A Posteriori *error estimation and adaptivity for coupled physics problems*

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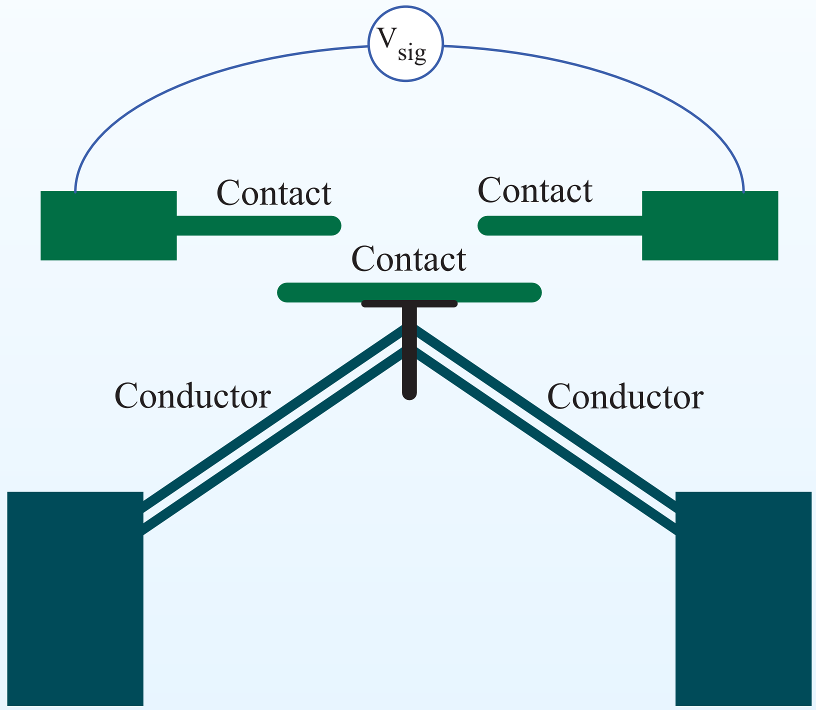

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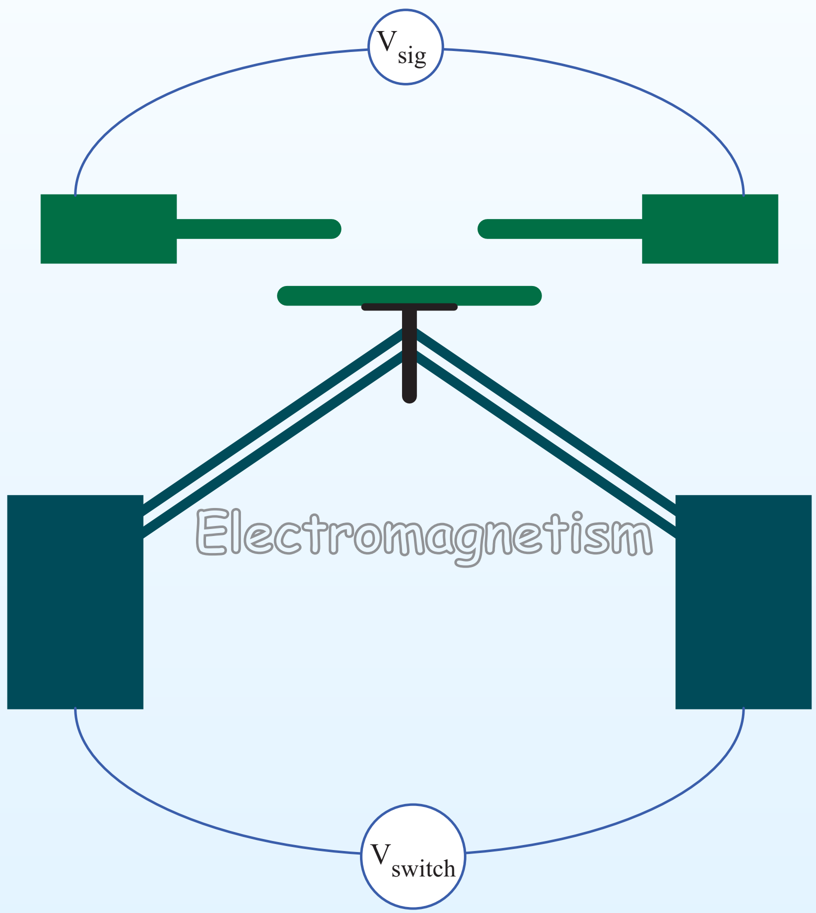

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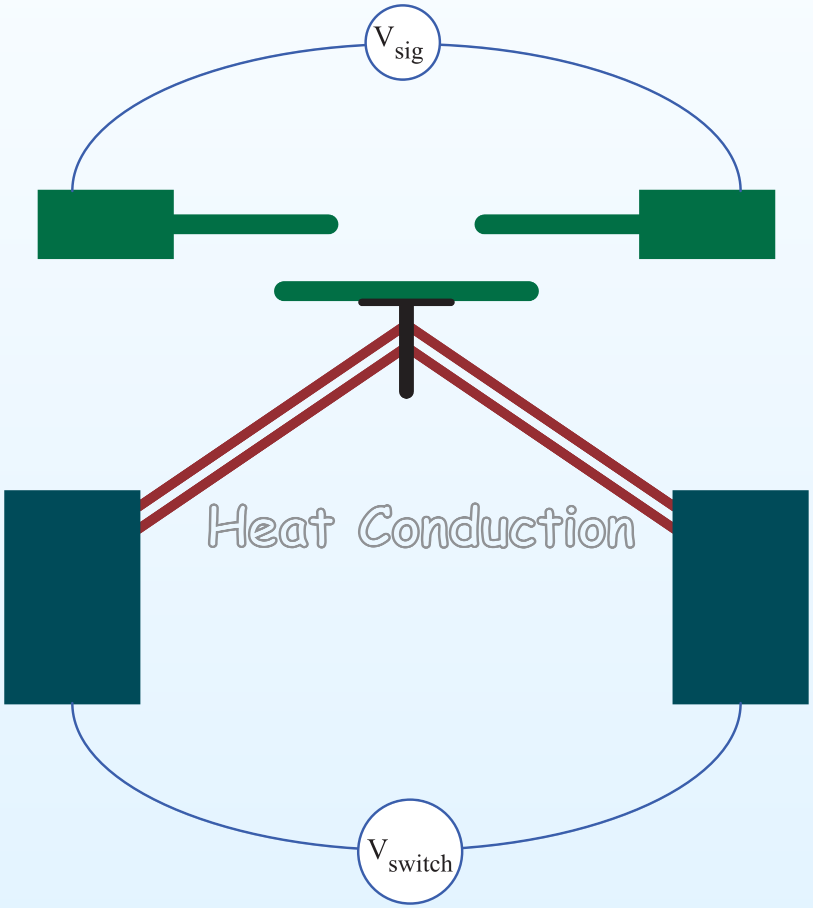

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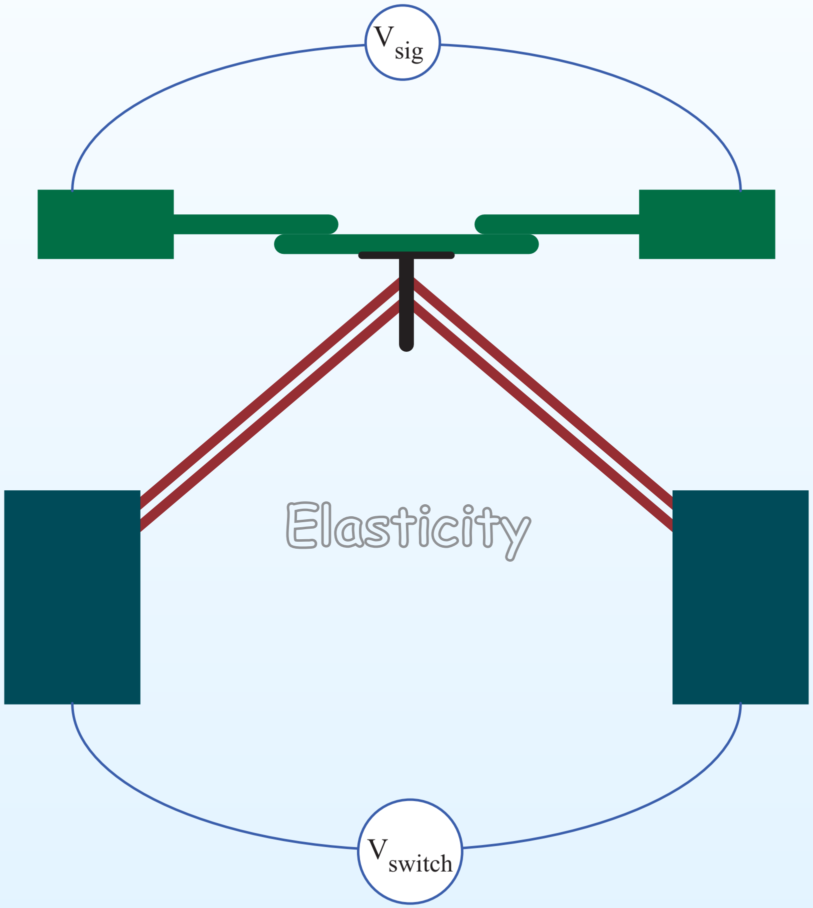


Coupling in the Thermal Actuator

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

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

Steady-state energy transport equation (Joule heating)

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

Steady-state momentum equations (linear elasticity)

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

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

In an operator decomposition approach, the problem is decomposed into three components, each of which is solved with a code specialized to the physics.

Philosophy and Goals

We wish to estimate the error in the solution of a multi-physics problem of the form

$$\mathcal{F}_1(x, u_1, Du_1, \ldots, u_n, Du_n) = 0\,,$$
$$\vdots$$
$$\mathcal{F}_n(x, u_1, Du_1, \ldots, u_n, Du_n) = 0\,,$$

and use this estimate to drive spatial adaptivity.

- We assume that a discretization of the entire system is infeasible.
- We want to solve only "single physics " problems and employ single physics residuals.
- Can we estimate the error due to the transfer of information?
- Can we estimate the effect of transferring information between representations on different discretizations?

Model Problem (one way coupling)

$$
\begin{aligned}
&-\nabla\cdot a_1\nabla u_1 + \mathbf{b}_1\cdot\nabla u_1 + c_1 u_1 = f_1, && u_1 = 0 \ \text{ on } \ \partial\Omega_1\\
&-\nabla\cdot a_2\nabla u_2 + \mathbf{b}_2\cdot\nabla u_2 + c_2 u_2 = f_2(x, u_1, Du_1), && u_2 = 0 \ \text{ on } \ \partial\Omega_2
\end{aligned}
$$

where a_i, b_i, c_i, f_i are smooth functions on bounded domains Ω_i in $\mathbb{R}^N$ where $\mathrm{meas}(\Omega_1 \bigcap \Omega_2) \neq 0$.

The particular example we will study is $\Omega_1 = \Omega_2 = \Omega$, and

$$
\begin{aligned}
-\Delta u_1 &= \sin(4\pi x)\sin(\pi y), && u_1 = 0 \ \text{ on } \partial\Omega\\
-\Delta u_2 &= \mathbf{b}\cdot\nabla u_1, && u_2 = 0 \text{ on } \partial\Omega
\end{aligned}
$$

where

$$
\mathbf{b} = \frac{2}{\pi}\begin{bmatrix} 25\sin(4\pi x) \\ \sin(\pi x) \end{bmatrix}.
$$

Quick Overview of A Posteriori *Error Analysis*

A Posteriori Analysis for a Linear Algebra Problem

Let U be an approximate solution of

$$\mathbf{A}u = b.$$

We seek to compute a quantity of interest given by a linear functional

$$(\psi, u).$$

The error

$$e = u - U$$

is not computable, but we can compute the residual R,

$$R = b - \mathbf{A}U.$$

A Posteriori Analysis for a Linear Algebra Problem

The adjoint problem for the generalized Green's vector is

$$\mathbf{A}^\top \phi = \psi.$$

Variational analysis gives the error representation

$$|(\psi, u) - (\psi, U)| = |(\psi, e)| = \left|(\mathbf{A}^\top \phi, e)\right| = \left|(\phi, \mathbf{A}e)\right| = |(\phi, R)|\,.$$

In the following bound

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

the stability factor $\|\phi\|$ is akin to a condition number.

To compute the estimate we solve for ϕ numerically.

A Posteriori Analysis for an Elliptic Problem

Let U be a Galerkin finite element approximation for

$$-\nabla \cdot a\nabla u + b \cdot \nabla u + cu = f \quad \text{on } \Omega.$$

The residual in weak form is

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

The adjoint problem for the generalized Green's function is

$$(a\nabla \phi, \nabla v) + (\mathrm{div}(b\phi), v) + (c\phi, v) = (\psi, v) \qquad \text{for all test functions } v.$$

The error representation is

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

where π_h is a projection into the space of U.

Operator Decomposition for a Linear Algebra Problem

Linear Algebraic Exposition

Consider an example from linear algebra which we use to motivate our later analysis of coupling error in the PDE system.

Let

$$\mathbf{A}u = \begin{pmatrix} \mathbf{A}_{11} & 0 \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

with approximate (numerical) solution U, where

$$U = \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} \approx \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = u.$$

We wish to estimate a linear functional of the error $e = u - U$.

Basic Problem

The block (lower) triangular structure of A yields

$$\mathbf{A}_{11} u_1 = b_1 \ ,$$

$$\mathbf{A}_{22} u_2 = b_2 - \mathbf{A}_{21} u_1 \ .$$

The corresponding residual for u_2 is

$$\mathcal{R}_2 = (b_2 - \mathbf{A}_{21} U_1) - \mathbf{A}_{22} U_2.$$

The residual of the numerical approximation U_2 involves U_1 rather than u_1, which is reasonable since U_2 is computed using U_1, not u_1.

Adjoint-Based Error Analysis

We wish to estimate the error in some quantity of interest based on u_2 only given by $(\psi_2^{(1)}, u_2)$.

Let $\phi^{(1)} = \begin{pmatrix} \phi_1^{(1)} \\ \phi_2^{(1)} \end{pmatrix}$ be the adjoint solution for data $\psi^{(1)} = \begin{pmatrix} 0 \\ \psi_2^{(1)} \end{pmatrix}$.

The global system is

$$\begin{pmatrix} 0 & 0 & \mathbf{A}_{11}^\top & \mathbf{A}_{21}^\top \\ 0 & 0 & 0 & \mathbf{A}_{22}^\top \\ \mathbf{A}_{11} & 0 & 0 & 0 \\ \mathbf{A}_{21} & \mathbf{A}_{22} & 0 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \phi_1^{(1)} \\ \phi_2^{(1)} \end{pmatrix} = \begin{pmatrix} 0 \\ \psi_2^{(1)} \\ b_1 \\ b_2 \end{pmatrix}.$$

Error Representation Formula

Solving the adjoint problem, the block (upper) triangular structure of $A^\top$ yields

$$\mathbf{A}_{22}^\top \phi_2^{(1)} = \psi_2^{(1)} \,,$$
$$\mathbf{A}_{11}^\top \phi_1^{(1)} + \mathbf{A}_{21}^\top \phi_2^{(1)} = 0 \Rightarrow \mathbf{A}_{11}^\top \phi_1^{(1)} = -\mathbf{A}_{21}^\top \phi_2^{(1)} \,.$$

The quantity of interest

$$\begin{aligned}
(\psi^{(1)}, e) &= (\psi_2^{(1)}, e_2) = (\mathbf{A}_{22}^\top \phi_2^{(1)}, e_2) \\
&= (\phi_2^{(1)}, \mathbf{A}_{22} u_2) - (\phi_2^{(1)}, \mathbf{A}_{22} U_2) \\
&= (\phi_2^{(1)}, b_2 - \mathbf{A}_{21} u_1) - (\phi_2^{(1)}, \mathbf{A}_{22} U_2) \\
&= (\phi_2^{(1)}, b_2 - \mathbf{A}_{21} U_1 - \mathbf{A}_{22} U_2) - (\phi_2^{(1)}, \mathbf{A}_{21}(u_1 - U_1)) \\
&= (\phi_2^{(1)}, \mathcal{R}_2) + (\phi_2^{(1)}, -\mathbf{A}_{21} e_1) \text{ where } e_i = u_i - U_i.
\end{aligned}$$

The blue term is computable, involving a weighted residual. The red term is the transfer error which is not immediately computable.

(Note that $\phi_1^{(1)}$ does not appear in the error representation formula!)

Secondary Adjoint Problem

We need to estimate the transfer error

$$(\phi_2^{(1)}, -\mathbf{A}_{21}e_1) = (-\mathbf{A}_{21}^\top \phi_2^{(1)}, e_1).$$

Observe that the transfer error is a linear functional of the error e_1 corresponding to adjoint data

$$\psi^{(2)} = \begin{pmatrix} \psi_1^{(2)} \\ 0 \end{pmatrix} = \begin{pmatrix} -\mathbf{A}_{21}^\top \phi_2^{(1)} \\ 0 \end{pmatrix}.$$

Solving the (block upper triangular) adjoint system with data $\psi^{(2)}$

$$\begin{aligned} \mathbf{A}_{22}^\top \phi_2^{(2)} &= 0 && \Rightarrow \phi_2^{(2)} = 0, \\ \mathbf{A}_{11}^\top \phi_1^{(2)} + \mathbf{A}_{21}^\top \phi_2^{(2)} &= \psi_1^{(2)} && \Rightarrow \mathbf{A}_{11}^\top \phi_1^{(2)} = \psi_1^{(2)} = -\mathbf{A}_{21}^\top \phi_2^{(1)}. \end{aligned}$$

Transfer Error

Hence

$$
\begin{aligned}
(\psi^{(2)}, e) = (\psi_1^{(2)}, e_1) \quad &= (-\mathbf{A}_{21}^\top \phi_2^{(1)}, e_1) \\
&= (\mathbf{A}_{11}^\top \phi_1^{(2)}, e_1) \\
&= (\phi_1^{(2)}, \mathbf{A}_{11} e_1) \\
&= (\phi_1^{(2)}, b_1 - \mathbf{A}_{11} U_1) \\
&= (\phi_1^{(2)}, \mathcal{R}_1)\,.
\end{aligned}
$$

The complete error representation is

$$
(\psi^{(1)}, e) = (\phi_2^{(1)}, \mathcal{R}_2) + (\phi_1^{(2)}, \mathcal{R}_1)\ ,
$$

which is a sum of weighted “single physics” residuals.

Operator Decomposition in the Model Elliptic System

PDE revisited

We now repeat this analysis for our PDE system

$$
\begin{aligned}
-\nabla \cdot a_1 \nabla u_1 + \mathbf{b}_1 \cdot \nabla u_1 + c_1 u_1 &= f_1, \quad u_1 = 0 \text{ on } \partial\Omega_1 \\
-\nabla \cdot a_2 \nabla u_2 + \mathbf{b}_2 \cdot \nabla u_2 + c_2 u_2 &= f_2(x, u_1, Du_1), \quad u_2 = 0 \text{ on } \partial\Omega_2
\end{aligned}
$$

Ω_i is a bounded domain in $\mathbb{R}^N$ and $\mathrm{meas}(\Omega_1 \bigcap \Omega_2) \neq 0$.

Weak Form

$$
\begin{aligned}
A_1(u_1, v_1) &= (a_1 \nabla u_1, \nabla v_1) + (\mathbf{b}_1 \cdot \nabla u_1, v_1) + (c_1 u_1, v_1) \\
&= (f_1, v_1) \ \forall v_1 \in \tilde{W}_2^1(\Omega_1), \\
A_2(u_2, v_2) &= (a_2 \nabla u_2, \nabla v_2) + (\mathbf{b}_2 \cdot \nabla u_2, v_2) + (c_2 u_2, v_2) \\
&= (f_2(x, u_1, Du_1), v_2) \ \forall v_2 \in \tilde{W}_2^1(\Omega_2).
\end{aligned}
$$

where $\tilde{W}_2^1(\Omega_i)$ is the subspace of $W_2^1(\Omega_i)$ with zero trace on $\partial\Omega_i$.

Adjoint Error Analysis

We wish to measure the error in a quantity of interest that only depends on u_2, thus $\psi^{(1)}$ for the adjoint problem can be written as $(0 \quad \psi_2^{(1)})^\top$.

Defining

$$\begin{aligned}
A_1^*(\phi_1, v_1) &= (a_1 \nabla \phi_1, \nabla v_1) - (\nabla \cdot (\mathbf{b}_1 \phi_1), v_1) + (c_1 \phi_1, v_1)\,, \\
A_2^*(\phi_2, v_2) &= (a_2 \nabla \phi_2, \nabla v_2) - (\nabla \cdot (\mathbf{b}_2 \phi_2), v_2) + (c_2 \phi_2, v_2)\,,
\end{aligned}$$

the adjoint equations are

$$\begin{aligned}
A_1^*(\phi_1^{(1)}, v_1) + (Lf_2(u_1)\phi_2^{(1)}, v_1) = 0 \; \forall v_1 \in \tilde{W}_2^1(\Omega_1) \\
A_2^*(\phi_2^{(1)}, v_2) = (\psi_2^{(1)}, v_2) \; \forall v_2 \in \tilde{W}_2^1(\Omega_2)\,.
\end{aligned}$$

The linearization term $Lf_2(u_1)\phi_2^{(1)}$ plays the same role as the upper triangular block $\mathbf{A}_{21}^\top$ in the linear algebraic exposition.

Error Representation Formula

We compute the quantity of interest

$$\begin{aligned}
\left(\psi^{(1)}, e\right) &= \left(\psi_2^{(1)}, e_2\right) \\
&= A_2^*(\phi_2^{(1)}, e_2) \\
&= A_2(e_2, \phi_2^{(1)}) \\
&= \left(f_2(x, u_1, Du_1), \phi_2^{(1)}\right) - A_2(u_{2,h}, \phi_2^{(1)}) \,.
\end{aligned}$$

Note that $\phi_1^{(1)}$ does not appear in the error representation formula, but $f_2(x, u_1, Du_1)$ is uncomputable!

Adding and subtracting $\left(f_2(u_{1,h}), \phi_2^{(1)}\right)$ and using Galerkin orthogonality

Error Representation Formula

$$
\begin{aligned}
\left(\psi^{(1)}, e\right) = {} & \left(f_2(u_1) - f_2(u_{1,h}), \phi_2^{(1)}\right) \\
& + \left(f_2(u_{1,h}), \phi_2^{(1)} - \Pi_h \phi_2^{(1)}\right) - A_2(u_{2,h}, \phi_2^{(1)} - \Pi_h \phi_2^{(1)}) \\
= {} & \left(f_2(u_1) - f_2(u_{1,h}), \phi_2^{(1)}\right) + \left(\mathcal{R}_2, \phi_2^{(1)} - \Pi_h \phi_2^{(1)}\right)
\end{aligned}
$$

- The blue term is a computable error representation for the discretization error in the second component and involves a single physics residual.
- The red term measures the transfer error between the components and is not computable.
- We solve a Secondary Adjoint Problem with quantity of interest $(f_2(u_1) - f_2(u_{1,h}), \phi_2^{(1)})$.

A Secondary Adjoint Problem

Noting that

$$\begin{aligned}\left(f_2(u_1) - f_2(u_{1,h}), \phi_2^{(1)}\right) &\approx \left(Lf_2(u_{1,h})e_1, \phi_2^{(1)}\right)\\ &= \left(Lf_2(u_{1,h})\phi_2^{(1)}, e_1\right)\\ &= \left(\psi^{(2)}, e\right),\end{aligned}$$

we pose a secondary adjoint problem

$$\begin{cases} A_1^*\left(\phi_1^{(2)}, v_1\right) + \left(Lf_2(u_{1,h})\phi_2^{(2)}, v_1\right) = \left(\psi_1^{(2)}, v_1\right) & \forall v_1 \in \tilde{W}_2^1(\Omega_1) \\ A_2^*\left(\phi_2^{(2)}, v_2\right) = 0 & \forall v_2 \in \tilde{W}_2^1(\Omega_2). \end{cases}$$

Since $\phi_2^{(2)} = 0$, this reduces to

$$A_1^*\left(\phi_1^{(2)}, v_1\right) = \left(\psi_1^{(2)}, v_1\right) \quad \forall v_1 \in \tilde{W}_2^1(\Omega_1).$$

Transfer Error Representation Formula

Using Galerkin orthogonality,

$$\begin{aligned}\left(\psi_1^{(2)}, e_1\right) &= A_1^*\left(\phi_1^{(2)}, e_1\right)\\ &= A_1\left(e_1, \phi_1^{(2)}\right)\\ &= \left(f_1, \phi_1^{(2)} - \Pi_h \phi_1^{(2)}\right) - A_1\left(u_{1,h}, \phi_1^{(2)} - \Pi_h \phi_1^{(2)}\right)\\ &= \left(\mathcal{R}_1, \phi_1^{(2)} - \Pi_h \phi_1^{(2)}\right).\end{aligned}$$

The full computable error representation is

$$\left(\psi^{(1)}, e\right) = \left(\mathcal{R}_2, \phi_2^{(1)} - \Pi_h \phi_2^{(1)}\right) + \left(\mathcal{R}_1, \phi_1^{(2)} - \Pi_h \phi_1^{(2)}\right) .$$

Each term on the RHS involves a computable single physics residual.

Example Problem $\Omega_1 = \Omega_2 = \Omega$

$$\begin{aligned} -\Delta u_1 &= \sin(4\pi x)\sin(\pi y), \quad u_1 = 0 \text{ on } \partial\Omega \\ -\Delta u_2 &= \mathbf{b}\cdot\nabla u_1, \quad u_2 = 0 \text{ on } \partial\Omega \quad \text{where} \quad \mathbf{b} = \frac{2}{\pi}\begin{bmatrix} 25\sin(4\pi x) \\ \sin(\pi x) \end{bmatrix}. \end{aligned}$$

The corresponding adjoint problem is

$$\begin{aligned} -\Delta\phi_1^{(1)} + Lf_2(u_1)\phi_2^{(1)} &= 0, \qquad \phi_1^{(1)} = 0 \text{ on } \partial\Omega \\ -\Delta\phi_2^{(1)} &= \delta_{\text{reg}}^x, \quad \phi_2^{(1)} = 0 \text{ on } \partial\Omega\,. \end{aligned}$$

The secondary adjoint problem is

$$\Delta\phi_1^{(2)} = \nabla\cdot(\mathbf{b}\phi_2^{(1)}), \quad \phi_1^{(2)} = 0 \text{ on } \partial\Omega\,.$$

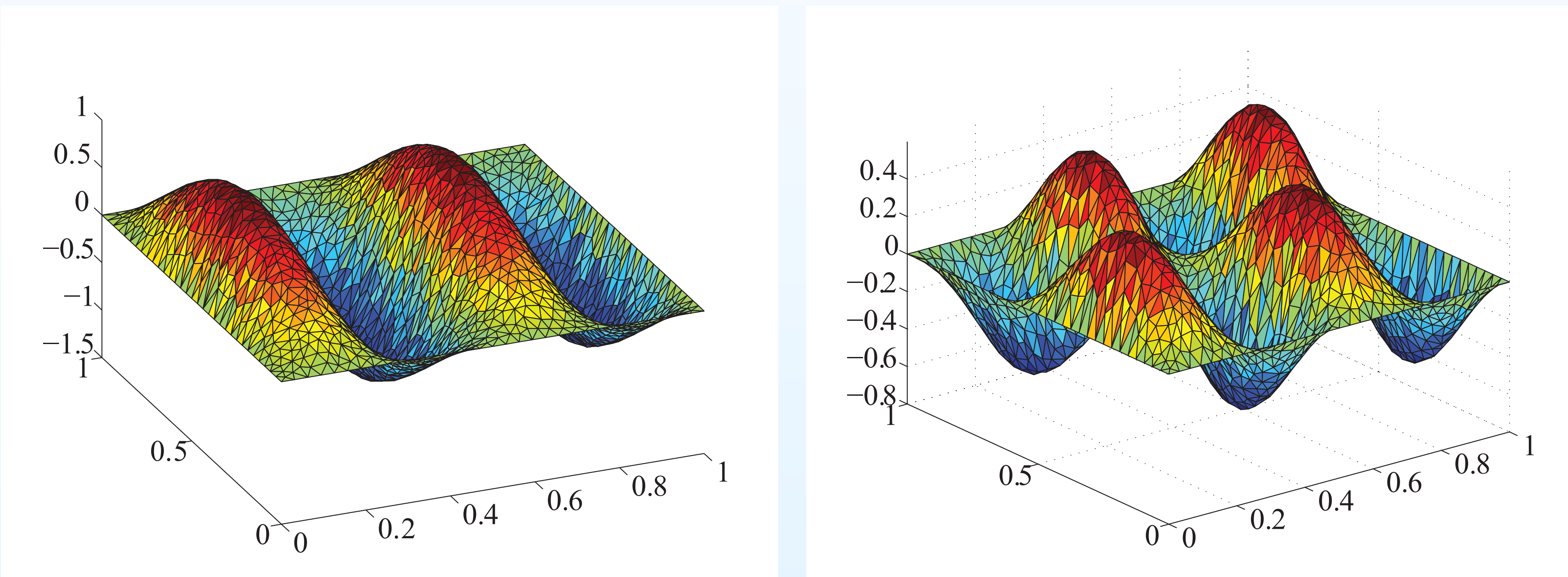
In the examples, linear elements were used to solve the forward problem, quadratic elements to solve the dual problem.

One way coupling example #1: First Computation

We use uniformly fine meshes for both components.

For the error in $u(.25, .25)$,

primary $\approx .0042$ transfer $\approx .0006$



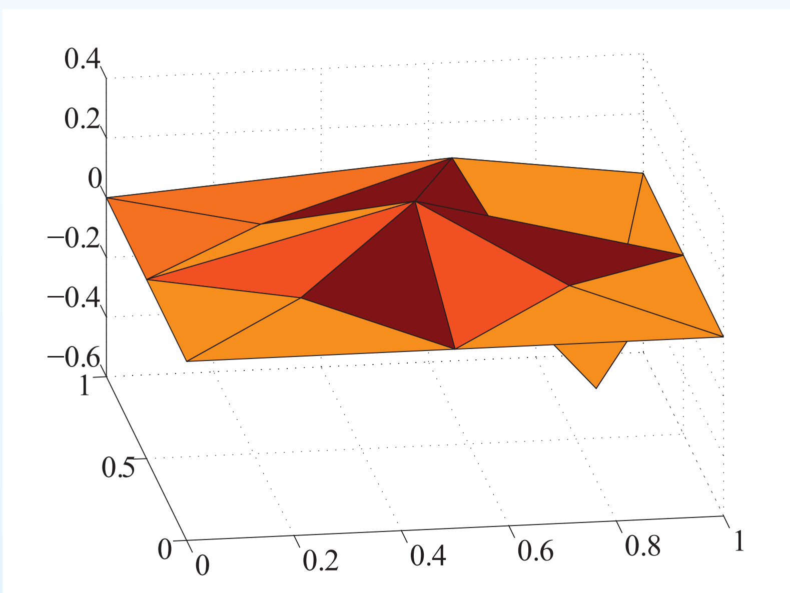
Solutions of components 1 and 2

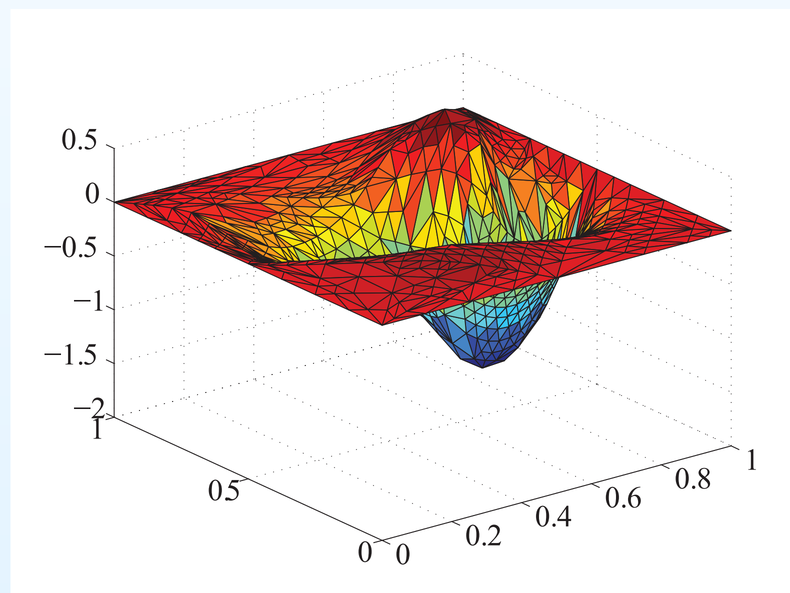
One way coupling example #1: Second Computation

Starting with coarse meshes, we adapt the mesh only for the second component to reduce the primary error while ignoring the transfer error.

For the average error,

primary error $\approx .0001$ transfer error $\approx .2244$



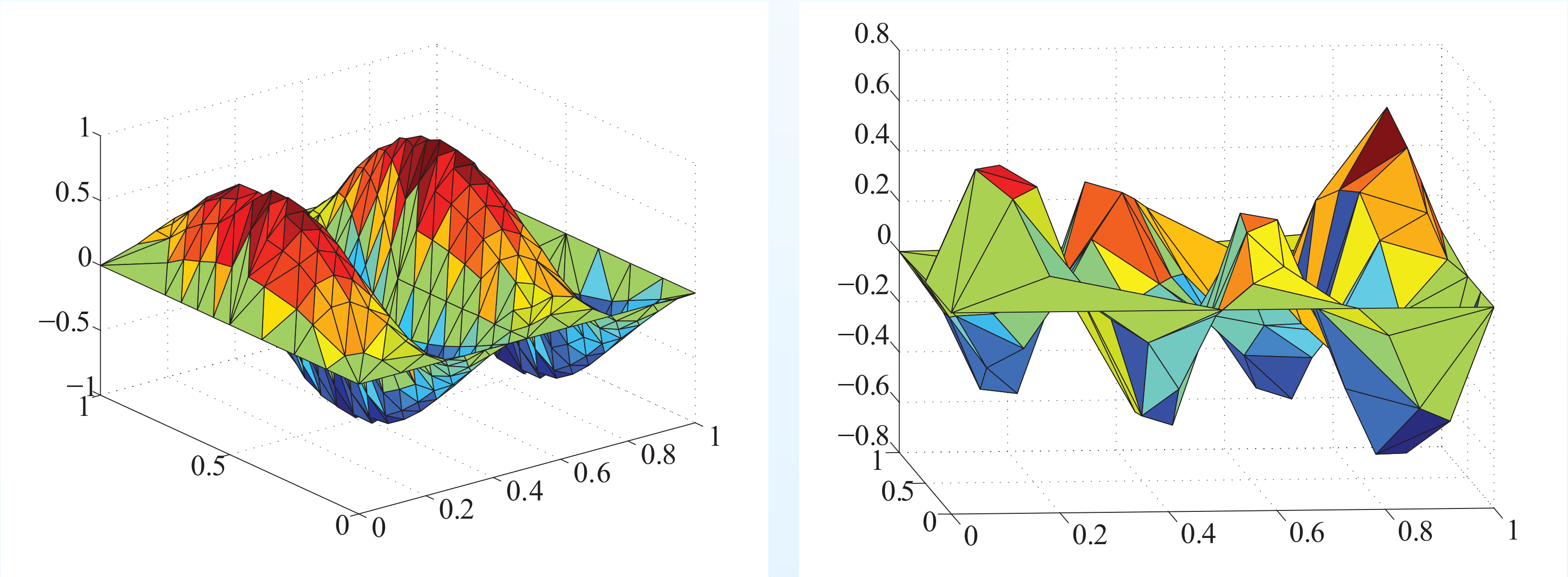


U_1 and U_2 following refinement based on discretization error of U_2 only

One way coupling example #1: Third Computation

We adapt the meshes for both components using the primary error representation for $u_{2,h}$ and the secondary representation for $u_{1,h}$ respectively.

Transferring the gradient $\nabla u_{1,h}$ leads to increased sensitivity to errors.



Final refined solutions for components 1 and 2

Further considerations

- Due to time limitations I will skip consideration of projection errors...
- Projection errors should not be trivialized however, since they can dominate the error.
- The blockwise adaptive method that will be discussed later was conceived in part as an attempt to minimize projection errors in time dependent problems.

Cardiac modeling

In its simplest form, a mathematical model of the whole heart involves

1. electrical activity
2. mechanical activity
3. coupling between soft tissue mechanics and the electrical activity.

These processes occur on widely differing length scales and timescales, challenging any single discretization technique.

Electrical activity

An adapted version of the Fitzhugh-Nagumo equations.

$$\begin{aligned}
\frac{\partial V}{\partial t} &= \nabla\cdot\left(D\nabla V\right) - \kappa V\left(V-a\right)\left(V-1\right) - rV + I_s, \\
\frac{\partial r}{\partial t} &= \left(\gamma + \frac{\eta_1 r}{\eta_2 + V}\right)\left(-r - \kappa V\left(V-b-1\right)\right), \\
\frac{\partial T_a}{\partial t} &= \varepsilon\left(V\right)\left(k_{T_a} V - T_a\right),
\end{aligned}$$

where

$$\varepsilon\left(V\right) = \frac{\varepsilon_0}{2}\left(11 - 9\tanh\left(\alpha\left(V - V_*\right)\right)\right).$$

Mechanical activity

Assuming,

1. inertial terms are negligible, so tissue deformation can be solved at a quasi-steady state
2. T_a acts only along tissue fibres
3. gravity can be neglected.

We begin with linear elasticity (nonlinear elasticity coming soon)

$$\nabla \cdot \boldsymbol{\sigma} = \hat{\mathbf{F}} T_a,$$

where $\hat{\mathbf{F}}$ is a vector giving the direction of the cardiac fibres, and

$$\sigma_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \delta_{ij} \frac{\partial u_k}{\partial x_k}, \qquad i, j = 1, 2,$$

where $\mathbf{u}$ is the displacement, λ and μ are the Lamé constants.

Construction of the adjoint system

Consider the simplified system

$$
\begin{aligned}
\dot{u}_1(t) + \mathbf{A}_{11} u_1(t) &= b_1 && t \in (0, T] \\
u_1(0) &= u_{1,0} \\
\mathbf{A}_{21} u_1(t) + \mathbf{A}_{22} u_2(t) &= b_2 && t \in (0, T]
\end{aligned}
$$

The residual at a particular time t_j is

$$R_2(t_j) = b_2 - \mathbf{A}_{21} U_1(t_j) - \mathbf{A}_{22} U_2(t_j),$$

and the coupling error at time t_j is

$$(\psi_2^{(1)}, e_2(t_j)) = \Big(R_2(t_j), \phi_2^{(1)}(t_j)\Big) + \Big(e_1(t_j), -\mathbf{A}_{21}^\top \phi_2^{(1)}(t_j)\Big) .$$

Construction of the adjoint system

The calculation of $e_1(t_j)$ requires the solution of an adjoint equation backwards in time

$$-\dot{\phi}_1(t) + \mathbf{A}_{11}^{\top}\phi_1(t) = 0 \qquad t \in [t_j, 0)$$

$$\phi_1(t_j) = -\mathbf{A}_{21}^{\top}\phi_2^{(1)}(t_j)$$

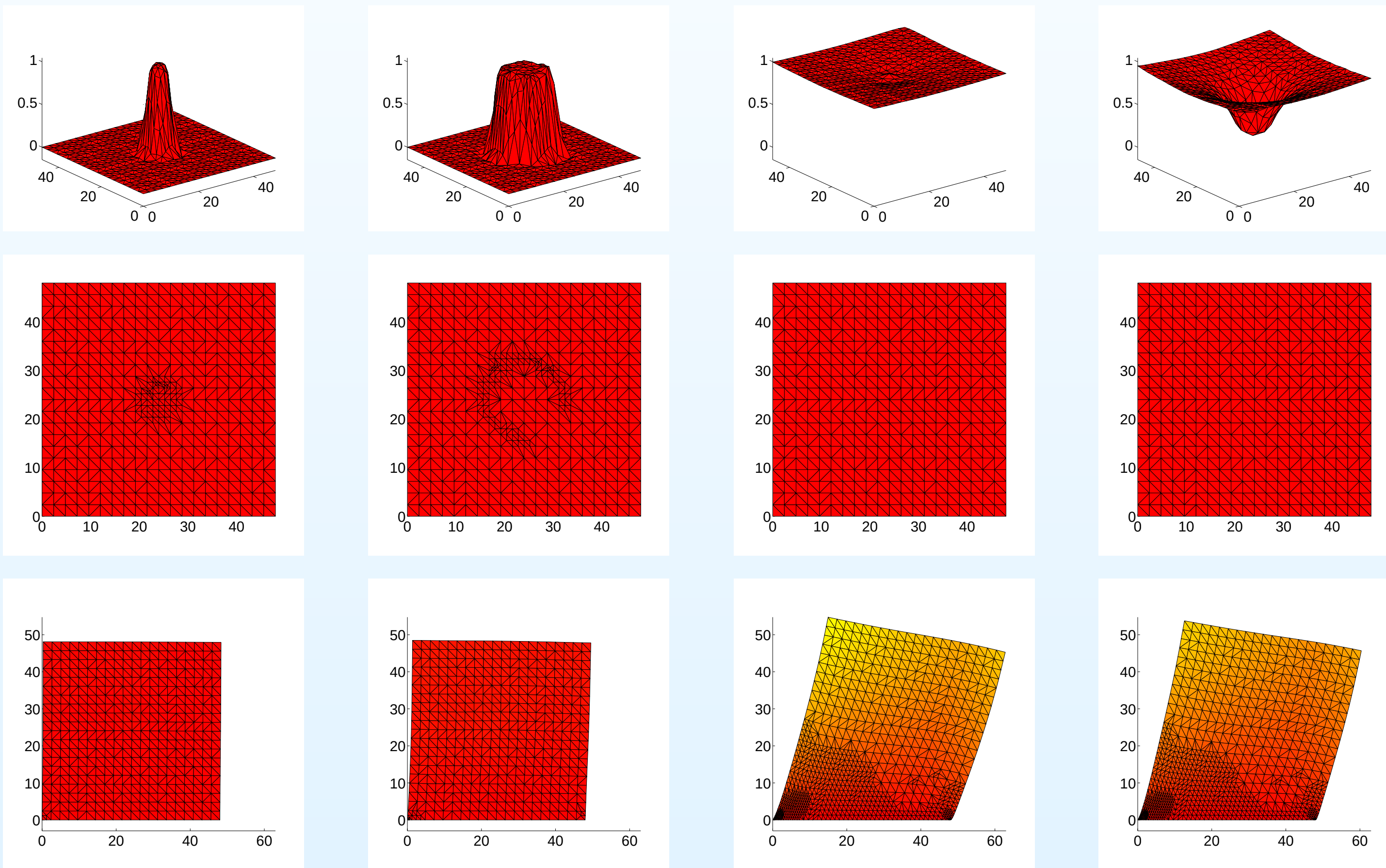
We took some “liberties” with the construction and solution of this adjoint problem.

Effectively we ignored the accumulation of error over time and considered the time integration over the current time step only. The effect of these quite severe approximations are under consideration.

One-way coupling in the heart

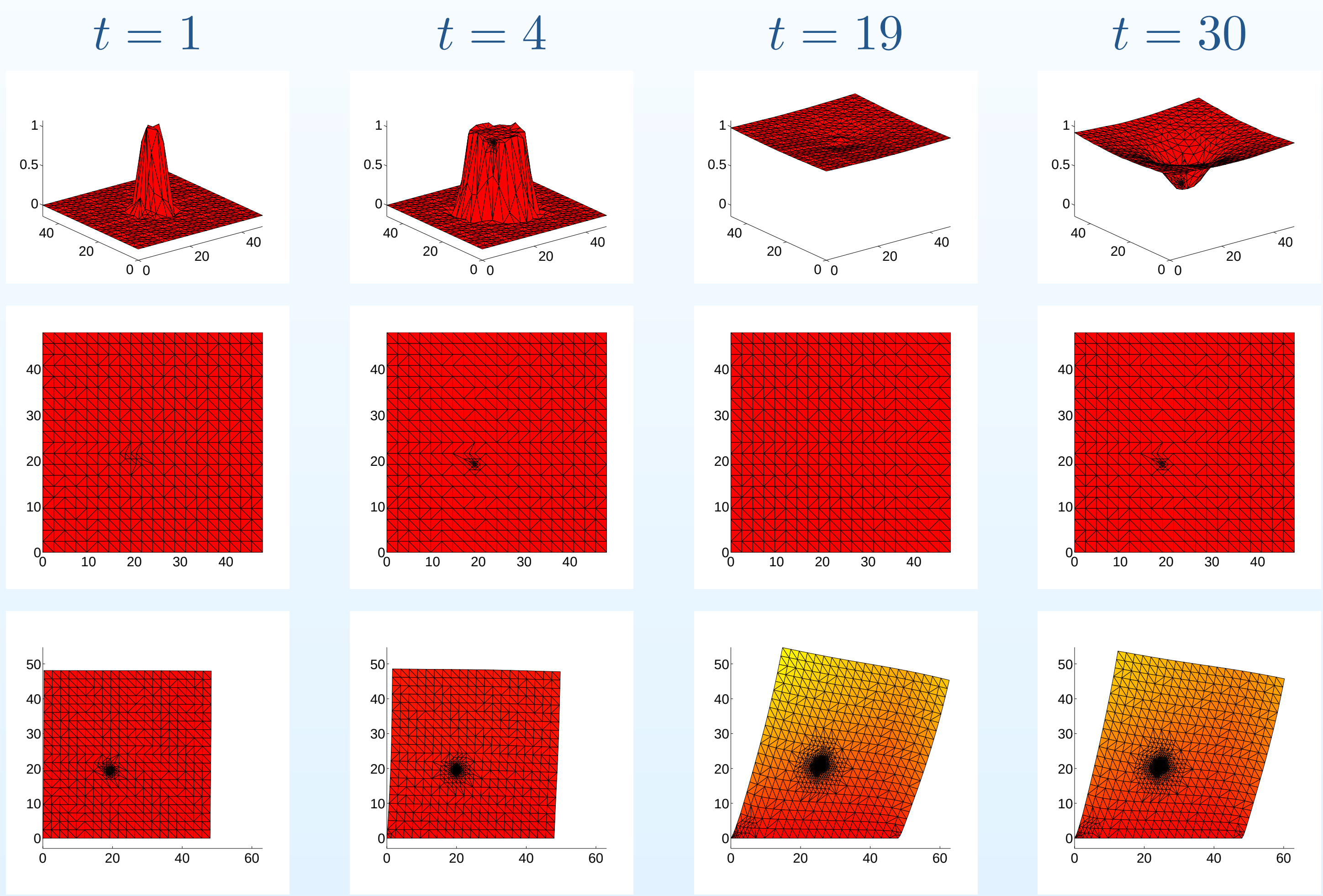
(top row) Transmembrane potential; (middle row) Mesh for electrophysiology; (bottom row) deformation; for a QoI equal to the average displacement.

$t = 1$ $\quad$ $t = 4$ $\quad$ $t = 19$ $\quad$ $t = 30$



One-way coupling in the heart

(top row) Transmembrane potential; (middle row) Mesh for electrophysiology; bottom row) deformation; for a QoI equal to the displacement at $(19.3, 19.3)$.



Two-way coupling

Coupled Systems

Consider an example from linear algebra. (The subsequent analysis of a fully coupled PDE system is the subject of another talk.)

Let

$$\mathbf{A}u = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

with approximate (numerical) solution U, where

$$U = \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} \approx \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = u.$$

Estimate a linear functional of the error $e = u - U$ assuming that $\mathbf{A}_{11}$ and $\mathbf{A}_{22}$ are nonsingular.

Coupled Systems

Assume the coupled system is solved via an "operator decomposition" by decomposing $\mathbf{A} = \mathbf{D} + \mathbf{C}$, where $\mathbf{D}$ is invertible, i.e.,

$$\mathbf{D} = \begin{pmatrix} \mathbf{A}_{11} & 0 \\ 0 & \mathbf{A}_{22} \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} 0 & \mathbf{A}_{12} \\ \mathbf{A}_{21} & 0 \end{pmatrix}.$$

The (Jacobi) solution procedure is to start with

$$(\mathbf{D} + \mathbf{C})u = b \Rightarrow \mathbf{D}u = b - \mathbf{C}u\,,$$

and then solve

$$\begin{cases} u^{(0)} = 0, \\ \mathbf{D}u^{(i)} = b - \mathbf{C}u^{(i-1)}, \quad i \geq 1. \end{cases}$$

The convergence depends on the spectral radius of $\mathbf{D}^{-1}\mathbf{C}$.

Coupled Systems (iteration vs discretization error)

We wish to estimate a linear functional of $e^{(i)} = u - U^{(i)}$. Note that

$$(u - U^{(i)}, \psi) = (u - u^{(i)}, \psi) + (u^{(i)} - U^{(i)}, \psi),$$

where

- $u - u^{(i)}$ is the theoretical iteration error which we assume approaches zero, i.e., we assume that the iteration converges,
- $u^{(i)} - U^{(i)}$ is the numerical error in solving the i^{th} step of the iterative procedure.

A similar argument to the previous one, yields

$$(x^{(i)} - X^{(i)}, \psi) = \sum_{j=1}^{i} (b - \mathbf{C}X^{(j-1)} - \mathbf{D}X^{(j)}, \phi^{(j)}).$$

Fully coupled elliptic system

Consider a two component fully coupled system of the form

$$\begin{cases} -\nabla \cdot a_1 \nabla u_1 + b_1 \cdot \nabla u_1 + c_1 u_1 = f_1(x, u_2, Du_2) \\ -\nabla \cdot a_2 \nabla u_2 + b_2 \cdot \nabla u_2 + c_2 u_2 = f_2(x, u_1, Du_1) \end{cases} \tag{1}$$

for $x \in \Omega$ with $u_1 = u_2 = 0 \text{ on } \partial\Omega$.

Non-iteration error for block Gauss-Seidel iteration

$$
\begin{aligned}
(\psi_2^{[1]}, e_2^{\{i\}}) &= \sum_{j=1}^{i} \mathcal{R}_2(U_2^{\{i-j+1\}}, \phi_2^{[j]}; U_1^{\{i-j+1\}}) \\
&+ \sum_{j=1}^{i} \mathcal{R}_1(U_1^{\{i-j+1\}}, \phi_1^{[j]}; U_2^{\{i-j\}})
\end{aligned} \tag{2}
$$

where $\phi^{[j]}$ satisfies

$$
\begin{cases}
\mathcal{A}_2^*(\phi_2^{[j]}, \chi) = (\psi_2^{[j]}, \chi), \\
\mathcal{A}_1^*(\phi_1^{[j]}, \chi) = (\psi_1^{[j]}, \chi),
\end{cases} \tag{3}
$$

with $\psi^{[j]}$ is defined recursively by

$$
\begin{cases}
(\psi_2^{[j]}, \chi) = (Df_1(U^{\{i-j\}})\chi, \phi_1^{[j-1]}), \\
(\psi_1^{[j]}, \chi) = (Df_2(U^{\{i-j+1\}})\chi, \phi_2^{[j]}),
\end{cases} \tag{4}
$$

and $\psi_2^{[1]}$ is a predetermined quantity of interest.

Fully coupled elliptic system

Consider the two-dimensional linearly-coupled elliptic system

$$\begin{cases} -\nabla \cdot (\alpha \nabla u_1) + b_1 \cdot \nabla u_1 = 85\pi^2(2\sin 4\pi x \sin \pi y + u_2) \\ -\Delta u_2 = b_2 \cdot \nabla u_1 \end{cases}, u_1 = u_2 = 0 \in \partial\Omega, \tag{5}$$

where

$$\begin{cases} \alpha = 10 + \pi^2(\frac{5}{13}\cos 4\pi x + \frac{1}{2}\cos \pi y) \\ b_1 = \frac{1}{\pi}\begin{bmatrix} \frac{8}{13}\sin 4\pi x & \frac{1}{2}\sin \pi y \end{bmatrix}^\top \\ b_2 = \frac{1}{\pi}\begin{bmatrix} \frac{1}{2}\sin 4\pi x & 2\sin \pi y \end{bmatrix}^\top. \end{cases}$$

This system has the exact solution

$$\begin{cases} u_1 = \sin 4\pi x \sin \pi y \\ u_2 = \pi^{-2}(\sin 8\pi x \sin \pi y/65 + \sin 4\pi x \sin 2\pi y/20). \end{cases}$$

Our quantity of interest is $u_2(x_0)$ where $x_0 = (0.15, 0.15)$.

Fully coupled elliptic system

Upon convergence of the Gauss-Seidel iteration we computed the four leading terms of the error representation formula. These were

(i) the "primary" error $\mathcal{R}_2(U_2^{\{n\}}, \Phi_2^{[1]}; U_1^{\{n\}})$,

(ii) the "transfer" error $\mathcal{R}_1(U_1^{\{n\}}, \Phi_1^{[1]}; U_2^{\{n-1\}})$,

(iii) the "inherited" error $\mathcal{R}_2(U_2^{\{n-1\}}, \Phi_2^{[2]}; U_1^{\{n-1\}})$, and

(iv) the "inherited transfer" error, $\mathcal{R}_1(U_1^{\{n-1\}}, \Phi_1^{[2]}; U_2^{\{n-2\}})$.

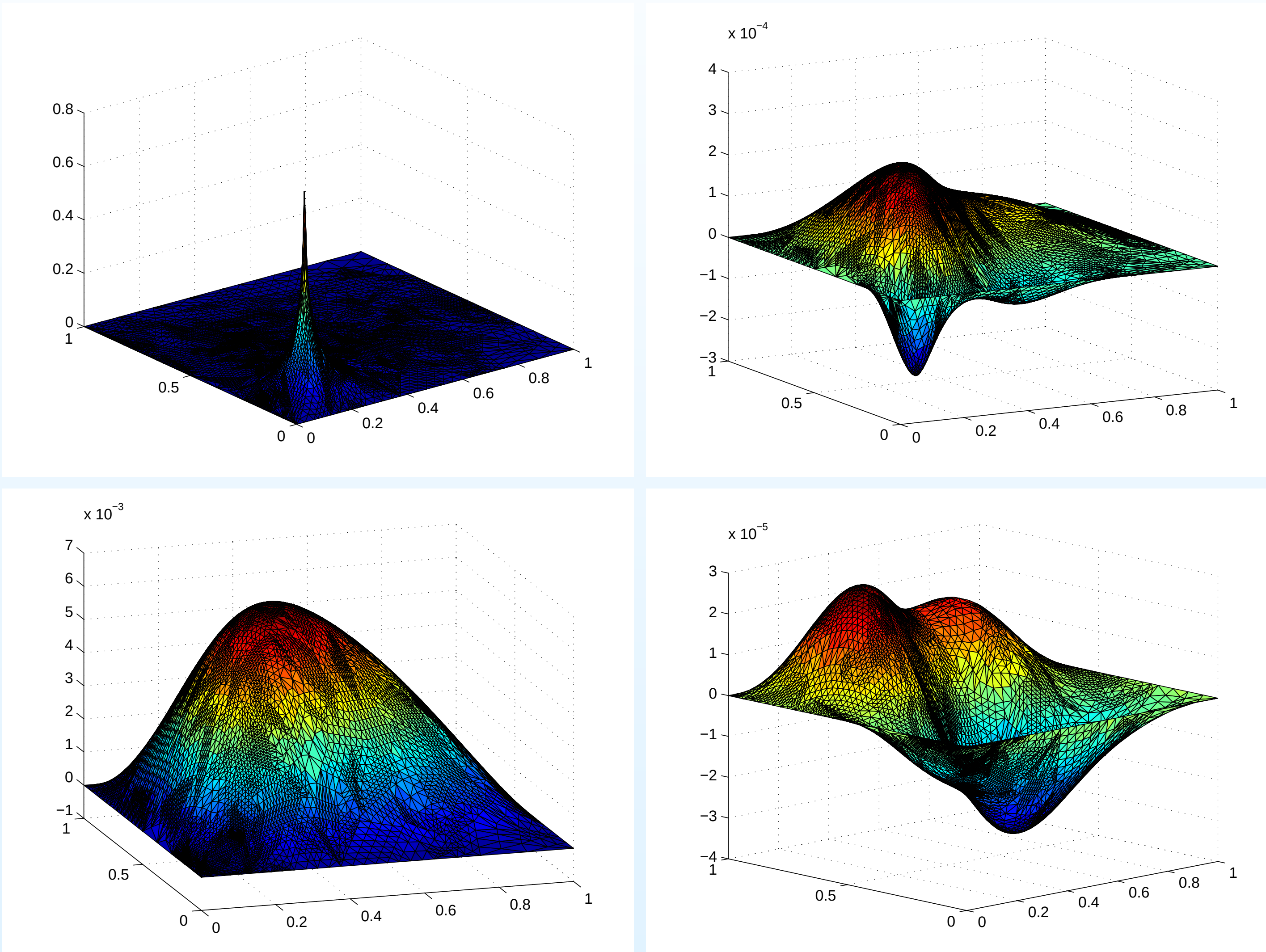
The adjoint problems used to compute these weighted residuals were

$$\begin{cases} A_2^*(\phi_2^{[1]}, \chi) = (\delta_{x_0}^{reg}, \chi) \\ A_1^*(\phi_1^{[1]}, \chi) = (-\mathrm{div}(b_2 \phi_2^{[1]}), \chi) \\ A_2^*(\phi_2^{[2]}, \chi) = (-\mathrm{div}(b_1 \phi_1^{[2]}), \chi) \\ A_1^*(\phi_1^{[2]}, \chi) = (-\mathrm{div}(b_2 \phi_2^{[2]}), \chi) \end{cases} \qquad \forall \chi \in \mathcal{S}_2^h(\Omega),$$

Piecewise linear elements for $U^{[i]}$, piecewise quadratics for $\Phi^{[i]}$.

Fully coupled elliptic system

Primary, transfer, inherited and inherited transfer errors respectively.



Fully coupled elliptic system

Primary error $\mathcal{R}_2(U_2^{\{n\}}, \Phi_2^{[1]}; U_1^{\{n\}})$	Transfer error $\mathcal{R}_1(U_1^{\{n\}}, \Phi_1^{[1]}; U_2^{\{n-1\}})$
0.5070×10^{-4}	0.0940×10^{-4}
Inherited error $\mathcal{R}_2(U_2^{\{n-1\}}, \Phi_2^{[2]}; U_1^{\{n-1\}})$	**Inherited transfer error** $\mathcal{R}_1(U_1^{\{n-1\}}, \Phi_1^{[2]}; U_2^{\{n-2\}})$
-0.0010×10^{-4}	0.0409×10^{-4}

Remarks

- Gauss-Seidel iteration leads to both *within iteration* (transfer) error and *between iteration* error.
- If the iteration corresponds to a coupled nonlinear PDE system, the matrices $\mathbf{D}$ and $\mathbf{C}$ will vary from iterate to iterate. The i^{th} error estimate requires the solution of i different adjoint problems.
- Each adjoint problem is computable, but their number is significant, which suggests that higher order iteration methods requiring fewer iterations (e.g. Newton iteration) are strongly preferred.

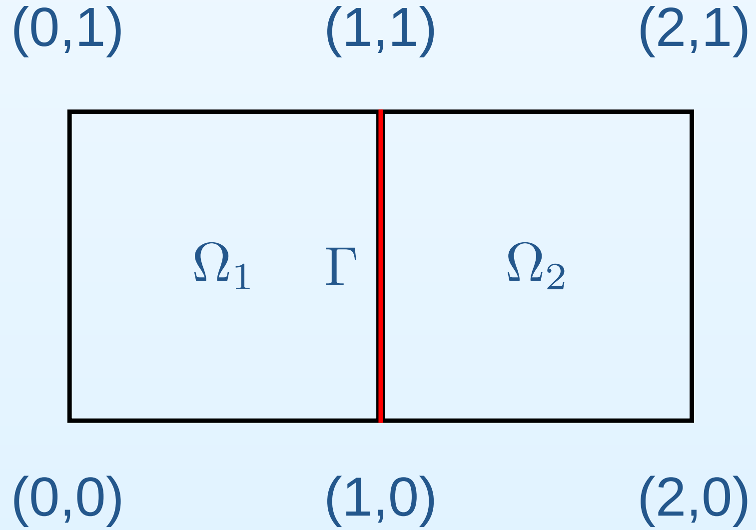
Coupling across a common interface

Operator Decomposition via a common interface

Consider the elliptic interface problem

$$\begin{cases} -\nabla \cdot (\nabla u_1) = f_1, & x \in \Omega_1 \\ \begin{cases} u_1 = u_2, \\ \boldsymbol{n} \cdot \nabla u_1 = \boldsymbol{n} \cdot \nabla u_2, \end{cases} & x \in \Gamma \\ -\nabla \cdot (\nabla u_2) = f_2, & x \in \Omega_2 \end{cases}$$

where $\Omega_1 = [0,1] \times [0,1]$ and $\Omega_2 = [1,2] \times [0,1]$.



A coupled parabolic problem

Consider a “monolithic” approach to the following coupled elliptic problem which uses a Lagrange multiplier construction to impose the continuity conditions along the common interface.

$$
\begin{aligned}
\dot{u}_i + \mathcal{L}_i u_i &= f_i && (x,t) \in \Omega_i \times (0,T],\ i=1,2 \\
u_i(x,0) &= u_{i,0}(x) && (x,t) \in \Omega_i \times \{0\},\ i=1,2 \\
u_i &= 0 && (x,t) \in \partial\Omega_i \backslash \Gamma \times (0,T],\ i=1,2 \\
u_1 &= u_2 && (x,t) \in \Gamma \times (0,T] \\
\lambda = k_1 \frac{\partial u_1}{\partial n} &= -k_2 \frac{\partial u_2}{\partial n} && (x,t) \in \Gamma \times (0,T]
\end{aligned}
\qquad (6)
$$

where

$\mathcal{L}_i u_i = -\nabla \cdot (k_i \nabla u_i) + c_i u_i, \quad k_i \geq k_{i,0} > 0$ and c_i, f_i sufficiently smooth.

A coupled parabolic problem

We define the bilinear form

$$a_i(u_i, v_i) = \int_{\Omega_i} \big(k_i \nabla u_i \nabla v_i + c_i u_i v_i\big) \,\mathrm{d}\Omega_i. \tag{7}$$

We partition $[0, T]$ as

$$0 = t_0 < t_1 < \cdots < t_n < \ldots t_N = T \tag{8}$$

and let

$$I_n = (t_{n-1}, t_n], \quad S_{i,n} = \Omega_i \times I_n, \quad \text{and} \quad \Gamma_n = \Gamma \times I_n.$$

A coupled parabolic problem

For

$$H^1_D(\Omega_i) = \{v : v \in H^1(\Omega_i) | v = 0 \text{ on } \partial\Omega_i \backslash \Gamma\}$$

we define

$$X^q_{i,n} = \{w(x,t) : w(x,t) = \sum_{j=0}^{q} t^j v_j(x), v_j \in V_i, (x,t) \in S_{i,n}\},$$

$$\text{for } i = 1, 2,\ n = 1, \dots, N,\ \text{where } V_i \subset H^1_D(\Omega_i)$$

and

$$Y^q_{i,n} = \{w(x,t) : w(x,t) = \sum_{j=0}^{q} t^j v_j(x), v_j \in W, (x,t) \in \Gamma_n\},$$

$$\text{for } n = 1, \dots, N,\ \text{where } W \subset H^{-1/2}(\Gamma).$$

Discontinuous Galerkin

Given $u_i(0)$, $i = 1, 2$ find $u_i \in X^q_{i,n}$, $i = 1, 2$, $\lambda \in Y^q_n$ such that

$$\int_{I_n} \big((\dot{u}_i, v_i)_{\Omega_i} + a_i(u_i, v_i)\big)\, \mathrm{d}t + \big([u_i]_{n-1}, v_i^+\big)_{\Omega_i} \mp \int_{I_n} \langle \lambda, v_i \rangle_\Gamma \, \mathrm{d}t$$
$$= \int_{I_n} (f_i, v_i)_{\Omega_i} \, \mathrm{d}t \; \forall v_i \in X^q_{i,n} \quad \text{for } n = 1, 2, \ldots, N, \; i = 1, 2,$$

$$\int_{I_n} \langle \nu, u_2 - u_1 \rangle_\Gamma \, \mathrm{d}t = 0 \; \forall \nu \in Y^q_n \quad \text{for } n = 1, 2, \ldots, N.$$

The adjoint problem

The adjoint problem is

$$
\begin{aligned}
-\dot{\phi}_i + \mathcal{L}_i^* u_i &= \psi_i & (x,t) &\in \Omega_i \times [0,T),\ i = 1,2 \\
\phi_i(x,T) &= 0 & (x,t) &\in \Omega_i \times \{T\},\ i = 1,2 \\
\phi_i &= 0 & (x,t) &\in \partial\Omega_i \backslash \Gamma \times [0,T),\ i = 1,2 \\
\phi_1 &= \phi_2 & (x,t) &\in \Gamma \times [0,T) \\
\mu = k_1 \frac{\partial \phi_1}{\partial n} &= -k_2 \frac{\partial \phi_2}{\partial n} & (x,t) &\in \Gamma \times [0,T)
\end{aligned}
$$

where for this self-adjoint problem $\mathcal{L}_i^* = \mathcal{L}_i,\ i = 1,2$.

Error representation formula

Summing over n and defining

$$
\begin{aligned}
(R_i, \phi_i) \quad &= \quad \sum_{n=1}^{N} \int_{I_n} \Big((f_i, \phi_i)_{\Omega_i} - (\dot{u}_i^h, \phi_i)_{\Omega_i} - a_i(u_i^h, \phi_i) - \left(\left[u_i^h \right]_{t_{n-1}}, \phi_i(t_{n-1}) \right)_{\Omega_i} \\
&\qquad \pm \langle \lambda^h, \phi_i \rangle_\Gamma \Big) \, \mathrm{d}t \\
\langle \mu, R_\lambda \rangle \quad &= \quad \sum_{n=1}^{N} \int_{I_n} \langle \mu, u_2^h - u_1^h \rangle_\Gamma \, \mathrm{d}t
\end{aligned}
$$

we have

$$
\int_0^T \Big((e_1, \psi_1)_{\Omega_1} + (e_2, \psi_2)_{\Omega_2} - \langle e_\lambda, \psi \rangle_\Gamma \Big) \, \mathrm{d}t = (R_1, \phi_1) + (R_2, \phi_2) + \langle \mu, R_\lambda \rangle.
$$

Studies of *effectivity ratio* for both coupled elliptic and coupled parabolic problems with known exact solutions are conclusive.

Block adaptivity

- IDEA: Employ a sequence of space/time “blocks” consisting of fixed, though non-uniform, space meshes as a way of implementing adaptive algorithms that are truly efficient in a high performance environment.
- By efficiency, we refer not only to accuracy, but also computational costs such as load balancing.
- A block adaptive strategy reduces the number of mesh changes that must be treated and makes the problem of quantifying the effects of mesh changes on accuracy computationally feasible.
- However, a major issue with a block-adaptive approach is determining block discretizations from coarse scale solution information that achieve the desired accuracy and efficiency.

Block adaptivity (examples)

- Coefficients, boundary conditions and right hand side were chosen so that the exact solution was

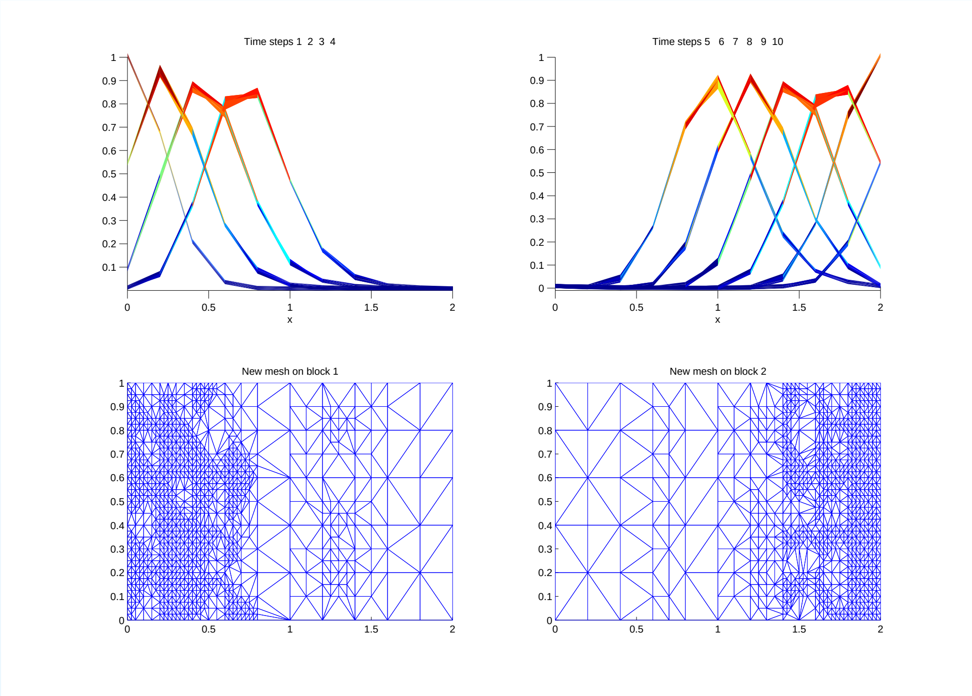
$$u = \exp(-10(x - 10t)^2)$$

  on

$$\Omega(x, y) \times (0, T] = (0, 2) \times (0, 1) \times (0, 0.25]$$

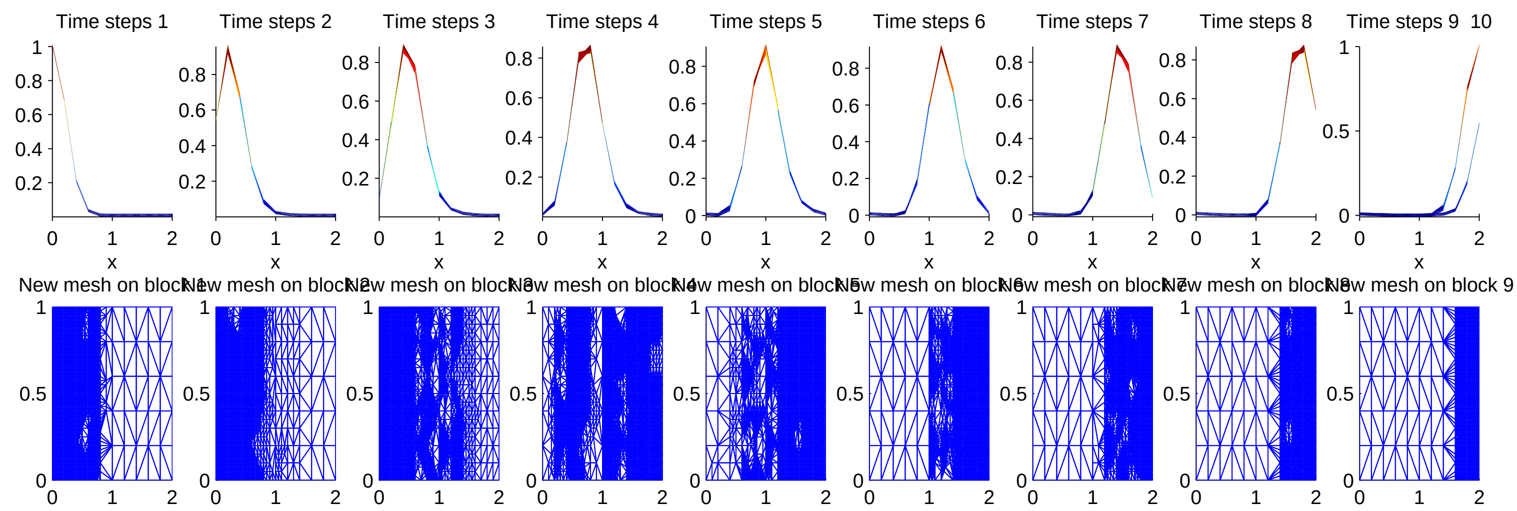
- The coarse forward solution was obtained on an 11×6 element uniform spatial mesh and 10 uniform time steps, using dG(0) in time
- The coarse adjoint problem was solved on a 44×24 element uniform spatial mesh and 10 uniform time steps, using dG(1) in time
- The maximum number of refinements allowed for an original element was three

Block adaptivity : Example # 1



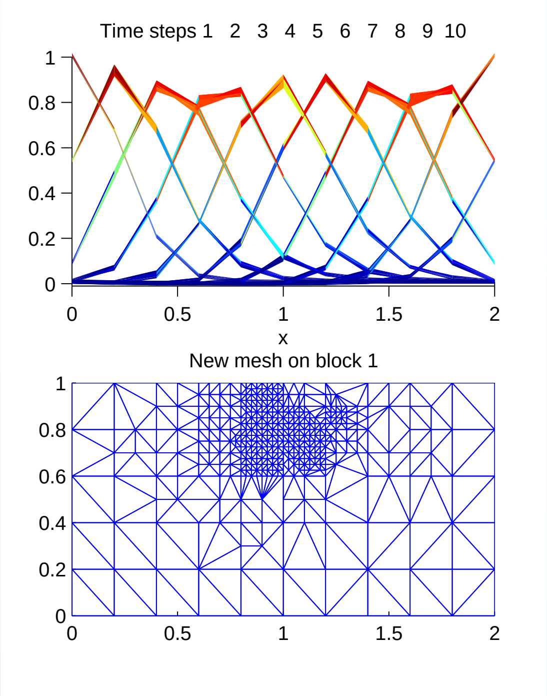
- QoI = average error in the whole domain (average in time, too)
- Global tolerance TOL = 1e-2, NMAX = 200
- Estimated error was reduced from $\approx 10^{-4}$ to $\approx 10^{-5}$

Block adaptivity: Example # 2



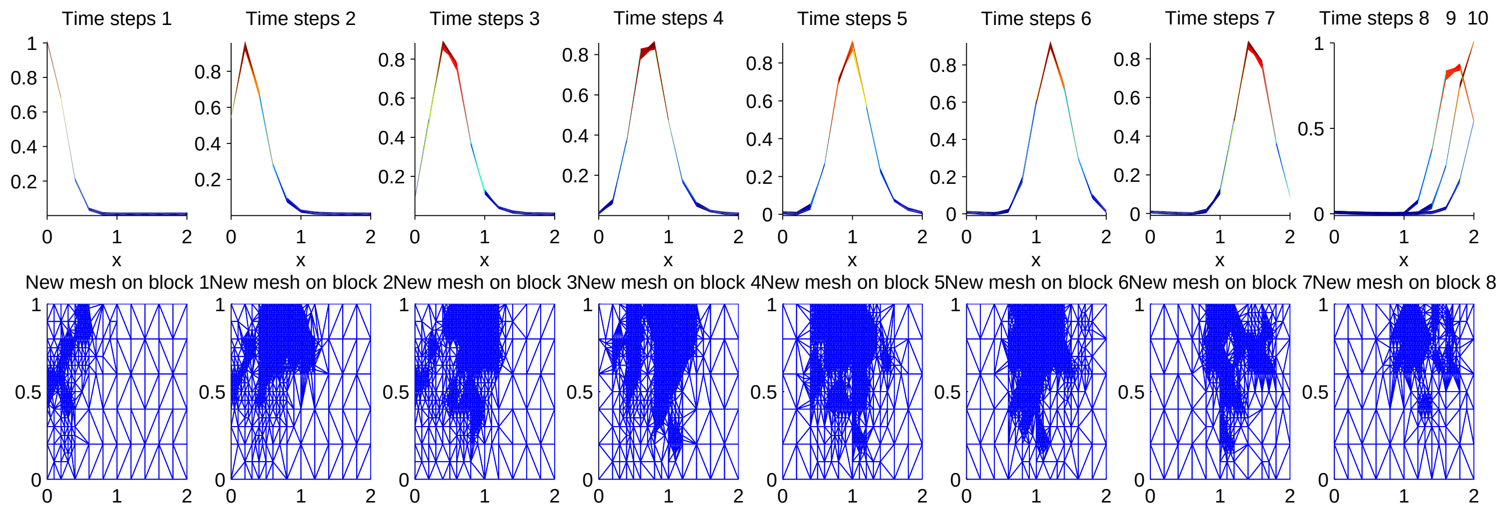
- QoI = average error in the whole domain (average in time, too)
- Global tolerance TOL = 10^{-3}, NMAX = 200
- Estimated error was reduced from $\approx 10^{-4}$ to $\approx 10^{-6}$

Block adaptivity: Example # 3



- QoI = λ over the [0.8,1] segment of the interface
- Global tolerance TOL = 10^{-1}, NMAX = 500
- The error was reduced to $\approx 10^{-4}$

Block adaptivity: Example # 4



- QoI = λ over the [0.8,1] segment of the interface
- Global tolerance TOL = 10^{-2}, NMAX = 500
- The error was reduced to $\approx 10^{-5}$

Mixed parabolic and elliptic systems

Again consider a “monolithic” approach to the following coupled parabolic and elliptic problem.

$$
\begin{aligned}
\dot{u}_1 + \mathcal{L}_1 u_1 &= f_1 & (x,t) &\in \Omega_1 \times (0,T] \\
u_1(x,0) &= u_{1,0}(x) & (x,t) &\in \Omega_1 \times \{0\} \\
u_1 &= 0 & (x,t) &\in \partial\Omega_1 \backslash \Gamma \times (0,T] \\
\mathcal{L}_2 u_2 &= f_2 & (x,t) &\in \Omega_2 \times (0,T] \\
u_2 &= 0 & (x,t) &\in \partial\Omega_2 \backslash \Gamma \times (0,T] \\
u_1 &= u_2 & (x,t) &\in \Gamma \times (0,T] \\
\lambda = k_1 \frac{\partial u_1}{\partial n} &= -k_2 \frac{\partial u_2}{\partial n} & (x,t) &\in \Gamma \times (0,T]
\end{aligned}
$$

where

$\mathcal{L}_i u_i = -\nabla \cdot (k_i \nabla u_i) + c_i u_i \quad k_i \geq k_{i,0} > 0$ and c_i, f_i sufficiently smooth.

Error representation formula

Substituting e_1, e_2 and e_λ as test functions in the weak form of the adjoint problem and proceeding as above, after defining

$$
\begin{aligned}
(R_1, \phi_1) &= \sum_{n=1}^{N} \int_{I_n} \Big((f_1, \phi_1)_{\Omega_1} - (\dot{u}_1^h, \phi_1)_{\Omega_1} - a_1(u_1^h, \phi_1) - \left(\left[u_1^h \right]_{t_{n-1}}, \phi_1(t_{n-1}) \right)_{\Omega_1} \\
&\qquad + \langle \lambda^h, \phi_i \rangle_\Gamma \Big) \, \mathrm{d}t, \\
(R_2, \phi_2) &= \sum_{n=1}^{N} \int_{I_n} \Big((f_2, \phi_2)_{\Omega_2} - a_2(u_2^h, \phi_2) - \langle \lambda^h, \phi_2 \rangle_\Gamma \Big) \, \mathrm{d}t, \\
\langle \mu, R_\lambda \rangle &= \sum_{n=1}^{N} \int_{I_n} \langle \mu, u_2^h - u_1^h \rangle_\Gamma \, \mathrm{d}t,
\end{aligned}
$$

we again have

$$
\int_0^T \Big((e_1, \psi_1)_{\Omega_1} + (e_2, \psi_2)_{\Omega_2} - \langle e_\lambda, \psi \rangle_\Gamma \Big) \, \mathrm{d}t = (R_1, \phi_1) + (R_1, \phi_1) + \langle \mu, R_\lambda \rangle.
$$

Fluid structure interaction problems

$$
\begin{aligned}
\rho\dot{v} + \nabla\cdot\sigma_{\text{fluid}} &= f_{\text{fluid}} && (x,t)\in\Omega_{\text{fluid}}\times(0,T] \\
\nabla\cdot v &= 0 && (x,t)\in\Omega_{\text{fluid}}\times(0,T] \\
v(x,0) &= v_0 && (x,t)\in\Omega_{\text{fluid}}\times\{0\} \\
v &= g_{\text{fluid}}^D && (x,t)\in\partial\Omega_{\text{fluid}}^D\times(0,T] \\
\sigma_{\text{fluid}}\cdot n &= g_{\text{fluid}}^N && (x,t)\in\partial\Omega_{\text{fluid}}^N\times(0,T] \\
\sigma_{\text{fluid}}\cdot n &= -\sigma_{\text{solid}}\cdot n && (x,t)\in\Gamma\times(0,T] \\
v &= \dot{u} && (x,t)\in\Gamma\times(0,T] \\
-\nabla\cdot\sigma_{\text{solid}} &= f_{\text{solid}} && (x,t)\in\Omega_{\text{solid}}\times(0,T] \\
\nabla\cdot u &= 0 && (x,t)\in\Omega_{\text{solid}}\times(0,T] \\
u(x,0) &= u_0 && (x,t)\in\Omega_{\text{solid}}\times\{0\} \\
u &= g_{\text{solid}}^D && (x,t)\in\partial\Omega_{\text{solid}}^D\times(0,T] \\
\sigma_{\text{solid}}\cdot n &= g_{\text{solid}}^N && (x,t)\in\partial\Omega_{\text{solid}}^N\times(0,T].
\end{aligned}
$$

Conclusions

- *A posteriori* error analyses can be developed for a range of coupled physics problems and provides impressive results on model problems
- For sophisticated models, the construction and solution of the adjoint systems can be challenging and may require some additional form of approximation
- Coarse forward and adjoint solutions can be used to develop effective block adaptive strategies for time-dependent problems
- Even with large teams, software development remains challenging