# Scalable Solution Methods via Optimal Control Reformulations

SAND2008-4280C

**Denis Ridzal**
Optimization and UQ
dridzal@sandia.gov

Pavel Bochev
Applied Math and Applications
pbboche@sandia.gov

Sandia National Laboratories, Albuquerque, NM, USA

July 2, 2008

**ECCOMAS 2008**

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94-AL85000.

# Outline

- Solution of Multi-Physics/Operator Problems: Diagnosis and Goal
- Our Optimization Approach and Related Work
- An Optimization-Based Solver for Advection-Dominated PDEs
- Numerical Results
- Summary

# Solution of Multiphysics Problems

## Diagnosis

- Predictive simulation of complex physical systems requires simultaneous component models with radically different mathematical properties.
- Incompatibility in the discrete numerical representation of individual physics operators remains the main challenge.

→ True for: single-domain/multiple-physics (e.g. advection-diffusion, MHD)
*and* multiple-domain/multiple-physics (e.g. porous flow, FSI)

- Two key aspects

(1) development of physics-coupling mechanisms (e.g. mortar methods)
(2) development of specialized solvers for algebraic systems (e.g. JFNK)

have been largely viewed as separate, disjoint thrust areas.

## Goal

- Unifying, mathematically rigorous approach to robust solution of multiphysics problems, based on ideas from optimization and control.
- Our approach integrates the development of scalable solvers with the formulation and analysis of physics-coupling strategies.

# Approach and Related Work

## Outline of the Idea

**Step 1.** The original composite problem is broken down into component physics problems for which scalable solvers are available.

**Step 2.** Components are coupled via distributed (SD/MP) and/or boundary control variables (MD/MP) and an objective functional.

**Step 3.** The resulting discrete optimization problem is solved as a fully coupled algebraic system or in the null space of PDE constraints.

$\longrightarrow$ **Preview:** *The solution of a nearly hyperbolic PDE is broken down into the sequential solution of several elliptic PDEs (efficiently handled by AMG!).*

## Related Work

- Lots of disjoint work on physics coupling and specialized MP solvers.
- Some work on the direct use of optimization formulations in solving PDEs: Gunzburger et al. *Optimization-Based DD for PDEs* (1997), Ben Dhia/Rateau *Arlequin Method* (2004).

# Application: Scalable Solvers for Advection-Dominated Elliptic PDEs

- Given an elliptic solver, such as algebraic multigrid, can we develop a scalable solution technique for advection-dominated PDEs?

$$-\epsilon\Delta y(x) + \vec{c}(x)\cdot\nabla y(x) = f(x), \qquad |\vec{c}| \approx 1,\ \ \epsilon \ll 1,\ \ \text{w.l.o.g.}$$

- Yes ...
  - Bank/Wan/Qu: *Kernel Preserving Multigrid (2006)*
  - Elman/Wu: *Comparison of Geometric and Algebraic MG (2006)*
- ... but can we accomplish this with a generic, off-the-shelf solver, i.e. *without problem-specific modifications*?
- Goals:
  - straightforward reuse of existing solver technologies
  - wider applicability (compared to specialized approaches)

# Method

**Step 1.** Decomposition.

$$-\epsilon\Delta y(x) + \vec{c}(x)\cdot\nabla y(x) = f(x)$$

$$\boxed{(1-\epsilon)\Delta y(x) - f(x)} \quad \boxed{-\Delta y(x) + \vec{c}(x)\cdot\nabla y(x) = 0}$$

**Step 2.** Coupling.

Minimize $$\frac{1}{2}\|y_1(x) - y_2(x)\|^2 + \frac{\alpha}{2}\|u(x)\|^2$$

subject to

$$\boxed{-(1-\epsilon)\Delta y_1(x) = u(x) - f(x)}$$
$$\boxed{-\Delta y_2(x) + \vec{c}(x)\cdot\nabla y_2(x) = u(x)}$$

**Step 3.** Solution.

- Express state variables $y_1$ and $y_2$ in terms of the control variables $u$.
- Formulate the reduced objective functional and solve the unconstrained minimization problem.

# The Discrete Problem

$$\text{Minimize} \quad \frac{1}{2}\begin{pmatrix}\vec{y}_1 & \vec{y}_2\end{pmatrix}^T \begin{pmatrix}\mathbf{Q} & -\mathbf{Q}\\ -\mathbf{Q} & \mathbf{Q}\end{pmatrix}\begin{pmatrix}\vec{y}_1\\ \vec{y}_2\end{pmatrix} + \frac{\alpha}{2}\vec{u}^T\mathbf{R}\,\vec{u}$$

subject to

$$\mathbf{A}_1\,\vec{y}_1 + \mathbf{B}\,\vec{u} = \vec{b}_1$$

$$\mathbf{A}_2\,\vec{y}_2 + \mathbf{B}\,\vec{u} = \vec{b}_2$$

- Reduced problem: Minimize $\frac{1}{2}\vec{u}^T\mathbf{H}\,\vec{u} + \vec{g}^T\vec{u}$
- Application of the reduced Hessian matrix $\mathbf{H}$ to a vector $\vec{u}$:
  1. Solve state eqn's: $\mathbf{A}_1\,\vec{y}_1 = \mathbf{B}\,\vec{u}$, $\mathbf{A}_2\,\vec{y}_2 = \mathbf{B}\,\vec{u}$
  2. Solve adjoint eqn's: $\mathbf{A}_1^T\,\vec{\lambda}_1 = \mathbf{Q}\,(\vec{y}_1 - \vec{y}_2)$, $\mathbf{A}_2^T\,\vec{\lambda}_2 = -\mathbf{Q}\,(\vec{y}_1 - \vec{y}_2)$
  3. $\mathbf{H}\,\vec{u} = \mathbf{B}\,(\vec{\lambda}_1 + \vec{\lambda}_2) + \alpha\,\mathbf{R}\,\vec{u}$
- Lemma: *The reduced Hessian matrix* $\mathbf{H}$ *is SPD.*

$\Longrightarrow$ The reduced problem is equivalent to solving $\mathbf{H}\,\vec{u} = \vec{g}$.

# Solver Setup

- The reduced problem can be solved using the conjugate gradient method. However:
  - control variables are distributed $\Rightarrow$ $\mathbf{H}$ is very large (and dense!)
  - $\mathbf{H}$ is not available explicitly $\Rightarrow$ inexactness in the application of $\mathbf{H}$ leads to immediate loss of symmetry
  - $\mathbf{H}$ has a "nice" spectrum (eigenvalue clusters!)

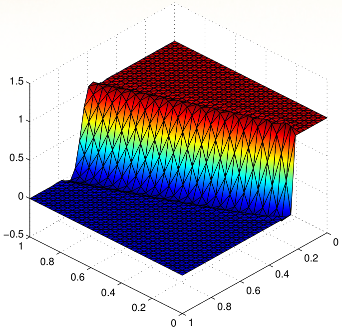
$\Rightarrow$ Think of the reduced problem as $\mathbf{H}\,\vec{u} = \vec{g}$ and solve it using GMRES.

- relative stopping tolerance: 1e-8 ($\ll$ discretization error)
- no preconditioning is necessary

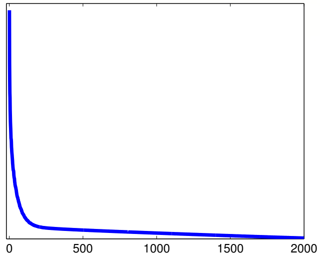
- Inner systems ($\mathbf{A}_1\,\vec{y}_1 = \mathbf{B}\,\vec{u}$, etc.) are solved using AMG/GMRES.
  - relative stopping tolerance for inner GMRES: 1e-12
  - preconditioner: ML (Trilinos)
    - 1 cycle, 2-level; 2nd-degree Chebyshev smoother (pre/post)
    - preconditioner setup is performed only once and all intermediate data, as well as intermediate data structures are reused

# Example 1: Hughes/Brooks

## Main features: Crosswind advection.




Spectrum of reduced Hessian.




AMG/GMRES applied to the original problem: DOES NOT CONVERGE!

**Optimization-based approach:**

Outer Iterations

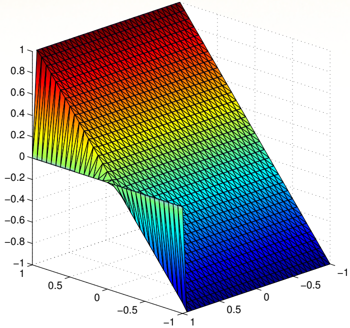
| $64 \times 64$ | $128 \times 128$ | $256 \times 256$ | $512 \times 512$ |
|---|---|---|---|
| 56 | 56 | 55 | 53 |

Inner AMG/GMRES Iterations

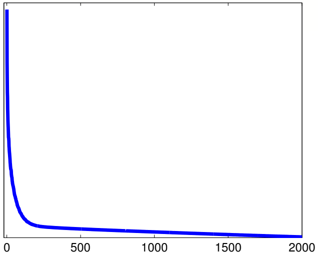
| Only 10–20 per solve! |
|---|
| (4 systems per outer iteration) |

# Example 2: Elman/Silvester/Wathen (1)

Main features: Constant vertical wind, exponential boundary layer.




Spectrum of reduced Hessian.




AMG/GMRES applied to the original problem: DOES NOT CONVERGE!

**Optimization-based approach:**

Outer Iterations

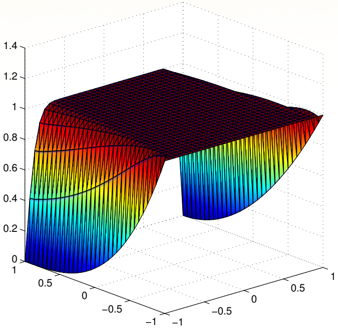
| 64 × 64 | 128 × 128 | 256 × 256 | 512 × 512 |
|---|---|---|---|
| 160 | 152 | 149 | 146 |

Inner AMG/GMRES Iterations

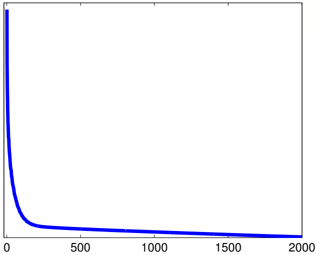
| Only 10–20 per solve! |
|---|
| (4 systems per outer iteration) |

# Example 3: Elman/Silvester/Wathen (2)

## Main features: Variable vertical wind, characteristic boundary layers.




Spectrum of reduced Hessian.




AMG/GMRES applied to the original problem: DOES NOT CONVERGE!

**Optimization-based approach:**

Outer Iterations

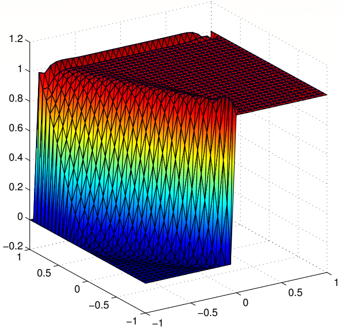
| 64 × 64 | 128 × 128 | 256 × 256 | 512 × 512 |
|---|---|---|---|
| 100 | 100 | 100 | 100 |

Inner AMG/GMRES Iterations

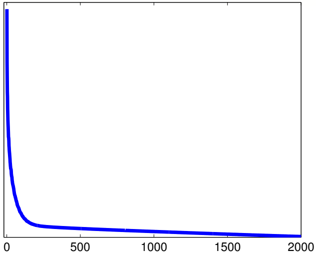
| Only 10–20 per solve! |
|---|
| (4 systems per outer iteration) |

# Example 4: Elman/Silvester/Wathen (3)

Main features: Constant wind at $30^\circ$, downstream and interior boundary layers.




Spectrum of reduced Hessian.




AMG/GMRES applied to the original problem: DOES NOT CONVERGE!

**Optimization-based approach:**

Outer Iterations

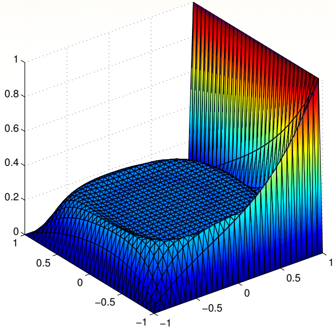
| $64 \times 64$ | $128 \times 128$ | $256 \times 256$ | $512 \times 512$ |
|---|---|---|---|
| 132 | 132 | 129 | 121 |

Inner AMG/GMRES Iterations

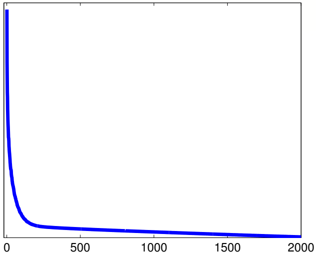
| |
|---|
| Only 10–20 per solve! |
| (4 systems per outer iteration) |

# Example 5: Elman/Silvester/Wathen (4)

Main features: recirculating wind, characteristic boundary layers.




Spectrum of reduced Hessian.




AMG/GMRES applied to the original problem: DOES NOT CONVERGE!

**Optimization-based approach:**

Outer Iterations

| 64 × 64 | 128 × 128 | 256 × 256 | 512 × 512 |
|---|---|---|---|
| 137 | 133 | 125 | 117 |

Inner AMG/GMRES Iterations

| Only 10–20 per solve! |
|---|
| (4 systems per outer iteration) |

# Summary

- Text-book solutions are recovered (no surprise).
- Inner systems are set up only once and solved very efficiently.
- Roughly constant number of outer iterations as problem size increases. $\Rightarrow$ SCALABILITY!
- Scalability unaffected by the size of the Peclet number $|\vec{c}|/\epsilon$ or by the advective direction.
- Easy to implement: A simple Matlab driver for the outer loop calls the off-the-shelf multigrid solver ML.