This is achieved

by combining extremely sophisticated mathematics in analysis and geometry with cutting edge numerical methodology.

The impact of the research related to this project is widespread, as can be seen in the greatly increasing levels of activity around the world on such problems. This is also evidenced by the number of invitations to speak, the number of funded interdisciplinary projects including a recent award of an extremely prestigious National Science Foundation Focused Research Group (FRG) award to Estep and Holst, the citation record (Estep's h-index is 15 and Holst's h-index is 20), and the high level of the involvement of the PI's in research environment through panels, reports, editing, and so on.

5.2. Impact on other disciplines

Developing reliable and accurate tools for carrying out predictive science and engineering for multiscale, multiphysics systems on complex domains and conducting uncertainty quantification in simulated results is the major problem of computational science and engineering at present. Addressing this challenge requires fundamental research in the mathematical sciences. This project is aimed at addressing a number of key research problems involved with simulating multiphysics systems. Along with theory, the PIs systematically implement the results into public software, and, along with their collaborators, use the software to tackle scientific and engineering research problems. This yields a direct transfer of the theoretical mathematical developments and software implementations to the application domain.

This is evidenced by the large number of interdisciplinary collaborations of the PIs and the substantial volume of interactions with Department of Energy laboratories and industry. Details are provided below.

5.3. Impact in the profession

5.4. Honors and awards

Estep was appointed (founding) Co-Editor in Chief of the SIAM / ASA Journal on Uncertainty Quantification

Estep won the University Scholarship Impact Award, Colorado State University, 2011

Estep was appointed University Interdisciplinary Research Scholar, Colorado State University in 2009

Estep received the Oliver P. Pennock Distinguished Service Award, Colorado State University in 2009

Estep was appointed Editor in Chief, SIAM Book Series on Computational Science and Engineering, 2009 - 2014

Holst received the CSU Distinguished Alumnus Award, 2009

Holst was appointed the Chancellor's Associates Endowed Chair in Mathematics and Physics at UC San Diego in 2012

5.5. Impact on the professional research community

Estep served as one of the Moderators for the SAMSI National SIAM and ASA Town Hall Meeting on Uncertainty Quantification, 2010

Estep served as the Co-Organizer and first Chair, SIAM Activity Group on Uncertainty Quantification, 2010

Estep served as a Program Leader for the SAMSI Program on Uncertainty Quantification, 2011-2012

Estep served as co-chair of the first SIAM/ASA/USACM Conference on Uncertainty Quantification (April, 2012)

Estep along with J. Berger (Duke) and M. Gunzburger (FSU) proposed a new Journal on Uncertainty Quantification to be jointly published by the ASA and SIAM

Estep serves on the Advisory Board for the Center for Advanced Modeling and Simulation, Idaho National Laboratory, 2009 - 2012

Estep serves on the Governing Board of the Statistical and Applied Mathematical Sciences Institute (SAMSI), 2009-2016

Estep served on the National Science Foundation Office of Cyberinfrastructure Grand Challenges Communities Task Force, 2009-2010 (co-author of final recommendation report)

Estep served as Breakout Lead and Report co-author, Uncertainty Quantification and Stochastic Systems, Department of Energy Cross-Cutting Technologies for Computing at the Exascale, 2010

Estep was an invited participant in the Fusion Simulation Program Definition Workshop, 2011

Estep serves on the American Mathematical Society Simmons Travel Grants Committee, 2011-2014

Estep serves as Moderator, Mathematics in the Geosciences Workshop, Northwestern University, 2011

Estep was co-author of *Multiphysics Simulations: Challenges and Opportunities*, Tech. Report ANL/MCS-TM-321, Argonne National Laboratory, 2011

Estep was co-author of *Fostering Interactions Between the Geosciences and Mathematics, Statistics, and Computer Science*, Technical Report TR-2012-02, Department of Computer Science, University of Chicago, 2012

Holst serves on the Executive Committee for the San Diego Supercomputer Center (SDSC), 2007-present

Holst is a Co-Organizer (with R. Bank) of 20th International Conference on Domain Decomposition (DD20), February 2011.

Holst is the Primary Organizer (with J. Hameed): Numerical Methods for Implicit Models in Biomolecular Systems, SIAM CS&E Conference Minisymposium, March 2011

Holst is the Primary Organizer (with A. Demlow, A. Gillette, Y. Zhu): Workshop on Exploiting Geometry in the Development of Numerical Methods for Partial Differential Equations, UCSD Workshop, San Diego, November 2011.

Holst is the Primary Organizer (with A. Demlow, R. Szypowski): Exploiting Geometry in the Development of Numerical Methods for Partial Differential Equations, SIAM Analysis of PDE Conference Minisymposium, November 2011.

Holst is the Primary Organizer (with D. Arnold, A. Gillette): AMS Joint Meeting FEEC Minisymposium, on New Developments in the Finite Element Exterior Calculus, January 2013.

Holst is the Primary Organizer (with A. Gillette, R. Szypowski): Workshop on Exploiting Geometry in the Development of Numerical Methods for Partial Differential Equations II, UCSD Workshop, San Diego, January 2013.

Holst and Estep regularly serve on Grant Review Panels for NSF and DOE, 2004-present

5.6. *Professional editorial appointments*

Estep: co Editor in Chief (founding), SIAM / ASA Journal on Uncertainty Quantification

Estep: Editor in Chief, SIAM Book Series on Computational Science and Engineering, 2009 - 2014

Estep: Associate Editor, SIAM Journal on Numerical Analysis, 2005-2011

Estep: Associate Editor, International Journal for Uncertainty Quantification, 2010-

Estep: Associate Editor, Multiphysics Modeling Book Series, A. A. Balkema Publishing, CRC Press, 2010-

Estep: Associate Editor, Journal of Applied Mathematics and Computing, 2008-2013

Holst: Associate Editor, Numerische Mathematik, 2008-present

Holst: Associate Editor, SIAM Book Series on Computational Science and Engineering, 2009-2014

5.7. *Impact on technology transfer*

The PIs maintain a very substantial interdisciplinary collaboration activity with scientists and engineers in universities, Department of Energy laboratories, and industry. These collaborations lead to direct injection of research ideas into practical use.

5.8. *Consulting and collaborative activities*

In this section, we report currently funded projects that involve substantial interdisciplinary collaborations and transfer of research results related to this project into applications.

Estep is co-PI on the project *Framework Application for Core-Edge Transport Simulations (FACETS)* funded by the Office of Advanced Scientific Computing Research and Office of Fusion Energy Sciences, Department of Energy, 2007-12. Collaborators include: R. H. Cohen, L. Diachin, and T. Epperly at Lawrence Livermore National Laboratory; J. Larson and L. McInnes at Argonne National Laboratory; M. R. Fahey and J. Cobb at Oak Ridge National Laboratory. Subject is development and analysis of numerical solution methods for coupled core-edge fusion simulations.

Estep is PI on the project *Collaborative Proposal: Transforming How Climate System Models are Used: A Global, Multi-Resolution Approach to Regional Ocean Modeling* funded by the Department of Energy, 2009-11. Collaborators include Todd Ringler at Los Alamos National Laboratory. Subject is development and analysis of numerical methods for multiscale ocean models.

Estep is PI on the project *Adjoint-based methods for uncertainty quantification* funded by the Lawrence Livermore National Laboratory, 2010-13. Collaborators are Carol Woodward and Jeff Hittinger at Lawrence Livermore National Laboratory. Duties include (1) pursue develop a posteriori error estimates for hyperbolic problems including shock behavior and (2) consult on uncertainty and error quantification with laboratory personnel

Estep is co-PI on the project *The Inverse Problem for Estimation of Structure of Biological Macromolecules from Small-Angle X-Ray Scattering* funded by the National Institutes of Health, 2010-2014. Collaborators include Jay Breidt (Statistics, CSU) and Karolin Luger (Biochemistry, CSU). Subject is determining the structure of biological macromolecules using small angle x-ray scattering data.

Estep is PI on the project *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* funded by the Department of Energy, 2010-2013. Collaborators include John Shadid (Sandia Nat. Lab.) and Victor Ginting (U. Wyom.). Subject is developing a posteriori error estimates for solutions of reacting flow and fusion reaction models.

Estep is co-PI on the project *Collaborative Research: A posteriori error analysis and adaptivity for discontinuous interface problems* funded by the National Science Foundation, 2010-2013. Collaborator is Simon Tavener (CSU). Purpose is developing and analyzing conservative solution methods for elliptic problems with coefficients that are discontinuous across complex interfaces.

Estep is PI on the CSU Subcontract from Multiscale Design Systems, LLC supported by an Air Force SBIR Phase II grant. Collaborators are Simon Tavener (CSU) and Jacob Fish (Columbia Uni.) in 2011. Purpose is developing fast methods for UQ for multiscale models of polymers in stressed environments.

Estep is PI on the project *Uncertainty Analysis for Multiscale Models of Nuclear Fuel Performance* supported by the Idaho National Laboratory from 2011-2014. Collaborators are Simon Tavener (CSU) and Michael Pernice (Idaho Nat. Lab.). Purpose is UQ for multiscale models of nuclear fuel.

Estep is PI on the project *11-2031: Multiscale modeling and uncertainty quantification for nuclear fuel performance*, Nuclear Energy University Programs, Department of Energy, 2011-14. Collaborators are Simon Tavener (CSU), Michael Pernice (INL), Peter Polyakov (Wyoming), Dongbin Xiu (Purdue), Anter el Azab (Purdue)

Estep is a co-PI on the project *Data-Driven Inverse Sensitivity Analysis for Predictive Coastal Ocean Modeling*, Computational and Data-Enabled Science and Engineering in Mathematical and Statistical Sciences (CDS&E-MSS), National Science Foundation, 2012-15. Collaborators are Troy Butler (CSU), Clint Dawson (U. Texas at Austin), and Joannes Westerink (Notre Dame)

Estep and Holst are co-PIs on the project *FRG: Error Quantification and Control for Gravitational Waveform Simulation* funded by the National Science Foundation, 2011-2014. The Project is concerned with estimating the error in computed wave forms obtained from LIGO data.

Holst is PIs on the project *FRG: Analysis of the Einstein Constraint Equations* funded by the National Science Foundation, 2013-2016. The Project is concerned with further extending the solution theory for the Einstein constraint equations.

Holst is PI on the project *MRI: Acquisition of a Parallel Computing and Visualization Facility to Enable Integrated Research and Training in Modern Computational Science, Mathematics, and Engineering* funded by National Science Foundation, 2008-2011. Collaborators include Randolph Bank (UCSD Mathematics), Scott Baden (UCSD Computer Science), and John Weare (UCSD Chemistry). The subject is the design and construction of a state-of-the-art parallel computing system with an excess of 1000 compute nodes, Infiniband high-speed network fabric, parallel filesystems, LCD vizualization walls, housed in a modern server room with raised floor and forced chilled air.

Holst is PI on the project *Adaptive Methods and Finite Element Exterior Calculus for Nonlinear Geometric PDE*, funded by National Science Foundation, 2012-2015. Co-PI is former student and postdoc Ryan Szypowski, now an assistant professor in mathematics at Cal Poly

Pomona. The subject is the design and analysis of adaptive methods for use with the finite element exterior calculus.

Holst is Co-PI on the project *Adaptive Radiotherapy Based on High Performance Computing* funded by the Department of Energy, Lawrence Livermore National Laboratory, and the University of California, 2009-2012. Collaborators include Steve Jian (UCSD Medical School), A. Majumdar (SDSC), and D.J. Choi (SDSC). The subject is realtime solution of coupled reaction-diffusion systems and the Boltzmann transport equation using a combination of parallel algorithms for partial differential equations, high-speed communication networks, and cluster computers.

Holst is Co-PI on the project *Scalable Adaptive Multilevel Solvers for Multiphysics Problems*, funded by the Department of Energy. The subject is the design and analysis of determinstic algorithms for use in physical simulation based on multilevel technologies.

Holst is Co-PI on the project *Applications of Quantum Computing in Aerospace Science and Engineering*, funded by the AirForce Office of Scientific Research. The subject is the design and analysis of quantum algorithms for use in physical simulation.

Holst is Co-PI and Core 1A lead on the project *National Biomedical Computation Resource (NBCR)* funded by the National Institutes of Health, 2009-2014. Collaborators include Andrew McCammon (UCSD Chemistry), Andrew McCulloch (UCSD Bioengineering), Mark Ellisman (UCSD Medical School), and Peter Arzberger (SDSC). The subject is multiscale modeling frameworks and adaptive finite element methods for complex multiscale and multiphysics problems arising in biomedical science.

Holst is Senior Scientist and founding member of the *NSF Physics Frontier Center for Theoretical Biological Physics (CTBP)*, funded by the National Science Foundation. Collaborators include Jose' Onuchic (UCSD Physics), Andrew McCammon (UCSD Chemistry), and Andy Kummel (UCSD Chemistry). The subject is multiscale modeling frameworks and adaptive finite element methods for complex multiscale and multiphysics problems arising in biophysics.

5.9. Transitions to technology applications

We report on current interactions with industry.

Estep was a Co-Principal Investigator in the Tech X, Inc. project *Framework Application for Core-Edge Transport Simulations (FACETS)*, funded by the Office of Advanced Scientific Computing Research and Office of Fusion Energy Sciences, Department of Energy. Estep's responsibilities include development and analysis of numerical solution methods for coupled core-edge fusion simulations. Algorithms developed in this program will be implemented into the FACETS high performance framework.

Estep was a subcontract in Phase II project for *Multiscale Design Systems, LLC* (Principal Officer: Jacob Fish, Rensselaer Polytechnic Institute) for the Air Force SBIR/STTR program. Estep's responsibilities include development of multiscale operator decomposition numerical methods and numerical methods for error estimation, uncertainty quantification and inverse problems for parameter identification for multiscale multiphysics models of hygro-thermo-mechano-oxidation-fatigue in polymer matrix composites used in aircraft applications. Algorithms developed in this program will be implemented into the Multiscale Design System for Continuum (MDS-C) and the Multiscale Design System for Discrete or atomistic medium (MDS-D) software packages.

Holst is collaborating with Eric Bylaska at Pacific Northwest National Laboratory on the incorporation of the Finite Element Toolkit (FETK, developed and maintained by the Holst Group) into several density functional modeling packages based at PNNL.

BLOCKWISE ADAPTIVITY FOR TIME DEPENDENT PROBLEMS BASED ON COARSE SCALE ADJOINT SOLUTIONS

V. CAREY *, D. ESTEP †, A. JOHANSSON ‡, M. LARSON §, AND S. TAVENER ¶

Abstract. We describe and test an adaptive algorithm for evolution problems that employs a sequence of "blocks" consisting of fixed, though non-uniform, space meshes. This approach offers the advantages of adaptive mesh refinement but with reduced overhead costs associated with load balancing, re-meshing, matrix reassembly, and the solution of adjoint problems used to estimate discretization error and the effects of mesh changes. A major issue with a block-adaptive approach is determining block discretizations from coarse scale solution information that achieve the desired accuracy. We describe several strategies to achieve this goal using adjoint-based *a posteriori* error estimates and we demonstrate the behavior of the proposed algorithms as well as several technical issues in a set of examples.

Key words. *a posteriori* error analysis, adaptive error control, adaptive mesh refinement, adjoint problem, discontinuous Galerkin method, duality, generalized Green's function, goal oriented error estimates, residual, variational analysis

AMS subject classifications. 65N15, 65N30, 65N50

1. Introduction.

We describe and test an adaptive algorithm for evolution problems that we call "blockwise adaptivity". This approach employs a sequence of "blocks" consisting of fixed, though non-uniform, space meshes, and is motivated by considerations of efficiency and accuracy. We balance the goal of achieving desired accuracy using discretizations with relatively few degrees of freedom against the computational costs associated with load balancing, re-meshing, matrix reassembly and in particular the cost of error estimation. A block adaptive strategy reduces the number of mesh changes that must be treated, which reduces the amount of computational time spent on re-meshing, assembly, and load balancing, and makes the problem of quantifying the effects of mesh changes on accuracy computationally feasible. A block adaptive strategy also provides a natural coarse scale discretization on which to solve the adjoint problem used to compute global *a posteriori* error estimates. This reduces the twin computational difficulties of storing a fine scale forward solution in order to form the adjoint problem and solving the adjoint problem on that fine scale discretization. However, a major issue with a block-adaptive approach is determining block discretizations from coarse scale solution information that achieve

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the desired accuracy and efficiency. We describe several strategies to achieve this goal using adjoint-based *a posteriori* error estimates.

To focus the discussion, we consider a reaction-diffusion equation for the solution u on an interval $[0,T]$,

$$\begin{cases} \dot{u} - \nabla \cdot (\epsilon(x,t)\nabla u) = f(u,x,t), & (x,t) \in \Omega \times (0,T], \\ u(x,t) = 0, & (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) = u_0(x), & x \in \Omega, \end{cases} \tag{1.1}$$

where Ω is a convex polygonal domain in $\mathbb{R}^d$ with boundary $\partial\Omega$, $\dot{u}$ denotes the partial derivative of u with respect to time, and there is a constant $\epsilon > 0$ such that

$$\epsilon(x,t) \geq \epsilon, \quad x \in \Omega,\ t > 0.$$

We also assume that ϵ and f have smooth second derivatives. The algorithms in this paper generalize to problems with different boundary conditions, convection, nonlinear diffusion coefficients, as well as systems, see [17, 15].

In terms of adaptive mesh refinement, the interesting situation is a solution of (1.1) that exhibits "regionalized" behavior in space and time. Considerations of efficiency suggests that time steps and space meshes should be locally refined to match the regional behavior, see the plot on the left in Fig. 1.1. Classic adaptive mesh refinement can be described as a constrained optimization problem, e.g., determine a discretization using the fewest degrees of freedom that yields a solution satisfying a given error criterion. In general, it is impossible to determine a closed-form solution of this optimization problem. An adaptive algorithm is an iterative procedure for determining a nearly optimal solution.

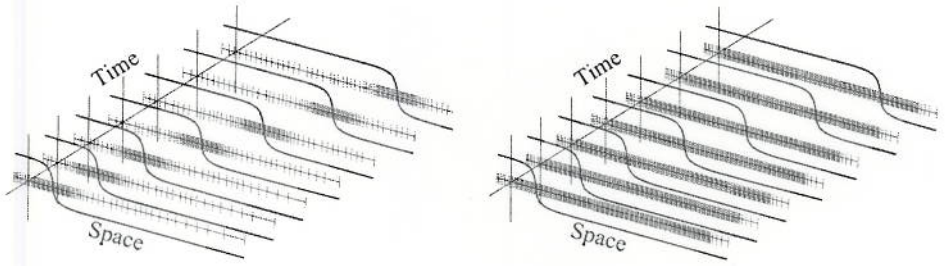

FIG. 1.1. *The evolution of a traveling front solution. Left: A computation using space meshes chosen by a standard adaptive strategy to control the spatial residual error at each time step. This entails re-meshing, re-assembly, load balancing, and projecting the solution on a new mesh at each step. Right: The uniform mesh that is required to achieve the same control over the residual. The computation is assembled and load balanced only once.*

We present a generic adaptive algorithm in Algorithm 1.1. An adaptive computation is generally started with an initial coarse mesh. The adaptive algorithm is then applied "real-time" as the integration proceeds so as to generate a new space mesh for each new time step, where the new space mesh is based on (or adapted from) the mesh for the current time step. In practice, the remeshing may be applied on intervals of a small number of steps.

While adaptive mesh refinement is appealing on an intuitional level, there are serious issues facing its use for evolution problems including the following.

Algorithm 1.1 Generic Adaptive Algorithm for an Evolution Problem

```
Choose an initial coarse mesh and time step
while the final time has not been reached do
    Compute a numerical solution using the current time step and space mesh
    Estimate the error of the computed solution
    while the error estimate is too large do
        Estimate local error contributions and adapt in space
        Estimate local error contributions and adapt in time
        Compute a numerical solution using the new time step and space mesh
        Estimate the error of the computed solution
    end while
    Increment time by the accepted time step
end while
```

1. ***Accuracy*** Each spatial mesh change requires a projection of the numerical solution onto the new mesh, and this can affect accuracy. In fact, this can destroy convergence altogether, see [8].
2. ***Overhead Costs*** Changing the spatial discretization requires generating a new mesh and reassembly of matrices. Significant mesh changes require a redistribution of unknowns among the processors to achieve load balancing. All of these tasks are computationally intensive.
3. ***Coarsening*** Un-refinement or coarsening of a mesh involves loss of information about a numerical solution that cannot be recovered. Currently, there is no theory for coarsening that guarantees that there is no loss of accuracy.
4. ***Global Error Estimation*** Efficient adaptive mesh refinement requires accurate error estimates of the true, global error, but cancelation of errors over both space and time makes choosing adapted meshes problematic.

Using a fixed spatial mesh eliminates the first three issues. But, the scale required of the mesh is determined by the finest scale required in any region where discretization impacts global accuracy, see Fig. 1.1. This necessarily increases computational time and solver costs and memory limits may make it impossible to use the necessary uniform mesh.

In this paper, we propose a "blockwise" adaptive algorithm that employs nonuniform meshes that remain fixed for discrete period of times, or "blocks", see Fig. 1.2. With the proper implementation, this strategy addresses the following key issues.

1. ***Accuracy*** The projections onto new meshes occur at a relatively small set of discrete times. We use *a posteriori* error estimates to predict the effect of the projections and choose overlaps in the meshes to reduce the error induced by the mesh changes.
2. ***Overhead Costs*** Re-meshing, assembly, and load balancing are required only at the discrete times demarcating blocks.
3. ***Coarsening*** There is ***no*** coarsening of a given mesh in the indicated strategy. Mesh changes are handled purely as projections between different meshes.

The idea of re-meshing only after a fixed number of steps is by no means new. However, this strategy depends critically upon choosing suitable block discretizations, and thus, ultimately, on accurately predicting the behavior of the solution. The choice of block discretizations is a difficult issue that requires balancing the inefficiency of using a fixed spatial mesh inside each block against the gain in accuracy achieved

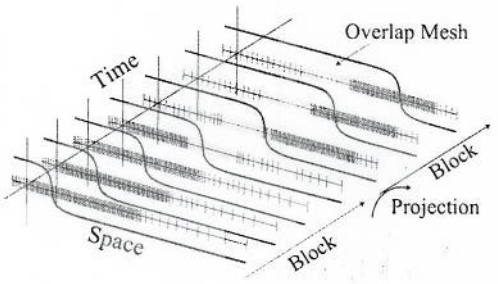

FIG. 1.2. *The evolution of a solution with a traveling front computed using blockwise adaptivity with two blocks. On each block, the space mesh is chosen to maintain the same level of control over the local residual as is achieved in the computation shown in Fig. 1.1. In addition, there is a sufficient degree of overlap between the two meshes (the lightly-shaded mesh region) to insure there is no loss of accuracy in projecting the solution between the two meshes. Re-meshing, assembly, and load balancing is only required twice, once for each block.*

by limiting projections between different meshes and the decrease in computational cost due to limiting the number of times at which re-meshing, re-assembly, and load balancing is required. This is partly a computer science problem of distributing available resources, e.g., memory and compute cycles, efficiently, and partly a numerical analysis problem, e.g., determining meshes for each block and projections between blocks.

In this paper, we focus on the problem of determining blocks, e.g., the length of times for each block, the meshes for each block that maintain accuracy in the desired information, and suitable overlap meshes for transitions between blocks from the coarse-scale adjoint solutions. The solutions of these problems require accurate estimates of the error in a specific quantity of interest. We use a computable *a posteriori* error estimate that yields robustly accurate estimates of the error in a specified quantity of interest in terms of a sum of space-time element contributions, see [9, 10, 17, 15, 3, 20]. The *a posteriori* error estimates are based on duality, adjoint problems, and variational analysis. Accurate error estimates are obtained by numerically solving the linear adjoint problem related to the desired quantity of interest.

Solving adjoint problems offers computational challenges such as the need to store the forward solution in order to form the adjoint problem and the cost of the adjoint solve. Our approach is to perform the adjoint solves using relatively coarse scale discretizations and using a coarse scale representation of the forward solution to form the adjoint problem, which reduces the memory overhead and the cost of the adjoint solve. This approach is motivated by the following observations.

1. Adjoint problems are linear and often present fewer numerical difficulties than the associated forward problems.
2. Solutions of adjoint problems tend to vary slowly on the scale of the discretization, whereas residuals of forward solutions tend to oscillate on the scale of the discretization
3. The accuracy required of the adjoint solution, which is being used only for error estimation, is orders of magnitude less than generally desired for the forward solution.

An enormous literature on adaptive methods for differential equations has devel-

oped over nearly six decades of activity and the major developments form a highly inter-connected web. We do not attempt to review the history of adaptive methods or to present a comprehensive list of references. Instead, we provide only a short list of references that either contain further references and/or address computational issues related to adaptive mesh refinement for evolution problems [8, 7, 5, 4, 18, 22, 9, 10, 17, 19, 15, 3, 1, 23, 24, 20, 2, 14].

This paper considers adaptive mesh refinement from a different point of view than much of the existing literature. Namely, we are concerned with trying to understand how to adapt discretizations based on under-resolved solutions on relatively coarse discretizations in order to obtain particular information, as opposed to analyzing adaptive mesh algorithms in the asymptotic limit of mesh refinement. This point of view is important for many large scale applications, for which such conditions are generic. In §2 we review the standard *a posteriori* error analysis and modify this for a block adaptive strategy. We review adaptive error control in §3 and introduce new features necessary for block adaptivity and several block adaptive strategies. One- and three-dimensional illustrative computational examples are provided in §4 and we draw conclusions in §5.

2. Discretization and error estimation. We begin by reviewing discretization and *a posteriori* error estimation for evolution problems and then describe the block-wise discretization and present the corresponding error estimate.

2.1. Discretization. We formulate the discretization as a space-time finite element method because that is convenient for deriving *a posteriori* error estimates based on variational analysis. However, we emphasize that the estimates can be extended to a wide range of discretizations, e.g. finite difference and finite volume methods, which can be written as equivalent finite element methods.

We describe two finite element space-time discretizations of (1.1) called the continuous and discontinuous Galerkin methods, see [11, 13, 12, 10, 17, 15]. We partition $[0,T]$ as $0 = t_0 < t_1 < t_2 < \cdots < t_n < \cdots < t_N = T$, denoting each time interval by $I_n = (t_{n-1}, t_n]$ and time step by $k_n = t_n - t_{n-1}$ and we construct a discretization $\mathcal{T}$ of Ω such that the union of the elements in $\mathcal{T}$ is Ω while the intersection of any two elements is either a common edge, node, or is empty. We assume that the smallest angle of any element is bounded below by a fixed constant. To measure the size of the elements of $\mathcal{T}$, we use a piecewise constant function h, the so-called mesh function, defined so $h|_\triangle = \operatorname{diam}(\triangle)$ for $\triangle \in \mathcal{T}$. Similarly, we use k to denote the piecewise constant function that is k_n on I_n.

The approximations are polynomials in time and piecewise polynomials in space on each space-time "slab" $S_n = \Omega \times I_n$. In space, we let $V \subset H_0^1(\Omega)$ denote the space of piecewise linear continuous functions defined on $\mathcal{T}$, where each function is zero on $\partial\Omega$. Then on each slab, we define

$$W_n^q = \left\{ w(x,t) : \, w(x,t) = \sum_{j=0}^{q} t^j v_j(x), \, v_j \in V, \, (x,t) \in S_n \right\}.$$

Finally, we let W^q denote the space of functions defined on the space-time domain $\Omega \times [0,T]$ such that $v|_{S_n} \in W_n^q$ for $n \geq 1$. Note that functions in W^q may be discontinuous across the discrete time levels and we denote the jump across t_n by $[w]_n = w_n^+ - w_n^-$ where $w_n^\pm = \lim_{s \to t_n^\pm} w(s)$.

We use a projection operator into V, $Pv \in V$, e.g. the L^2 projection satisfying $(Pv, w) = (v, w)$ for all $w \in V$, where $(\cdot, \cdot)$ denotes the $L_2(\Omega)$ inner product. We

use the $\|\ \|$ for the L_2 norm. We also use a projection operator into the piecewise polynomial functions in time, denoted by $\pi_n : L^2(I_n) \to \mathcal{P}^q(I_n)$, where $\mathcal{P}^q(I_n)$ is the space of polynomials of degree q or less defined on I_n. The global projection operator π is defined by setting $\pi = \pi_n$ on S_n.

DEFINITION 2.1. *The* **discontinuous Galerkin** *dG(q) approximation $U \in W^q$ satisfies $U_0^- = Pu_0$ and*

$$\int_{t_{n-1}}^{t_n} \big((\dot{U}, v) + (\epsilon \nabla U, \nabla v)\big)\, dt + \big([U]_{n-1}, v^+\big) = \int_{t_{n-1}}^{t_n} (f(U), v)\, dt \quad \text{for all } v \in W_n^q, \quad 1 \le n \le N. \tag{2.1}$$

We also use a related method for solving the adjoint problem:

DEFINITION 2.2. *The* **continuous Galerkin** *cG(q) approximation $U \in W^q$ satisfies $U_0^- = Pu_0$ and*

$$\begin{cases} \displaystyle\int_{t_{n-1}}^{t_n} \big((\dot{U}, v) + (\epsilon \nabla U, \nabla v)\big)\, dt = \int_{t_{n-1}}^{t_n} (f(U), v)\, dt \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{for all } v \in W_n^{q-1}, \quad 1 \le n \le N, \\ U_{n-1}^+ = U_{n-1}^-. \end{cases} \tag{2.2}$$

Note that U is continuous across time nodes when the space mesh is fixed.

With appropriate use of quadrature to evaluate the integrals in the variational formulation, these Galerkin methods yield standard difference schemes. If the lumped mass quadrature is used in space, then the discrete system yielding the dG(0) approximation is the same as the system obtained for the nodal values of the "backward Euler in time"-"second order centered difference scheme in space" finite difference scheme. Likewise, the cG(1) method is related to the Crank-Nicolson scheme, and the dG(1) method is related to the third order sub-diagonal Padé difference scheme. Under general assumptions, the cG(q) and dG(q) have order of accuracy $q + 1$ in time at any point and a superconvergence order of $2q + 1$ and $2q$ respectively at time nodes.

2.2. An *a posteriori* error estimate. We begin by defining a suitable adjoint problem for error analysis. A more detailed description is given in [15]. The adjoint problem is a parabolic problem with coefficients obtained by linearization around an average of the true and approximate solutions.

$$\bar{f} = \bar{f}(u, U) = \int_0^1 \frac{\partial f}{\partial u}(us + U(1 - s))\, ds. \tag{2.3}$$

The regularity of u and U typically imply that $\bar{f}$ is piecewise continuous with respect to t and a continuous, H^1 function in space.

Written out pointwise for convenience, the adjoint problem to (1.1) for the generalized Green's function associated to the data ψ, which determines the quantity of interest,

$$\int_0^T (u, \psi)\, dt,$$

is

$$\begin{cases} -\dot{\phi} - \nabla \cdot (\epsilon \nabla \phi) - \bar{f}\phi = \psi, & (x,t) \in \Omega \times (T,0], \\ \phi(x,t) = 0, & (x,t) \in \partial\Omega \times (T,0], \\ \phi(x,T) = 0, & x \in \Omega, \end{cases} \tag{2.4}$$

This choice for the adjoint yields the following error representation formula for the dG method.

THEOREM 2.3. *dG A Posteriori Error Estimate*

$$\int_0^T (e,\psi)\,dt = ((I-P)u_0, \phi(0)) + \sum_{n=1}^{N} \big([U]_{n-1}, (\pi P\phi - \phi)^+_{n-1}\big) + \int_0^T \big((\dot{U}, \pi P\phi - \phi) + (\epsilon(U)\nabla U, \nabla(\pi P\phi - \phi)) - (f(U), \pi P\phi - \phi)\big)\,dt. \tag{2.5}$$

The initial error is $e^-(0) = (I-P)u_0$.

In practice, we compute a numerical solution of the linear adjoint problem obtained from (2.4) by replacing u with the computed approximate solution U in the definition of $\bar{f}$ and solve using a higher order method in space and time, see [15]. We denote the approximate adjoint solution by Φ. We focus on the dG method, while application to the cG method is analogous.

COROLLARY 2.4. *The approximate a posteriori error estimate for the dG method is*

$$\left|\int_0^T (e,\psi)\,dt\right| \approx E(U) = E(U;\psi) = \Big|((I-P)u_0, \Phi(0)) + \sum_{n=1}^{N} \big([U]_{n-1}, (\pi P\Phi - \Phi)^+_{n-1}\big) + \int_0^T \big((\dot{U}, \pi P\Phi - \Phi) + (\epsilon(U)\nabla U, \nabla(\pi P\Phi - \Phi)) - (f(U), \pi P\Phi - \Phi)\big)\,dt\Big|. \tag{2.6}$$

2.3. Blockwise discretization. We describe the blockwise formulation of the discontinuous Galerkin method. We partition $[0,T]$ into time blocks $0 = T_0 < T_1 < T_2 < \cdots < T_b < \cdots < T_B = T$. We discretize each block $[T_{b-1}, T_b]$ by $T_{b-1} = t_{b,0} < t_{b,1} < \cdots < t_{b,N_b} = T_b$, denoting each subinterval by $I_{b,n} = (t_{b,n-1}, t_{b,n}]$ and time step by $k_{b,n} = t_{b,n} - t_{b,n-1}$. To each block $[T_{b-1}, T_b]$, we associate a discretization $\mathcal{T}_b$ of Ω arranged so the union of the elements in $\mathcal{T}_b$ is Ω while the intersection of any two elements is either a common edge, node, or is empty. We assume that the smallest angle of any element is bounded below by a fixed constant. To measure the size of the elements of $\mathcal{T}_b$, we use the mesh function h_b.

The approximations are polynomials in time and piecewise polynomials in space on each space-time "slab" $S_{b,n} = \Omega \times I_{b,n}$. In space, we let $V_b \subset H_0^1(\Omega)$ denote the space of piecewise linear continuous functions defined on $\mathcal{T}_b$, where each function is zero on $\partial\Omega$. Then on each slab, we define

$$W^q_{b,n} = \left\{ w(x,t) : w(x,t) = \sum_{j=0}^{q} t^j v_{b,j}(x),\ v_{b,j} \in V_b,\ (x,t) \in S_{b,n} \right\}.$$

Finally, we let W^q denote the space of functions defined on the space-time domain $\Omega \times [0,T]$ such that $v|_{S_{b,n}} \in W^q_{b,n}$ for $b,n \geq 1$. Note that functions in W^q may be

discontinuous across the discrete time levels and we denote the jump across $t_{b,n}$ by $[w]_{b,n} = w^+_{b,n} - w^-_{b,n}$.

To compute the dG approximation on the new block, we project the final value of the approximation from the previous block onto the new mesh. We use a projection operator $P_b v \in V_b$ and a projection operator into the piecewise polynomial functions in time, denoted by $\pi_{b,n} : L^2(I_{b,n}) \to \mathcal{P}^q(I_{b,n})$. We then define π_b as $\pi_b = \pi_{b,n}$ on $S_{b,n}$. Finally, we define global projections P and π which on each block are P_b and π_b respectively.

DEFINITION 2.5. *The blockwise discontinuous Galerkin dG(q) approximation $U \in W^q$ satisfies $U^-_{b,0} = P_1 u_0$ and for $b = 1, 2, \cdots, B$,*

$$\int_{t_{b,n-1}}^{t_{b,n}} \big((\dot{U}, v) + (\epsilon \nabla U, \nabla v)\big)\, dt + \big([U]_{b,n-1}, v^+\big) = \int_{t_{b,n-1}}^{t_{b,n}} (f(U), v)\, dt$$
$$\text{for all } v \in W^q_{b,n}, \quad 1 \le n \le N_b. \quad (2.7)$$

2.4. A blockwise *a posteriori* error estimate. Adapting the standard argument that yields (2.5), we obtain a blockwise *a posteriori* error estimate.

THEOREM 2.6. *Blockwise A Posteriori Error Estimate*

$$\int_0^T (e, \psi)\, dt \approx ((I - P_0)u_0, \Phi(0)) + \sum_{b=1}^{B} \big((I - P_b)U, \Phi(T_{b-1})\big)$$
$$+ \sum_{b=1}^{B} \Big(\int_{T_{b-1}}^{T_b} \big((\dot{U}, \pi P_b \Phi - \Phi) + (\epsilon(U)\nabla U, \nabla(\pi P_b \Phi - \Phi)) - (f(U), \pi P_b \Phi - \Phi)\big)\, dt$$
$$+ \sum_{n=1}^{N_b} \big([U]_{b,n-1}, (\pi P_b \Phi - \Phi)^+_{b,n-1}\big)\Big). \quad (2.8)$$

The second term on the right measures the effects of changing meshes on the accuracy of the approximation. A similar "jump" term already appears in the estimate for the standard dG method at each time step. In this case of transitions between blocks, the "jump" arises because of mesh changes between blocks. Note that the adjoint weight does not involve the projection of Φ into the approximation space (i.e. Galerkin orthogonality). Instead, the contributions from the projections accumulate in the same way as an initial error.

Our purpose is to use the *a posteriori* bounds $Æ_x, Æ_t$ to choose block times $\{T_b\}$ and corresponding meshes $\mathcal{T}_b$ and timesteps $k_{b,i}$. An important issue is the effect of transferring solutions between the meshes of adjacent blocks on the accuracy of the computed information, and so we address the computation of a bound on the second term on the right in (2.8),

$$\Xi(U) = \sum_{b=1}^{B} \big|\big((I - P_b)U, \Phi(T_{b-1})\big)\big|. \quad (2.9)$$

3. Adaptive error control. We start off by describing some standard approaches to adaptive error control and the relation to adaptive error control based on *a posteriori* error estimates. We then turn to the problem of choosing blocks for a block discretization and generating the corresponding spatial and temporal discretizations for each block.

3.1. Goal oriented adaptive error control. The aim of goal oriented adaptive error control is to generate a mesh with a nearly minimal number of elements such that for a given tolerance TOL and data ψ,

$$\left| \int_0^T (e, \psi)\, ds \right| \lesssim \text{TOL}. \tag{3.1}$$

We note that (3.1) cannot be verified in practice because the error is unknown, so instead we use an estimate or a bound for the error in the quantity of interest. Different ways to generate an acceptable mesh vary by the estimate or bound used for the quantity of interest as well as the strategy for mesh refinement.

For example using the *a posteriori* estimate (2.6), the goal of adaptive error control is to determine a discretization so that a mesh acceptance criterion,

$$E(U) \lesssim \text{TOL}, \tag{3.2}$$

is satisfied. If (3.2) is not satisfied, then we refine the mesh in order to compute a new solution for which the criterion is met. Refinement decisions require identifying the contributions to the error from discretization on each element. We can write $E(U)$ as a sum over space-time elements,

$$E(U) = \Big| \sum_{\triangle\in\mathcal{T}} ((I-P)u_0, \Phi(0))_\triangle + \sum_{n=1}^{N} \sum_{\triangle\in\mathcal{T}} \left([U]_{n-1}, (\pi P\Phi - \Phi)^+_{n-1}\right)_\triangle$$
$$+\sum_{n=1}^{N} \sum_{\triangle\in\mathcal{T}} \int_{t_{n-1}}^{t_n} \left((\dot{U}, \pi P\Phi - \Phi)_\triangle + (\epsilon(U)\nabla U, \nabla(\pi P\Phi - \Phi))_\triangle - (f(U), \pi P\Phi - \Phi)_\triangle\right) dt \Big|,$$

where $(\ ,\ )_\triangle$ denotes the L^2 inner product on element $\triangle$. This clearly identifies possible element contributions.

However, a major difficulty is that the error estimate generally involves a large amount of cancelation among the element contributions, which makes determining a truly efficient refinement strategy extremely difficult.

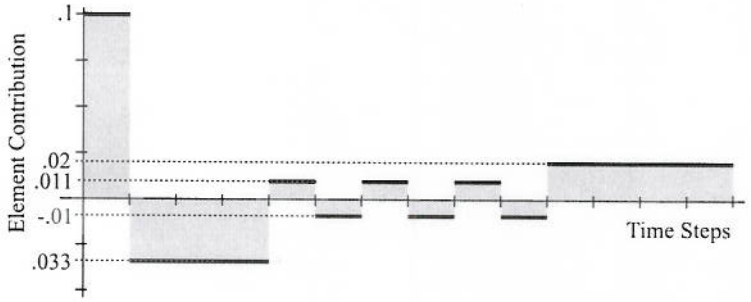

FIG. 3.1. *The element contributions to the error in integration.*

EXAMPLE 3.1. We consider a first order accurate numerical solution that has the element contributions shown in Fig. 3.1.

The first time step has the largest contribution. The next three steps each contribute -0.033, so cancelation means that the total contribution from the first four

steps is 0.001. Likewise, the next six steps contribute +0.003 in total. The last four steps contribute 0.08 in total. The total error is therefore

$$.1 - 3 \times .033 + .011 - .01 + .011 - .01 + .011 - .01 + 4 \times .02 = 0.084$$

If we use a standard approach of refining only some fraction of the elements with the largest contributions, we are likely to refine the first four steps. For simplicity, we assume that the elements marked for refinement are divided into two time steps. The resulting integration will have accuracy

$$\frac{1}{2^2} \times 2 \times .1 - \frac{1}{2^2} \times 6 \times .033 + .011 - .01 + .011 - .01 + .011 - .01 + 4 \times .02 \approx 0.0835.$$

Note that the individual element contributions decrease at a second order rate. The problem is that even though the element contributions in the first four steps are individually large, there is significant cancelation and refinement in this region and refinement does not decrease the error significantly. On the other hand, if we refine the last four time steps instead, we obtain

$$.1 - 3 \times .033 + .011 - .01 + .011 - .01 + .011 - .01 + \frac{1}{2^2} \times 8 \times .02 \approx 0.044.$$

While this is a non-standard approach, it decreases the error significantly.

In the adjoint-weight approach, the issue of cancelation of error is neglected in a sense by replacing the *accurate* error estimate $E(U)$ by an inaccurate upper bound,

$$E(U) \leq \text{Æ}(U) = \text{Æ}(U;\psi), \tag{3.3}$$

where we define $\text{Æ}(U;\psi)$ by summing bounds over each element.

DEFINITION 3.2. *Element-wise upper bound on the total error*

$$\text{Æ}(U;\psi) = \sum_{\Delta\in\mathcal{T}} \left|((I-P)u_0, \Phi(0))_\Delta\right| + \sum_{n=1}^{N}\sum_{\Delta\in\mathcal{T}} \left|\left([U]_{n-1}, (\pi P\Phi - \Phi)^+_{n-1}\right)_\Delta\right|$$
$$+\sum_{n=1}^{N}\sum_{\Delta\in\mathcal{T}} \left| \int_{t_{n-1}}^{t_n} (\dot{U}, \pi P\Phi - \Phi)_\Delta + (\epsilon(U)\nabla U, \nabla(\pi P\Phi - \Phi))_\Delta - (f(U), \pi P\Phi - \Phi)_\Delta \, dt \right|.$$

Thus, if (3.2) is not satisfied, the mesh is refined in order to achieve

$$\text{Æ}(U) \lessapprox \text{TOL}. \tag{3.4}$$

The adaptive error control problem can now be profitably posed as a constrained minimization problem, namely to find a mesh with a minimal number of degrees of freedom on which the approximation satisfies the bound (3.4). Using the fact that the bound Æ is a sum of positive terms and assuming the solution is asymptotically accurate, a calculus of variations argument yields the generic (see e.g. [9, 10, 3, 2]).

> ***Principle of Equidistribution*** An approximate solution of the constrained optimization problem for an optimal mesh for an upper bound on the error is achieved when the elements contributions to the bound are approximately equal.

The Principle of Equidistribution has been used in various forms at least since the seventies (and probably earlier in industry). However, experience with a wide range of problems suggest that the bound $Æ(U)$ is generically several orders of magnitude larger than the estimate $E(U)$. A strategy based on the Principle of Equidistribution that optimizes computational cost with respect to a error *bound* and not the actual error can therefore result in significant over-refinement.

In general, there are many solutions of the constrained minimization problem associated with (3.4). An adaptive mesh algorithm is a procedure for computing an acceptable solution. Traditionally, different approaches are used for spatial and temporal adaption. A global "compute-estimate-mark-adapt" algorithm (see for example 1.1) is typically used for spatial meshes. This is an iterative approach in which only some fraction of the elements on which the contribution to the error bound is largest are refined during each iteration and whole cycle is iterated until a prescribed tolerance is achieved. Temporal approaches to mesh adaption, e.g., local error control [21], tend to use a "sweeping" strategy from initial to final time, where a solution is advanced past each time step only when the step contribution is estimated to be lower than an acceptable fraction of the total error. This may be viewed as a generally pessimistic way to achieve the Principle of Equidistribution because it removes positive effects of cancelation of error altogether. As a consequence of these differences, element contributions to the error estimate or bound typically vary in size quite considerably while contributions from different time intervals are more nearly equal.

We use a strategy that treats space and time discretizations more equitably. In the case of a parabolic problem, it is straightforward to distinguish the time and space contributions to the bound $Æ$. We define the time and space bounds as follows.

DEFINITION 3.3. *Element-wise temporal and spatial error bounds*

$$\begin{aligned} Æ_t(U) = &\sum_{n=1}^{N}\sum_{\triangle\in\mathcal{T}}\left|\left([U]_{n-1},((\pi-I)P\Phi)^+_{n-1}\right)_{\triangle}\right| \\ &+\sum_{n=1}^{N}\sum_{\triangle\in\mathcal{T}}\left|\int_{t_{n-1}}^{t_n}(\dot{U},(\pi-I)P\Phi)_{\triangle}+(\epsilon(U)\nabla U,\nabla(\pi-I)P\Phi)_{\triangle}\right. \\ &\qquad\left.-(f(U),(\pi-I)P\Phi)_{\triangle}\,dt\right|, \end{aligned} \tag{3.5}$$

$$\begin{aligned} Æ_x(U) = &\sum_{\triangle\in\mathcal{T}}|((I-P)u_0,\Phi(0))_{\triangle}|+\sum_{n=1}^{N}\sum_{\triangle\in\mathcal{T}}n\left|\left([U]_{n-1},(P\Phi-\Phi)^+_{n-1}\right)_{\triangle}\right| \\ &+\sum_{n=1}^{N}\sum_{\triangle\in\mathcal{T}}\left|\int_{t_{n-1}}^{t_n}(\dot{U},P\Phi-\Phi)_{\triangle}+(\epsilon(U)\nabla U,\nabla(P\Phi-\Phi))_{\triangle}\right. \\ &\qquad\left.-(f(U),P\Phi-\Phi)_{\triangle}\,dt\right|. \end{aligned} \tag{3.6}$$

We see that the time bound is precisely the *a posteriori* bound for the dG approximation for the "method of lines" initial value problem resulting after discretization in space. The adjoint weight depends on the projection of the adjoint solution into the time finite element space. On the other hand, the adjoint weight in the space bound depends on the projection of the adjoint solution into the spatial finite element space.

We split the error between the time and space contributions and refine the current mesh in order to achieve

$$Æ_x(U) \lessapprox \frac{\mathrm{TOL}}{2} \text{ and } Æ_t(U) \lessapprox \frac{\mathrm{TOL}}{2}. \tag{3.7}$$

On a given time interval, this requires an iteration during which both the space mesh and time steps are refined.

3.2. Goal oriented block adaptive error control. For the purpose of developing a block adaptive algorithm, we treat adaptivity with respect to space and time in the same way. The reason is that we determine the blocks by predicting the local element sizes (or number of sub-elements) that are required in the final mesh. We create a block by grouping together a set of coarse-scale space-time slabs that are adjacent in time and satisfy some criteria, e.g. similar spatial meshes are predicted for the space-time slabs in the block or a maximal number of elements are predicted to be required in the block.

3.2.1. Choosing a global tolerance for the error bound. We want the predictions of the element sizes required in an acceptable fine scale mesh to be as accurate as possible. We recall that an acceptable mesh need only satisfy the estimate criterion (3.2) and not the more stringent bound criterion (3.4). We define the overestimation factor for a given mesh,

$$\gamma = \frac{Æ(U)}{E(U)},$$

and the corresponding absolute tolerance for Æ,

$$\mathrm{ATOL} = \gamma \times \mathrm{TOL}.$$

We replace (3.4) by

$$Æ_x(U) \lessapprox \frac{\mathrm{ATOL}}{2} \text{ and } Æ_t(U) \lessapprox \frac{\mathrm{ATOL}}{2}. \tag{3.8}$$

Note that ATOL $\approx$ TOL when there is little cancelation among the element contributions and ATOL $>$ TOL otherwise. In this way, we attempt to mitigate the inefficiency that is introduced by replacing an accurate error estimate by an inaccurate bound in decisions about mesh refinement. This approach for setting tolerances is discussed further in [16].

3.2.2. Predicting refinement in space. Given a local space-time element $\mathfrak{S} = \mathfrak{S}(\triangle, n) = \triangle \times [t_{n-1}, t_n]$ in the n^{th} space-time slab that is marked for refinement, we show how to predict the number of space-time elements that are needed to meet the acceptance criterion. We assume that in the current mesh, there are N time steps and M space elements in each space-time slab, giving a total of NM space-time elements. We define a local absolute tolerance

$$\mathrm{LATOL} = \frac{\mathrm{ATOL}}{2NM}.$$

By the Principle of Equidistribution, we adopt the goal of refining each space-time element so that the local element contribution is approximately LATOL.

Using *a priori* convergence analysis, see [15], it is possible to show that there is a constant C such that

$$Æ_x|_{\mathfrak{S}(\triangle,n)} \sim C(h_\triangle)^p \tag{3.9}$$

as $h_\triangle \to 0$, where p is related to the order of the finite element method in space and $h_\triangle$ is the element size. Likewise, we can show constant C such that

$$Æ_t|_{\mathfrak{S}(\triangle,n)} \sim Ck^q \tag{3.10}$$

as $k \to 0$, where q is related to the order of the finite element method in time.

Now suppose that an element $\mathfrak{S}_{\text{new}}$ in the final mesh is obtained from $\mathfrak{S}_{\text{old}}$ in the current mesh by refinement. We have

$$\text{LATOL} \approx Æ_x|_{\mathfrak{S}_{\text{new}}} \approx Æ_x|_{\mathfrak{S}_{\text{old}}} \times \left(\frac{h_{\triangle_{\text{new}}}}{h_{\triangle_{\text{old}}}}\right)^p. \tag{3.11}$$

This yields a prediction for the new mesh size,

$$h_{\triangle_{\text{new}}} \approx \left(\frac{\text{LATOL}}{Æ_x|_{\mathfrak{S}_{\text{old}}}}\right)^{1/p} \times h_{\triangle_{\text{old}}}. \tag{3.12}$$

Recalling that d is the space dimension, this predicts that the element $\triangle_{\text{old}}$ should be refined into roughly

$$\left(\frac{h_{\triangle_{\text{old}}}}{h_{\triangle_{\text{new}}}}\right)^d = \left(\frac{Æ_x|_{\mathfrak{S}_{\text{old}}}}{\text{LATOL}}\right)^{d/p} \tag{3.13}$$

sub-elements.

3.2.3. Predicting refinement in time. For refinement in time,

$$Æ_t|_{\mathfrak{S}_{\text{new}}} \approx Æ_t|_{\mathfrak{S}_{\text{old}}} \times \left(\frac{k_{\text{new}}}{k_{\text{old}}}\right)^q \approx \text{LATOL}. \tag{3.14}$$

This yields a prediction for the new mesh size,

$$k_{\text{new}} \approx \left(\frac{\text{LATOL}}{Æ_t|_{\mathfrak{S}_{\text{old}}}}\right)^{1/q} \times k_{\text{old}}. \tag{3.15}$$

This predicts that the time step k_{old} should be refined into roughly

$$\frac{k_{\text{old}}}{k_{\text{new}}} = \left(\frac{Æ_t|_{\mathfrak{S}_{\text{old}}}}{\text{LATOL}}\right)^{1/q} \tag{3.16}$$

sub-intervals.

3.2.4. Determining overlaps for meshes on adjacent blocks. After the meshes for each block are determined based on the *a posteriori* prediction of error, we need to estimate the effects of transferring the solution between meshes on adjacent blocks. See § 4.1 for an example that illustrates this point. Recall that (2.9) provides a bound on these effects. The difficulty with using (2.9) is that we do not have the fine scale numerical solution U required for that expression until after solving on the fine scale, whereas ideally we could predict a reasonable overlap before computing the expensive fine scale solution.

We list three strategies for mitigating the possibility of projection error in our block adaptive framework.

1. There is a very simple strategy. In forming the space mesh for the block $[T_{b-1}, T_b] \times \Omega$, we guide refinement by using the maximum of the element contributions on each individual element, taking the maximum over the time intervals included in the block. We may simply include the maximum over the last time interval included in the previous block, $[T_{b-2}, T_{b-1}]$, i.e., over the interval $[t_{b-1,N_{b-1}-1}, t_{b-1,N_{b-1}}]$. We can be even more conservative by including some number of the last time steps in the maximum computation.
2. We can use gradient recovery [6] to compute an approximate solution on the fine scale mesh in each block using the solution from the last time interval contained in each block. We can then directly compute $(I - P_b)U$ for each b and evaluate (2.9).
3. We can evaluate (2.9) *a posteriori* by evaluating $(I - P_b)U$ using the fine scale forward solution and the coarse scale adjoint solution.

3.3. Block adaptive algorithms. Using the development above, we present a generic block adaptive algorithm in Algorithm 3.1. We provide a detailed algorithm in Appendix A.

Algorithm 3.1 Block Adaptive Algorithm

1: Choose the "coarse" mesh and time step
2: Compute the coarse scale numerical solution
3: Estimate the element contributions to the error for the current solution
4: Predict the number of space-time elements into which each current space-time element is to be divided using (3.13) and (3.16)
5: Build block discretizations by constructing meshes satisfying the requirements for groups of neighboring time steps
6: Compute the fine scale numerical solution using the block discretizations

We note that the Block Adaptive Algorithm 3.1 can be iterated, so that the fine scale becomes the new coarse scale, and a new fine scale is subsequently computed. In crude terms, the block adaptive Algorithm 3.1 is analogous to the core estimate-mark-refine algorithm at the heart of the generic Algorithm 1.1, but is different in the mark and refine steps. The critical step defining the block adaptive algorithm Algorithm 3.1 is the strategy used to create block discretizations. Once the blocks are identified, we can use any adaptive mesh refinement strategy for producing the actual meshes. We describe several strategies for determining block discretizations.

3.3.1. A memory-bound strategy. In the first strategy, we assume there is a target number of elements `Nmax` in space that is maximal in some sense, e.g., the largest number of elements that can be stored in core. We form blocks by creating a

union of adjacent coarse-scale space-time slabs, one slab at a time, until the projected space mesh for the block uses `Nmax` elements. To create the block mesh, we use the maximum of the predicted number of elements `Nelem_children` on each individual element (given by equation (3.13)) in the union forming the block. We illustrate in Fig. 3.2. The parameter θ governs how often the mesh is replaced by a coarser mesh, where $\theta \approx 10$ works well in practice.

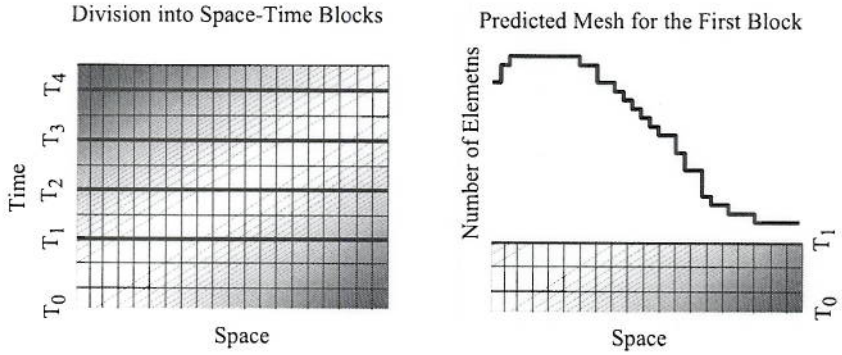

FIG. 3.2. *The memory bound strategy is used for a traveling pulse that moves with constant speed from left to right. Left: The original uniform mesh and a contour plot of the number of predicted elements of new sub-elements* `Nelem_children`. *The scale is from dark (low) to white (high). Right: The predicted number of new sub-elements* `Nelem_children` *for the first block, which consists of three adjacent space-time slabs from the original discretization.*

3.3.2. A correlation strategy. In the second strategy, we aim to choose blocks in order to use a relatively small number of elements, so `Nmax` may be considerably smaller than for the first algorithm. This strategy forms a block by grouping together adjacent coarse-scale space-time slabs whose predicted number of elements `Nelem_children` are close.

In [14], we consider the problem of detecting significant overlap of local element contributions for different computations. Following the approach there, given two vectors $\vec{v}, \vec{w}$ whose coefficients are element contributions to an error estimate, we define their *correlation* to be $c(\vec{v}, \vec{w}) = \vec{v} \cdot \vec{w}$. We say that $\vec{v}$ is significantly correlated with $\vec{w}$ if

$$\frac{c(\vec{v}, \vec{w})}{\|\vec{w}\|^2} > \gamma_1 \text{ and } \frac{\|\vec{w} - \frac{c(\vec{v}, \vec{w})}{\|\vec{v}\|^2}\vec{v}\|}{\|\vec{w}\|} < \gamma_2,$$

where $0 < \gamma_1, \gamma_2$. The first condition insures that $\vec{v}$ has a suitable large projection onto $\vec{w}$ while the second condition corrects for differences in scale between $\vec{v}$ and $\vec{w}$ (consider $\|\vec{v}\| \gg \|\vec{w}\|$ so that $c(\vec{v}, \vec{w}) \gg \|\vec{w}\|$).

We implement the new criterion for creating blocks by choosing to add the next time slab to a current block based on the correlation criterion.

3.3.3. Global strategies. In the first two strategies for creating blocks, we sweep through time. We can also use a bisection search beginning with the original large block and subdividing to find acceptable blocks. In analog to the difference between the standard global strategy for space mesh refinement to achieve the Principle of Equidistribution and the local-error control approach, the bisection search is a global strategy that can be a more efficient way to achieve equidistribution.

4. Computational Examples. We apply the block adaptive algorithms to several prototypical examples in one and three space dimensions. The one dimensional examples illustrate several key points when implementing block-adaptive methods, while the three dimensional examples include a traveling wave front, a solution that undergoes time- and space-localized perturbations, and a periodic motion in a convection-dominated flow.

The forward problems and adjoint problems are solved with linear and quadratic elements in space and dG0 and cG1 in time respectively. The one dimensional examples are computed using the Matlab code ACES [25]. The three dimensional examples are performed on a hexahedral mesh using a trilinear spatial basis for the forward problem and a triquadratic basis for the adjoint. Local mesh refinement is accomplished by the use of hanging nodes where one hanging node per edge or face is allowed. Conformity of the basis is obtained by interpolation of the surrounding regular nodes. The use of an hierarchical octree-based data structure assists refinement but also allows for de-refinement when the element indicators are small. For the convection driven flow problem, SUPG is employed for both the forward and adjoint problems, with parameter

$$\delta = \frac{1}{(1/\Delta t + U/h)},$$

where Δt is the time step and U is the speed of the convection field at the current time, i.e., $U = ||\beta||_2$ in (4.5). This is not an obstacle for the block-adaptive framework, as we simply modify the theoretical convergence rate p in the computation of `Nelem_children` in (3.13).

4.1. Example One: Projection errors between blocks. We illustrate the necessity for addressing the effect of transferring solutions between space-time blocks with a simple one-dimensional example involving a traveling wave.

$$\begin{cases} u_t - u_{xx} = f(x,t), & 0 < x < 1,\ 0 < t, \\ u(0,t) = u(1,t) = \beta(t), & 0 < t, \\ u(x,0) = \tanh(\alpha(x-0.2)), & 0 < x < 1, \end{cases} \tag{4.1}$$

where $\alpha = 50$ and f and β are chosen to give an exact solution $u = \tanh(\alpha(x-t-0.2))$. We solve with a coarse mesh using $h = 0.1$ and time step $k = 0.05$ from initial time 0 to final time 0.6. The quantity of interest is the average space-time error. We compute a fine scale solution using two blocks derived from the coarse scale solution. The first block, $t = [0, 0.3]$, uses a finer spatial mesh in the region $x \in [0.1, 0.6]$, while the second block uses a fine mesh in the region $[0.5, 1]$, so the overlap is minimal and and the predictions for refinement areas are incorrect. Consequently, the approximate traveling wave travels too quickly. The first block solution at $t = 0.3$ and its projection onto the second block at $t = 0.3$ is displayed in Fig. 4.1.

In Fig. 4.1 we illustrate the *a posteriori* use of (2.9) to correct the projection error. Block 1 is computed using the predicted fine scale mesh. Block 2 is tested for significant projection error using (2.9) using the fine scale solution for Block 1 and the mesh for Block 2 is refined if the elementwise projection error exceeds $LATOL$. We note that the overlap strategy for the projection error in §3.2.4 also works well in this particular example.

4.2. Example Two: Coarse scale resolution. Since we are using the coarse scale discretization to predict the global behavior of the solution on the fine scale,

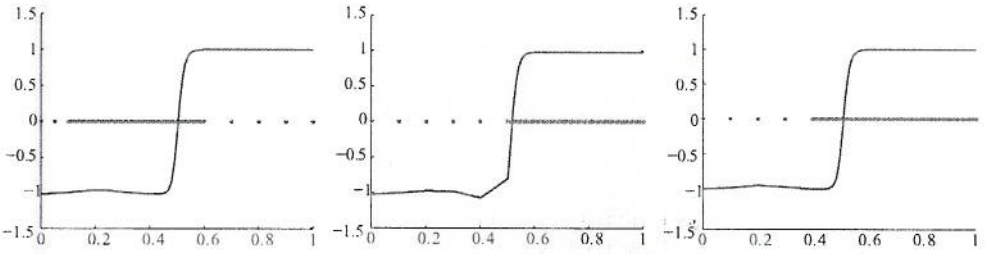

FIG. 4.1. *Problem (4.1). The circles indicate the spatial meshes used in each of the two blocks. Left: the solution on Block 1. Middle: the projection of the approximate solution in block 1 onto the mesh in block 2. Right: the solution onto Block 2 after using the projection error estimate (2.9) to correct significant projection errors between the two blocks. This demonstrates the possible consequences when the meshes for neighboring blocks do not overlap sufficiently.*

it is important to insure that the coarse scale discretization is not too coarse. (This is a difference between the block adaptive approach and a standard adaptive mesh refinement, which is generally started with a very coarse mesh.) This issue is especially important for nonlinear problems since linearization is used to define the adjoint problem, which in turn provides the means to quantify the effects of cancelation and accumulation of errors.

Consider the one-dimensional nonlinear parabolic equation

$$\begin{cases} u_t - \frac{1}{2\alpha} u_{xx} = \alpha(u-1)(1-u^2), & -1 < x < 1,\ 0 < t < 0.6, \\ u(0,t) = -1,\ u(1,t) = 1, & 0 < t, \\ u(x,0) = \tanh(\alpha(x-0.2)), & -1 < x < 1, \end{cases} \tag{4.2}$$

We choose α to obtain the same solution as the example in § 4.1, $u = \tanh(\alpha(x - t - 0.2))$. The quantity of interest is the average space-time error. For the coarse discretization, we use $h = 0.05$ and $k = 0.05$. These choices provide an excellent coarse scale discretization for the linear example in § 4.1 but does not work well for the nonlinear version. We show two snapshots of the solution u in Fig. 4.2 at $t = 0.3$ and $t = 0.6$. The wave-speed is predicted inaccurately, which leads to a poor block selection and this subsequently affects the fine scale accuracy. Using a coarse scale discretization with $h = 0.1$ and $k = 0.1$ yields inaccurate results.

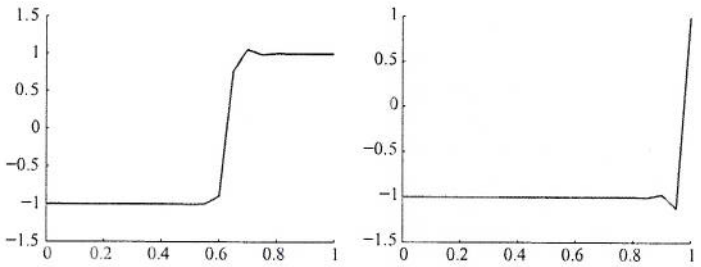

FIG. 4.2. *Problem (4.2). Correlation strategy with an insufficiently accurate coarse-scale solution. Solution on the adapted mesh at $t = 0.3$ and $t = 0.6$ respectively.*

The poor predictions based on the coarse-scale discretization can be avoided by slightly enriching the discretization with a finer time step. We use a coarse discretiza-

tion with $h = 0.05$ and $k = 0.01$ and the correlation strategy to produce blocks. The approximate solution on the adapted mesh at $t = 0.45$ is shown in Fig. 4.3.

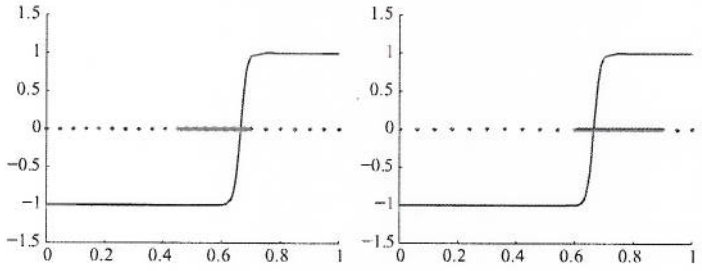

FIG. 4.3. *Problem (4.2). Correlation strategy with an improved coarse-scale solution. Solution on the adapted mesh at $t = 0.45$ on blocks 3 and 4 respectively.*

4.3. Example three: A traveling wave solution. This example is a wave propagating along the main diagonal of the unit cube ($\Omega = [0,1] \times [0,1] \times [0,1]$). The governing equation is

$$\begin{cases} u_t - \Delta u = f(x,t), & x \in \Omega,\ 0 < t, \\ u(x,t) = 0, & x \in \partial\Omega, 0 < t, \\ u(x,0) = (x_1 - x_1^2)(x_2 - x_2^2)(x_3 - x_3^2)\arctan(\frac{c\sqrt{3}}{3}\sqrt{x_1^2 + x_2^2 + x_3^2}), & x \in \Omega, \end{cases} \tag{4.3}$$

where $c = 75$ and f is constructed to yield the exact solution

$$u = \frac{\sqrt{3}}{3}\arctan(\frac{c\sqrt{3}}{3}\sqrt{x_1^2 + x_2^2 + x_3^2} - t).$$

The coarse block solution u_C is constructed on an $8 \times 8 \times 8$ uniform mesh using hexahedral meshes with an initial time step of 0.1. The quantity of interest is the time average of the solution value. The memory bound strategy is used to construct the discretization blocks with $ATOL = 0.000178$ and `Nmax`=50000. Block information is given in Table 4.1. As might be expected, all of the blocks use approximately the same number of elements. We show contour plots of the solution on "slices" of some of the block meshes along the plane $x = 0.5$ in Fig. 4.4.

Block	T_{b-1}	T_b	# vertices	# hexahedra
1	0	0.4	58711	50394
2	0.4	0.6	63219	54503
3	0.6	0.7	72267	61265
4	0.7	0.8	62626	52368
5	0.8	1	64764	54860
6	1	1.1	62790	54377

TABLE 4.1
Problem (4.3). Blocks resulting from the memory bound strategy.

4.4. Example Four: Localized forcing in space and time. This example contrasts the difference in the blocks produced by the memory bound and correlation

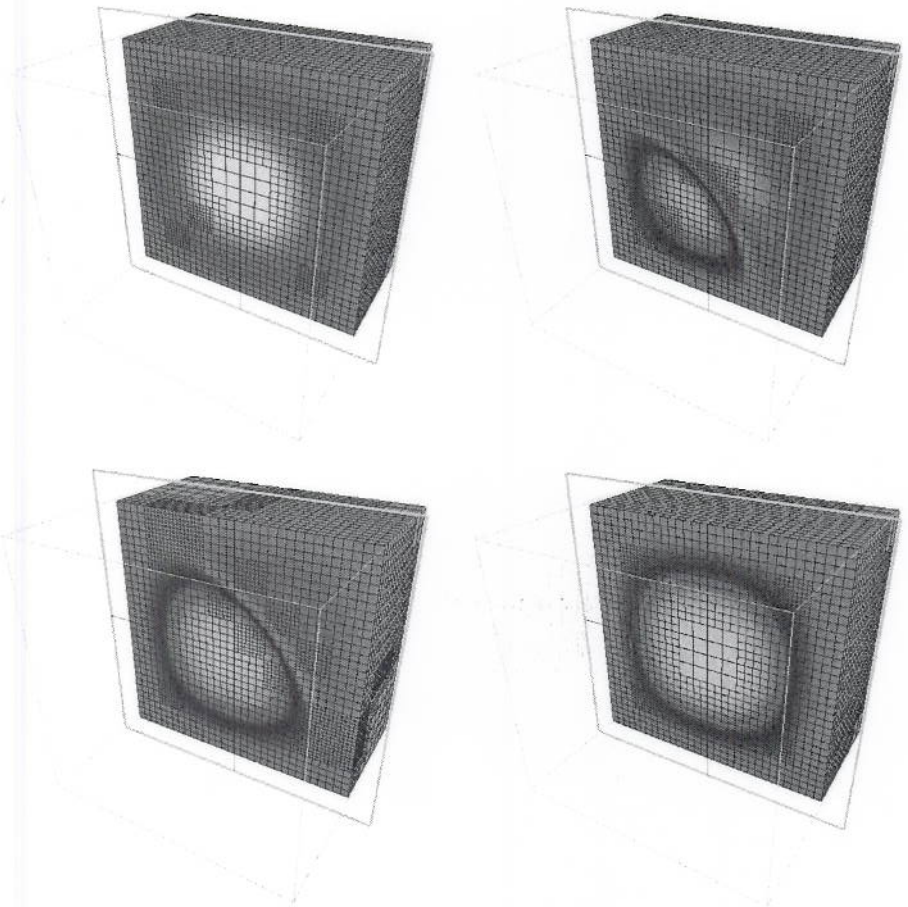

FIG. 4.4. *Problem (4.3). Memory bound strategy. Slices through the mesh perpendicular to the x-axis at $x = 0.5$. Upper left: $t = 0$ (block 1). Upper right: $t = 0.44$ (block 2). Lower left: $t = 0.6$ (block 3). Lower right: $t = 1.1$ (block 6).*

strategies when solving an equation with source terms that are localized in space and time. The governing equation on the unit cube Ω is

$$\begin{cases} u_t - \Delta u = 50e^{-(\alpha_1(x-x_1)^2+(t-t_1)^2)} + 20e^{-(\alpha_2(x-x_2)^2+(t-t_2)^2)}, & x \in \Omega, 0 < t, \\ u(x,0) = 0, & x \in \Omega, \end{cases} \tag{4.4}$$

with homogeneous Neumann boundary conditions on all the sides except the bottom where a homogeneous Dirichlet condition is imposed. We choose $\alpha_1 = 50$, $\alpha_2 = 10$, $t_1 = 1$, $t_2 = 10$, $x_1 = (0.125, 0.125, 0.125)$ and $x_2 = (0.75, 0.5, 0.75)$. The quantity of interest is the time average of the solution value.

We use a coarse discretization consisting of an $8 \times 8 \times 8$ uniform hexahedral mesh and time step of 0.1. With $ATOL = 0.00010044$ and `Nmax` $= 50000$ we show the block information for the memory bound and correlation strategies respectively in Table 4.2 and Table 4.3. The algorithms lead to significantly different block meshes.

Block	T_{b-1}	T_b	# vertices	# hexahedra
1	0	1.1	59465	54125
2	1.1	1.2	63112	57772
3	1.2	2.4	45359	40958
4	2.4	11.9	12383	10165
5	11.9	14.9	2029	1478

TABLE 4.2
Problem (4.4). Blocks resulting from the memory bound strategy.

Block	T_{b-1}	T_b	# vertices	# hexahedra
1	0	1.1	63112	57772
2	1.1	1.2	63112	57772
3	1.2	1.6	45359	40958
4	1.6	2.5	9611	8037
5	2.5	2.9	1968	1436
6	2.9	8.5	966	652
7	8.5	9	2617	1926
8	9	10.8	12651	10382
9	10.8	11.3	7363	5860
10	11.3	12.6	3139	2360
11	12.6	14.9	729	512

TABLE 4.3
Problem (4.4). Blocks resulting from the correlation strategy.

The correlation strategy chooses many more blocks, but many of the blocks have very low numbers of elements.

We show planar slices near x_1 and x_2 of the meshes for Blocks 1 and 3 in Fig. 4.5. For comparison, we show planar slices perpendicular to the x-axis near x_1 and x_2 of the meshes for blocks constructed using the two strategies in Fig. 4.6. Both strategies result in similar meshes near x_2 at time $t = 10$. However at $t = 8.8$, the correlation strategy leads to coarse meshes that are not produced by the memory bound strategy. The mesh resulting from the memory bound strategy retains the refinement resulting from the earlier perturbation near x_1 at $t = 1$.

4.5. Example Five: Periodic motion in a convection-dominated flow. This example has a heat source with a forced oscillating convective term within the unit cube Ω to produce an "orbiting" zone of perturbation. The governing equation is

$$\begin{cases} u_t + \beta \cdot \nabla u - \Delta u = f, & x \in \Omega, 0 < t < 1, \\ u(x,t) = 0, & x \in \partial\Omega, 0 < t < 1, \\ u(x,0) = 0, & x \in \Omega, \end{cases} \tag{4.5}$$

with $\beta = (20(\cos(\pi t)\sin(2\pi t), \sin(\pi t)\sin(2\pi t), \cos(2\pi t))$ and $f(x) = e^{-50(x_1^2+x_2^2+x_3^2)}$. The quantity of interest is the time average value. The coarse discretization used 4913 vertices and at time step of 0.01. The blocks constructed by the memory-bound strategy using $ATOL = 0.00044$ and `Nmax`=50000 are described in Table 4.4.

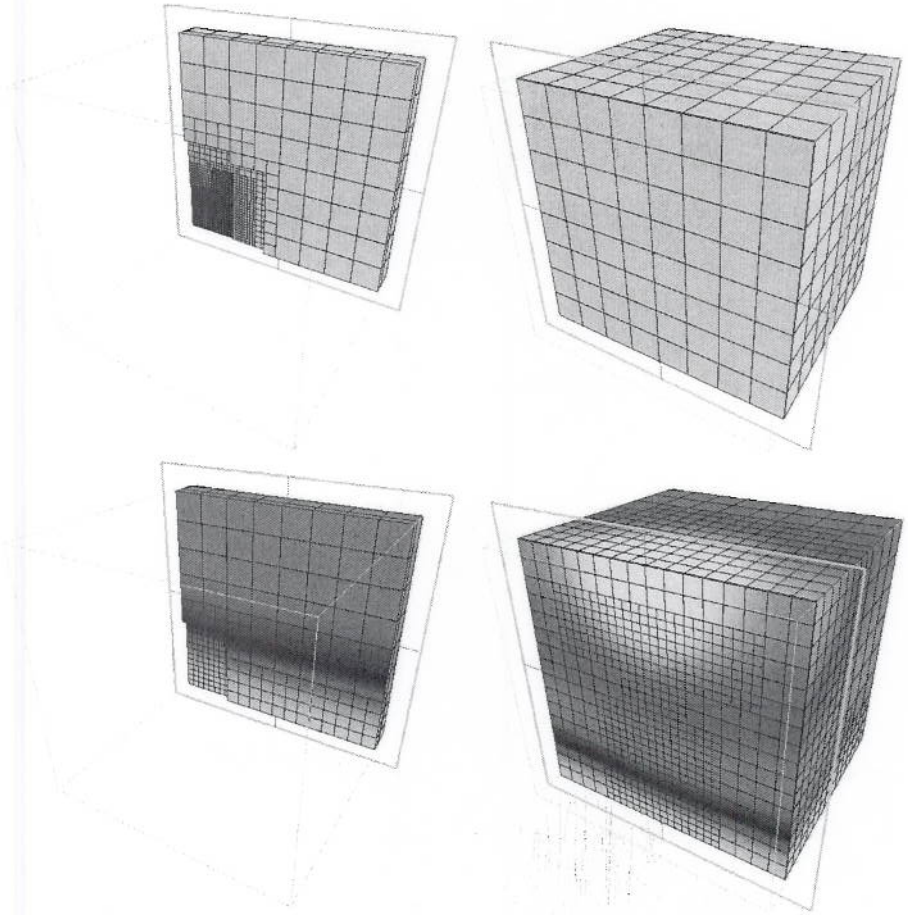

FIG. 4.5. *Problem (4.4). Memory bound strategy. Slices through the mesh perpendicular to the x-axis. Upper left: Slice near x_1 at $t = 1$ (block 1). Upper right: Slice near x_2 at $t = 1$ (block 1). Lower left: Slice near x_1 at $t = 10$ (block 4). Lower right: Slice near x_2 at $t = 10$ (block 4).*

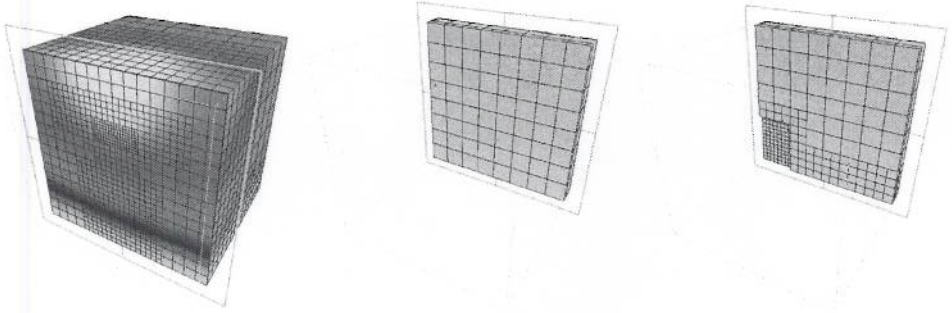

FIG. 4.6. *Problem (4.4). Slices through the mesh perpendicular to the x-axis. Left: Correlation strategy. Slice near x_2 at $t = 10$ (block 8). Middle: Correlation strategy. Slice near x_1 at $t = 8.8$ (block 7). Right: Memory bound strategy. Slice near x_1 at $t = 8.8$ (block 4).*

Block	T_b	T_{b+1}	# vertices	# hexahedra
1	0	0.09	58799	51066
2	0.09	0.15	58424	50289
3	0.15	0.27	58393	50359
4	0.27	0.61	59102	50744
5	0.61	0.99	28395	23388

TABLE 4.4
Problem (4.5). Blocks resulting from the memory bound strategy.

We provide "slices" through the mesh that are perpendicular to the x-axis at $x = 0.5$ for four representative times in Fig. 4.7.

5. Conclusions. In this paper, we consider adaptive algorithms for evolution problems that use a sequence of "blocks" in time which employ fixed, non-uniform space meshes. Blockwise adaptive algorithms provide a way to balance the goal of achieving desired accuracy using discretizations with relatively few degrees of freedom with the computational overhead associated with load balancing, re-meshing, matrix reassembly and error estimation. Block adaptive algorithms achieve this balance by minimizing the number of mesh changes. However, a major issue is determining block discretizations from coarse scale solution information that achieve the desired accuracy and efficiency. We describe several strategies to achieve this goal using adjoint-based *a posteriori* error estimates. We demonstrate the behavior of the proposed algorithms as well as several technical issues in a set of examples.

REFERENCES

[1] I. BABUŠKA AND T. STROUBOULIS, *The Finite Element Method and its Reliability*, Clarendon Press, New York, 2001.

[2] W. BANGERTH AND R. RANNACHER, *Adaptive Finite Element Methods for Differential Equations*, Birkhauser Verlag, 2003.

[3] R. BECKER AND R. RANNACHER, *An optimal control approach to* a posteriori *error estimation in finite element methods*, Acta Numerica, (2001), pp. 1–102.

[4] M. BERGER AND P. COLELLA, *Local adaptive mesh refinement for shock hydrodynamics*, J. Comput. Phys., 82 (1989), pp. 64–84.

[5] M. BIETERMAN, J. FLAHERTY, AND P. MOORE, *Adaptive refinement methods for non-linear parabolic partial differential equations*, in Accuracy Estimates and Adaptive Refinements in Finite Element Computations, John Wiley and Sons, Ltd., New York, 1986.

[6] V. CAREY, D. ESTEP, AND S. TAVENER, *Averaging based projections in operator decomposition methods for elliptic systems.* In preparation, 2009.

[7] S. F. DAVIS AND J. E. FLAHERTY, *An adaptive finite element method for initial-boundary value problems for partial differential equations*, SIAM J. Sci. Stat. Comput., 3 (1982), pp. 85–107.

[8] T. DUPONT, *Mesh modification for evolution equations*, Math. Comp., 39 (1982), pp. 85–107.

[9] K. ERIKSSON, D. ESTEP, P. HANSBO, AND C. JOHNSON, *Introduction to adaptive methods for differential equations*, Acta Numerica, (1995), pp. 105–158.

[10] ———, *Computational Differential Equations*, Cambridge University Press, New York, 1996.

[11] K. ERIKSSON AND C. JOHNSON, *Adaptive finite element methods for parabolic problems I: A linear model problem*, SIAM J. Numer. Anal., 28 (1991), pp. 43–77.

[12] D. ESTEP, *A posteriori error bounds and global error control for approximations of ordinary differential equations*, SIAM J. Numer. Anal., 32 (1995), pp. 1–48.

[13] D. ESTEP AND D. FRENCH, *Global error control for the continuous Galerkin finite element method for ordinary differential equations*, RAIRO Modél. Math. Anal. Numér., 28 (1994), pp. 815–852.

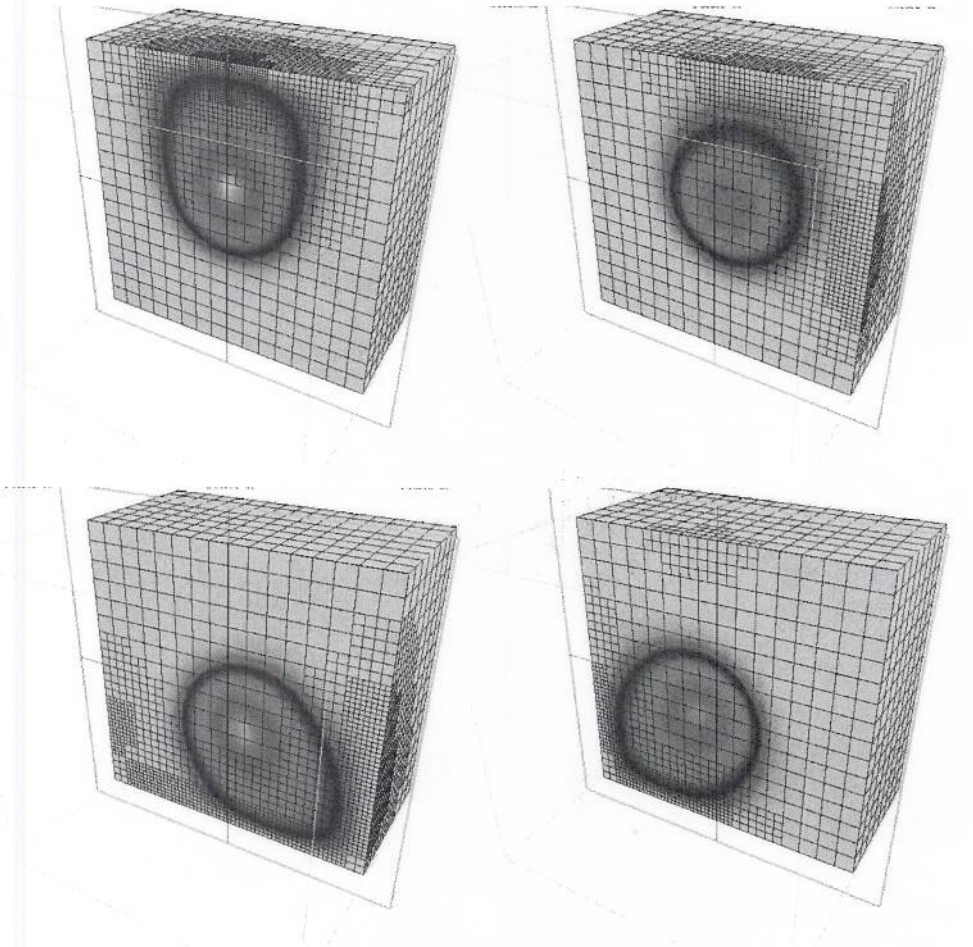

FIG. 4.7. *Problem (4.5). Memory bound strategy. Slices through the mesh perpendicular to the x-axis at* $x = 0.5$. *Upper left:* $t = 0.04$ *(block 1). Upper right:* $t = 0.16$ *(block 3). Lower left:* $t = 0.42$ *(block 4). Lower right:* $t = 0.62$ *(block 5).*

[14] D. ESTEP, M. HOLST, AND M. LARSON, *Generalized Green's functions and the effective domain of influence*, SIAM J. Sci. Comput., 26 (2005), pp. 1314–1339.

[15] D. ESTEP, M. LARSON, AND R. WILLIAMS, *Estimating the error of numerical solutions of systems of reaction-diffusion equations*, Memoirs A.M.S., 146 (2000), pp. 1–109.

[16] D. ESTEP AND J. SANDELIN, *Cancelation of error and adaptive error control for ordinary differential equations*. In preparation, 2009.

[17] D. ESTEP AND R. WILLIAMS, *Accurate parallel integration of large sparse systems of differential equations*, Math. Models Meth. Appl. Sci., 6 (1996), pp. 535–568.

[18] R. E. EWING, R. D. LAZAROV, AND A. T. VASSILEV, *Adaptive techniques for time-dependent problems*, Comput. Methods Appl. Mech. Engrg., 101 (1992), pp. 113–126.

[19] J. E. FLAHERTY, R. M. LOY, C. OZTURAN, M. S. SHEPHARD, B. K. SZYMANSKI, J. D. TERESCO, AND L. H. ZIANTZ, *Parallel structures and dynamic load balancing for adaptive finite element computation*, Appl. Numer. Math., 26 (1998), pp. 241–263.

[20] M. GILES AND E. SÜLI, *Adjoint methods for PDEs: A posteriori error analysis and postprocessing by duality*, Acta Numerica, (2002), pp. 145–236.

[21] E. HAIRER, S. NORSETT, AND G. WANNER, *Solving Ordinary Differential Equations I*, Springer-Verlag, New York, 1987.

[22] P. K. MOORE AND J. E. FLAHERTY, *Adaptive local overlapping grid methods for parabolic-systems in 2 space dimensions*, J. Comput. Phys., 98 (1992), pp. 54–63.
[23] J.-F. REMACLE, O. KLAAS, J. E. FLAHERTY, AND M. S. SHEPHARD, *Parallel algorithm oriented mesh database*, Engineering with Computers, 18 (2002), pp. 274–284.
[24] J. R. STEWART AND H. C. EDWARDS, *Parallel adaptive application development using the SIERRA framework*, in Proceedings of the First MIT Conference in Computational Fluid and Solid Mechanics, Elsevier, Amsterdam, 2001.
[25] T. WILDEY, *Adaptive Coupled Equation Solver (ACES)* `http://users.ices.utexas.edu/~twildey/software`.

Appendix A. Detailed description of a block adaptive algorithm.

The notation used in our block adaptive algorithm is as follows.

1. `Ntimestep` = current number of time steps
2. `Nelem(j)` = number of space elements in timestep j, i.e., for $t \in [t_{j-1}, t_j]$
3. `Ntimestep_children(j)` = number of subintervals into which timestep j is to be divided
4. `Nelem_children(i,j)` = number of subelements into which finite element i is to be divided in timestep j
5. The bth "block" is time interval $[T_{b-1}, T_b] = [t_{b,0}, t_{b,N_b}]$
6. The bth "block" comprises timesteps $j_{b-1}, \ldots, j_b$, i.e., $N_b = j_b - j_{b-1}$, $t_{b,0} = t_{j_{b-1}}$ and $t_{b,N_b} = t_{j_b}$.
7. `block(i,b)` = number of intervals the parent element i will be divided into on block b.
8. `Nelem_block(b)` = number of elements in block b.
9. We use the MATLAB colon operator : to denote the full row or column.
10. The parameter θ governs how often a mesh is coarsened; $\theta \approx 10$ works well.

Algorithm A.1 A memory-bound strategy

Input error tolerance `TOL`, maximum number of elements in any block `Nmax`, the initial coarse-scale discretization for the forward problem, and the coarse-scale discretization for the adjoint problems
Solve forward problem (1.1) for U on $[0, T]$
Project forward solution onto coarse-scale adjoint problem mesh
Solve adjoint problem (2.4) on coarse scale mesh and compute $E(U)$
Compute LATOL, $Æ_x$, $Æ_t$ (3.6),(3.5)
for $j = 1, \ldots,$ `Ntimesteps` **do**
    Compute `Ntimestep_children(j)` (3.13)
    for $i = 1, \ldots,$ `Nelem(j)` **do**
        Compute `Nelem_children(i,j)` (3.16)
    end for
end for
`Ntimesteps` $\leftarrow \sum_{j=1}^{\texttt{Ntimesteps}}$ `Ntimestep_children(j)`
Each subinterval of $[t_{j-1}, t_j]$ inherits `Nelem_children(i,j)`
$b = 1$, $T_0 = 0$, $T_1 = k_1$, $j_0 = 1$, $j = 2$
`block(:,b)` $\leftarrow$ `Nelem_children(:,1)`
`Nelem_block(b)` $\leftarrow \sum_i$ `block(i,b)`
while $T_b < T$ **do**
    while `Nelem_block(b)` $<$ `Nmax` **and**
        `Nelem_block(b)` $< \theta \times \sum_{i=1}^{\texttt{Nelem(j)}}$ `Nelem_children(i,j)` **do**
        $j_b \leftarrow j$
        $T_b \leftarrow T_b + k_j$
        `block(:,b)` $\leftarrow \max$[`block(:,b)`, `Nelem_children(:,j)`]
        `Nelem_block(b)` $= \sum_i$ `block(i,b)`
        $j \leftarrow j + 1$
    end while
    $b \leftarrow b + 1$
end while
for $i = 1, \ldots, b$ **do**
    Compute new mesh for block b
    Optional: Estimate projection error and correct predicted meshes if necessary
end for
for $i = 1, \ldots, b$ **do**
    Solve forward problem on block b for U
    Project U onto mesh for block $b + 1$
    Optional: Compute projection error between blocks and correct meshes
end for

To implement the correlation-based strategy, we alter the block selection criteria ($\sum$ `block`$(b) \leq$ `Nmax`) with a step which accepts a block if `block`$(:, b)$ is correlated to `Nelem_children`$(:, j)$ and `Nelem_block(b)` is less than `Nmax`.

The algorithm assumes that the blocks are always generated (even on repeat solve cycles) using the coarse mesh as a base. The algorithm may be easily modified to work recursively on the blocks. It may also be modified, with a little more care, to allow merging and splitting of blocks during repeated solves.

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