Final Report

A Posteriori Analysis of Adaptive Multiscale Operator Decomposition Methods for Multiphysics Problems

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1 Introduction

This is the final report for the research project,

> ***"A Posteriori Analysis of Interface Effects in the Discretization of Multi-Scaled and Multi-Physics Problems by Decomposition Techniques," Office of Science, Department of Energy, $940,972, 2004-2008, ending October 30, 2009.***

1.1 Fundamental issues arising in multiscale, multiphysics models

This project was concerned with the solution of multiphysics, multiscale systems that couple different physical processes acting across a large range of scales relevant to the interests of the DOE. Multiscale, multiphysics models are characterized by intimate interactions between different physics across a wide range of scales. This poses significant computational challenges, e.g.

Accurate and efficient computation Computing information that depends on solution behavior occurring at very different scales is problematic. It is rarely possible to simply use a discretization sufficiently fine to resolve the finest scale behavior.

Complex stability A multiphysics problem generally offers a complex stability picture that results from a fusion of the stability properties of different physics, for example, consider a reacting fluid that combines fluid flow with the dynamical properties of reaction-diffusion equations.

Linking different physics Understanding the significance of linkages between physical components and how those affect model output is another complicated issue. In many situations, the output of one physical component must be transformed and/or scaled to obtain information relevant to the other components.

1.2 Multiscale operator decomposition

The research in this project focussed on ***Multiscale Operator Decomposition (MOD)*** methods for solving multiphysics problems. The general approach is to decompose a multiphysics problem into components involving simpler physics over a relatively limited range of scales, and then to seek the solution of the entire system through some sort of iterative procedure involving solutions of the individual components. This approach is appealing for several reasons;

- Many multiphysics models are built component-by-component, and the level of physical understanding and detail often varies enormously between components,
- It provides a way to accommodate multiple scales and multiple discretization methods in one problem,
- It provides a way to seamlessly combine multiple levels of description of physical phenomena,
- There is generally a good understanding of how to solve a broad spectrum of single physics problems accurately and efficiently, especially on high performance platforms,
- It provides a way to utilize the enormous investment in code developed for single physics problems.

MOD is a very widely used technique for solving multiphysics, multiscale problems; it is heavily used throughout the DOE computational landscape.

Example 1.2.1 *A classic example of MOD is* operator splitting *for a reaction-diffusion equation,*

$$\begin{cases} \dfrac{\partial u}{\partial t} = \nabla \cdot (a(x,u)\nabla u) + f(x,u), & x \in \Omega, 0 < t, \\ \textit{suitable boundary conditions}, & x \in \partial\Omega, 0 < t, \\ u(\cdot, 0) = u_0(\cdot) \end{cases} \tag{1}$$

where a and f are smooth functions with $a(\cdot,\cdot) \geq a_0 > 0$ and $\Omega \subset \mathbb{R}^d$ is a spatial domain. The generic picture is a relatively fast, destabilizing reaction component interacting with a relatively slow, stabilizing diffusion component. Accuracy considerations dictate the use of relatively small steps to integrate the reaction component. On the other hand, stability considerations over moderate to long time intervals suggests the use of implicit, dissipative numerical methods for integrating diffusion problems. Such methods are expensive to use per step, but relatively large steps can be used on a purely dissipative problem. If the reaction and diffusion components are integrated together, then the small steps required for accurate resolution of the reaction lead to an expensive computation. In a high performance setting, operator decomposition means that the reaction solves are completely local.

If we discretize in space using a continuous, piecewise linear finite element method with M elements, we obtain the initial value problem: find $y \in \mathbb{R}^M$ such that

$$\begin{cases} \dot{y} = Ay(t) + F(y(t)), & 0 < t \leq T, \\ y(0) = y_0, \end{cases} \tag{2}$$

where A is an $l \times l$ constant matrix representing a "diffusion component" and $F(y) = (F_1(y), F_2(y), \cdots, F_l(y))^\top$ is a vector of nonlinear functions representing a "reaction component".

We first discretize $[0,T]$ into $0 = t_0 < t_1 < t_2 < \cdots < t_N = T$ with diffusion *time steps $\{\Delta t_n\}_{n=1}^N$, $\Delta t_n = t_n - t_{n-1}$, and $\Delta t = \max_{1 \leq n \leq N}(\Delta t_n)$. We define a piecewise continuous approximate solution $\tilde{y}(t)$ with nodal values $\{\tilde{y}_n\}$ obtained from the procedure described in Alg. 1.*

Algorithm 1 Operator Decomposition for Reaction-Diffusion Equations

Set $\tilde{y}_0 = y_0$
for $n = 1, \cdots, N$ **do**
Compute $y^r(t_n^-)$ satisfying the reaction component

$$\begin{cases} \dot{y^r} = f(y^r(t)), & t_{n-1} < t \leq t_n, \\ y^r(t_{n-1}^+) = \tilde{y}_{n-1} \end{cases} \tag{3}$$

Compute $y^d(t_n^-)$ satisfying the diffusion component

$$\begin{cases} \dot{y^d} = Ay^d(t), & t_{n-1} < t \leq t_n, \\ y^d(t_{n-1}^+) = y^r(t_n^-) \end{cases} \tag{4}$$

Set $\tilde{y}_n = y^d(t_n^-)$
end for

This algorithm has the potential to be a multiscale solution procedure since we can now resolve the solution of each component on independent scales. We consider the time steps introduced above, $\{\Delta t_n\}_{n=1}^N$*, to be* diffusion *time steps. For each diffusion step, we choose a (small) time step* $\Delta s_n = \Delta t_n / M_n$ *with* $\Delta s = \max_{1\le n\le N} \Delta s_n$*, and the nodes* $t_{n-1} = s_{0,n} < s_{1,n} < \cdots < s_{M_n,n} = t_n$ *(see Fig. 1). We associate the time intervals* $I_n = [t_{n-1}, t_n]$ *and* $I_{m,n} = [s_{m-1,n}, s_{m,n}]$ *with these discretizations. In practice, it is not uncommon to use reaction steps significantly smaller (e.g.*

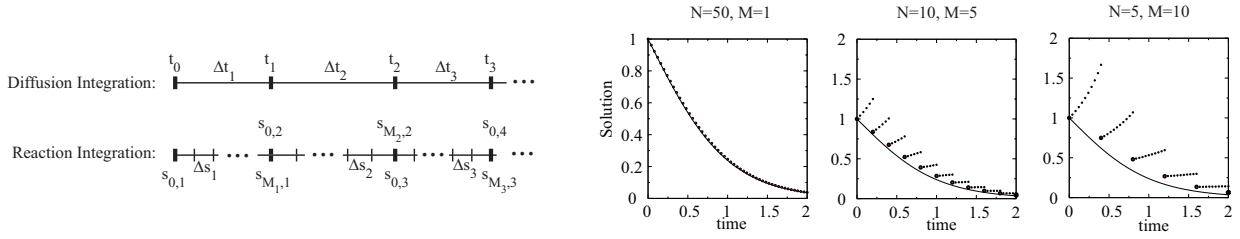


Figure 1: Left: Discretization of time used for MOD. Right: Plots of the approximation $\tilde{Y}$ and the true solution for Ex. 1.2.2. The nodal values of $\tilde{Y}$ are denoted by the larger points while the smaller points denote node values of the reaction component Y^r.

factor of 10^{-5}*) than the diffusion steps. We use a numerical scheme of order* q_r *to solve the reaction component (3) on each diffusion interval using steps* Δs_n*, then use a numerical scheme of order* q_d *to solve the diffusion component 4) using step* Δt_n*. We let* $\tilde{Y}(t)$ *denote the piecewise continuous, linear approximation of the MOD solution that joins the nodal values* $\tilde{Y}_n$*. Adapting standard convergence analysis techniques, we can show that if* f *is Lipschitz continuous, on a fixed time interval, there are constants* C_1, C_2, C_3 *such that,*

$$|y_N - \tilde{Y}_N| \le C_1 \Delta t + C_2 \Delta t^{q_d} + C_3 \Delta s^{q_r}.$$

If we use a higher order splitting method, the first term on the right is $\mathbf{O}(\Delta t^2)$*.*

Moving past this example, we use "multiscale operator decomposition" to denote a very general class of discretization methodologies for coupled physics problems. Computational procedures including

- Solving a coupled physics problems using different discretization methods and discretization scales for the different components,
- Incomplete iteration and the use of approximate Jacobians in nonlinear and fully implicit methods,
- Processing solution information from one component for use in other components,

are all procedures that may seriously affect both error and stability in similar ways, and, viewed in this way, are examples of MOD.

The ability to use different discretization methods and scales for different components is a key benefit of MOD. It allows for truly efficient solution of complex problems. Unfortunately, MOD can have unforseen effects on both accuracy and stability of solutions. The reason is that we have discretized the instantaneous interaction between the different physical components.

Example 1.2.2 *We consider a problem in which the reaction component exhibits finite time blow up when undamped by the diffusion component. The problem is*

$$\begin{cases} \dot{y} + \lambda y = y^2, & t > 0, \\ y(0) = y_0 \in \mathbb{R}, \end{cases} \qquad \Longrightarrow \qquad y(t) = \frac{\lambda y_0}{y_0 - (y_0 - \lambda)\, e^{\lambda t}}, \ \textit{for } \lambda \neq 0. \tag{5}$$

The exact solution exists for all time and tends to zero as $t \to \infty$ when $\lambda > y_0$. On the other hand, there is finite time blow up, e.g. $y \to \infty$ at a finite time, if $\lambda < y_0$.

Applying MOD to (5), the solutions of the two components and the MOD solution are,

$$y^r(t) = \frac{y^{d-}_{n-1}}{1 - y^{d-}_{n-1}(t - t_{n-1})}, \quad y^d(t) = e^{-\lambda(t-t_{n-1})}\, y^{r-}_n, \quad \tilde{y}_n = \frac{e^{-\lambda \Delta t_n} \tilde{y}_{n-1}}{1 - \Delta t_n\, \tilde{y}_{n-1}},$$

when the reaction component is defined. We see that decoupling the smoothing effect provided by instantaneous interaction with the diffusion component means that the reaction component can blow up in finite time. This affects the numerical solution.

We solve the components (3), (4) using the forward and backward Euler method respectively,

$$Y^{r-}_{m,n} = Y^{r-}_{m-1,n} + f(Y^{r-}_{m-1,n})\, \Delta s_n, \quad Y^{d-}_n = Y^{d-}_{n-1} + A Y^{d-}_n\, \Delta t_n.$$

We compute a piecewise linear discrete approximation $\tilde{Y}$ using the nodal values of Y^d.

In Fig. 1, we show the results obtained for a sequence of numerical solutions with increasing diffusion steps and correspondingly an increase in the number of reaction steps per diffusion step. With one reaction step per diffusion step, we obtain reasonable accuracy. As we increase the scale differences in the integration of the components, the effects of MOD become increasingly important, eventually to the point of ruining convergence altogether.

Note that we are not advocating the use of operator splitting for reaction-diffusion equations. Our point of view is that because splitting is frequently used in DOE-related computations, it is important to conduct an analysis of its effects. In general, we emphasize that the error in this example is just one example of the kinds of instability that can be introduced by MOD and we show below that MOD commonly affects both accuracy and stability in a wide variety of contexts. Given the benefits and dangers of MOD, our assertion is that

> ***It is absolutely essential to quantify the effects on accuracy and stability introduced by multiscale operator decomposition solution of multiphysics problems.***

2 Progress Report on Current Project

After briefly describing *a posteriori* error estimation using adjoint operators and variational analysis, we present three examples of MOD solution of multiphysics problems and the related *a posteriori* error analysis. These three examples (all three are papers in SINUM [7, 2, 17]) represent a major advance in the analysis of the solution of multiscale, multiphysics problems. Together, these three examples set the general picture for the proposed research project.

We then give a brief survey of the results obtained in the current project, the people involved, and the ways in which the project team contributed to the DOE mission.

2.1 A posteriori analysis using adjoint operators

The proposed research relies on *a posteriori* analysis involving computable residuals to measure local introduction of error and the generalized Green's function solving the adjoint problem that measure the global effects of accumulation and propagation of error on a quantity of interest. Duality and adjoint operators have a long history in the analysis of models. Applying these tools to error estimation was originally pioneered by Estep, Johnson and collaborators .

We describe the ideas formally. We assume that the goal is to compute a quantity of interest (x, ψ) from the solution x of a linear system $Ax = b$, where ψ is a specified data vector, A is an invertible operator, and b is given data. If $X \approx x$ denotes an approximate solution, then the unknown error is $e = X - x$ and the residual is $R = AX - b$. Since the residual of the true solution is zero, the error is related to the residual by the *perturbation relation*

$$Ae = R. \tag{6}$$

The *generalized Green's vector* ϕ satisfies the dual or adjoint problem

$$A^\top \phi = \psi. \tag{7}$$

A variational argument shows that

$$e \cdot \psi = e \cdot A^\top \phi = Ae \cdot \phi = R \cdot \phi.$$

This gives the *a posteriori* error estimate on a projection of the error

$$|e \cdot \psi| = |R \cdot \phi|. \tag{8}$$

The generalized Green's vector ϕ provides quantitative information on relevant stability properties of the computed information obtained from the solution. To use (8), we numerically approximate the generalized Green's function, which yields extremely accurate estimates in general.

The analysis for nonlinear problems is more complicated because there is not a unique definition of an adjoint operator. The most useful definition depends on the goal of the analysis and the properties of the operators involved. There is a standard approach that is useful under certain limitations. Suppose the problem is $f(x) = b$, so that the perturbation relation for the approximate solution $X \approx x$ is

$$f(X) - f(x) = R = f(X) - b. \tag{9}$$

We use the integral mean value theorem to write the perturbation relation as

$$Ae = \int_0^1 f'(sX + (1-s)x)\, ds\; e = f(X) - f(x) = R,$$

where f' is the Frechet derivative of f. Introducing the linear adjoint problem associated to the average derivative A, the analysis proceeds as above. In practice, under the assumption that the error is small, A is replaced by $f'(X)$.

We briefly describe the *a posteriori* estimate for the continuous Galerkin space-time finite element method for a nonlinear reaction-diffusion equation,

$$\dot{u} - \nabla \cdot (a(u, x, t)\nabla u) = f(u, x, t) \tag{10}$$

with homogeneous Dirichlet boundary conditions and suitable initial conditions. We emphasize

Our approach is to analyze the specific numerical methods used by our engineering and scientific collaborators in universities, national laboratories, and industry working on DOE-related projects.

We generally represent these numerical methods in the finite element-variational analysis framework so that we can apply tools such as adjoint operators. But, the analysis is altered specifically to treat the methods used in practice.

The time axis is partitioned $t_0 < t_1 < t_2 < \cdots$ with intervals $I_n = [t_{n-1}, t_n]$. On each interval, the space domain is triangulated by $\mathcal{T}_n$ in the usual way. The approximation U is a continuous piecewise linear polynomial in time with coefficients in the space of continuous piecewise linear functions V_n associated to $\mathcal{T}_n$. On each interval, U solves

$$\int_{I_n} (\dot{U}, W)\, dt + \int_{I_n} (a(U)\nabla U, \nabla W)\, dt = \int_{I_n} (f(U), W)\, dt, \tag{11}$$

for all $W \in V_n$, where $(\ ,\ )$ denotes the L_2 inner product in space. The data at t_{n-1} is the last value of U from the previous interval projected on the new mesh. With appropriate choices of quadrature to evaluate the integrals in (11) on a uniform mesh in two dimensional space, this method is equivalent to the standard finite difference scheme using the trapezoidal difference method in time and five point stencil difference method in space.

The generalized Green's function solves the adjoint problem corresponding to data ψ,

$$\begin{cases} -\dot{\phi} - \nabla \cdot \bar{\epsilon}\nabla\phi + \bar{\beta} \cdot \nabla\phi = \bar{f}\phi, & t_n > t > 0, \\ \phi(t_n) = \psi, \end{cases} \tag{12}$$

where we have linearized $\bar{\epsilon} = \int_0^1 \epsilon(us + U(1-s))\, ds$, $\bar{\beta} = \int_0^1 \epsilon'(us + U(1-s))\nabla(us + U(1-s))\, ds$, and $\bar{f} = \int_0^1 f'(us + U(1-s))\, ds$. In this case, the boundary conditions are the same as for the original problem. Carrying out a straightforward variational analysis, entirely analogous to the standard analysis for a Green's function, yields the *error representation formula,*

$$(e(t_n), \psi) = \sum_{m=1}^{n} \int_{t_{m-1}}^{t_m} \left((\dot{U}, \pi P\phi - \phi) + (\epsilon(U)\nabla U, \nabla(\pi P\phi - \phi)) - (f(U), \pi P\phi - \phi) \right) dt, \tag{13}$$

where P and π denote projections into the space and time finite element spaces respectively. We can use (13) directly to compute accurate error estimates. This involves computing an approximate solution of the adjoint problem formed typically by linearizing around the computed solution. We can also further manipulate (13) to get an estimate more suitable for adaptive error control in which different sources of error are distinguished.

2.1.1 Computing the information that is desired and needed

A fundamental aspect of this analytic approach is the focus on the precise information, or quantity of interest, that is to be computed in the model. This includes both the overall quantities to be obtained from the model as well as auxiliary information that are passed between components of a multiphysics problem.

The sensitivity of particular information obtained from a solution of a differential equation can be much different than the the sensitivity of the solution as a whole, i.e. in some global norm.

Goal-oriented a posteriori error estimates can translate to a tremendous gain in computational efficiency. This is a particularly important consideration in multiscale, multiphysics problems in which it may be computationally infeasible to obtain solutions that are accurate uniformly everywhere in space-time.

Example 2.1.1 *To illustrate, we consider the chaotic Lorenz problem,*

$$\begin{cases} \dot{u}_1 = -10u_1 + 10u_2, \\ \dot{u}_2 = 28u_1 - u_2 - u_1u_3, \quad 0 < t, \\ \dot{u}_3 = -\frac{8}{3}u_3 + u_1u_2. \end{cases} \tag{14}$$

Nearly all solutions exhibit the same qualitative behavior. There are two non-zero steady state solutions and a generic solution is either "orbiting" one of these solutions or transitioning between orbits, see Fig. 2. Chaos is often described as "sensitivity to initial conditions", which means that solutions that begin close by to each other eventually move apart.

The chaotic behavior affects numerical solutions as well, see Fig. 2. The pointwise numerical

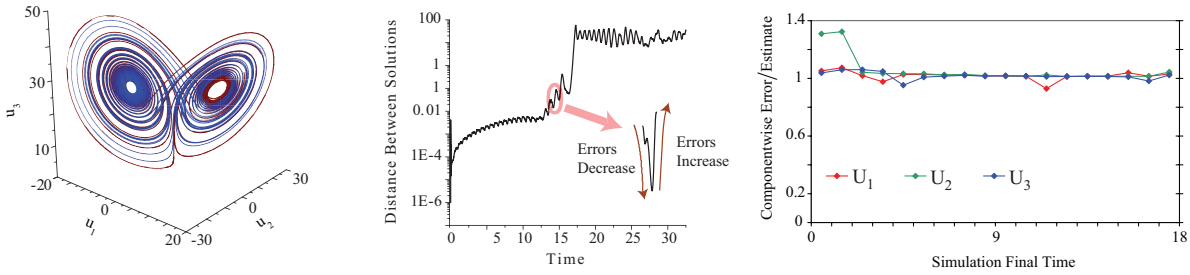
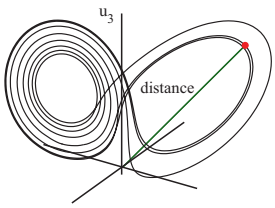


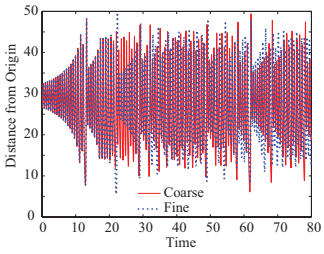
Figure 2: Left: Two numerical approximations of the same Lorenz solution with different accuracies. Middle: The pointwise difference between the numerical solutions. Right: The pointwise error/estimate ratios for each component versus time at many time points for the inaccurate solution.

error follows an increasing trend, but actually decreases during some short periods of time. Typical convergence analysis does not take into account the potential cancellation of error and changing stability of a solution, hence tends to greatly overestimate the actual error. Using the a posteriori error estimation techniques described above, we can compute robustly accurate estimates of the error in specific quantities of interest. In Fig. 2, we demonstrate the accuracy of the a posteriori error estimate.

A little reflection suggests considering the pointwise behavior of Lorenz solutions is not physically motivated. Originally derived to explain the unpredictability of the weather, the Lorenz problem is certainly not a pointwise model! Rather, it is more reasonable to consider a quantity of interest that better represents qualitative behavior of all solutions.

This is important because it turns out that the effect of perturbations depends strongly on the information being computed. Motivated by the fact that all solutions must remain in a large neighborhood of the origin, we consider the average distance and its variance from a solution of the Lorenz problem to the origin. In Fig. 3, we compare results for numerical solutions with a coarse time step .001 *and fine time step* .0001 *along with results obtained from an ensemble of* 100 *accurate solutions computed using time step* .0001 *for* 15 *time units. Similar results are obtained over any time interval checked from* 15 *to* 320*. The accuracy of the numerical solution appears to have little effect on the accuracy of the average distance and its variance.*





	Coarse Solution		Fine Solution		Ensemble Average	
End Time	Ave	Var	Ave	Var	Ave	Var
320	26.3	83.7	26.3	83.0	26.3	83.7

Figure 3: Left: The quantity of interest is the average distance from the solution to the origin. Middle: the average distance for solutions with time steps .001 and .0001. Right: Average and variance of distance for the two solutions and an ensemble average of accurate solutions.

2.1.2 Difficulties with analysis of MOD for nonlinear problems

The underlying assumption in the analysis for nonlinear problems outlined in Sec. 2.1 is that the residual of the approximate solution is very small, i.e. the approximate solution X is very nearly a solution of the nonlinear problem. This argument breaks down if the procedure to produce X involves significant perturbation of the original operator f, e.g. as a consequence of multiscale operator decomposition. One of the main achievements of the current project is to develop techniques for dealing with this issue.

To give a rough idea of the issues, we consider again the finite dimensional example in Sec. 2.1. Let x solve

$$f(x) = b,$$

and suppose that $\tilde{x}$ solves a perturbed problem

$$\tilde{f}(\tilde{x}) = b. \tag{15}$$

Such a perturbation might be introduced by a MOD decomposition. We let $\tilde{X} \approx \tilde{x}$ denote a computed solution of (15). We have the perturbation relation for the perturbed problem,

$$\tilde{f}(\tilde{X}) - \tilde{f}(\tilde{x}) = \tilde{f}(\tilde{X}) - b = \tilde{R},$$

and we can apply the *a posteriori* analysis for nonlinear problems in Sec. 2.1 to the perturbed problem to estimate $\tilde{X} - \tilde{x}$.

However, we wish to estimate $\tilde{X} - x$. We can write

$$\tilde{f}(\tilde{X}) - f(x) = \tilde{f}(\tilde{X}) - b = \tilde{R},$$

but we can no longer apply the integral Mean Value Theorem to linearize the left hand side as we did above.

2.2 Three examples of analysis of MOD methods

We present MOD solution methods and the analysis for three examples. The examples illustrate the general approach to analyzing the effects of MOD developed under the current project, as well as the particular difficulties that must be overcome in specific cases.

2.2.1 Reaction-diffusion problems

A reaction-diffusion-convection problem (1) combines three physical effects, i.e. diffusion, convection, and reaction, in a single system of equations. MOD is used when these three components are treated independently in some fashion, e.g. the classic operator splitting algorithm 1.

In Ex. 1.2.2, we present a simple example in which MOD affects the stability. Such effects can take a myriad of forms.

Example 2.2.1 *We illustrate another kind of instability resulting from MOD applied to the Brusselator model of chemical dynamics,*

$$\begin{cases} \frac{\partial u_1}{\partial t} - k_1 \frac{\partial^2 u_1}{\partial x^2} = \alpha - (\beta+1)u_1 + u_1^2 u_2, & x \in (0,1), t > 0, \\ \frac{\partial u_2}{\partial t} - k_2 \frac{\partial^2 u_2}{\partial x^2} = \beta u_1 - u_1^2 u_2, & x \in (0,1), t > 0, \\ u_1(0,t) = u_1(1,t) = \alpha,\ u_2(0,t) = u_2(1,t) = \beta/\alpha, & t > 0, \\ u_1(x,0) = u_{1,0}(x),\ u_2(x,0) = u_{2,0}(x), & x \in (0,1), \end{cases} \tag{16}$$

where u_1 and u_2 are the concentrations. Solutions exhibit a wide range of behavior depending on parameter values. Below, we use $\alpha = 2$, $\beta = 5.45$, $k_1 = 0.008$, $k_2 = 0.004$ and initial conditions $u_1(x,0) = \alpha + 0.1\sin(\pi x)$ and $u_2(x,0) = \beta/\alpha + 0.1\sin(\pi x)$, which yields an oscillatory, mildly unstable solution.

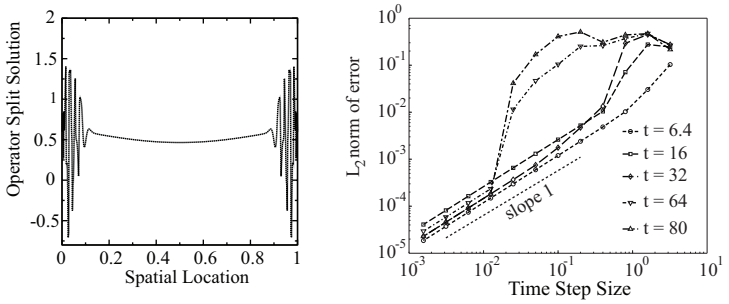


Figure 4: The lefthand plot illustrates typical instability that can arise from MOD applied to Brusselator problem. Solution is shown at time 80. On the right, we show plots of the error in the L_2 norm versus time step size at different times.

We discretize in space using a second order finite element method with 500 elements, and apply a standard first order splitting scheme using the trapezoidal rule for the diffusion with time step of .2 and backward Euler for the reaction with time step of .004. In Fig. 4, we show a numerical solution that exhibits nonphysical oscillations that develop after some time. We also show plots of the error versus time steps at different times, which show there is a critical time step above which the instability develops. It turns out that refining the space discretization actually makes the error accumulation worse.

The *a posteriori* analysis distinguishes the effects of MOD from the effects of numerical discretization of the components. The numerical error arising in each component can be treated with the standard *a posteriori* analysis discussed above applied componentwise. Estimating the error arising from the MOD requires a new approach.

A main technical issue is the definition of a suitable adjoint problem because the standard approach used for nonlinear problems described in Sec. 2.1 fails. Indeed, the adjoint operator

corresponding to the solution operator for a MOD discretization is typically different than the adjoint operator associated with the true solution operator. This difference takes the form of "residuals" between certain adjoint operators associated with the fully coupled problem and the discretization. A practical difficulty is that solving the adjoint for the fully coupled problem poses the same multiphysics challenges as solving the original forward problem. We develop a new hybrid *a priori - a posteriori* estimate that combines a computable leading order expression obtained using *a posteriori* arguments with a provably higher order remainder, see [7].

We begin with the decomposition

$$\tilde{Y} - y = (\tilde{Y} - \tilde{y}) + (\tilde{y} - y), \tag{17}$$

where y solves (2), $\tilde{y}$ is computed via the abstract operator splitting Alg. 1 and $\tilde{Y}$ is the numerical counterpart.

The first expression on the right of (17) is the error of $\tilde{Y}$ as a solution of the operator split problem. This expression can be estimated using the standard *a posteriori* error analysis. To this purpose, we let ϑ^d denote solution of the adjoint associated with the diffusion component (4),

$$\begin{cases} -\dot{\vartheta^d} = A^\top \vartheta^d(t), \quad t_n > t \geq t_{n-1}, \\ \vartheta^d(t_n^-) = \psi_n. \end{cases}$$

Furthermore, we let ϑ^r denote the solution of the the adjoint associated with the reaction component (3),

$$\begin{cases} -\dot{\vartheta^r} = (\hat{F}'(y^r, Y^r))^\top \vartheta^r(t), \quad s_{m,n} > t \geq s_{m-1,n}, \\ \vartheta^r(s_{m,n}) = \psi^r_{m,n}, \end{cases}$$

for $m = M_n, \cdots, 1$, with ${\psi^r}_{M_n,n} = {\vartheta^d}^+_{n-1}$, ${\psi^r}_{m,n} = \vartheta^r_{m,n}$ for $m < M_n$, and

$$\hat{F}'(y^r, Y^r) = \int_0^1 F'(sy^r + (1-s)Y^r)\, ds.$$

Thus ϑ^r is continuous across the internal reaction time nodes $s_{m,n}$, $m = 1, \cdots, M_n - 1$.

The second expression on the right of (17) is the analytic error of MOD. The nonlinearity complicates the analysis because we have to use linearization to define unique adjoint problems, which raises the issue of choosing a trajectory around which to linearize. We cannot use the standard approach of linearizing the error representation described in Sec. 2.1 because of MOD. Instead, we assume that both the original problem and the MOD version have a common solution and we linearize each problem in a neighborhood of this common solution. For example, we assume that $y = 0$ is a steady state solution of both problems, which can be achieved by assuming that $F(0) = 0$, and we linearize in a region around 0. In terms of applications to reaction-diffusion problems, there are mathematical reasons for making the homogeneity assumption and it is satisfied in a great many applications. However, we can modify the analysis to allow for linearization around any known common solution.

On time interval (t_{n-1}, t_n), we consider the linearized problem,

$$\begin{cases} \dot{y} = A\, y(t) + \overline{F'(y)}\, y(t), \quad t_{n-1} < t \leq t_n, \\ y(t_{n-1}) = y_{n-1}, \end{cases}$$

where

$$\overline{F'(y)} = \int_0^1 F'(sy)\, ds.$$

We note that $\overline{F'(y)}y = F(y)$ because $F(0) = 0$. The generalized Green's function φ satisfies the adjoint problem

$$\begin{cases} -\dot{\varphi} = A^\top \varphi(t) + \overline{F'(y)}^\top \varphi(t), & t_n > t \geq t_{n-1}, \\ \varphi(t_n) = \varphi(t_n^+), \end{cases} \tag{18}$$

where $A^\top$ and $\overline{F'(y)}^\top$ denote the transpose of A and $\overline{F'(y)}$, respectively. The local adjoint problems are coupled by the choice of data, resulting in a simple representation of the solution values

$$(y_n, \psi_n) = (y_{n-1}, \varphi_{n-1}),\ n = 1, 2, \cdots, N \implies (y_N, \psi_N) = (y_0, \varphi_N). \tag{19}$$

We use analogs for (19) for solutions of each component in the MOD discretization. For $n = 1, \cdots, N$, we define the three adjoint problems. The diffusion problem is simpler because it is linear,

$$\begin{cases} -\dot{\varphi^d} = A^\top \varphi^d(t), & t_n > t \geq t_{n-1}, \\ \varphi^d(t_n^-) = \psi_n^d. \end{cases} \tag{20}$$

It is convenient to let Φ_n^d denote the solution operator, so $\varphi^d(t_{n-1}) = \Phi_n^d \psi_n^d$.

We require two adjoint problems to treat the reaction component. The difference between the problems is the function around which they linearized,

$$\begin{cases} -\dot{\varphi_1^r} = \overline{F'(\tilde{Y})}^\top \varphi_1^r(t), & t_n > t \geq t_{n-1}, \\ \varphi_1^r(t_n^-) = \psi_n^r, \end{cases} \qquad \begin{cases} -\dot{\varphi_2^r} = \overline{F'(Y^r)}^\top \varphi_2^r(t), & t_n > t \geq t_{n-1}, \\ \varphi_2^r(t_n^-) = \psi_n^r, \end{cases} \tag{21}$$

where $\psi_n^r = \varphi_{n-1}^{d+}$. If $\Phi_n^r(z)$ denotes the solution operator for the problem linearized around a function z, then we have $\varphi_1^r(t_{n-1}) = \Phi_n^r(\tilde{Y})\psi_n^r$ and $\varphi_2^r(t_{n-1}) = \Phi_n^r(Y^r)\psi_n^r$.

Theorem 2.2.1 (Computable *a posteriori* error estimate) *A hybrid* a posteriori - a priori *error estimate for the MOD dG finite element method is*

$$\begin{aligned} (\tilde{Y}_N - y_N, \psi_N) = &\sum_{n=1}^{N} \sum_{m=1}^{M_n} \left(\int_{I_{m,n}} (\dot{Y^r} - F(Y^r), \vartheta^r - \Pi\vartheta^r)\, dt + ([Y^r]_{m-1,n}, \vartheta^{r+}_{m-1,n} - \Pi\vartheta^{r+}_{m-1,n}) \right) \\ &+ \sum_{n=1}^{N} \left(\int_{I_n} (\dot{Y^d} - AY^d, \vartheta^d - \Pi\vartheta^d)\, dt + ([Y^d]_{n-1}, \vartheta^{d+}_{n-1} - \Pi\vartheta^{d+}_{n-1}) \right) \\ &+ \sum_{n=1}^{N} (\tilde{Y}_{n-1}, (E_1 + E_2)\psi_n) + \mathbf{O}(\Delta t^{q_d+2}) + \mathbf{O}(\Delta t\, \Delta s^{q_r+1}), \end{aligned}$$

where

$$E_1 = \frac{1}{2}\Delta t_n \left(A^\top \mathcal{F}(\tilde{Y}) - \mathcal{F}(\tilde{Y}) A^\top \right),\ \mathcal{F}(\tilde{Y}) = \int_{I_n} \overline{F'(\tilde{Y})}\, dt,$$

$$E_2 = \left(\Phi_n^r(\tilde{Y}) - \Phi_n^r(Y^r) \right) \Phi_n^d,$$

and and q_d and q_r are the degrees of the methods for the numerical solutions of the diffusion and reaction components respectively.

The first expression on the right is the error introduced by the numerical solution of the reaction component. Likewise, the second expression on the right is the error introduced by the numerical solution of the diffusion component. The third expression on the right measures the effects of MOD. The expression E_1 is a leading order estimate for the effects of MOD while E_2 accounts for issues arising from the differences in linearizing around the global computed solution as opposed to the solution of the reaction component. Both of these quantities are scaled by the solution itself. Finally, the higher order terms represent bounds on terms that are not computable but are higher order. In practice, we neglect those terms when computing an estimate.

Using the estimate requires the solution of five adjoint problems. But we avoid the need to solve an adjoint problem corresponding to linearization around the true solution by deriving the hybrid estimate.

Example 2.2.2 *The first example is partial differential equation version of Ex. 1.2.2,*

$$\begin{cases} \frac{\partial u}{\partial t} - 0.05\,\frac{\partial^2 u}{\partial x^2} = u^2, & x \in (0,1), t > 0, \\ u(0,t) = u(1,t) = 0, & t > 0, \\ u(x,0) = 4x(1-x), & x \in (0,1). \end{cases}$$

The solution of the reaction component exhibits finite time blow up when undamped by the diffusion component. This is perhaps the most extreme form of instability. Table 1 shows the ratio of the error to the estimate computed at the final time $T = 1$. We used 20 elements in space. We see that the estimate is very accurate for a range of time steps.

Δt	M	Exact Err (%)	Error/Estimate
.1	100	11.07	1.0286
.01	10	1.35	1.0067
.001	1	0.45	1.0020

Table 1: Error estimate for the blow up problem at $T = 1$, reaction time step $= 10^{-3}$

Example 2.2.3 *We next consider the Brusselator problem (16) with $\alpha = 2$, $\beta = 5.45$, $k_1 = 0.008$, $k_2 = 0.004$ and initial conditions $u_1(x,0) = \alpha + 0.1\sin(\pi x)$ and $u_2(x,0) = \beta/\alpha + 0.1\sin(\pi x)$, which yields an oscillatory solution. In this case, the reaction is very mildly unstable. We note that in original form, the reaction terms do not satisfy the requirement $F(0) = 0$ so we linearize around the steady state solution c with with $c_i = \alpha$ for $i = 1, \cdots, N_e - 1$ and $c_i = \beta/\alpha$ for $i = N_e, \cdots, 2N_e - 2$, so that $F(c) = 0$.*

Fig. 5 compares the exact errors computed using $\Delta t = 0.01$ and $M = 10$ reaction time steps to the hybrid a posteriori *error estimates for a 32 node spatial finite element discretization. We show results for $[0, 2]$, when the solution is still in a transient stage, and at $T = 40$ when the solution has become periodic. All the results show that the exact and estimated errors are in remarkable agreement.*

2.2.2 Systems of elliptic problems coupled through parameters

Another example are systems of elliptic equations coupled through "parameter passing", in which the solution of each component equation is used to create parameters for the other component

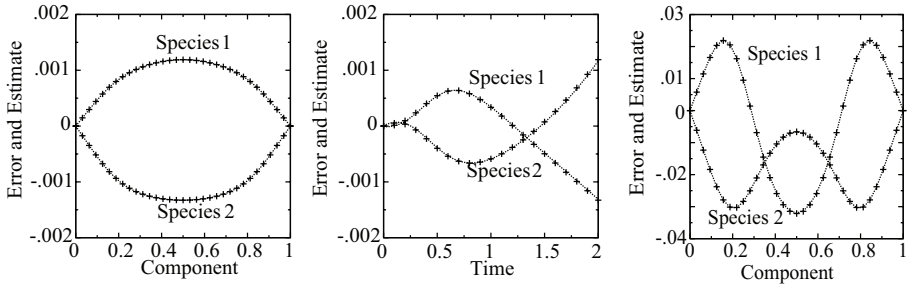


Figure 5: Brusselator results. Left: comparison of errors against the spatial location at $T = 2$. Middle: time history of errors at the midpoint location on $[0, 2]$. Right: comparison of errors against the spatial location at $T = 40$. The dotted line is the exact error and the (+) is the estimated error

equations. Such a system can be written on a domain Ω as

$$\begin{cases} \mathcal{L}_1(x, u_1, Du_1, \cdots, u_n, Du_n) = 0 \\ \qquad\qquad \vdots \qquad\qquad\qquad\qquad , \ x \in \Omega. \\ \mathcal{L}_n(x, u_1, Du_1, \cdots, u_n, Du_n) = 0 \end{cases} \tag{22}$$

A natural form of MOD is to split the global multi-physics problem into n "single-physics" components that are solved individually. In general, the solution of each component requires knowledge of the solutions of all the other components; the full problem requires some form of iteration to obtain the solution.

Example 2.2.4 *Our work is motivated by a model of a MEMS thermal actuator investigated by engineers at Sandia National Laboratory. A contact rests on thin braces composed of a conducting material. When a current is passed through the braces, they heat up and consequently expand to close the contact. The system is modeled by a system of three coupled equations. The first is an electrostatic current equation*

$$\nabla \cdot (\sigma \nabla u_1) = 0, \tag{23}$$

governing potential u_1 (where the current is $J = -\sigma \nabla u_1$), the second is a steady-state energy equation

$$\nabla \cdot (\kappa(u_2) \nabla u_2) = \sigma(\nabla u_1 \cdot \nabla u_1), \tag{24}$$

for the governing temperature u_2, and a linear elasticity equation giving the steady-state displacement u_3,

$$\nabla \cdot \left(\lambda \, tr(E) I + 2\mu E - \beta(u_2 - u_{2,ref}) I\right) = 0, \quad E = \left(\nabla u_3 + \nabla u_3^{\top}\right)/2. \tag{25}$$

Using MOD, the complete system (23-25) is decomposed into three components, each of which is solved with a code specialized to the particular type of physics.

We can capture the essential features of the thermal actuator model using a two component "triangular" system

$$\begin{cases} -\nabla \cdot a_1 \nabla u_1 + b_1 \cdot \nabla u_1 + c_1 u_1 = f_1(x), & x \in \Omega, \\ -\nabla \cdot a_2 \nabla u_2 + b_2 \cdot \nabla u_2 + c_2 u_2 = f_2(x, u_1, Du_1), & x \in \Omega, \\ u_1 = u_2 = 0, & x \in \partial\Omega, \end{cases} \tag{26}$$

where a_i, b_i, c_i, f_i are smooth functions, with $a_1, a_2 \geq \alpha > 0$ on a bounded domain Ω in $\mathbb{R}^N$ with boundary $\partial\Omega$, and α is a constant. The problems are coupled through f_2 and the "lower triangular" form of this system means that we can either solve it as a coupled system or we can solve the first equation and then use the solution to generate the parameters for the second problem.

The weak form of the first component of (26) reads: find $u_1 \in \tilde{W}_2^1(\Omega)$ satisfying

$$\mathcal{A}_1(u_1, v_1) = (a_1 \nabla u_1, \nabla v_1) + (b_1 \cdot \nabla u_1, v_1) + (c_1 u_1, v_1) = (f_1, v_1), \text{ for all } v_1 \in H_0^1(\Omega), \tag{27}$$

where $H_0^1(\Omega)$ is the subspace of functions in $H^1(\Omega)$ that are zero on $\partial\Omega$. Likewise the weak formulation of the second component of (26) reads: find $u_2 \in H_0^1(\Omega)$ satisfying

$$\mathcal{A}_2(u_2, v_2) = (a_2 \nabla u_2, \nabla v_2) + (b_2 \cdot \nabla u_2, v_2) + (c_2 u_2, v_2) = (f_2(x, u_1, Du_1), v_2), \text{ for all } v_2 \in H_0^1(\Omega). \tag{28}$$

We introduce the finite element space $\mathcal{S}_{h,1}(\Omega) \subset H_0^1(\Omega)$, corresponding to a discretization $\mathcal{T}_{h,1}$ of Ω for the first component, and another finite element space $\mathcal{S}_{h,2}(\Omega) \subset H_0^1(\Omega)$, on a different mesh $\mathcal{T}_{h,2}$, for the second component. We introduce projections $\Pi_{i\to j}$ from $\mathcal{S}_{h,i}$ to $\mathcal{S}_{h,j}$, e.g. interpolants or an L^2 orthogonal projection, and apply these in order to evaluate the equations defining the approximations.

Algorithm 2 Multiscale Operator Decomposition for Triangular Systems of Elliptic Equations

Construct discretizations $\mathcal{T}_{h,1}, \mathcal{T}_{h,2}$ and corresponding spaces $\mathcal{S}_{h,1}, \mathcal{S}_{h,2}$

Compute $U_1 \in \mathcal{S}_{h,1}(\Omega)$ satisfying

$$\mathcal{A}_1(U_1, v_1) = (f_1, v_1), \text{ for all } v_1 \in \mathcal{S}_{h,1}(\Omega). \tag{29}$$

Compute $U_2 \in \mathcal{S}_{h,2}(\Omega)$ satisfying

$$\Big\{ \mathcal{A}_2(U_2, v_2) = (f_2(x, \Pi_{1\to 2} U_1, \Pi_{1\to 2} DU_1), v_2), \quad \text{for all } v_2 \in \mathcal{S}_{h,2}(\Omega). \tag{30}$$

We observe that any errors made in the solution of the first component affect the solution of the second component. This turns out to be a crucial fact for *a posteriori* error analysis.

Example 2.2.5 *We solve a system*

$$\begin{cases} -\Delta u_1 = \sin(4\pi x)\sin(\pi y), & x \in \Omega \\ -\Delta u_2 = b \cdot \nabla u_1, & x \in \Omega, \\ u_1 = u_2 = 0, & x \in \partial\Omega, \end{cases} \qquad b = \frac{2}{\pi} \begin{pmatrix} 25\sin(4\pi x) \\ \sin(\pi x) \end{pmatrix} \tag{31}$$

using a standard piecewise linear, continuous finite element method, where $\Omega = [0,1] \times [0,1]$*, in order to compute the quantity of interest* $u_2(.25, .25)$ *involving the second component. We allow for independent meshes for* U_1 *and* U_2*.*

Using the same mesh for both components and evaluating the standard a posteriori error estimate for the second component problem, ***ignoring error in the first component solution****, yields an error estimate of* $\approx .0042$*. The true error is* $\approx .0048$ *and there is discrepancy of* $\approx .0006$ $(\approx 13\%)$*. This is a consequence of MOD, which effects we have* ***not*** *estimated.*

If we adapt the mesh for the solution of the second component based on the standard a posteriori error estimate, again neglecting any error inherited from the first component, the discrepancy becomes alarmingly worse. For example, we can refine the mesh until the estimate of the error in the second component is $\approx .0001$*. But, we find that the true error is* $\approx .2244$*!*

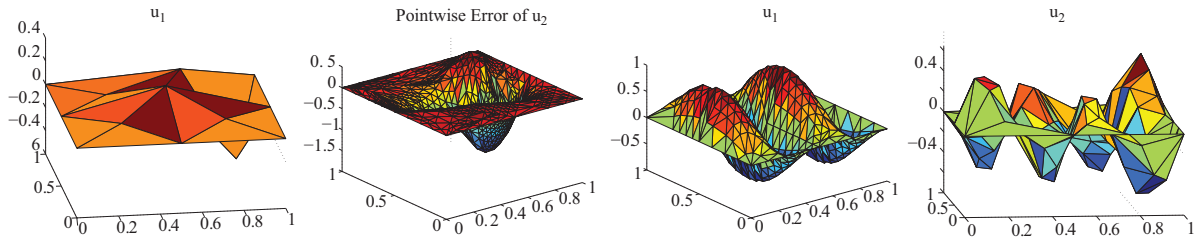


Figure 6: Left two plots: First component solution and pointwise error in the second component solution after refining mesh using estimate of the error only in the second component. Right two plots: Solutions obtained from adaptive refinement using the full estimate (36).

We assume that the goal is to compute a functional $(u_2, \psi_2^{(1)})$ of the solution of the second component. For the *a posteriori* analysis, we define the weak residuals for component, namely

$$\mathcal{R}_i(U_i, v) = (f_i(\nu), v) - \mathcal{A}_i(U_i, v), \quad i = 1, 2,$$

for a test function v.

The primary adjoint problem, reflecting the stability of each component with respect to its discretization, is

$$\left\{ \mathcal{A}_2^*(\phi_2^{(1)}, v_2) = (\psi_2^{(1)}, v_2), \qquad \text{for all } v_i \in \tilde{W}_2^1(\Omega), \right. \tag{32}$$

where

$$\begin{cases} \mathcal{A}_1^*(\phi_1^{(1)}, v_1) = (a_1 \nabla \phi_1^{(1)}, \nabla v_1) - (\mathrm{div}(b_1 \phi_1^{(1)}), v_1) + (c_1 \phi_1^{(1)}, v_1) \\ \mathcal{A}_2^*(\phi_2^{(1)}, v_2) = (a_2 \nabla \phi_2^{(1)}, \nabla v_2) - (\mathrm{div}(b_2 \phi_2^{(1)}), v_2) + (c_2 \phi_2^{(1)}, v_2). \end{cases}$$

We next account for the effect that error in u_1 has on the second component. We use the approximation

$$\left(\psi_1^{(2)}, e_1\right) = \left(e_1, Df_2(U_1)\Pi_{2\to 1}\phi_2^{(1)}\right) \approx (f_2(x, u_1, Du_1) - f_2(x, U_1, DU_1), \Pi_{2\to 1}\phi_2^{(1)}), \tag{33}$$

to define a new quantity of interest that describes the effect of errors in U_1 on the quantity of interest, and we construct a secondary adjoint problem to estimate the transfer error,

$$\mathcal{A}_1^*(\phi_1^{(2)}, v_1) = \left(\psi_1^{(2)}, v_1\right) \text{ for all } v_1 \in \tilde{W}_2^1(\Omega). \tag{34}$$

Note that using different discretizations for the components affects both the forward solution and the definition of the adjoint problems.

Finally, we define an adjoint problem to estimate the error arising from projecting solutions between the discretizations of the two component. The quantity of interest is defined

$$\left(\psi_1^{(3)}, e_1\right) = \left(Df_2(U_1) \times e_1, (I - \Pi_{2\to 1})\phi_2^{(1)}\right),$$

and the adjoint problem is

$$\mathcal{A}_1^*(\phi_1^{(3)}, v_1) = \left(\psi_1^{(3)}, v_1\right) \text{ for all } v_1 \in \tilde{W}_2^1(\Omega). \tag{35}$$

The error representation is finally

$$\begin{aligned} (\psi_2^{(1)}, e_2) = \mathcal{R}_2(U_2, (I - \Pi_2)\phi_2^{(1)}; U_1) + \mathcal{R}_1(U_1, (I - \Pi_1)(\phi_1^{(2)} + \phi_1^{(3)})) \\ + \left(\Pi_{1\to 2} f_2(U_1) - f_2(\Pi_{1\to 2} U_1), \phi_2^{(1)}\right) + \left((I - \Pi_{1\to 2}) f_2(U_1), \phi_2^{(1)}\right). \end{aligned} \tag{36}$$

The first term on the right measures the contribution to the error from the numerical solution of the second component. The second term measures the contribution arising from transferring error in the first component into the second component. Finally, the last two terms measure the effects of projecting between different discretizations.

Example 2.2.6 *We consider the problem in Ex. 2.2.5 with the quantity of interest equal to the average value of u_2 over the whole domain and initial coarse meshes as before, but now use the full estimate (36) to adapt the mesh for both U_1 and U_2 so that the estimated error is smaller than 10^{-4}. The complete a posteriori estimates the true error very accurately, and the true error is controlled. The resulting meshes are shown in Fig. 6. Note that the mesh for U_1 is actually more refined than the mesh for U_2.*

Space limitations preclude a description of the *a posteriori* analysis for a fully coupled problem (22). Given an iterative scheme for the solution, the analysis has two aspects, the transfer of information between the components during each iteration and the transfer of information between subsequent iterations. The first aspect is treated as described for the one-way coupled system. Similarly, the error passed between iterations is treated by defining suitable functionals for the information that is passed between iterations and solving auxiliary adjoint problems. However, the errors from all the previous iterations generally affect the solution at the current iteration level, and so the estimate has a "history" of estimates for errors from previous iterations. The effect of the error at any given iteration level decays in influence as the iteration converges in general, but may still be a persistent effect in some circumstances.

2.2.3 Coupling through boundaries: Conjugate heat transfer

The next class of problems we discuss involve models posed on domains consisting of distinct components that are joined at an interface boundary. There is a differential equation model posed on each component of the domain and the solutions on the different components are related through the boundary conditions imposed on the interface boundary.

Example 2.2.7 *Consider a model of heat in an object Ω composed of two materials occupying regions Ω_1, Ω_2 with $\Omega = \Omega_1 \cup \Omega_2$ and Γ denoting the common boundary $\Omega_1 \cap \Omega_2$. The stationary model for conjugate heat transfer between the components is*

$$\begin{cases} -\nabla \cdot (a_1 \nabla u_1) = f_1,\ x \in \Omega_1, \quad u_1 = 0,\ x \in \partial\Omega_1 \setminus \Gamma, \\ -\nabla \cdot (a_2 \nabla u_2) = f_2,\ x \in \Omega_2, \quad u_2 = 0,\ x \in \partial\Omega_2 \setminus \Gamma, \end{cases} \tag{37}$$

where the solutions are coupled by imposing continuity of value and normal flux on the interface boundary,

$$u_1 = u_2, \quad a_1 \nabla u_1 \cdot \boldsymbol{n} = a_2 \nabla u_2 \cdot \boldsymbol{n}, \quad x \in \Gamma.$$

Other important examples of such coupling are fluid-solid conjugate heat transfer [21] and models of fusion reactors involving coupling of the "core" and "edge" dynamics.

We can implement a MOD method for this problem using an iterative approach where boundary values are passed back and forth between the components during the solution.

Example 2.2.8 *For simplicity, we describe one iterative algorithm for a stationary problem*

Algorithm 3 Multiscale Operator Decomposition for Conjugate Heat Transfer

Construct space discretizations $\mathcal{T}_1, \mathcal{T}_2$ and finite element spaces $\mathcal{S}_1, \mathcal{S}_1$ for Ω_1, Ω_2
Choose an initial value $U_{n,2}^{(0)}$ on Γ
for $i = 1, \cdots, I$ **do**
Compute a finite element approximation $U_1^{(i)} \in \mathcal{S}_{n,1}$ for

$$-\nabla \cdot (a_1 \nabla u_1) = f_1,\ x \in \Omega_1, \qquad u_1 = 0,\ x \in \partial\Omega_1 \setminus \Gamma, \quad u_1 = U_2^{(i-1)},\ x \in \Gamma.$$

Compute a finite element approximation $U_2^{(i)} \in \mathcal{S}_{n,2}$ for

$$-\nabla \cdot (a_2 \nabla u_2) = f_2,\ x \in \Omega_2, \qquad u_2 = 0,\ x \in \partial\Omega_2 \setminus \Gamma, \quad a_2 \nabla u_2 \cdot \boldsymbol{n} = a_1 \nabla U_1^{(i)} \cdot \boldsymbol{n},\ x \in \Gamma.$$

end for

There are many other ways to iterate between components of course, and these different approaches have different convergence properties. We may also employ relaxation in order to yield more robust convergence. When solving an evolution problem, we employ an iteration such as Alg. 3 on each time step.

We attack the analysis of such problems using the same approach as used for MOD for elliptic systems outlined in Sec. 2.2.2. We identify the information that is passed between components as auxiliary quantities of interest and solve the corresponding adjoint problems in addition to the adjoint problem associated with the information to be computed from the solution of the model. The analysis includes estimates of the contributions of the error in the computed information transferred between components, the effects of using different discretizations in the components, and the effects of iteration error in the solution, resulting in very accurate estimates. The analysis has some special features because the auxiliary quantities of interest involve boundary values.

An interesting consequence of transferring gradient information is that the MOD solution suffers a loss of one order of convergence. If we simply apply the *a posteriori* error estimate to guide adaptive mesh refinement, the algorithm "compensates" by refining heavily near the interface boundary so as to reduce that source of error, which is inefficient. However, a careful examination of the *a posteriori* error estimate reveals that there is one expression that causes the loss of order. We adapt the "boundary flux recovery" technique developed by Wheeler and Carey to postprocess the finite element solution as to remove the offending term in the estimate, and this turns out to restore the order of convergence of the numerical approximation at a very low computational cost.

Example 2.2.9 *We illustrate using (37) with* Ω_1=$[0,1] \times [0,1]$ *and* $\Omega_2 = ([1,2] \times [0,1])$, $a_1 = 1$, $a_2 = 3$, *and* f_1 *and* f_2 *chosen so the true solutions are* $u_2 = \sin(2\pi x)\sin(2\pi y)$ *and* $u_1 = 3u_2$. *The quantity of interest equal to the value of* u_2 *at the point* $(1.75, 0.25)$. *In Fig. 7, we show a typical adapted mesh after three refinement steps. We also show the first order convergence for the MOD solution on a sequence of uniform meshes along with the second order convergence of the "flux corrected" solutions on the same meshes.*

2.3 Overview of results obtained in current project

We present a brief overview of the activity and results obtained in the current project. We divide the research papers into three large groups.

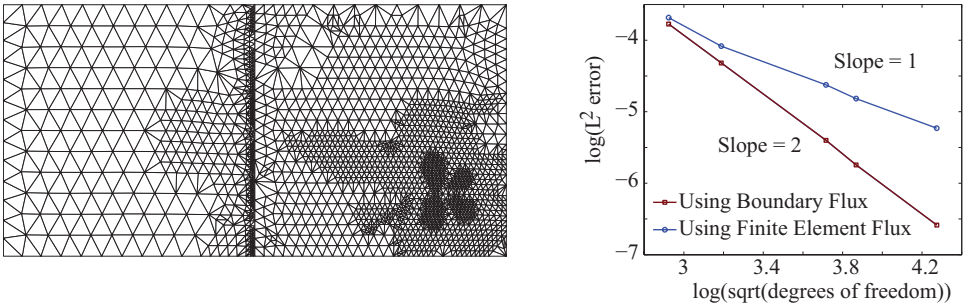


Figure 7: Adaptive mesh for the quantity of interest equal to the value of u_2 at the point $(1.75, 0.25)$ for the MOD solution and orders of convergence for the MOD solution and the flux corrected solution on a sequence of uniform meshes.

2.3.1 Analysis of multiscale, operator decomposition solution of multiphysics problems

The central achievement of the current project is the development of a systematic approach to *a posteriori* error analysis of MOD solutions of multiphysics problems. This represents a major contribution to the solution of multiscale, multiphysics problems. We applied this analysis to three particular problems.

- *An a posteriori-a priori analysis of multiscale operator splitting [7].* In this paper, we analyze a multiscale operator splitting method for reaction-diffusion equations. We present a new type of hybrid *a priori – a posteriori* error analysis pinpoints the effects that MOD has on accuracy and stability.

- *A posteriori analysis and adaptive error control for multiscale operator decomposition solution of elliptic systems I: Triangular systems [2].* We conduct an *a posteriori* analysis of a MOD finite element method for the solution of a triangular system of coupled elliptic problems. We focus on the propagation of errors arising from the solution of one component to another and the transfer of information between different representations of solution components. We discuss the use of Monte-Carlo integration for transferring information between solutions on different meshes.

- *A posteriori analysis and adaptive error control for multiscale operator decomposition solution of elliptic systems II: Fully coupled systems [3].* We extend the analysis in Part I to fully coupled problems, focusing on issues related to solving a nonlinear system and the effects on accuracy.

- *A posteriori analysis and improved accuracy for an operator decomposition solution of a conjugate heat transfer problem [17].* We conduct an *a posteriori* analysis of a MOD method for a conjugate heat transfer problem consisting of two materials coupled through a common boundary. We use boundary flux correction to improve accuracy in an efficient way.

- *A posteriori error analysis for a transient conjugate heat transfer problem [20].* We conduct an *a posteriori* analysis of a MOD method for a time-dependent conjugate heat transfer problem consisting of two materials coupled through a common boundary. We use boundary flux correction to improve accuracy in an efficient way.

- *A posteriori error estimation and adaptive mesh refinement for a multi-discretization operator decomposition approach to fluid-solid heat transfer [21].* We analyze a MOD finite element method for a conjugate heat transfer problem consisting of a fluid and a solid coupled through a common boundary.

- *Error estimation for multiscale methods* to appear in in *Bridging the Scales in Science and Engineering*, J. Fish, Ed., Oxford University Press [6]. We present a general introduction to the newly developed approach to *a posteriori* error estimation for multiscale, multiphysics problems.

- *A posteriori error analysis for elliptic problems with rough data* [9]. In this article we develop a number of a posteriori error estimates for elliptic problems with extremely rough data, using both standard Galerkin formulations as well as H^{-1}-type formulations. This work is based on a supporting rough data analysis framework for nonlinear elliptic systems recently developed in [23].

2.3.2 Nonparametric density estimation for partial differential equations with randomly perturbed parameters

The current project was initially focussed on *a posteriori* error estimation for coupled physics problems. The project had to expand to tackle broader questions of uncertainty quantification in order to keep the project relevant to our laboratory partners for several reasons, including

- Using multiphysics models to address practical scientific and engineering work always involves data, and hence any attempt to quantify error must include the effect of measurement error and uncertainty in data.

- In a MOD solution, each component inherits numerical errors transferred from the other components. These inherited errors resemble modeling error, e.g. they cannot typically be corrected by refinement in the current component.

Adjoint-based analysis provides powerful tools for sensitivity analysis that are foundational for uncertainty quantification. In this sequence of papers, we derive new methods for nonparametric density estimation. We focus on nonparametric density estimation because our experience suggests that the probability distributions associated with quantities of interest computed from many physical models tend to be highly complex and hence accessible only through sampling. Reasons include for example the effects of nonlinearity and the inclusion of multiple bifurcation points in typical parameter domains. Since physical models are often very expensive to evaluate, developing methods for density estimation that require minimal sampling is an important problem.

We explore two approaches in the work below. One approach uses the fact that the adjoint operator provides a relatively inexpensive way to compute the gradient of a quantity of interest with respect to parameters. This approach provides an elegant representation of the distribution associated with a random output quantity in terms of convolution of the corresponding adjoint solution with the distributions placed on the input data and parameters. Furthermore, the derivative information provides the basis for several adaptive sampling and variance reduction procedures. The second set of papers deal with elliptic problems in which the diffusion coefficients are randomly perturbed by a variable for which very limited information is known.

- *Fast and reliable methods for determining the evolution of uncertain parameters in differential equations [14].* We use derivative information about a quantity of interest obtained by solving

the adjoint problem to devise new, fast methods for nonparametric density estimation. These include a higher order representation of the response surface (HOPS) and an error estimate for a representation that can be used to guide adaptive sampling (FAPS). Both the higher order method and the adaptive sampling method are generally orders of magnitude faster than Monte-Carlo methods in the case that the parameter space is not too high dimensional.

- *Fast methods for determining the evolution of uncertain parameters in reaction-diffusion equations [15].* We extend the previous work to systems of reaction-diffusion problems and use the new methods to analyze the parameter sensitivity of a predator-prey model with a Holling II functional response that has six parameters.

- *Nonparametric density estimation for elliptic problems with random perturbations I: Computational method and a posteriori analysis [12].* We develop two efficient methods for computing solutions to the Poisson equation with randomly perturbed data and coefficient. The first method is designed to treat random right hand side and boundary condition and is based on solving a single corresponding adjoint problem, then constructing realizations of a linear functional of the solution by multiplying the adjoint solution with the data. The second method deals with a piecewise constant random perturbation in the coefficient. The Monte Carlo finite element method is combined with a domain decomposition algorithm such that the random perturbation is constant on the domains. Then a power series is used to approximate the inverse matrix on each domain, yielding a very fast method. We provide analysis of both techniques.

- *Nonparametric density estimation for elliptic problems with random perturbations II: Adaptive computation [12].* We devise an adaptive computation procedure for nonparametric density estimation for elliptic problems with random perturbations. The procedure balances the computational work between sampling, error in representation of the effects of variation, and the numerical error in the solution of the differential equation.

- *Nonparametric density estimation for elliptic problems with random perturbations III: Convergence analysis [11].* The nonparametric density estimation technique in Part I of this series relies a non-overlapping domain decomposition. In this paper, we examine the convergence properties of this domain decomposition.

2.3.3 General results in the solution and analysis of differential equations

We pursued a number of smaller projects to support the primary research of the project.

- *Iterative techniques for the solution of coupled multi-physics problems [19].* We investigate the iterative solution of multiphysics problems using a MOD approach. We derive an approach based on an inner Newton-Krylov iteration and the solution of a variational system, and show that this approach is a generalization of a preconditioning technique used in domain decomposition. We demonstrate that this approach can significantly reduce the overall cost.

- *A posteriori error estimation of approximate boundary fluxes [18].* We derive an *a posteriori* estimate of the error in the flux of a finite element solution of an elliptic problem on a piece of the boundary of the domain. We investigate the effects of smoothing the data corresponding to the quantity of interest and explore the effective domain of dependence of the quantity.

- *Generalized Green's functions and the effective domain of influence [8].* We use the generalized's Greens function to develop a new approach to domain decomposition for the efficient solution of elliptic problems when the goal either involves multiple quantities of interest or quantities of interest corresponding to global information such as average values over the domain.

- *Global error estimation and adaptive error control for ordinary differential equations [16].* We design and implement new global error control mechanisms based on *a posteriori* error estimates for quantities of interest for evolution problems. These approaches allow for the effects of cancellation of errors, resulting in greatly improved reliability and efficiency in many situations.

- *Adaptive error control for an elliptic optimization problem [10].* We consider optimization of parameters of elliptic problems and derive *a posteriori* error estimates for the error in the gradients used in search algorithms that are computed from finite element solutions of the problem. We devise an adaptive algorithm to refine and unrefine the finite element mesh at each step in the descent search algorithm.

- *Analysis techniques for weak solutions to coupled nonlinear elliptic problems with rough data [23].* We analyze the Joule heating problem, which is modeled as a coupled nonlinear elliptic system with rough data. We first develop a number of supporting results such as *a priori* L^∞-bounds for the individual potential and temperature fields. Based on these results, we then develop a topological fixed-point argument giving the first existence result for this system in the 3D case with mixed boundary conditions. The results required the development of techniques for dealing with rough data, which we are now employing in the development of adaptive numerical techniques for such problems [9].

- *New convergence proof techniques for adaptive methods [4, 5].* In [4], we analyze the convergence properties of an adaptive finite element method (AFEM) applied to a coupled indefinite linear elliptic system, and establish one of the first convergence (and optimality) results using quasi-orthoginality and differential complex techniques. In [5], we do a similar convergence analysis for adaptive finite element methods applied to a nonlinear elliptic problem with supercritical monotone nonlinearity and rough data. We first derive a number of supporting results such as *a priori* L^∞ and other estimates for a multiscale splitting of the solution. These results, together with some simple and realizable mesh conditions, then allow us to establish analogous discrete estimates. The AFEM algorithm we employ is then described, and convergence is shown using energy arguments. We have since improved this convergence proof technology to allow for non-monotone nonlinearities [24].

- *Multiresolution geometric meshing algorithms and software for multiscale modeling [30, 28, 29, 1].* In this work, we have developed a number of surface and volume geometric modeling and meshing algorithms for producing (or improving) surface and volume simplex mesh models of geometric data with multiscale features. The algorithms, which are all implemented in the GAMer module in the FETK software package [22], allow for a large variety of input data (point sets, distance functions or other level set information, boundary triangulations, or molecular data in PDB format) and produce high-fidelity surface and volume triangulations with low memory and computational complexity. Features of the algorithms include the ability to produce quality volume simplex meshes which match complex surface triangulations,

and the ability to produce multiresolution mesh hierarchies using quality mesh decimation algorithms.

2.4 Personnel involved in the current project

The following people were supported in the current project.

2.4.1 Principal Investigators

- Donald Estep, Department of Mathematics and Department of Statistics, Colorado State University
- Michael Holst, Department of Mathematics, University California San Diego
- Simon Tavener, Department of Mathematics, Colorado State University

2.4.2 Postdocs

- Varis Carey, in progress
- Victor Ginting, currently Assistant Professor, University of Wyoming
- Axel Malqvist, currently Assistant Professor, University of Uppsala
- Jeff Sandelin, in progress

2.4.3 Graduate Students

- D. Neckels, Thesis, 2005: "Variational Methods for Uncertainty Quantification". Currently, National Center for Atmospheric Research
- J. Sandelin, Thesis, 2006: "Global Estimate and Control of Model, Numerical, and Parameter Error". Currently, PRIMES postdoc, Colorado State University
- T. Wildey, Thesis, 2007: "A Posteriori Analysis of Operator Decomposition on Interface Problems". Currently, ICES Postdoctoral Fellow, University of Texas at Austin.
- T. Butler, Department of Mathematics, Colorado State University, in progress
- S. Lee, Department of Mathematics, Colorado State University, in progress
- R. Mckeown, Department of Forestry, Rangeland, and Watershed Stewardship, Colorado State University, in progress

2.5 Software developed in the current project

As part of the current project, the Estep group developed two software packages that have the capability to compute *a posteriori* error estimates based on solving adjoint problems and include adaptive mesh refinement.

- *GAASP* (Globally Accurate, Adaptive Sensitivity Package [13])

  Authors: Estep, Mckeown, Neckels, Sandelin

  This package has two parts: an adaptive ordinary differential equation solver that uses adjoints and includes both probabilistic and optimization error control mechanisms and a wrapper that allows for sensitivity analysis of an ordinary differential equation. The solver incorporates a number of sophisticated features to facilitate the formation and solution of adjoint problems. The user need only supply a righthand side, data, and quantities of interest. The sensitivity package employs both HOPS and FAPS [] density estimation techniques. GAASP is a C++ code.

- *ACES* (Adaptive Coupled Equation Solver [27])

  Author: Wildey

  ACES is a MATLAB/C software package designed to solve stationary and time-dependent multiphysics systems with a flexible framework that handles both coupling through parameters and coupling through boundary values for problems posed on multiple domains. It allows different numerical methods to be used for different components of the multiphysics system. ACES incorporates a number of error estimation and adaptive refinement techniques as well as boundary flux corrections.

Estep's group has also established strong working collaborations with code developers at Sandia. We have collaborated in particular with developers of SIERRA, CALORE, ARIA, and RHYTHMOS.

The Holst group has continued to develop and extend the FETK [22] software package. The FETK project is based at UCSD, but is developed collaboratively by personnel involved in this proposal and by other colleagues around the world. As described in detail on the FETK website [22], FETK consists of several independent packages which are developed using a common "object-oriented C" programming framework provided by one of the FETK libraries called MALOC. The libraries forming FETK are primarily: MALOC (Minimal Abstraction Layer for Object-oriented C); PUNC (Portable Understructure for Numerical Computing); SG (Socket Graphics); and MC (Manifold Code). As part of the current project, the Holst group developed a new library for FETK called GAMer, and further extended the core finite element library MC.

- *GAMer* (Geometry-preserving Adaptive MeshER)

  Author: Yu, Holst

  GAMer is a Geometry-preserving Adaptive MeshER that produces high-quality simplex meshes of surfaces and volumes, given a number of different types of input data. It is built on top of two state-of-the-art mesh generators: Triangle (for 2D constrained Delaunay meshes in the plane) and Tetgen (for 3D constrained Delaunay meshes in space), combined with a collection of algorithms for generating, improving, refining, and decimating surface triangulations of imbedded interior or exterior domain surfaces. GAMer and the algorithms it employs are described in detail in [30, 28, 29, 1].

- *MC* (Manifold Code)

  Author: Holst and collaborators

  MC (Manifold Code) is a parallel adaptive multilevel finite element software package designed to be used collaboratively with several related research FETK tools such as MALOC, GAMer,

and SG. MC is designed to numerically approximate the solutions of covariant divergence-form second-order nonlinear elliptic systems of partial differential equations with multiscale features on domains with the structure of Riemannian two- and three-manifolds. To accomplish this task as accurately and efficiently as possible, MC employs simplex triangulations of the domain manifold, Petrov-Galerkin finite element methods, *a posteriori* error estimation, adaptive mesh refinement and un-refinement, continuation, Newton methods, multilevel methods, and a recently-developed low-communication approach in parallel adaptive finite element methods. Extensions made to MC as part of the current project include the ability to form and solve large sparse linearized dual problems for producing duality-type *a posteriori* error indicators, and the development and implementation of new types of error indicator and marking algorithms as derived in [4, 5, 24] that guarantee AFEM convergence. In addition, a collection of decoupling iteration-type algorithms for multiphysics problems have been developed and implemented; cf. [1, 25, 32, 26, 31].

2.6 Exposure and service related to the current project

The research in the current project has garnered significant attention. This is an overview of activity relevant to the project during the period of the current project.

2.6.1 D. Estep

- Computational and Mathematical Methods in Sciences and Engineering (CMMSE) Prize, 2005
- Invited short course, 4th Montreal Scientific Computing Days, University of Montreal, Montreal, Canada, 2007
- 15 invited lectures at professional meeting, including two plenary talks and one keynote lecture
- 17 seminars and colloquia at universities and DOE laboratories
- Co-organizer of six professional workshops and minisymposia
- Served on two DOE review panels
- Co-Organizer, Second DOE Workshop on Multiscale Mathematics, 2004, with J. Shadid and S. Tavener. Co-editor and co-author for final report
- Panel Co-Leader, Panel on Validation, Verification, Uncertainty Analysis and Decision Optimization, Department of Energy Computational Subsurface Sciences Workshop, 2007. Coordinator for Priority Research Direction report "Uncertainty Representation, Uncertainty Propagation, and Sensitivity Analysis for Subsurface System". Contributor on two other Priority Research Direction reports.
- Department of Energy, Office of Advanced Scientific Computing, Applied Mathematics Strategic Plan Recommendation Panel, 2007.

2.6.2 M. Holst

- 25 invited lectures at professional meetings, including three keynote and plenary lectures.
- 17 seminars and colloquia at universities, DOE laboratories, and industry
- Co-organizer of five professional workshops and minisymposia, including workshops at IPAM, IMA, and MSRI.
- Served on DOE panel on Optimization and Complex Systems

2.6.3 S. Tavener

- Co-Organizer, Second DOE Workshop on Multiscale Mathematics, 2004, with D. Estep and J. Shadid. Co-editor and co-author for final report.
- Served on one DOE review panel
- Attended Department of Energy Computational Subsurface Sciences Workshop, 2007
- Six seminars and lectures at professional meetings

2.6.4 D. Estep's Research Group

Members of D. Estep's research group presented over 26 talks at professional meetings and seminars at universities and DOE laboratories.

2.6.5 Cooperation with and outreach to DOE laboratories

The research team has maintained an extremely active and close collaboration with personnel at Sandia National Laboratories in Albuquerque, New Mexico. The chief collaborators include P. Bochev, B. Carnes, T. Coffey, K. Copps, S. Domino, R. Lehoucq, C. Newman, J. Shadid, and J. Stewart. This collaboration has been sustained by a program of frequent visits by the investigators, postdocs, and students to Sandia and vice versa by periodic visits by Sandia researchers to Colorado State University.

Highlights of these exchanges during the period of the current project include:

- D. Estep made at least seven visits to Sandia. These visits often included members of his group
- Members of D. Estep's group made a number of visits to Sandia on their own, including a summer long visit by T. Wildey
- Sandia researchers made a number of visits to CSU
- D. Neckels took a LTE position at Sandia after graduating
- S. Tavener made 3 visits to Sandia
- M. Holst made 2 visits to Sandia, and made multiple short and long-term visits to CSU
- The First Colorado State Multiall Workshop (Fort Collins, 9/05) included 10 people from Sandia

- The Second Colorado State Multiall Workshop (Fort Collins, 9/06) included 14 people from Sandia

D. Estep also established ties to researchers at other national laboratories. During the period of this project, D. Estep visited Los Alamos, Lawrence Livermore and Idaho National Laboratories, and he has active (funded) collaborations with researchers at LLNL, INL, and ANL.

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