Adjoint-Fueled Advances in Error Estimation for Multiscale, Multiphysics Systems

Donald Estep

Department of Mathematics

Department of Statistics

Colorado State University

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Multiphysics, Multiscale Systems

Multiphysics, Multiscale Systems

Much of the work of my group is concerned with error estimation and uncertainty quantification for multiphysics, multiscale systems

Application drivers for our work:

- Fusion and fission reactors
- Reacting fluids and fluid-solid interactions
- Advanced materials, nano-manufacturing
- Biological systems, drug design and delivery
- Environmental, climate, ecological models

Analysis for Multiphysics, Multiscale Systems

In the last few years, there has been a breakthrough in the analysis for multiphysics, multiscale systems

Features

- The analysis estimates the errors passed between physical components
- The analysis takes into account the effects from changing scale and processing information between physical components
- The analysis quantifies the complicated stability properties of numerical methods

Example 1: MEMS-Scale Thermal Actuator

Electrostatic current equation ($J = -\sigma \nabla V$)

$$\nabla \cdot (\sigma \nabla V) = 0$$

Steady-state energy equation

$$\nabla \cdot (\kappa(T) \nabla T) = \sigma (\nabla V \cdot \nabla V)$$

Steady-state displacement (linear elasticity)

$$\hat{\nabla} \cdot \left(\lambda \, \mathrm{tr}(E) I + 2\mu E - \beta (T - T_{ref}) I \right) = 0$$

$$E = \left(\hat{\nabla} d + \hat{\nabla} d^{\top} \right) / 2$$

This is an example of “parameter passing”, in which the solution of one component is used to compute the parameters and/or data for another component.

Example 2: Reaction-Diffusion Equations

The Brusselator problem

$$\begin{cases} \frac{\partial u_1}{\partial t} - \epsilon\,\Delta u_1 = \alpha - \beta u_1 + u_1^2 u_2, \\ \frac{\partial u_2}{\partial t} - \epsilon\,\Delta u_2 = \gamma u_1 - u_1^2 u_2, \\ \text{suitable initial and boundary conditions} \end{cases}$$

The Brusselator is a simple model of the reaction kinetics of the two main species in an autocatalytic reaction taking place in solution

Tight coupling of different physical components with different scales and stability properties, e.g. reaction and diffusion, in the same equations

Example 3: Fluid-Solid Conjugate Heat Transfer

$$
\begin{cases}
-\mu\Delta u + \rho_0 \left(u \cdot \nabla\right) u + \nabla p + \rho_0 \beta T_F g = \rho_0 \left(1 + \beta T_0\right) g, \\
-\nabla \cdot u = 0, \\
-k_F \Delta T_F + \rho_0 c_p (u \cdot \nabla T_F) = Q_F, \\
\text{interface} \begin{cases} T_S = T_F, \\ k_F (n \cdot \nabla T_F) = k_S (n \cdot \nabla T_S), \end{cases} \\
-k_S \Delta T_S = Q_S,
\end{cases}
$$

Physics in different regions are coupled through a common interface

Example 4: Physics in a Fusion Reactor

R. Cohen simplified model for core-edge coupling

$$\begin{cases} \frac{\partial T_c}{\partial t} = \frac{\partial}{\partial x}\chi_c \frac{\partial T_c}{\partial x} + S_c, & \text{core region} \\ \frac{\partial T_m}{\partial t} = \frac{\partial}{\partial x}\chi_m \frac{\partial T_m}{\partial x} + S_m - \nu_{md}\left(T_m - T_d\right), & \text{edge midplane region} \\ \frac{\partial T_d}{\partial t} = \frac{\partial}{\partial x}\chi_d \frac{\partial T_d}{\partial x} + S_d + \nu_{md}\left(T_m - T_d\right) & \\ \qquad\qquad -\nu_{el} T_d \theta(x - x_s), & \text{edge divertor region} \end{cases}$$

The edge and core regions are coupled through a common boundary:

$$\begin{cases} T_c = \frac{1}{2}\left(T_m + T_d\right), \\ \chi_c \nabla T_c \cdot \boldsymbol{n} = \frac{1}{2}\left(\chi_m \nabla T_m \cdot \boldsymbol{n} + \chi_d \nabla T_d \cdot \boldsymbol{n}\right) \end{cases}$$

with $S_c = S_m + S_d$ and $\chi_c = \chi_m + \chi_d$ at the interface

The physics is coupled across scales in space and time

Multiscale Operator Decomposition

Multiscale Operator Decomposition

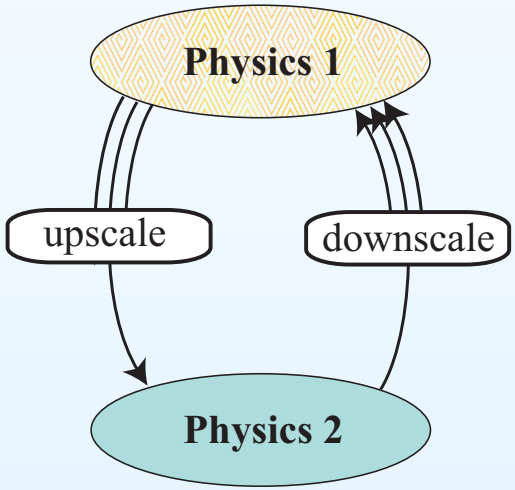
Multiscale operator decomposition methods are widely used for solving multiphysics, multiscale systems

The system is decomposed into components representing relatively simple physics and/or single scales and a global solution is sought by iterating solutions of the components

Multiscale Operator Decomposition

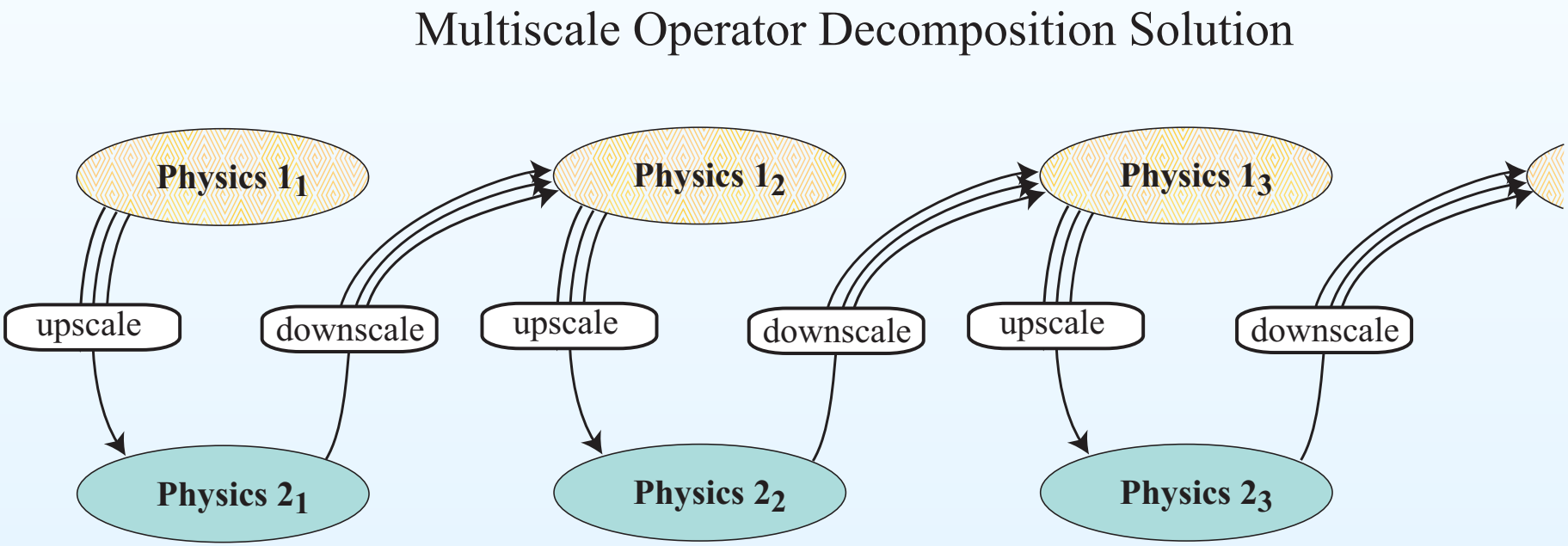
Multiscale operator decomposition methods are widely used for solving multiphysics, multiscale systems

Fully Coupled



Multiscale Operator Decomposition

Multiscale operator decomposition methods are widely used for solving multiphysics, multiscale systems



Multiscale operator decomposition takes many forms

MOD for a Coupled Elliptic System

A simplified Thermal Actuator model:

$$\begin{cases} -\nabla \cdot a_1 \nabla u_1 + \mathbf{b}_1 \cdot \nabla u_1 + c_1 u_1 = f_1(x), & x \in \Omega, \\ -\nabla \cdot a_2 \nabla u_2 + \mathbf{b}_2 \cdot \nabla u_2 + c_2 u_2 = f_2(x, u_1, Du_1), & x \in \Omega, \\ u_1 = u_2 = 0, & x \in \partial\Omega, \end{cases}$$

Ω is a bounded domain with boundary $\partial\Omega$

The coefficients are smooth functions and a_1, a_2 are bounded away from zero

We wish to compute information depending on u_2

MOD for a Coupled Elliptic System

Algorithm

- Construct discretizations $\mathcal{T}_{h,1}, \mathcal{T}_{h,2}$ and finite element spaces $\mathcal{S}_{h,1}, \mathcal{S}_{h,2}$
- Compute a finite element solution $U_1 \in \mathcal{S}_{h,1}(\Omega)$ of the first equation
- Project $U_1 \in \mathcal{S}_{h,1}(\Omega)$ into the space $\mathcal{S}_{h,2}(\Omega)$
- Compute a finite element solution $U_2 \in \mathcal{S}_{h,2}(\Omega)$ of the second equation

The projection between the finite element spaces is a crucial step

In a fully coupled system, U_2 would next be projected into the space for U_1 for the next iteration

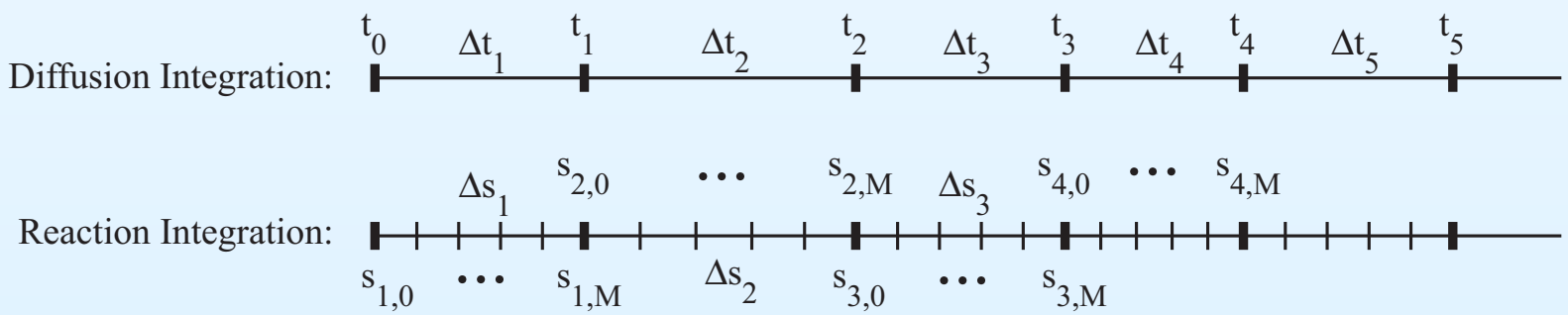
MOD for a Reaction-Diffusion Equation

We consider the reaction-diffusion problem

$$\begin{cases} \frac{du}{dt} = \Delta u + F(u), \quad 0 < t, \\ u(0) = u_0 \end{cases}$$

The diffusion component Δu induces stability and change over long time scales while the reaction component F induces instability and change over short time scales

The reaction component is solved using many time steps inside each diffusion step



MOD for a Reaction-Diffusion Equation

Multiscale Operator-Splitting Algorithm

- On $(t_{n-1}, t_n]$, use the fine mesh to solve

$$\begin{cases} \frac{du^R}{dt} = F(u^R), & t_{n-1} < t \leq t_n, \\ u^R(t_{n-1}) = u^D(t_{n-1}) \end{cases}$$

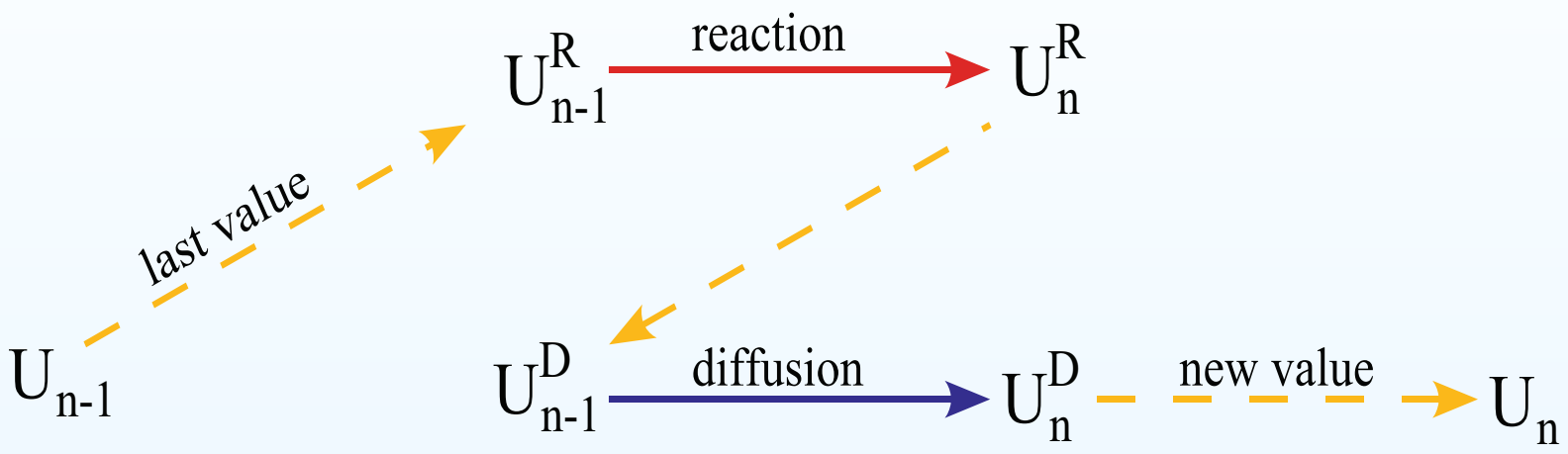
- On $(t_{n-1}, t_n]$, use the coarse mesh to solve

$$\begin{cases} \frac{du^D}{dt} - \Delta(u^D) = 0, & t_{n-1} < t \leq t_n, \\ u^D(t_{n-1}) = u^R(t_n) \end{cases}$$

- Advance to the next diffusion step

The operator split approximation is $u(t_n) \approx u^D(t_n)$

MOD for a Reaction-Diffusion Equation



MOD for Coupling Through a Boundary

A parabolic interface problem

$$\begin{cases} \frac{\partial u_1}{\partial t} - \nabla \cdot (\chi_1 \nabla u_1) = f_1, & x \in \Omega_1 \\ \frac{\partial u_2}{\partial t} - \nabla \cdot (\chi_2 \nabla u_2) = f_2, & x \in \Omega_2 \end{cases}$$

with coupling conditions

$$\begin{cases} u_1 = u_2, \\ \chi_1 \nabla u_1 \cdot \boldsymbol{n} = \chi_2 \nabla u_2 \cdot \boldsymbol{n}, \end{cases} \qquad x \in \Gamma$$

We use different space and time discretizations for the two components

We introduce projections between the discrete spaces on the two sides of the interface Γ

MOD for Coupling Through a Boundary

Let T_i^n denote an approximation at time t_n.

"Gauss-Seidel" Algorithm

- Given u_2^{n-1}, solve for u_1^n with $u_1^n = u_2^{n-1}$ on the interface
- Given u_1^n, solve for u_2^n with $\chi_2 \nabla u_2^n \cdot \boldsymbol{n} = \chi_1 \nabla u_1^n \cdot \boldsymbol{n}$ on the interface
- Move on to t_{n+1}

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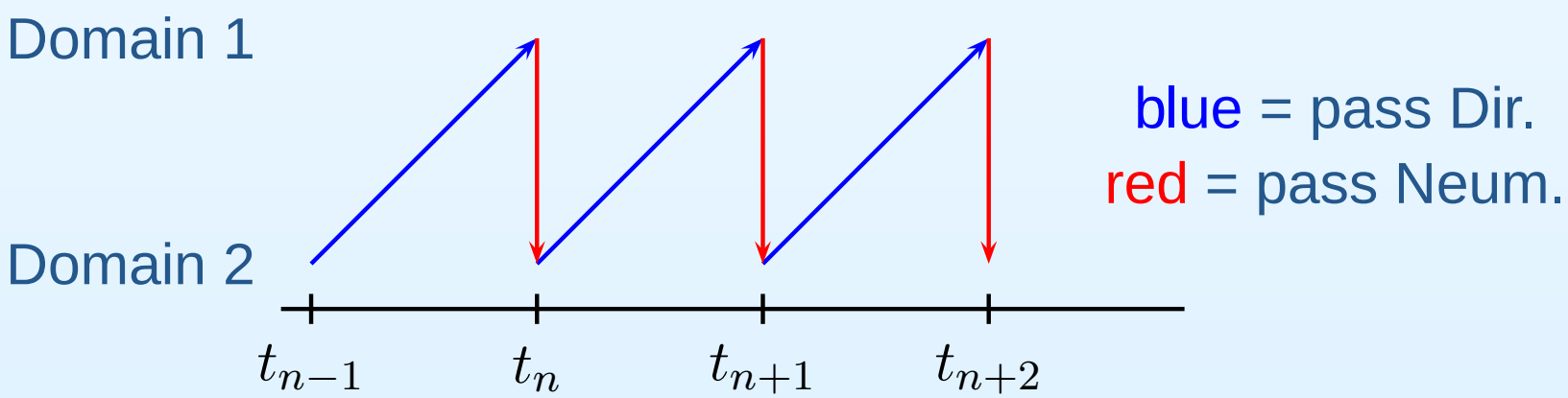
Illustration



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- Move on to t_{n+1}

There are many other ways to arrange iterations between components and timesteps

What Can Go Wrong with Multiscale Operator Decomposition?

Issues with Multiscale Operator Decomposition

Multiscale operator decomposition discretizes the instantaneous interactions between the component physics

The price:

- Transfer of computed information between components affects the accuracy of the numerical solution and the order of convergence
- New forms of instability, some of which are very subtle, arise

Even if each physical component is resolved accurately, coupling may cause the overall simulation to lose fidelity

These consequences are often not apparent on either the component or global level.

A Simple Thermal Actuator

Consider

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

where $\Omega = [0,1] \times [0,1]$

We consider the quantity of interest

$$u_2(.25, .25)$$

We solve for u_1 first and then solve for u_2 using independent meshes

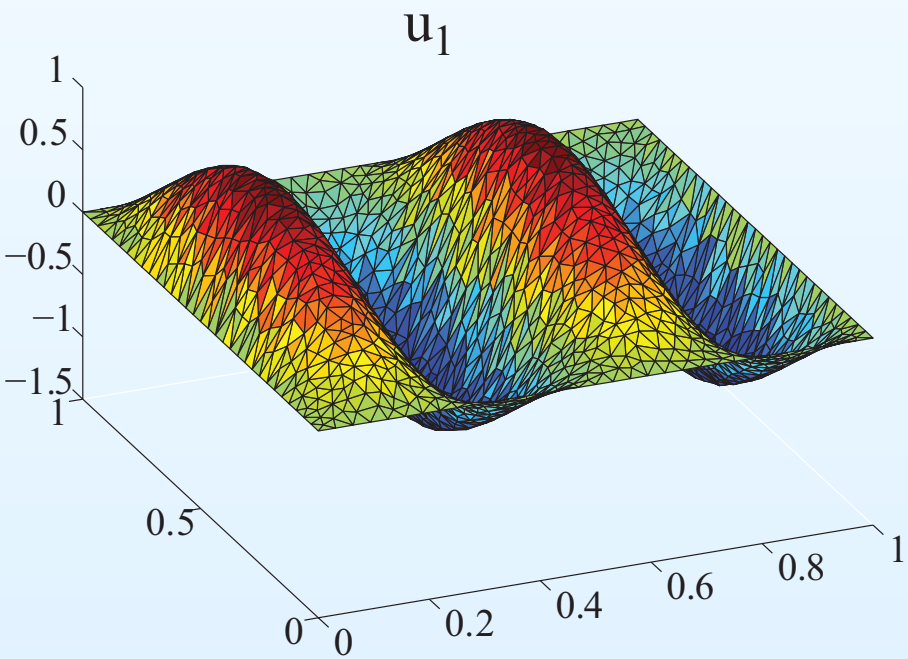
A Simple Thermal Actuator

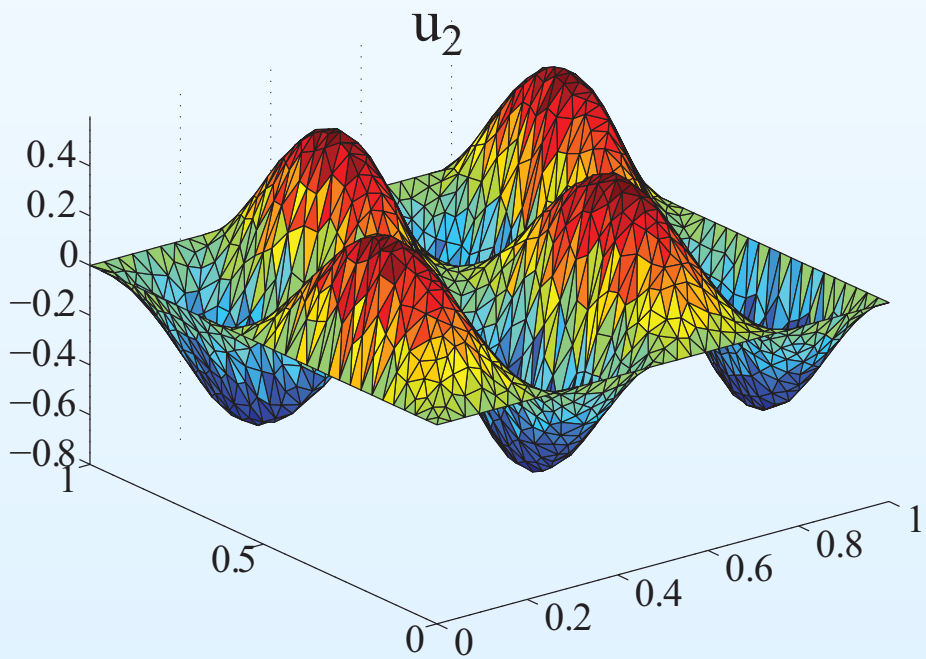
Using uniform meshes, an *a posteriori* error estimate yields

estimate of the error in the quantity of interest $\approx .0042$

true error $\approx .0048$

discrepancy in estimate $\approx .0006$ $(\approx 13\%)$



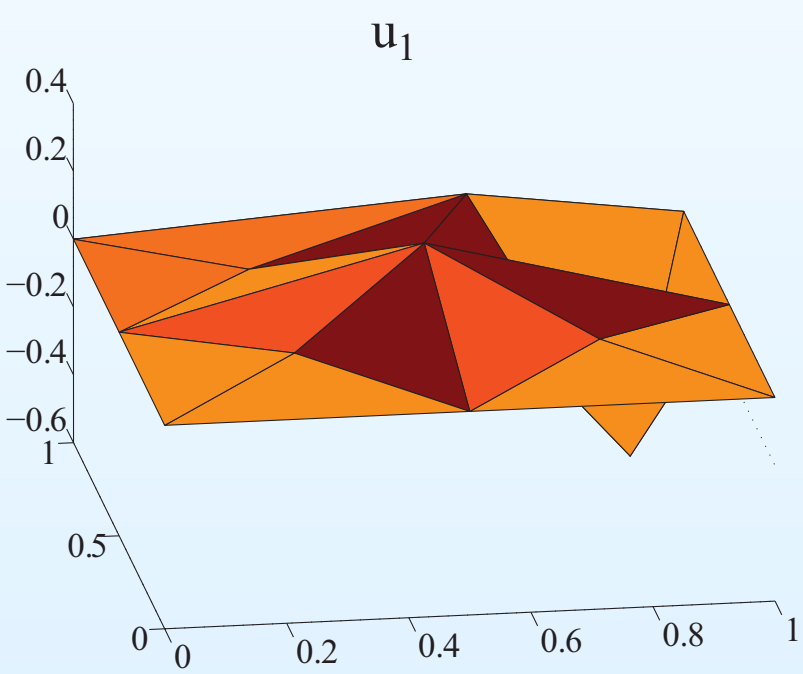


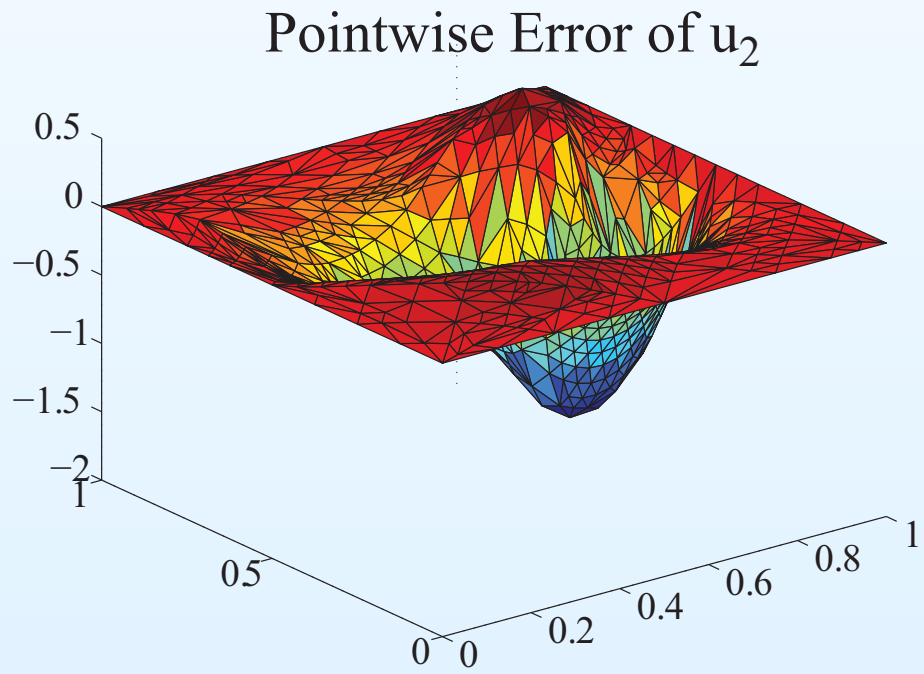
A Simple Thermal Actuator

Adapting the mesh using only an error estimate for the second component causes the discrepancy to become alarmingly worse

estimate of the error in the quantity of interest $\approx .0001$

true error $\approx .2244$



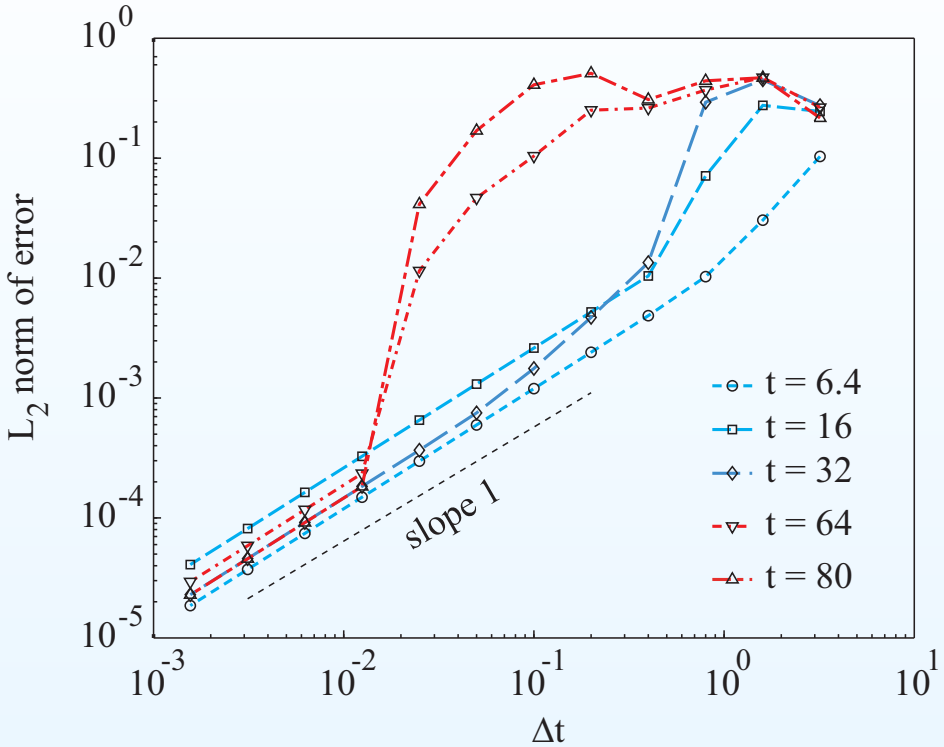


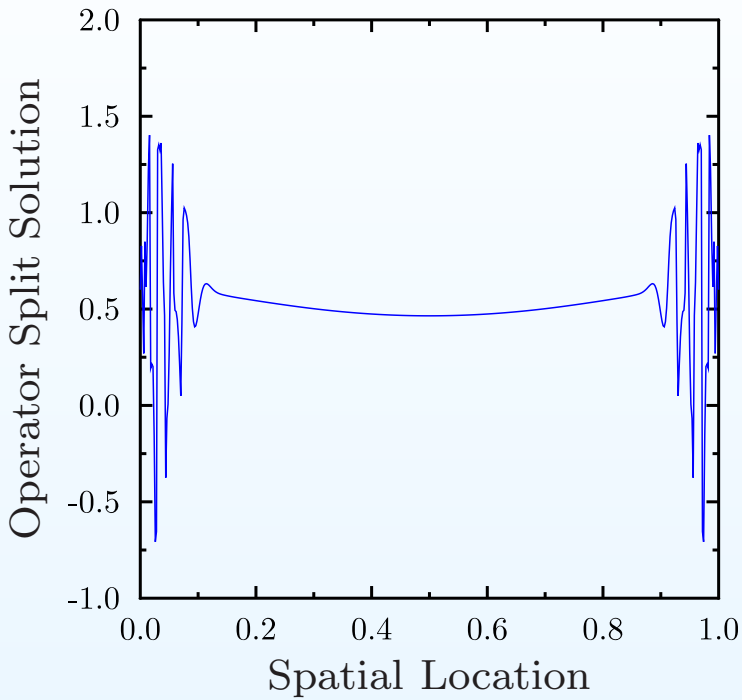
The Brusselator Problem

$$\begin{cases} \frac{\partial u_1}{\partial t} - 0.025\,\Delta u_1 = f_1(u_1, u_2) = 0.6 - 2u_1 + u_1^2 u_2, \\ \frac{\partial u_2}{\partial t} - 0.025\,\Delta u_2 = f_2(u_1, u_2) = 2u_1 - u_1^2 u_2, \\ \text{suitable initial and boundary conditions} \end{cases}$$

- Linear finite element method in space with 500 elements
- A standard first order splitting scheme
- Trapezoidal Rule for the diffusion and Backward Euler for the reaction with 50 reaction steps for each diffusion step

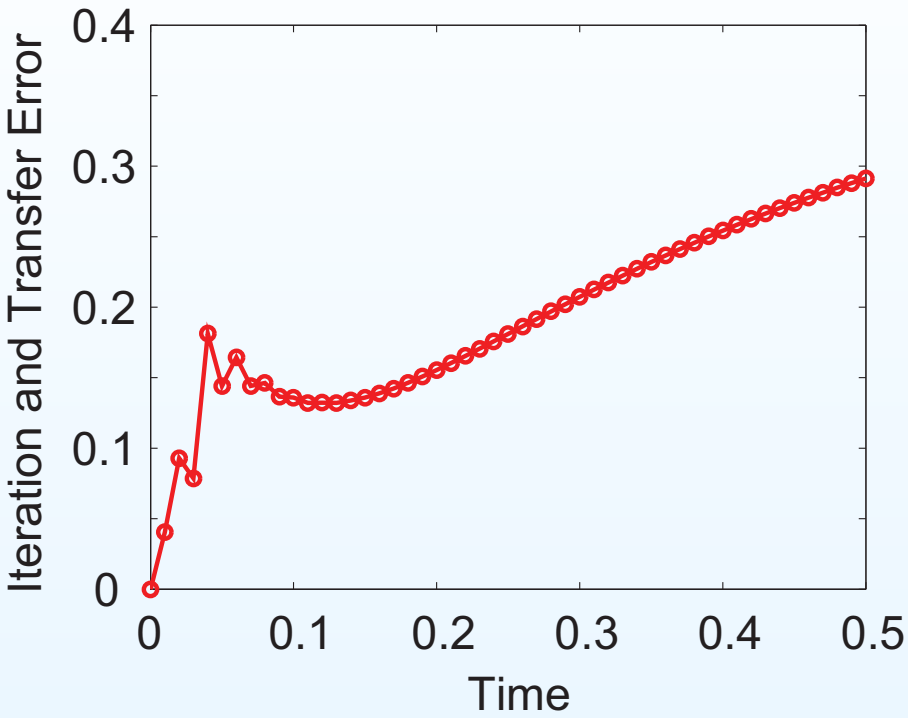
The Brusselator Problem





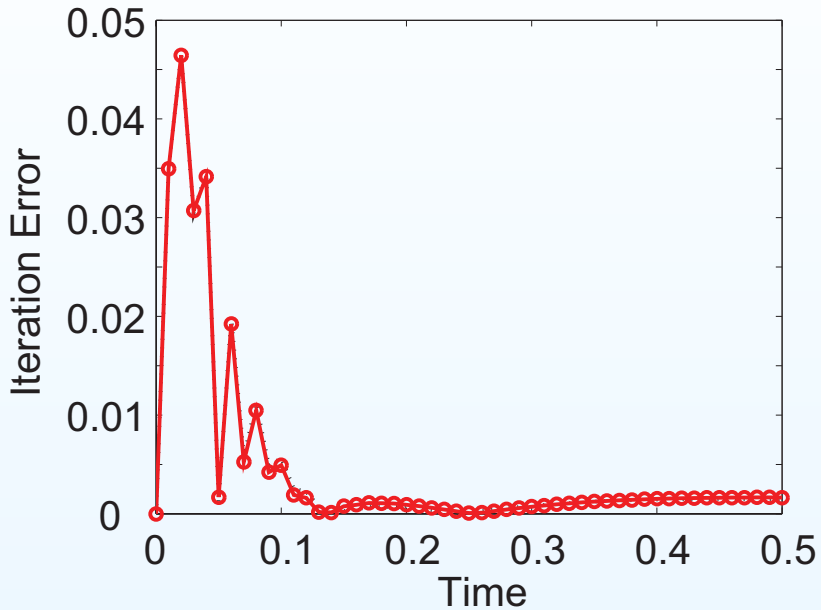
On moderate to long time intervals, there is a critical time step above which convergence fails

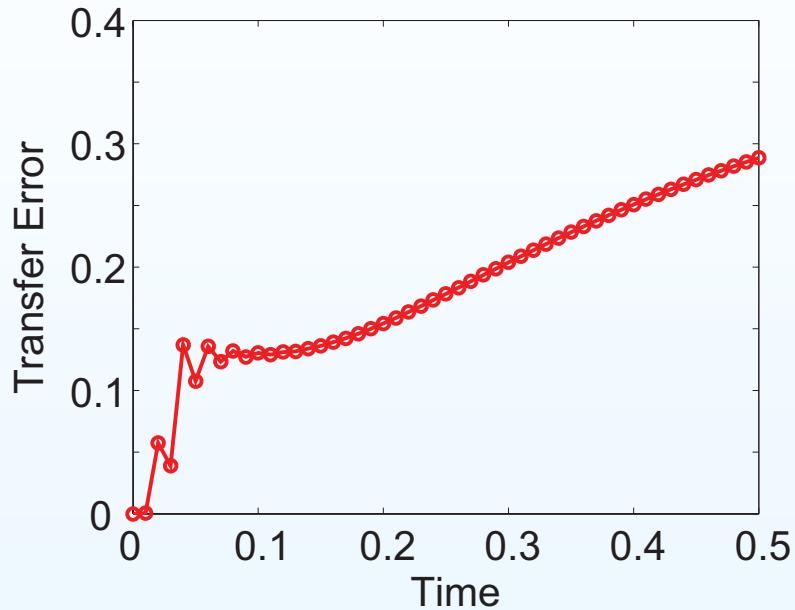
R. Cohen's Model with Coupling Through a Boundary



Using $\Delta t = 10^{-3}$, the total error of the approximation increases with time

R. Cohen's Model with Coupling Through a Boundary

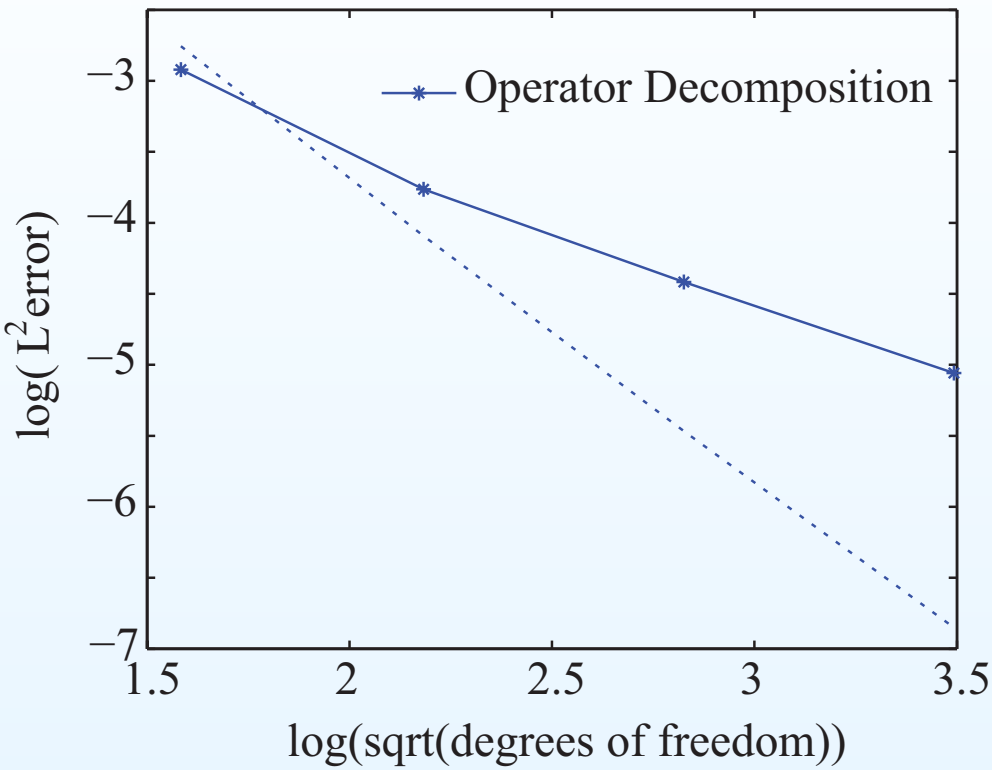




The error arising from incomplete iteration on each step becomes negligible as time passes

The transfer error accumulates with time and becomes the largest source of error

R. Cohen's Model with Coupling Through a Boundary



Though we use second order accurate methods for each component, the error in the operator decomposition approximation is only first order in space

Adjoint-Fueled Analysis of Differential Equations

Adjoint Operators and Differential Equations

Much of our research is aimed at error analysis and uncertainty quantification for differential equations

We use adjoint operators and variational analysis

The stability properties of an operator are fundamentally tied to the properties of its adjoint

The adjoint also provides a cheap way to compute derivative information

A Posteriori Error Analysis

Estimate the error in a quantity of interest computed from a numerical solution of a differential equation

We assume that the quantity of interest can be represented as a linear functional of the solution

We solve the adjoint problem associated with the linear functional

A Linear Algebra Example

Problem	$\mathbf{A}y = b$
Quantity of interest	(y, ψ)
Approximate solution	$Y \approx y$
Error	$(e, \psi) = (y - Y, \psi)$
Residual	$R = \mathbf{A}Y - b$
Adjoint problem	$\mathbf{A}^* \phi = \psi$

Analysis

$$\begin{aligned} |(e, \psi)| &= |(e, A^* \phi)| \\ &= |(Ae, \phi)| \\ &= |(R, \phi)| \end{aligned}$$

We solve for ϕ numerically to compute the estimate

Condition Numbers and Adjoint Solutions

The classic error bound is

$$\|e\| \leq C\kappa(\mathbf{A})\|R\|$$

The condition number $\kappa(\mathbf{A}) = \|\mathbf{A}\|\,\|\mathbf{A}^{-1}\|$ is a measure of stability

The *a posteriori* estimate yields

$$|(e,\psi)| \leq \|\phi\|\,\|R\|$$

The stability factor $\|\phi\|$ is a weak condition number for the quantity of interest

We can obtain κ from $\|\phi\|$ by taking the $\sup$ over all $\|\psi\| = 1$

Condition Numbers and Adjoint Solutions

Example Compute (y, e_1) from the solution of

$$\mathbf{A}y = b$$

where $\mathbf{A}$ is a random 800×800 matrix

Condition number of $\mathbf{A}$ is 6.7×10^4

estimate of the error in the quantity of interest $\approx 1.0 \times 10^{-15}$

a posteriori error bound for the quantity of interest $\approx 5.4 \times 10^{-14}$

traditional error bound for the error $\approx 3.5 \times 10^{-5}$

This kind of discrepancy between bounds and estimates is generic for differential equations

Abstract *A Posteriori* Error Analysis

We solve a differential equation

$$L(u) = f$$

for a quantity of interest given by a linear functional

$$(u, \psi) \qquad \psi \text{ determines the quantity of interest}$$

$(\, , \,)$ denotes the L^2 inner product over space and time

We compute a numerical approximation

$$U \approx u$$

The local resolution of the approximation is measured using the residual

$$R(U) = L(U) - f$$

Abstract *A Posteriori* Error Analysis

To build an error estimate, we solve a linear adjoint problem

$$(DL)^*\phi = \psi$$

We obtain the error representation

$$(U - u, \psi) = (R(U), \mathcal{W}(\phi))$$

for a suitable adjoint weight $\mathcal{W}(\phi)$

- The adjoint weight reflects stability by scaling residuals to create local contributions to the error
- The estimate accounts for the accumulation, cancellation, and propagation of local error contributions to the global error

The stability information is specific to the quantity of interest

A Posteriori Analysis for an Elliptic Problem

Let U be a Galerkin finite element approximation for

$$-\nabla \cdot a\nabla u + b \cdot \nabla u + cu = f \quad on\ \Omega$$

The residual in weak form is

$$(\mathcal{R}, v) = (a\nabla U, \nabla v) + \big(b \cdot \nabla U + cU - f, v\big) \quad for\ all\ test\ functions\ v$$

Obtained by integration by parts, the formal adjoint problem is

$$-\nabla \cdot a\nabla \phi - \text{div}(b\phi) + c\phi = \psi \quad on\ \Omega$$

The estimate is

$$(e, \psi) = \big(a\nabla U, \nabla(I - \pi_h)\phi)\big) + \big(b \cdot \nabla U + cU - f, (I - \pi_h)\phi\big)$$

π_h is a projection into the space of U

Goal-Oriented Adaptive Error Control

We write the error estimate as a sum of element contributions

$$(U-u,\psi) = (R(U),\mathcal{W}(\phi)) = \sum_{\text{elements } \Delta} (R(U),\mathcal{W}(\phi))_\Delta$$

where $(\ ,\ )_\Delta$ is the inner product over the element

In most cases, the signs of the element contributions $(R(U),\mathcal{W}(\phi))_\Delta$ vary

We replace the estimate by a bound

$$|(error,\psi)| \leq \sum_{elements\ \Delta} \left|(R(U),\mathcal{W}(\phi))_\Delta\right|$$

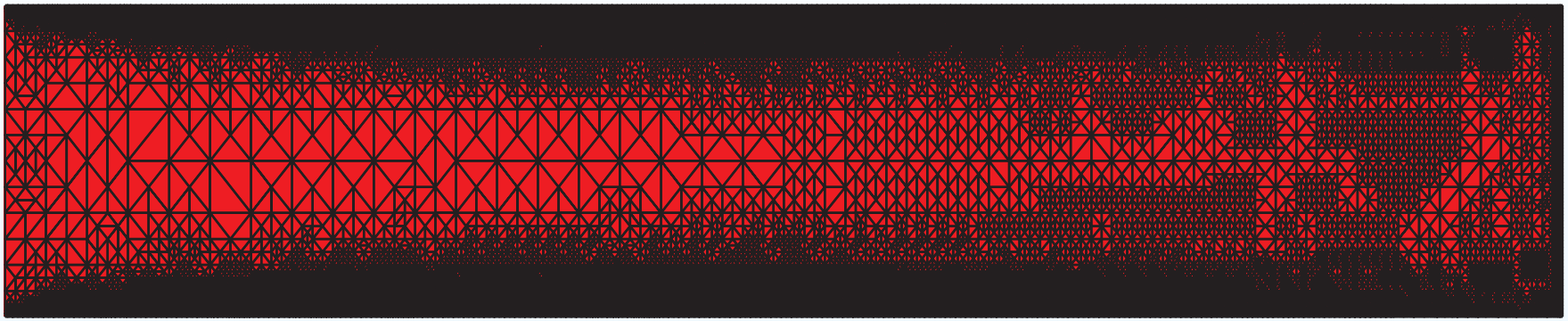
which has no inter-element cancellation

Goal-Oriented Adaptive Error Control

Example

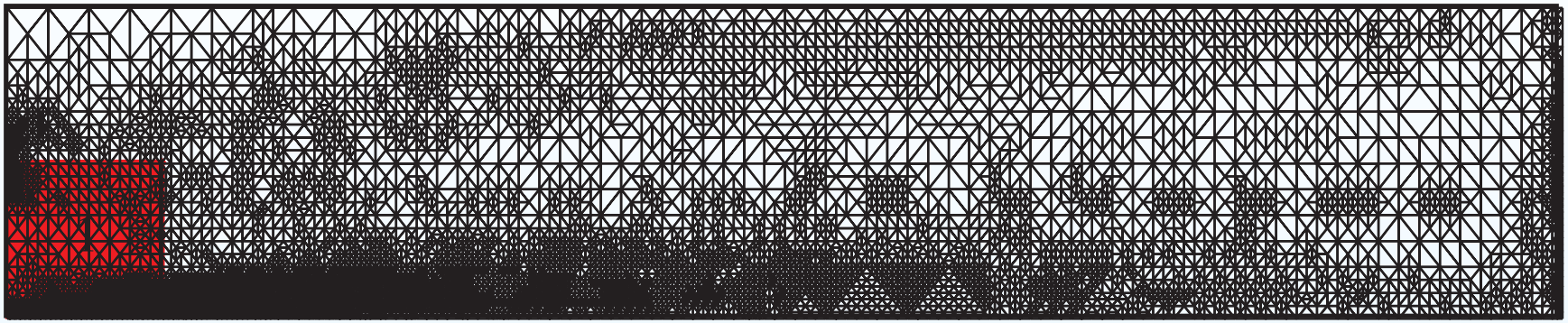
$$\begin{cases} -\nabla \cdot \Big((.05 + \tanh(10(x-5)^2 + 10(y-1)^2)) \nabla u \Big) \\ \qquad\qquad\qquad\qquad + \begin{pmatrix} -100 \\ 0 \end{pmatrix} \cdot \nabla u = 1, \quad (x,y) \in \Omega = [0,10] \times [0,2], \\ u = 0, \quad (x,y) \in \partial\Omega \end{cases}$$

Goal-Oriented Adaptive Error Control



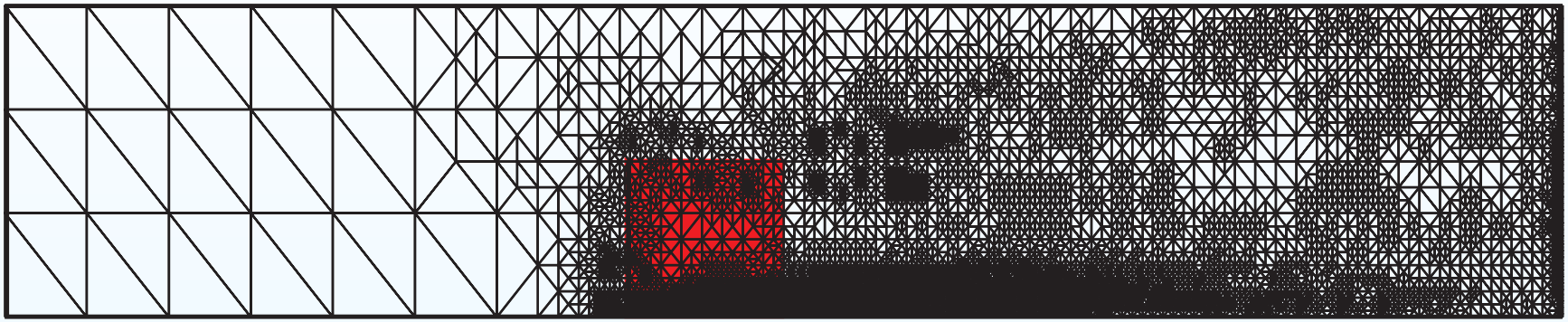
Final mesh for an average error of 4% (24,000 elements)

Goal-Oriented Adaptive Error Control



Final mesh for an average error in a patch (7,300 elements)

Goal-Oriented Adaptive Error Control



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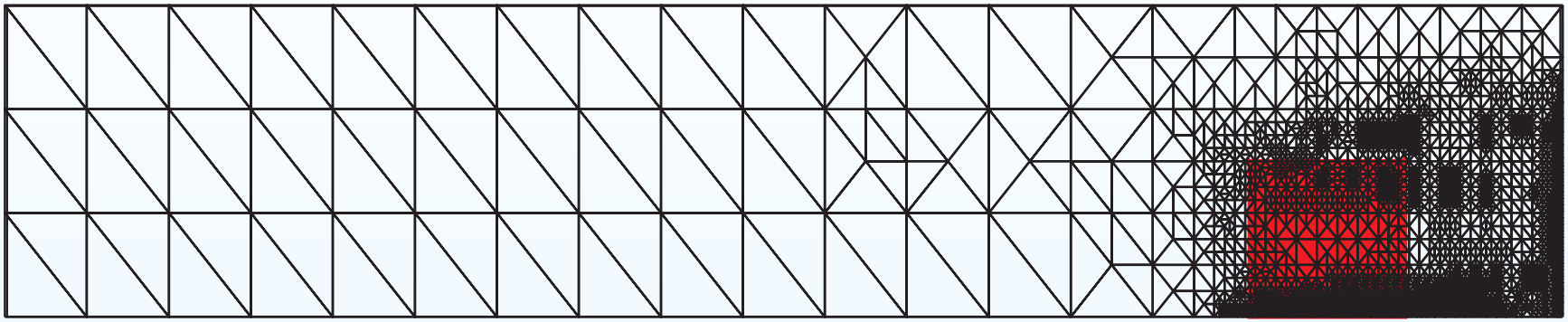
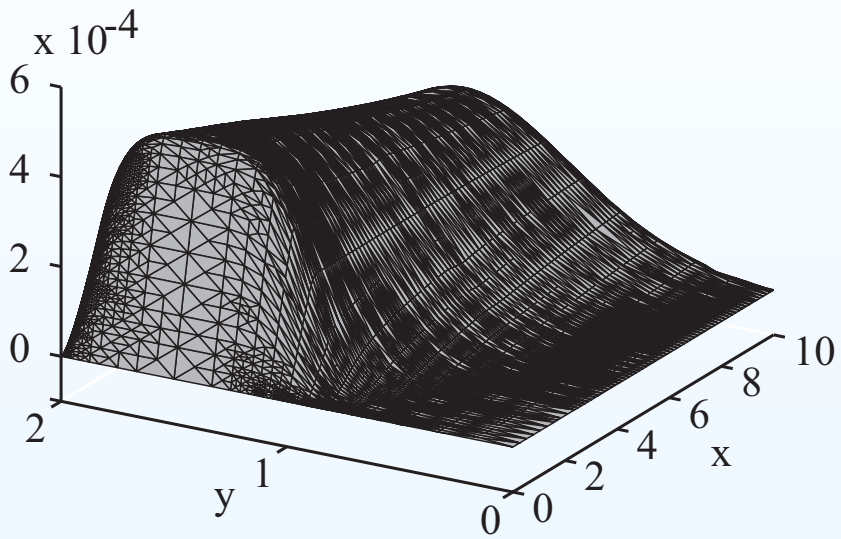
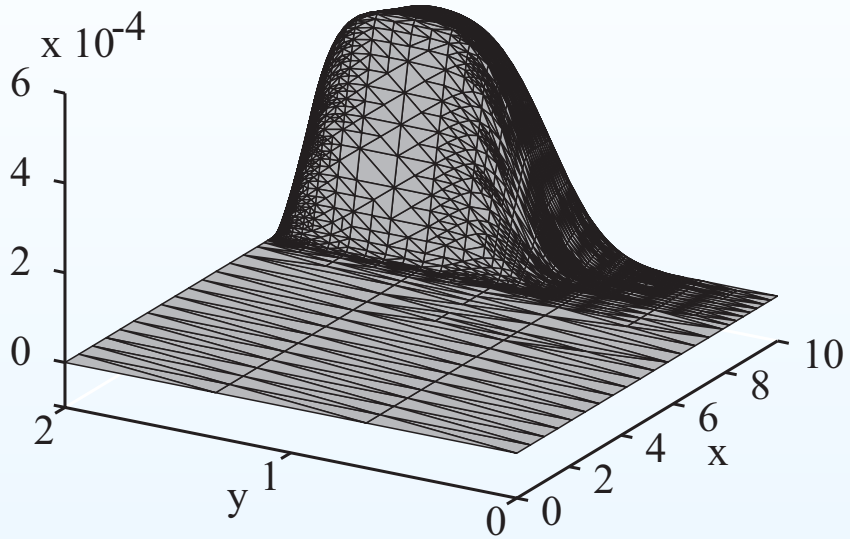


Final mesh for an average error in a patch (3,500 elements)

Goal-Oriented Adaptive Error Control





Adjoint solutions for the first and last patches

The Effect of Cancellation of Error

Adaptivity in an elliptic problem

+.001	+.001	+.001	+.01	+.01
+.001	+.001	+.001	+.01	+.01
+.001	+.001	+.001	+.001	+.001
-.0333	-.0333	+.001	+.001	+.001
+.1	-.0333	+.001	+.001	+.001

+.001	+.001	+.001	+.01	+.01
+.001	+.001	+.001	+.01	+.01
+.001	+.001	+.001	+.001	+.001
-.0333	-.0333	+.001	+.001	+.001
+.1	-.0333	+.001	+.001	+.001

Element contributions and two refinement strategies

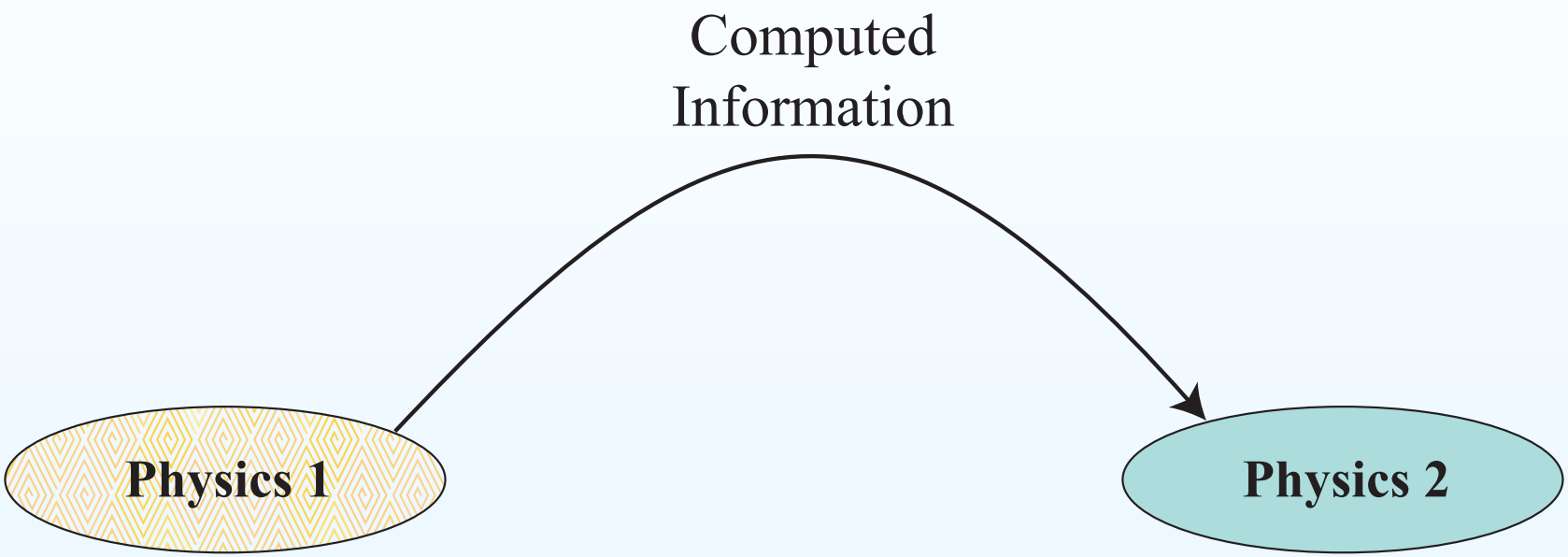
The total estimate is .0571.

Standard refinement strategy $\rightarrow$ .057025

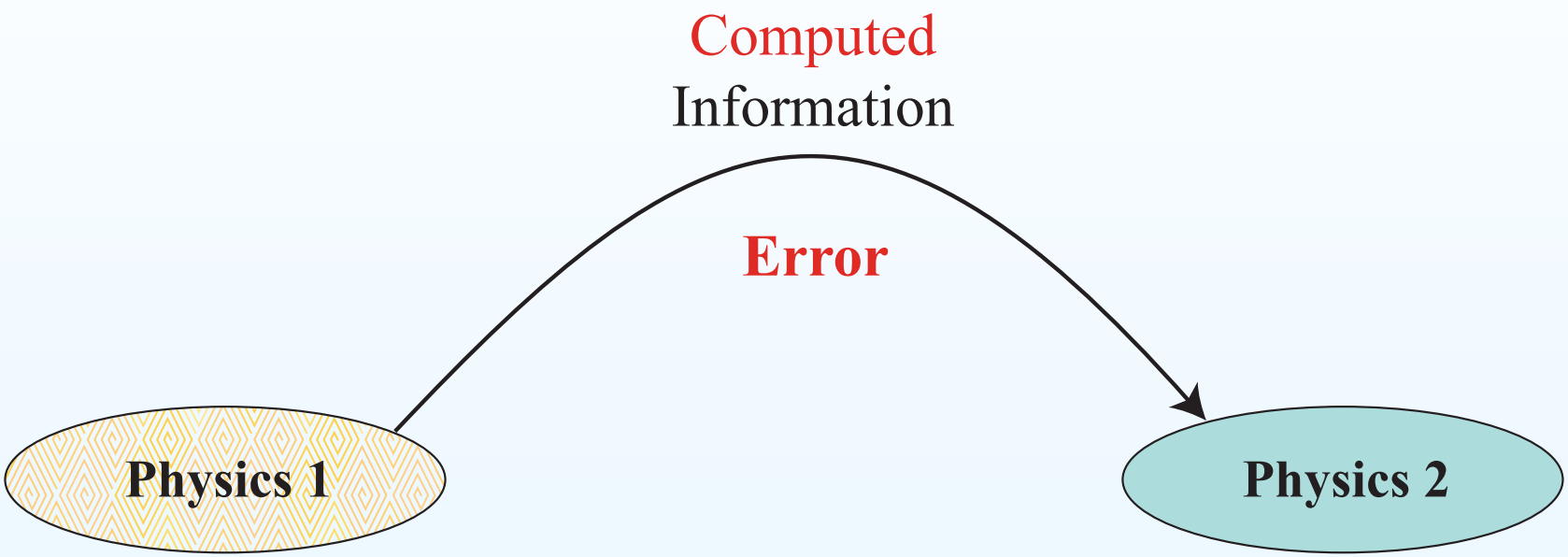
The nonstandard refinement strategy $\rightarrow$ .0271

Analysis of Multiphysics, Multiscale Systems

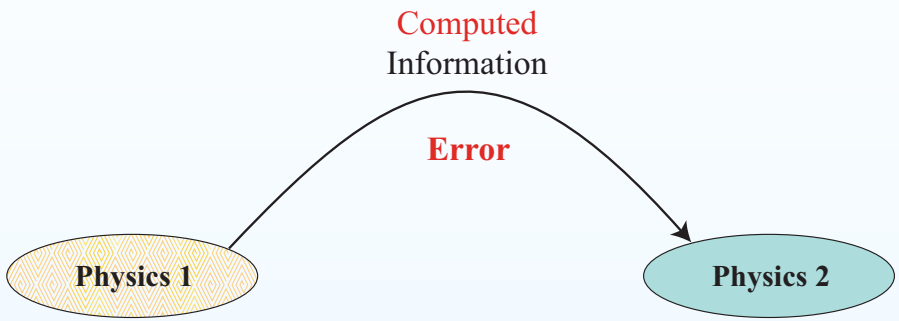
Multiscale Operator Decomposition: Issue 1



Multiscale Operator Decomposition: Issue 1



Multiscale Operator Decomposition: Issue 1



We define auxiliary quantities of interest corresponding to information passed between components

We solve auxiliary adjoint problems to estimate the error in that information

In an iterative scheme, we also estimate the “history” of errors passed from one iteration level to the next

We can also estimate the effect of processing, .e.g up and down scaling, the information

The Simple Thermal Actuator

Recall that neglecting the effects of operator decomposition leads to disturbing results

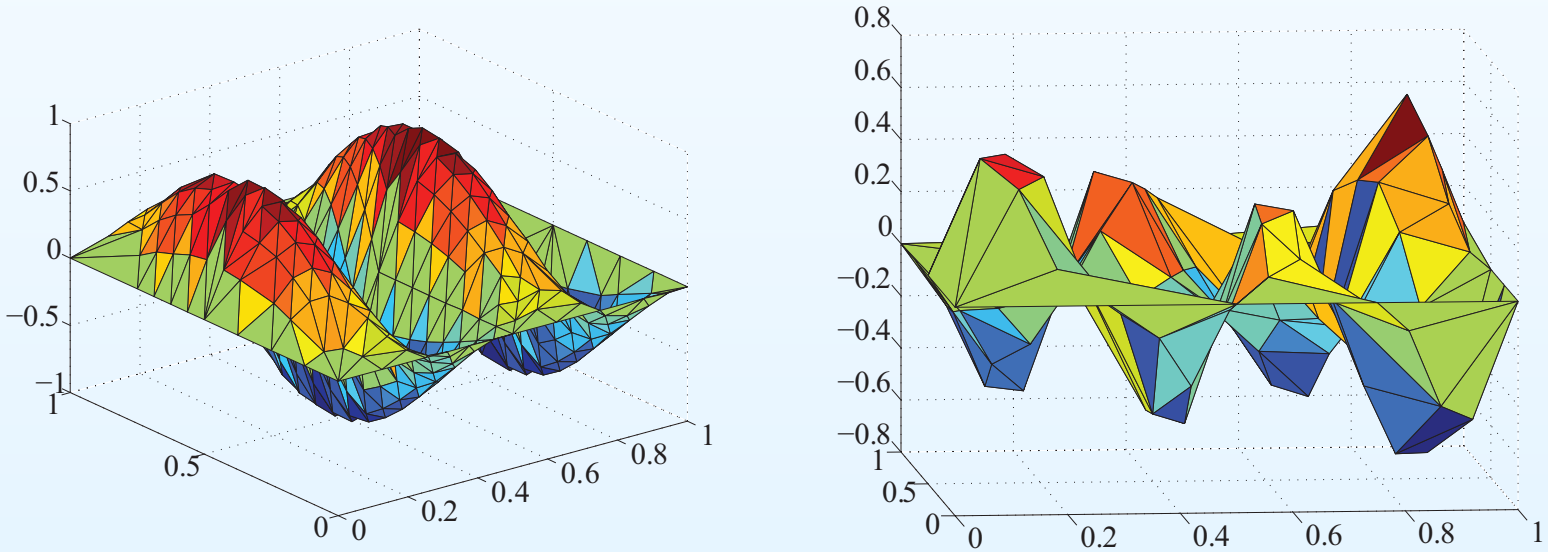
Theorem

$$(\psi, e) = \mathcal{R}_2(U_2, (I - \Pi_2)\phi_2^{(1)}; U_1) + \mathcal{R}_1(U_1, (I - \Pi_1)(\phi_1^{(2)} + \phi_1^{(3)}))$$
$$+\left(\Pi_{1\to 2} f_2(U_1) - f_2(\Pi_{1\to 2} U_1), \phi_2^{(1)}\right) + \left((I - \Pi_{1\to 2}) f_2(U_1), \phi_2^{(1)}\right)$$

The Simple Thermal Actuator

Recall that neglecting the effects of operator decomposition led to disturbing results

If we adapt the meshes the full analysis, we can drive the error below $.0001$



We actually refine the mesh for u_1 more than the mesh for u_2

Multiscale Operator Decomposition: Issue 2

The adjoint operator associated to a multiscale operator decomposition solution is generally different than the adjoint operator associated with the full problem

There are difficult technical issues about defining the appropriate adjoint operators

The estimates for MOD include terms that quantify the “error” in the adjoint operator

This measures the impact on stability properties

Additional work is needed to obtain a computable estimate

Reaction-Diffusion Equations

We derive a new type of hybrid *a priori* - *a posteriori* estimate

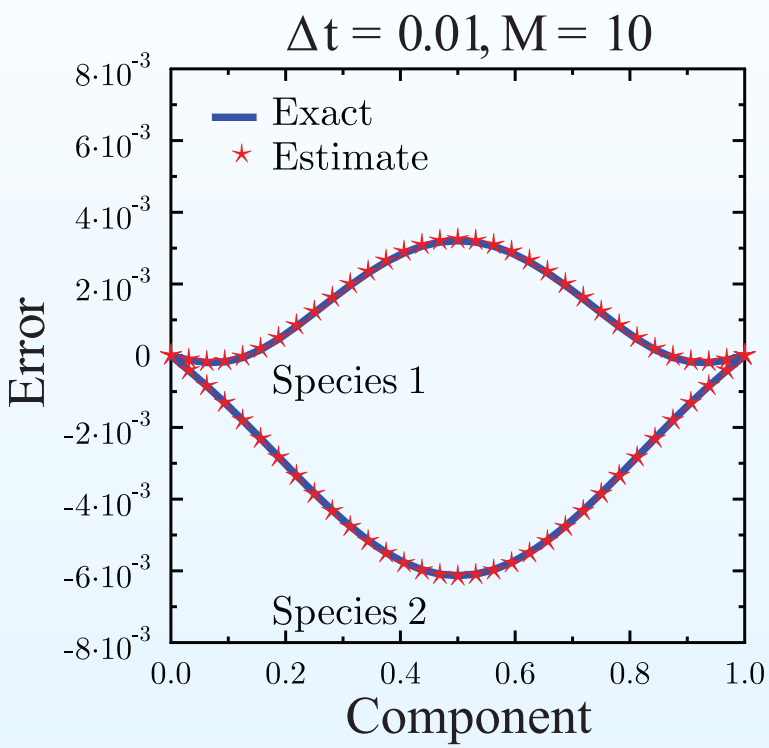
Theorem

$$\text{Error in a Q. of I.} \approx \mathcal{Q}_1 + \mathcal{Q}_2 + \mathcal{Q}_3$$

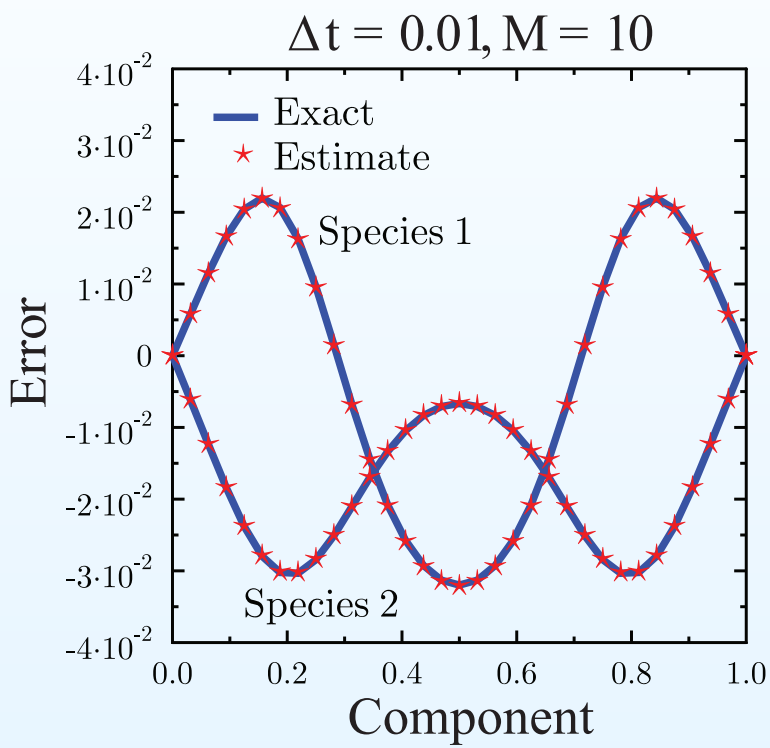
- $\mathcal{Q}_1$ estimates the error of the numerical solution of each component
- $\mathcal{Q}_2 \approx \sum_{n=1}^{N}(U_{n-1}, E_{n-1}), \quad E \approx$ a computable estimate for the error in the adjoint arising from operator decomposition
- $\mathcal{Q}_3 = \mathbf{O}(\Delta t^2)$ is an *a priori* expression that is provably higher order

The Brusselator Problem

Accuracy of the error estimate



T = 8



T = 40

Conjugate Heat Transfer

Theorem

$$
\begin{aligned}
(\psi, e) = {} & (f, \phi - \pi_V \phi) - a_1(u_h^{\{k\}}, \phi - \pi_V \phi_1) - c_1(u_h^{\{k\}}, u_h^{\{k\}}, \phi - \pi_V \phi) \\
& -b(\phi - \pi_V \phi, p_h) - d(T_{F,h}^{\{k\}}, \phi - \pi_V \phi) - b(u_h^{\{k\}}, z - \pi_Z z) \\
& + (Q_F, \theta_F - \pi_{W_F} \theta_F) - a_2(T_{F,h}^{\{k\}}, \theta_F - \pi_{W_F} \theta_F) \\
& -c_2(u_h^{\{k\}}, T_{F,h}^{\{k\}}, \theta_F - \pi_{W_F} \theta_F) + (Q_S, \theta_S - \pi_{W_S} \theta_S) - a_3(T_{S,h}^{\{k\}}, \theta_S - \pi_{W_S} \theta_S) \\
& + \left(T_{S,h}^{\{k\}} - \pi_S T_{F,h}^{\{k\}}, k_S(n \cdot \nabla \theta_S)\right)_{\Gamma_I} + \left(\pi_S T_{F,h}^{\{k\}} - T_{F,h}^{\{k\}}, k_S(n \cdot \nabla \theta_S)\right)_{\Gamma_I} \\
& + \left(k_S(n \cdot \nabla T_{S,h}^{\{k\}}), \pi_{W_F} \theta_F\right)_{\Gamma_I} + \left(Q_S, \pi_{W_S} \theta_S\right) - a_3\left(T_{S,h}^{\{k\}}, \pi_{W_S} \theta_S\right)
\end{aligned}
$$

The estimate involves auxiliary quantities of interest and adjoint problems measuring errors passed between components and between iteration levels

Conjugate Heat Transfer

One specific term in the estimate causes the observed loss of order of accuracy

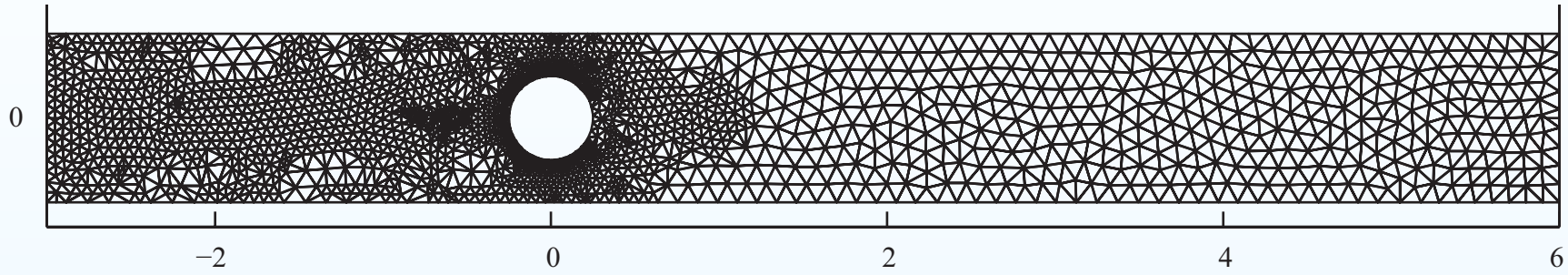
It arises from passing numerical fluxes at the interface

We can mitigate this several ways

- Use higher order elements or highly refined meshes
- Compute a discrete boundary flux correction for the error in the derivative on the interface

The last post-processing approach is very cheap and can be applied easily to existing codes

Conjugate Heat Transfer Between a Fluid and a Solid



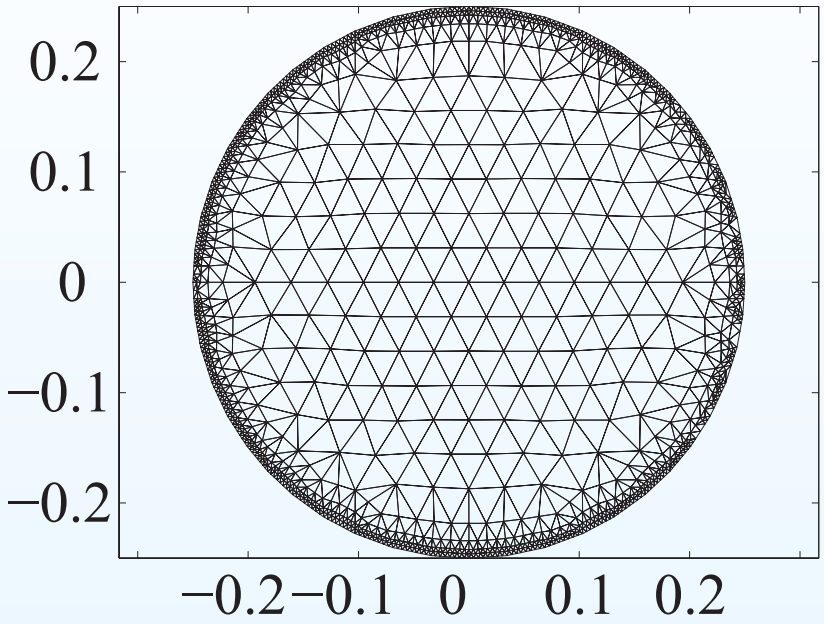
Quantity of interest is the temperature at a small region in the center of the cylinder

No flux correction is applied

Conditions are set to simulate the flow of water past a cylinder made from stainless steel

We use Taylor-Hood elements to solve the fluid and standard finite element methods for the solid with independent meshes

Conjugate Heat Transfer Between a Fluid and a Solid

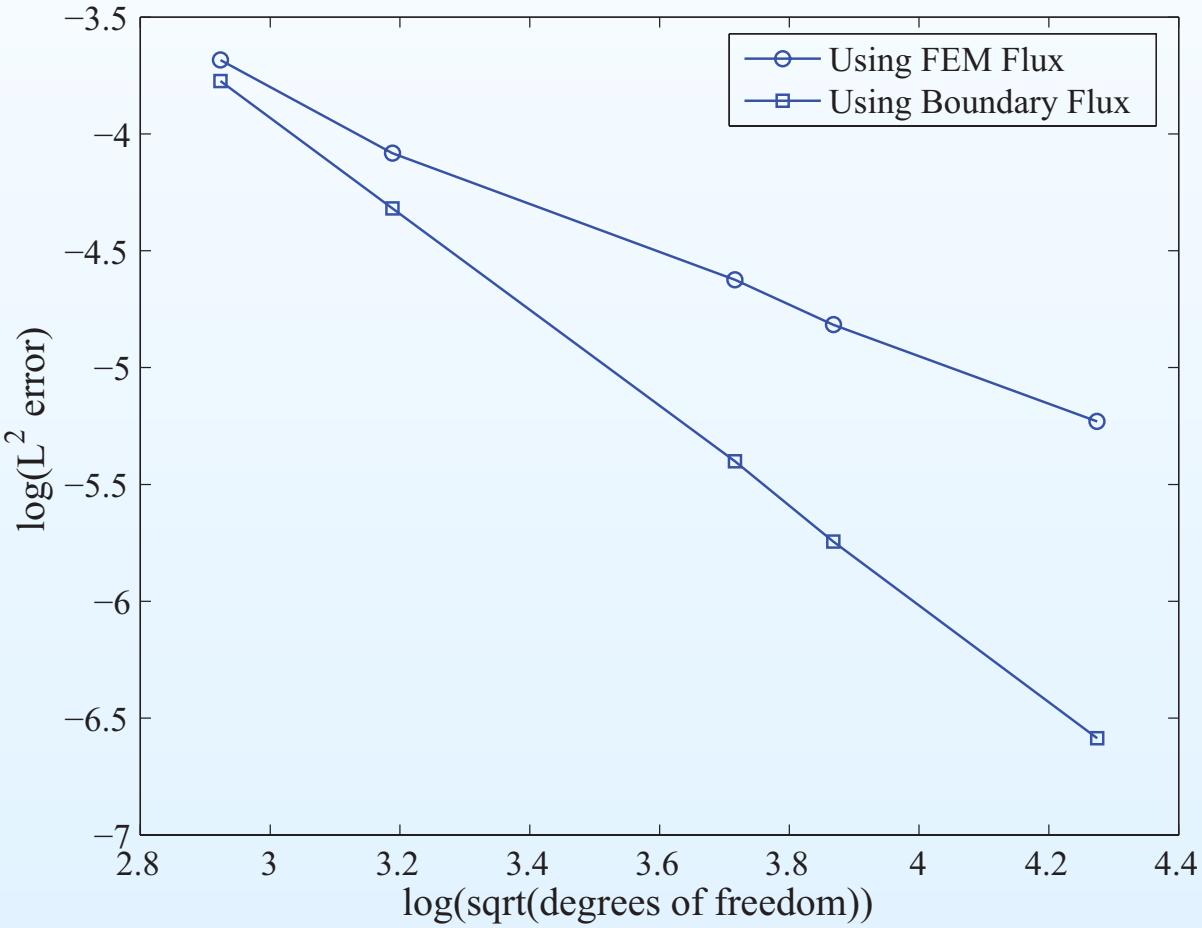


Quantity of interest is the temperature at a small region in the center of the cylinder

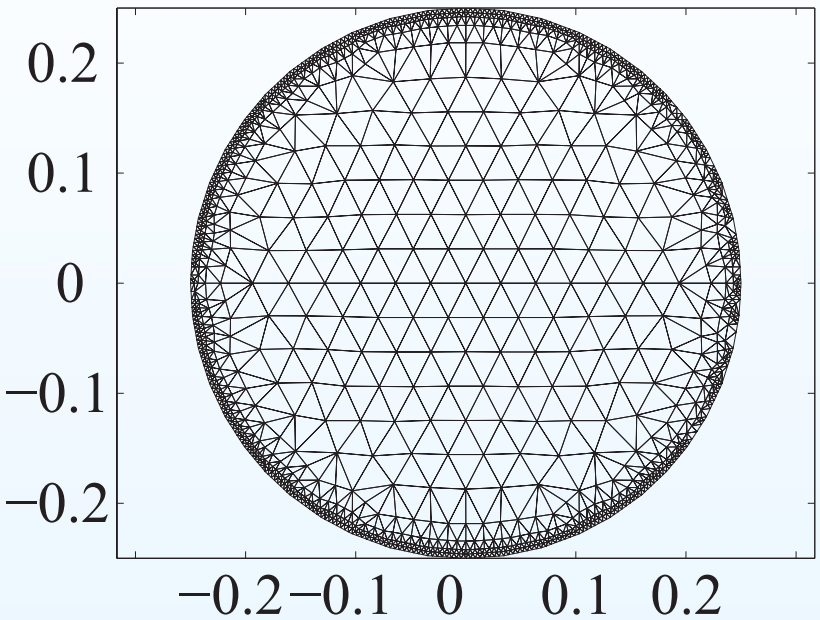
No flux correction is applied

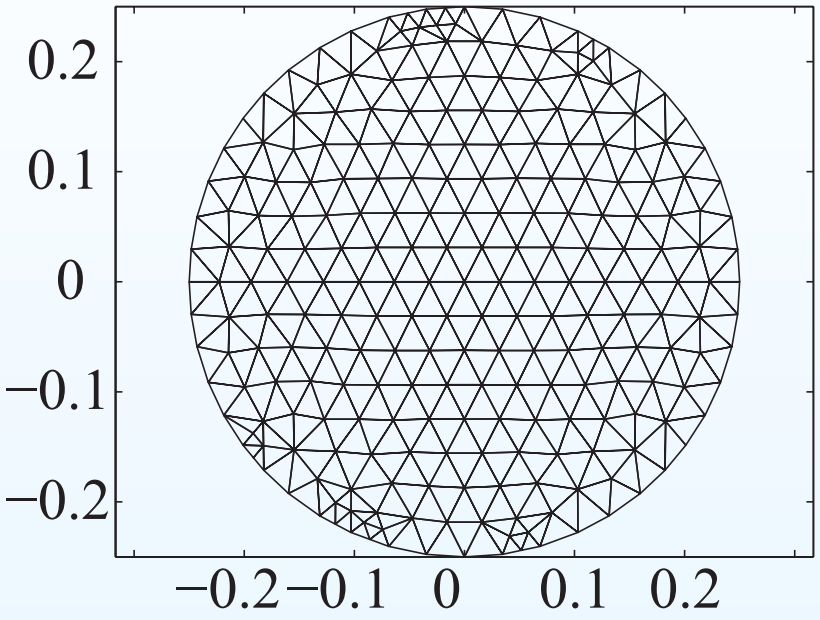
Conjugate Heat Transfer Between a Fluid and a Solid

Using the inexpensive boundary flux correction regains second order accuracy



Conjugate Heat Transfer Between a Fluid and a Solid





Quantity of interest is the temperature at a small region in the center of the cylinder

Flux correction is applied for the computation on the right

Conclusion

Related Work

We have analyzed other MOD schemes, e.g.

- Fully coupled elliptic systems
- Multiscale time integration methods

We note that adjoint problems are useful for other computations, e.g.

- Optimization
- Fast methods for nonparametric density estimation
- Inverse problems

Summary

We have developed a powerful analysis framework for *a posteriori* analysis of multiscale operator decomposition methods

It accounts for various sources of error:

- The solution of each component
- Information that is passed between components
- Incomplete iteration
- Differences between the adjoints to the original problem and a multiscale operator decomposition discretization

The analysis typically involves solving auxiliary adjoint problems as a way of quantifying the effect on stability

Additional work is required to obtain computable estimates