

Multigrid preconditioners for linear systems arising in PDE constrained optimization

Andrei Draganescu

Department of Mathematics and Statistics
University of Maryland, Baltimore County

March 5, 2013

Acknowledgments

- *Former collaborators:*
Todd Dupont (U Chicago), Volkan Akçelik (Exxon),
George Biros (U Texas), Omar Ghattas (U Texas),
Judith Hill (ORNL), Cosmin Petra (ANL), Bart van Bloemen
Waanders (Sandia).
- *Current collaborators:* (UMBC)
Mona Hajghassem, Jyoti Saraswat , Ana Maria Soane
- *Grants:*
 - NSF awards DMS-1016177 and DMS-0821311.
 - DOE contract no: DE-SC0005455.

Outline

- 1 Model problems
- 2 Unconstrained problems with linear PDE constraints
- 3 Nonlinear constraints, control constraints
 - A semilinear elliptic constrained problem
 - Control-constrained problems
 - Optimal control problems constrained by the Stokes equations

Abstract problem formulation

$$\left\{ \begin{array}{l} \text{minimize} \quad J(y, u) = \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + R(u, y), \\ \text{subj. to} \quad u \in U_{ad} \subset U, \quad y \in Y_{ad} \subset Y, \\ \quad \quad \quad e(y, u) = 0. \end{array} \right. \quad (1)$$

- U_{ad} and Y_{ad} – sets of admissible controls resp. states (convex, closed, non-empty).
- Ex.: $U_{ad} = \{u \in U : \underline{u} \leq u \leq \bar{u}\}$, $Y_{ad} = \{y \in Y : \underline{y} \leq y \leq \bar{y}\}$.
- Equality constraint is a well-posed PDE:
for all $u \in U$ there is a unique $y \in Y$ (depending continuously on u), so that

$$e(y, u) = 0, \quad y \stackrel{\text{def}}{=} K(u).$$

Reduced problem formulation

If $U_{ad} = U$ and $Y_{ad} = Y$, problem can be reformulated as unconstrained:

$$\min_{u \in U} J(u) = \frac{1}{2} \|K(u) - y_d\|^2 + \frac{\beta}{2} \|Lu\|^2, \quad u \in U_{ad}. \quad (2)$$

- If $\beta \ll 1$, essentially we want solve

$$K(u) = y_d.$$

- However, problems of interest are ill-posed, need regularization:
 - $L = I \Rightarrow$ find u of smallest norm ;
 - $L = \nabla \Rightarrow$ find u of smallest variation.

Motivating applications

1. Reverse advection-diffusion problems (source inversion):

- $T > 0$ fixed “end-time”, y_d end-time state, u initial state
- $z(\cdot, t)$ transported quantity subjected to:

$$\begin{cases} \partial_t z - \nabla \cdot (a \nabla z + bz) + cz = 0 & \text{on } \Omega \\ z(\mathbf{x}, t) = 0 & \text{for } \mathbf{x} \in \partial\Omega, t \in [0, T] \\ z(\mathbf{x}, 0) = u(\mathbf{x}) & \text{for } \mathbf{x} \in \Omega \end{cases}$$

- $K = S(T)$: initial - to - final

$$K u = S(T)u \stackrel{\text{def}}{=} z(\cdot, T)$$

Further motivating applications

2. Elliptic optimal control problem:

- PDE-constrained optimal control problem

$$\left\{ \begin{array}{l} \text{minimize} \quad \frac{1}{2} \|y - y_d\|^2 + \frac{\beta}{2} \|u\|^2, \\ \text{subj to:} \quad -\Delta y = u, \quad u|_{\partial\Omega} = 0, \\ \quad \quad \quad \underline{u} \leq u \leq \bar{u}. \end{array} \right.$$

- If unconstrained, then $K = (-\Delta)^{-1}$.

The case of linear constraints

Assume K linear, $U_{ad} = U$:

$$\min_u J(u) = \frac{1}{2} \|Ku - y_d\|^2 + \frac{\beta}{2} \|u\|^2$$

- Newton's method gives the solution explicitly in one step:

$$u^{\min} = u_0^{\text{guess}} - G^{-1} \nabla J(u_0^{\text{guess}}),$$

where

$$G = G(\beta) = I + \beta^{-1} K^* \cdot K,$$

$$\nabla J(u) = u + \beta^{-1} K^* (Ku - y_d).$$

- Formulation is equivalent to the regularized normal equations

$$(\beta I + K^* \cdot K)u = K^* y_d.$$

Strategy: discretize-then-optimize

- Natural FE discretization for the operator K :

$$\min_u J(u) = \frac{1}{2} \|K_h u - y_d\|^2 + \frac{\beta}{2} \|u\|^2.$$

- Solution of discrete problem:

$$u_h^{\min} = u_{0,h}^{\text{guess}} - G_h^{-1} \nabla J_h(u_{0,h}^{\text{guess}}),$$

where

$$G_h = G_h(\beta) = I + \beta^{-1} K_h^* \cdot K_h,$$

$$\nabla J_h(u) = u + \beta^{-1} K_h^* (K_h u - \pi_h y_d),$$

π_h is the orthogonal projection onto the finite element space V_h

- **Main problem: need to invert the operator G_h efficiently.**

Main issues

- The matrix representing the linear operator G_h is dense, potentially large, and not available.
- Matrix-vector product cost is comparable to two forward computations (expensive, but feasible):

$$G_h \cdot u = u + \beta^{-1} K_h^* \cdot K_h u .$$

- Gradient computation also costs as much as two forward computations (only done once):

$$\nabla J_h(u) = u + \beta^{-1} K_h^* (K_h u - \pi_h y_d) .$$

- Need iterative methods.

Solution using conjugate gradient

- Eigenvalues of G_h cluster around 1 \Rightarrow
CG is a good choice for solving inverting G_h :
the number of iterations
 - is independent of the resolution;
 - grows only logarithmically with $\beta \rightarrow 0$.

- A measure of success: speedup over CG.

Multigrid strategies

- major differences between G_h and an elliptic operator A_h :

G_h	A_h
smoothing	roughening
nonlocal	local
$\text{cond}(G_h)$ bounded	$\text{cond}(A_h) \rightarrow \infty$ as $h \rightarrow 0$

- Related multigrid work:

- Hackbusch (1981), King (1992), Rieder (1997), Hanke and Vogel (1999), Kaltenbacher (2003), Donatelli (2005), Biros and **Dogan** (2008), Draganescu and Dupont (2008), Borzi and Kunisch (2005).
- Lewis and Nash (2000)
- overview: Borzi and Schultz (SIAM review, 2009)
- more recent: Wathen, Stoll, Rees, Dollar, Draganescu and Soane, etc

Two-grid approximation (heuristics)

“smooth” functions

“rough” functions

$$\bullet V_h = \underbrace{V_{2h}}_{\text{smooth}} \oplus \underbrace{W}_{\text{rough}}$$

- denote $\pi = \pi_{2h}$, $\rho = I - \pi_{2h}$

$$G_h = \underbrace{\pi G_h \pi}_{M_1} + \underbrace{\rho G_h \pi}_{M_2} + \underbrace{\pi G_h \rho}_{M_3} + \underbrace{\rho G_h \rho}_{M_4}$$

- since $G_h \rho = (I + \beta^{-1} K_h^* K_h) \rho \approx \rho$

$$M_2 \approx 0$$

$$M_3 \approx 0$$

$$M_1 \approx G_{2h} \pi$$

$$M_4 \approx \rho$$

- conclusion:

$$G_h \approx M_h \stackrel{\text{def}}{=} G_{2h} \pi_{2h} \oplus (I - \pi_{2h}).$$

Two-grid approximation (heuristics)

“smooth” functions “rough” functions

$$\bullet V_h = \underbrace{V_{2h}}_{\text{smooth}} \oplus \underbrace{W}_{\text{rough}}$$

$$\bullet \text{denote } \pi = \pi_{2h}, \rho = I - \pi_{2h}$$

$$G_h = \underbrace{\pi G_h \pi}_{M_1} + \underbrace{\rho G_h \pi}_{M_2} + \underbrace{\pi G_h \rho}_{M_3} + \underbrace{\rho G_h \rho}_{M_4}$$

$$\bullet \text{since } G_h \rho = (I + \beta^{-1} K_h^* K_h) \rho \approx \rho$$

$$M_2 \approx 0$$

$$M_3 \approx 0$$

$$M_1 \approx G_{2h} \pi$$

$$M_4 \approx \rho$$

• conclusion:

$$G_h \approx M_h \stackrel{\text{def}}{=} G_{2h} \pi_{2h} \oplus (I - \pi_{2h}).$$

Two-grid approximation (heuristics)

“smooth” functions “rough” functions

$$\bullet V_h = \underbrace{V_{2h}}_{\text{smooth}} \oplus \underbrace{W}_{\text{rough}}$$

$$\bullet \text{denote } \pi = \pi_{2h}, \rho = I - \pi_{2h}$$

$$G_h = \underbrace{\pi G_h \pi}_{M_1} + \underbrace{\rho G_h \pi}_{M_2} + \underbrace{\pi G_h \rho}_{M_3} + \underbrace{\rho G_h \rho}_{M_4}$$

$$\bullet \text{since } G_h \rho = (I + \beta^{-1} K_h^* K_h) \rho \approx \rho$$

$$M_2 \approx 0$$

$$M_1 \approx G_{2h} \pi$$

$$M_3 \approx 0$$

$$M_4 \approx \rho$$

• conclusion:

$$G_h \approx M_h \stackrel{\text{def}}{=} G_{2h} \pi_{2h} \oplus (I - \pi_{2h}).$$

Two-grid approximation (heuristics)

“smooth” functions “rough” functions

$$\bullet V_h = \underbrace{V_{2h}}_{\text{smooth}} \oplus \underbrace{W}_{\text{rough}}$$

$$\bullet \text{denote } \pi = \pi_{2h}, \rho = I - \pi_{2h}$$

$$G_h = \underbrace{\pi G_h \pi}_{M_1} + \underbrace{\rho G_h \pi}_{M_2} + \underbrace{\pi G_h \rho}_{M_3} + \underbrace{\rho G_h \rho}_{M_4}$$

$$\bullet \text{since } G_h \rho = (I + \beta^{-1} K_h^* K_h) \rho \approx \rho$$

$$M_2 \approx 0$$

$$M_3 \approx 0$$

$$M_1 \approx G_{2h} \pi$$

$$M_4 \approx \rho$$

• conclusion:

$$G_h \approx M_h \stackrel{\text{def}}{=} G_{2h} \pi_{2h} \oplus (I - \pi_{2h}).$$

Two-grid approximation (heuristics)

“smooth” functions “rough” functions

$$\bullet V_h = \underbrace{V_{2h}}_{\text{smooth}} \oplus \underbrace{W}_{\text{rough}}$$

$$\bullet \text{denote } \pi = \pi_{2h}, \rho = I - \pi_{2h}$$

$$G_h = \underbrace{\pi G_h \pi}_{M_1} + \underbrace{\rho G_h \pi}_{M_2} + \underbrace{\pi G_h \rho}_{M_3} + \underbrace{\rho G_h \rho}_{M_4}$$

$$\bullet \text{since } G_h \rho = (I + \beta^{-1} K_h^* K_h) \rho \approx \rho$$

$$M_2 \approx 0$$

$$M_3 \approx 0$$

$$M_1 \approx G_{2h} \pi$$

$$M_4 \approx \rho$$

• conclusion:

$$G_h \approx M_h \stackrel{\text{def}}{=} G_{2h} \pi_{2h} \oplus (I - \pi_{2h}).$$

Multigrid for our problem

two-grid approximation (results)

Proposed preconditioner:

$$L_h \stackrel{\text{def}}{=} (M_h)^{-1} = G_{2h}^{-1} \pi_{2h} + (I - \pi_{2h}).$$

Theorem (A.D., Dupont 2004):

For h sufficiently small and $u \in V_h$

$$1 - C \frac{h^p}{\beta} \leq \frac{\langle (M_h)^{-1} u, u \rangle}{\langle (G_h)^{-1} u, u \rangle} \leq 1 + C \frac{h^p}{\beta},$$

where p is the order of the discrete method.

From two-grid to multigrid

natural extension (V-cycle)

- Natural extension to multigrid is suboptimal:

$$L_h = G_{2h}^{-1} \pi_{2h} + (I - \pi_{2h}) \approx G_h^{-1}$$

$$\Downarrow \text{ (since } L_{2h} \approx G_{2h}^{-1} \text{)}$$

$$L_h \stackrel{\text{def}}{=} L_{2h} \pi_{2h} + (I - \pi_{2h})$$

Corollary:

For h, h_0 small enough and $u \in V_h$

$$1 - C \frac{h_0^p}{\beta} \leq \frac{\langle L_h u, u \rangle}{\langle (G_h)^{-1} u, u \rangle} \leq 1 + C \frac{h_0^p}{\beta}.$$

From two-grid to multigrid

natural extension (V-cycle)

- Natural extension to multigrid is suboptimal:

$$L_h = G_{2h}^{-1} \pi_{2h} + (I - \pi_{2h}) \approx G_h^{-1}$$

$$\Downarrow \text{ (since } L_{2h} \approx G_{2h}^{-1} \text{)}$$

$$L_h \stackrel{\text{def}}{=} L_{2h} \pi_{2h} + (I - \pi_{2h})$$

Corollary:

For h, h_0 small enough and $u \in V_h$

$$1 - C \frac{h_0^p}{\beta} \leq \frac{\langle L_h u, u \rangle}{\langle (G_h)^{-1} u, u \rangle} \leq 1 + C \frac{h_0^p}{\beta}.$$

From two-grid to multigrid

natural extension (V-cycle)

- Natural extension to multigrid is suboptimal:

$$L_h = G_{2h}^{-1} \pi_{2h} + (I - \pi_{2h}) \approx G_h^{-1}$$

$$\Downarrow \text{ (since } L_{2h} \approx G_{2h}^{-1} \text{)}$$

$$L_h \stackrel{\text{def}}{=} L_{2h} \pi_{2h} + (I - \pi_{2h})$$

Corollary:

For h, h_0 small enough and $u \in V_h$

$$1 - C \frac{h_0^p}{\beta} \leq \frac{\langle L_h u, u \rangle}{\langle (G_h)^{-1} u, u \rangle} \leq 1 + C \frac{h_0^p}{\beta} .$$

From two-grid to multigrid

Newton extension (W-cycle)

- essential ingredient: use Newton's method for the nonlinear operator equation

$$X^{-1} - G_h = 0$$

- basic idea:

X_1 (below) is an improved approximation of $(G_h)^{-1}$ over X_0

$$X_1 = \mathcal{N}_{G_h}(X_0) \stackrel{\text{def}}{=} 2X_0 - X_0 \cdot G_h \cdot X_0$$

-

$$L_h \stackrel{\text{def}}{=} \mathcal{N}_{G_h}(L_{2h}\pi_{2h} + (I - \pi_{2h}))$$

From two-grid to multigrid

Newton extension (W-cycle)

- essential ingredient: use Newton's method for the nonlinear operator equation

$$X^{-1} - G_h = 0$$

- basic idea:

X_1 (below) is an improved approximation of $(G_h)^{-1}$ over X_0

$$X_1 = \mathcal{N}_{G_h}(X_0) \stackrel{\text{def}}{=} 2X_0 - X_0 \cdot G_h \cdot X_0$$



$$L_h \stackrel{\text{def}}{=} \mathcal{N}_{G_h}(L_{2h}\pi_{2h} + (I - \pi_{2h}))$$

From two-grid to multigrid

Newton extension (W-cycle)

- essential ingredient: use Newton's method for the nonlinear operator equation

$$X^{-1} - G_h = 0$$

- basic idea:

X_1 (below) is an improved approximation of $(G_h)^{-1}$ over X_0

$$X_1 = \mathcal{N}_{G_h}(X_0) \stackrel{\text{def}}{=} 2X_0 - X_0 \cdot G_h \cdot X_0$$

-

$$L_h \stackrel{\text{def}}{=} \mathcal{N}_{G_h}(L_{2h}\pi_{2h} + (I - \pi_{2h}))$$

From two-grid to multigrid

Newton extension (result)

Theorem (A.D., Dupont 2004):

For h, h_0 sufficiently small and $u \in V_h$

$$1 - C \frac{h^p}{\beta} \leq \frac{\langle L_h u, u \rangle}{\langle (G_h)^{-1} u, u \rangle} \leq 1 + C \frac{h^p}{\beta} .$$

Numerical results

First test case: one dimensional advection-diffusion equation

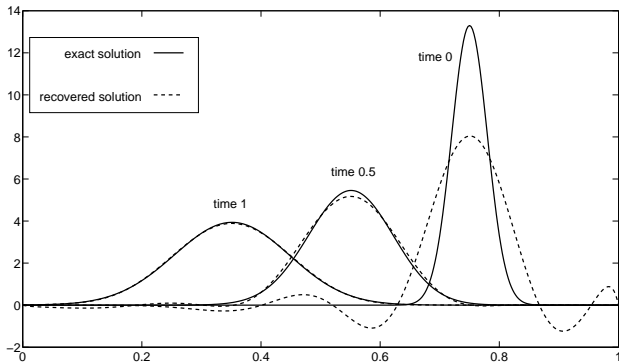
- Forward problem:

$$\partial_t z - \partial_x(a\partial_x z + bz) + cz = 0, \text{ on } (0, 1), \quad z(\cdot, 0) = u.$$

- We will test multigrid with up to 6 levels vs. conjugate gradient.
- Measures of success:
 - measure 1: cost(inverse problem) / cost(forward problem)
 - measure 2: cost(inverse problem) / cost(CG solve)

Numerical results

First test case: one dimensional advection-diffusion equation



Numerical results

First test case: one dimensional advection-diffusion equation

Table: Iteration count (I/F) for the W-cycle; $\beta = 10^{-3}$.

N	1		2		3		4		5		6	
200	15	(32.3)	11	(61.1)	9	(29.6)	7	(19.4)	6	(16.2)	5	(13.7)
400	16	(34.1)	9	(48)	7	(22.8)	6	(16.8)	5	(13.8)		
800	16	(34)	7	(38)	6	(19.8)	5	(14.4)				
1600	16	(34)	6	(32)	5	(16.9)						
3200	17	(36)	5	(26.7)								

Outline

- 1 Model problems
- 2 Unconstrained problems with linear PDE constraints
- 3 **Nonlinear constraints, control constraints**
 - **A semilinear elliptic constrained problem**
 - Control-constrained problems
 - Optimal control problems constrained by the Stokes equations

Semilinear elliptic constraints (with Jyoti Saraswat)

- Optimal control problem:

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \|y - y_d\|^2 + \frac{\beta}{2} \|u\|^2, \\ & \text{subj to:} && Ay + c_0 y + f(y) = u, \quad u \in L^2(\Omega). \end{aligned} \tag{3}$$

Assumptions and basic facts

- A is a uniformly elliptic operator on $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) with sufficiently smooth coefficients, $c_0 \geq 0$ is in L^∞ .
- $f : \mathbb{R} \rightarrow \mathbb{R}$ is increasing, sufficiently smooth (C^3 will do).
- Monotone operator theory guarantees unique solution $u \rightarrow y(u) \in H_0^1$.
- Stampacchia technique produces L^∞ -estimates for $y(u)$ independent of c_0 , f : $\|y(u)\|_{L^\infty} \leq C_\infty \|u\|_{L^2}$.
- Full elliptic regularity is assumed: $y(u) \in H^2$.
- Mesh to allow for discrete FE maximum principle.

Reduced form of control problem

- Unconstrained optimal control problem:

$$\text{minimize } \frac{1}{2} \|y(u) - y_d\|^2 + \frac{\beta}{2} \|u\|^2 \quad (4)$$

- Existence of optimal control $\bar{u} \in L^2(\Omega)$ guaranteed by standard techniques: optimal state $\bar{y} = y(\bar{u}) \in H^2(\Omega) \cap H_0^1(\Omega)$.
- Uniqueness of the optimal control \bar{u} is not guaranteed in general.
- The optimal control problem may not be convex.

Solving the control problem

- The state is twice differentiable with respect to the control so the cost functional is twice differentiable.
- Apply Newton's method to solve the control problem:

$$u_{n+1} = u_n - \text{Hessian}^{-1} \text{gradient} .$$

- *Grid-sequencing* used to obtain good initial guess.
- *Adjoint methods* used to obtain gradients and the Hessian-vector multiplication.

Gradient and Hessian using adjoints

- $L = L(u) = A + f'(u)$ is the linearization of the semilinear operator at y .
- Gradient: $\nabla_u J(u) = (L^*)^{-1}(y(u) - y_d) + \beta u$.
- Hessian-vector multiplication:

$$G(u)v = L^{*-1}(1 - f''(u)q(u))L^{-1}v + \beta v,$$

where

$$q = q(u) = (L^*)^{-1}(y(u) - y_d).$$

- Cost of Hessian-vector multiplication is equivalent to two linear elliptic solves.

Mesh independence of Newton's method

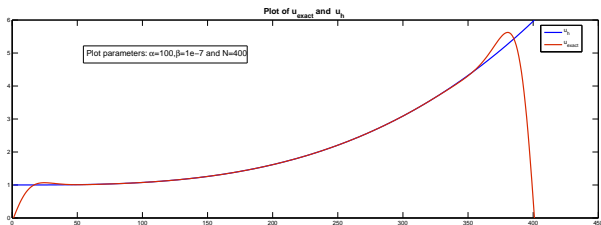


Table: Newton iterations

Resolution	50	100	200	250	300	350
Newton's iterations	4	4	4	4	4	4

Hessian and preconditioner

The Hessian:

$$G(u) = L^{*-1}(1 - f''(u)q(u))L^{-1} + \beta I$$

- As before, the Hessian is smoothing.
- Proposed two grid preconditioner:

$$M_h = \beta \rho + G_{2h}(\pi u) \pi$$

Two-grid preconditioner

Theorem (J. Saraswat, A.D., 2012)

On a quasi-uniform mesh and under usual elliptic regularity assumptions

$$\|(G_h(u) - M_h(u))v\| \leq Ch^2 \|v\|, \quad \forall v \in L^2(\Omega),$$

C independent of h .

Remark:

- Optimal order in h

One dimensional, in-vitro experiments

Table: Joint spectrum analysis in 1D: $f(y) = \alpha y^3$

N	$z_k = \max(\text{abs}(\ln d))$	ratio = $\frac{z_k}{z_{k+1}}$
10	2.426486	N/A
20	0.569206	4.262924
40	0.134355	4.236559
80	0.034536	3.890306
160	0.008709	3.965544
320	0.002182	3.990972
640	0.000545	3.997717

Here $d = \text{eig}(G_h, T_h)$.

The spectral distance between constructed preconditioner and Hessian is $O(h^2)$, which is the optimal rate.

Two-dimensional, in-vivo experiments with $f(y) = \alpha y^3$

Table: $\alpha = 1, \beta = 10^{-4}$

iterate N	16	32	64	128
1	7 (12)	6 (12)	4 (12)	4 (12)
2	7 (11)	5 (11)	4 (11)	4 (11)
3	4 (5)	3 (5)	2 (6)	1 (6)

Table: $\alpha = 1, \beta = 10^{-5}$

iterate N	16	32	64	128
1	11 (21)	8 (21)	5 (21)	4 (21)
2	10 (20)	8 (20)	5 (20)	4 (20)
3	5 (9)	4 (9)	2 (9)	2 (9)

Two-dimensional, in-vivo experiments

Table: $\alpha = 10, \beta = 10^{-5}$

iterate N	16	32	64	128
1	11 (21)	8 (21)	5 (21)	4 (21)
2	11 (20)	8 (20)	5 (20)	4 (20)
3	10 (16)	5 (16)	5 (16)	4 (16)
4	4 (8)	2 (8)	2 (8)	1 (8)

Table: $\alpha = 10, \beta = 10^{-7}$

iterate N	16	32	64	128
1	40 (76)	21 (93)	9 (99)	5 (98)
2	39 (65)	16 (72)	6 (71)	5 (71)
3	33 (50)	13 (48)	6 (49)	5 (46)
4	13 (12)	2 (12)	2 (12)	2 (12)

Outline

- 1 Model problems
- 2 Unconstrained problems with linear PDE constraints
- 3 Nonlinear constraints, control constraints**
 - A semilinear elliptic constrained problem
 - Control-constrained problems**
 - Optimal control problems constrained by the Stokes equations

Problem formulation

- Model problem:

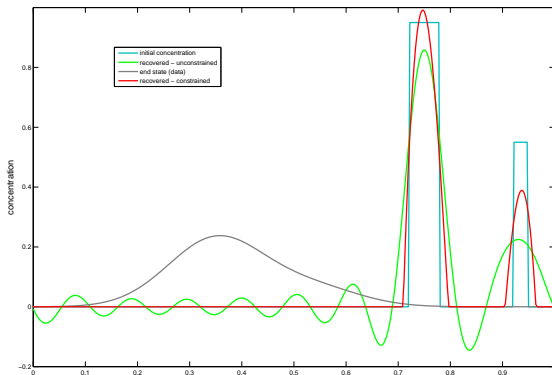
$$K : L^2(\Omega) \rightarrow L^2(\Omega) \text{ compact, linear, } f \in L^2(\Omega)$$

Optimal control problem

$$\begin{aligned} &\text{minimize} && \frac{1}{2} \|Ku - y_d\|^2 + \frac{\beta}{2} \|u\|^2 \\ &\text{subj to:} && u \in L^2(\Omega), \quad a \leq u \leq b \end{aligned} \tag{5}$$

Why bound-constraints ?

- Physically meaningful, other qualitative considerations
- Example: solution is localized if the “true” solution is so



Discrete problem formulation

- Norms: discrete norm $\|u\|_h^2 = \sum w_i u^2(P_i)$
- Inequality constraints: $a \leq u \leq b$, enforced at nodes (strong enforcement)

Discrete optimal control problem

$$\begin{array}{ll}
 \text{minimize} & \frac{1}{2} \|K_h u - y_{d,h}\|_h^2 + \frac{\beta}{2} \|u\|_h^2 \\
 \text{subj to:} & u \in V_h, \quad a_h(P) \leq u(P) \leq b_h(P), \quad \forall \text{ node } P
 \end{array} \tag{6}$$

Discrete problem formulation

- Norms: discrete norm $\|u\|_h^2 = \sum w_i u^2(P_i)$
- Inequality constraints: $a \leq u \leq b$, enforced at nodes (strong enforcement)

Discrete optimal control problem

$$\begin{aligned}
 &\text{minimize} && \frac{1}{2} \|K_h u - y_{d,h}\|_h^2 + \frac{\beta}{2} \|u\|_h^2 \\
 &\text{subj to:} && u \in V_h, \quad a_h(P) \leq u(P) \leq b_h(P), \quad \forall \text{ node } P
 \end{aligned} \tag{6}$$

Discrete problem formulation

- Norms: discrete norm $\|u\|_h^2 = \sum w_i u^2(P_i)$
- Inequality constraints: $a \leq u \leq b$, enforced at nodes (strong enforcement)

Discrete optimal control problem

$$\begin{array}{ll}
 \text{minimize} & \frac{1}{2} \|K_h u - y_{d,h}\|_h^2 + \frac{\beta}{2} \|u\|_h^2 \\
 \text{subj to:} & u \in V_h, \quad a_h(P) \leq u(P) \leq b_h(P), \quad \forall \text{ node } P
 \end{array} \tag{6}$$

Optimization methods

- Optimization algorithms (outer iteration):
 - Semi-smooth Newton methods (active-set type strategies)
 - Interior point methods (IPM)
- Require: solving few linear systems at each outer iteration
 - semi-smooth Newton: subsystem (principal minor)
 - IPM: modified, same-size system
- Goals:
 - small # of outer iterations (prefer mesh-independence)
 - **here**: fast solvers for the linear systems:
of linear iterations **to decrease with increasing resolution**

Optimization methods

- Optimization algorithms (outer iteration):
 - Semi-smooth Newton methods (active-set type strategies)
 - Interior point methods (IPM)
- Require: solving few linear systems at each outer iteration
 - semi-smooth Newton: subsystem (principal minor)
 - IPM: modified, same-size system
- Goals:
 - small # of outer iterations (prefer mesh-independence)
 - **here**: fast solvers for the linear systems:
of linear iterations **to decrease with increasing resolution**

Optimization methods

- Optimization algorithms (outer iteration):
 - Semi-smooth Newton methods (active-set type strategies)
 - Interior point methods (IPM)
- Require: solving few linear systems at each outer iteration
 - semi-smooth Newton: subsystem (principal minor)
 - IPM: modified, same-size system
- Goals:
 - small # of outer iterations (prefer mesh-independence)
 - **here**: fast solvers for the linear systems:
of linear iterations **to decrease with increasing resolution**

A. Primal-dual interior point methods (with Cosmin Petra)

For fixed resolution V_h and uniform grids:

- solve perturbed KKT system for $\mu \downarrow 0$:

$$\begin{aligned}(\beta \mathbf{I} + \mathbf{K}^T \mathbf{K}) \mathbf{u} - \mathbf{v} &= -\mathbf{K}^T \mathbf{y}_d \\ \mathbf{u} \cdot \mathbf{v} &= \mu \mathbf{e} \\ \mathbf{u}, \mathbf{v} &> \mathbf{0}\end{aligned}$$

- Mehrotra's predictor-corrector IPM

$$\begin{aligned}(\beta \mathbf{I} + \mathbf{K}^T \mathbf{K}) \Delta \mathbf{u} - \Delta \mathbf{v} &= \mathbf{r}_c \\ \mathbf{V} \Delta \mathbf{u} + \mathbf{U} \Delta \mathbf{v} &= \mathbf{r}_a\end{aligned}$$

- reduced system

$$(\beta \mathbf{I} + \mathbf{U}^{-1} \mathbf{V} + \mathbf{K}^T \mathbf{K}) \Delta \mathbf{u} = \mathbf{r}_c - \mathbf{U}^{-1} \mathbf{r}_a$$

with \mathbf{U}, \mathbf{V} diagonal, positive

A. Primal-dual interior point methods (with Cosmin Petra)

For fixed resolution V_h and uniform grids:

- solve perturbed KKT system for $\mu \downarrow 0$:

$$\begin{aligned}(\beta \mathbf{I} + \mathbf{K}^T \mathbf{K}) \mathbf{u} - \mathbf{v} &= -\mathbf{K}^T \mathbf{y}_d \\ \mathbf{u} \cdot \mathbf{v} &= \mu \mathbf{e} \\ \mathbf{u}, \mathbf{v} &> \mathbf{0}\end{aligned}$$

- Mehrotra's predictor-corrector IPM

$$\begin{aligned}(\beta \mathbf{I} + \mathbf{K}^T \mathbf{K}) \Delta \mathbf{u} - \Delta \mathbf{v} &= \mathbf{r}_c \\ \mathbf{V} \Delta \mathbf{u} + \mathbf{U} \Delta \mathbf{v} &= \mathbf{r}_a\end{aligned}$$

- reduced system

$$(\beta \mathbf{I} + \mathbf{U}^{-1} \mathbf{V} + \mathbf{K}^T \mathbf{K}) \Delta \mathbf{u} = \mathbf{r}_c - \mathbf{U}^{-1} \mathbf{r}_a$$

with \mathbf{U}, \mathbf{V} diagonal, positive

A. Primal-dual interior point methods (with Cosmin Petra)

For fixed resolution V_h and uniform grids:

- solve perturbed KKT system for $\mu \downarrow 0$:

$$\begin{aligned}(\beta \mathbf{I} + \mathbf{K}^T \mathbf{K}) \mathbf{u} - \mathbf{v} &= -\mathbf{K}^T \mathbf{y}_d \\ \mathbf{u} \cdot \mathbf{v} &= \mu \mathbf{e} \\ \mathbf{u}, \mathbf{v} &> \mathbf{0}\end{aligned}$$

- Mehrotra's predictor-corrector IPM

$$\begin{aligned}(\beta \mathbf{I} + \mathbf{K}^T \mathbf{K}) \Delta \mathbf{u} - \Delta \mathbf{v} &= \mathbf{r}_c \\ \mathbf{V} \Delta \mathbf{u} + \mathbf{U} \Delta \mathbf{v} &= \mathbf{r}_a\end{aligned}$$

- reduced system

$$(\beta \mathbf{I} + \mathbf{U}^{-1} \mathbf{V} + \mathbf{K}^T \mathbf{K}) \Delta \mathbf{u} = \mathbf{r}_c - \mathbf{U}^{-1} \mathbf{r}_a$$

with \mathbf{U}, \mathbf{V} diagonal, positive

The systems

- the matrix: $(\beta \mathbf{I} + \mathbf{U}^{-1} \mathbf{V} + \mathbf{K}^T \mathbf{K})$
- $\mathbf{U}^{-1} \mathbf{V}$ represents a relatively smooth function
- need to invert

$$(D_{\beta+\lambda} + \underbrace{\mathbf{K}^T \mathbf{K}}_{\mathbf{K}^* \mathbf{K}})$$

with $D_{\beta+\lambda} = \beta \mathbf{I} + \mathbf{U}^{-1} \mathbf{V}$

- ... and further

$$D_{\sqrt{\beta+\lambda}} \left(\mathbf{I} + \underbrace{\mathbf{A} \mathbf{K}^T \mathbf{K} \mathbf{A}}_{(\mathbf{K} \mathbf{A})^* (\mathbf{K} \mathbf{A})} \right) D_{\sqrt{\beta+\lambda}}$$

with $\mathbf{A} = D_{\sqrt{1/(\beta+\lambda)}}$

The systems

- the matrix: $(\beta \mathbf{I} + \mathbf{U}^{-1} \mathbf{V} + \mathbf{K}^T \mathbf{K})$
- $\mathbf{U}^{-1} \mathbf{V}$ represents a relatively smooth function
- need to invert

$$(D_{\beta+\lambda} + \underbrace{\mathbf{K}^T \mathbf{K}}_{\mathbf{K}^* \mathbf{K}})$$

with $D_{\beta+\lambda} = \beta \mathbf{I} + \mathbf{U}^{-1} \mathbf{V}$

- ... and further

$$D_{\sqrt{\beta+\lambda}} \left(\mathbf{I} + \underbrace{\mathbf{A} \mathbf{K}^T \mathbf{K} \mathbf{A}}_{(\mathbf{K} \mathbf{A})^* (\mathbf{K} \mathbf{A})} \right) D_{\sqrt{\beta+\lambda}}$$

with $\mathbf{A} = D_{\sqrt{1/(\beta+\lambda)}}$

The systems

- the matrix: $(\beta \mathbf{I} + \mathbf{U}^{-1} \mathbf{V} + \mathbf{K}^T \mathbf{K})$
- $\mathbf{U}^{-1} \mathbf{V}$ represents a relatively smooth function
- need to invert

$$(D_{\beta+\lambda} + \underbrace{\mathbf{K}^T \mathbf{K}}_{\mathbf{K}^* \mathbf{K}})$$

with $D_{\beta+\lambda} = \beta \mathbf{I} + \mathbf{U}^{-1} \mathbf{V}$

- ... and further

$$D_{\sqrt{\beta+\lambda}} \left(\mathbf{I} + \underbrace{\mathbf{A} \mathbf{K}^T \mathbf{K} \mathbf{A}}_{(\mathbf{K} \mathbf{A})^* (\mathbf{K} \mathbf{A})} \right) D_{\sqrt{\beta+\lambda}}$$

with $\mathbf{A} = D_{\sqrt{1/(\beta+\lambda)}}$

The systems

- Need good preconditioner for

$$G_h = I + (K_h A_h)^* (K_h A_h) = I + (L_h)^* (L_h)$$

$$\text{with } A_h = D \sqrt{1/(\beta + \lambda_h)}$$

- Assume $\lambda_h = \text{interpolate}(\lambda)$

$$L_h \stackrel{\text{def}}{=} K_h A_h$$

$$L \stackrel{\text{def}}{=} K D \sqrt{1/(\beta + \lambda)}$$

Key facts

- $G_h = I + L_h^* L_h$ is **dense**, available only matrix-free
- $\text{cond}(I + L_h^* L_h) = O(\beta^{-1})$, mesh-independent, large
- $A_h = D_{\sqrt{1/(\beta + \lambda_h)}}$ neutral with respect to smoothing
- $L_{(h)} = K_{(h)} A_{(h)}$ same smoothing properties as $K_{(h)}$

Two-grid preconditioner

Theorem (A.D. and Petra, 2009)

On a uniform grid

$$\rho(I - M_h^{-1}G_h) \leq Ch^2 \|(\beta + \lambda)^{-\frac{1}{2}}\|_{W_\infty^2}$$

Remarks:

- optimal order in h
- quality expected to decay as $\mu \downarrow 0$ since λ only L^2 in general
- for fixed $\beta \neq 0$ linear iterations/outer iteration expected to decrease with $h \downarrow 0$
- M_h is slightly non-symmetric

Backwards advection-diffusion problem example

Optimal control problem

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \|S(T)u - y_d\|^2 + \frac{\beta}{2} \|u\|^2 \\ & \text{subj to:} && u \in L^2(\Omega), \quad 0 \leq u \leq 1 \end{aligned} \quad (7)$$

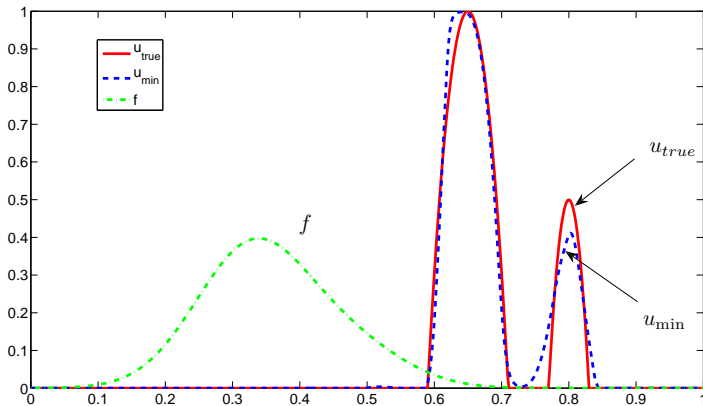
- $z(\cdot, t)$ transported quantity subjected to:

$$\begin{cases} \partial_t z - \nabla \cdot (a \nabla z + bz) + cz = 0 & \text{on } \Omega \\ z(x, t) = 0 & \text{for } x \in \partial\Omega, \quad t \in [0, T] \\ z(x, 0) = u(x) & \text{for } x \in \Omega \end{cases}$$

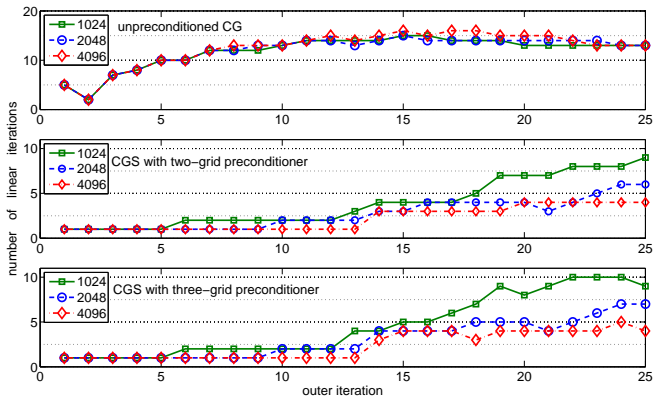
- $K = S(T)$: initial - to - final

$$K u = S(T)u \stackrel{\text{def}}{=} z(\cdot, T)$$

Solution

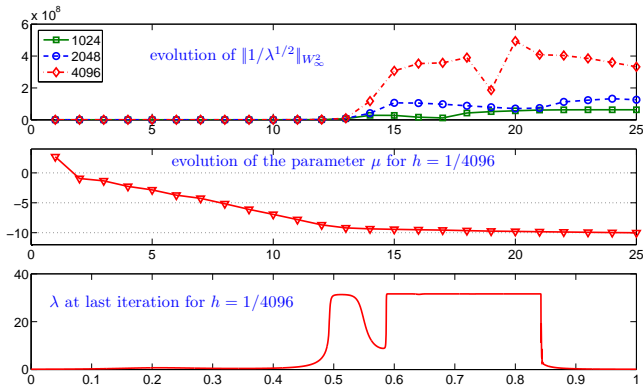


Iteration count / predictor-step linear systems



Evolution of quantities of interest

- Evolution of $\|\lambda^{-\frac{1}{2}}\|_{W_\infty^2}$, μ , and last λ_h :



Another measure of success

Total number of finest-level mat-vecs (application of K)

$h \setminus$ levels	1	2	3
1/1024	728	581	661
1/2048	740	463	489
1/4096	764	403	425
1/8192	768	377	403

Elliptic-constrained problem

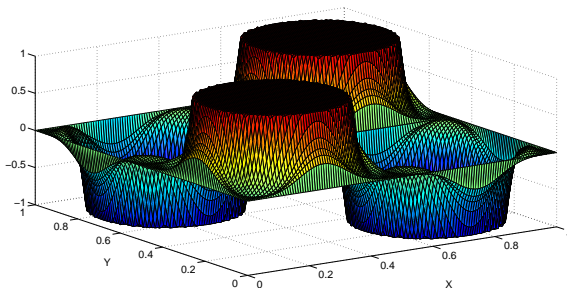
minimize

$$\frac{1}{2} \|y - f\|^2 + \frac{\beta}{2} \|u\|^2$$

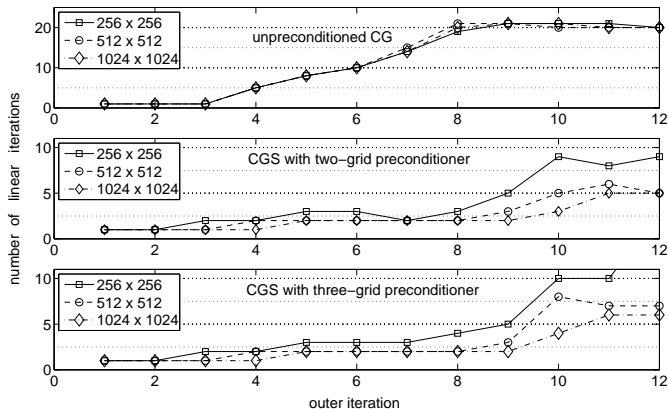
subj to:

$$-\Delta y = u, \quad -1 \leq u \leq 1$$

$$\Delta f = \frac{3}{2} \sin(2\pi x) \sin(2\pi y), \quad \beta = 10^{-6}$$



Iteration count / predictor-step linear systems



Mat-vecs count

Total number of finest-level mat-vecs (Poisson solves)

$h \setminus$ levels	1	2	3	4
1/256	354	282	572	—
1/512	355	220	250	452
1/1024	355	198	210	224
1/2048	363	172	174	174

B. Semismooth Newton methods

- KKT system (unperturbed):

$$\begin{aligned}(\beta \mathbf{I} + \mathbf{K}^T \mathbf{K})\mathbf{u} - \mathbf{v} &= -\mathbf{K}^T \mathbf{y}_d \\ \mathbf{u} \cdot \mathbf{v} &= \mathbf{0} \\ \mathbf{u}, \mathbf{v} &\geq \mathbf{0}\end{aligned}$$

- Reformulate as a semismooth nonlinear system:

$$\begin{aligned}(\beta \mathbf{I} + \mathbf{K}^T \mathbf{K})\mathbf{u} - \mathbf{v} &= -\mathbf{K}^T \mathbf{y}_d \\ \mathbf{v} - \max(\mathbf{0}, \mathbf{v} - \beta \mathbf{u}) &= \mathbf{0}.\end{aligned}$$

Active set strategy

- Define the *active index-set* by

$$\mathcal{A} = \{i \in \{1, \dots, N\} : (\mathbf{v} - \beta \mathbf{u})_i > 0\}$$

and the *inactive index-set* by

$$\mathcal{I} = \{i \in \{1, \dots, N\} : (\mathbf{v} - \beta \mathbf{u})_i \leq 0\} .$$

- The semismooth Newton method produces a sequence of active/inactive sets $(\mathcal{A}_k, \mathcal{I}_k)_{k=1,2,\dots}$ that approximate $(\mathcal{A}, \mathcal{I})$.

Linear systems

- The critical system to be solved is at each semismooth Newton iterate has the form

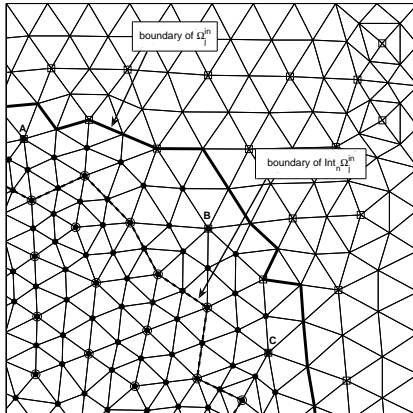
$$\mathbf{G}^{\mathcal{I}} \mathbf{u}_{\mathcal{I}} \stackrel{\text{def}}{=} (\beta \mathbf{I} + \mathbf{K}^{\mathbf{T}} \mathbf{K})^{\mathcal{I}\mathcal{I}} \mathbf{u}_{\mathcal{I}} = \mathbf{b}_{\mathcal{I}} .$$

where \mathcal{I} is the current guess at the inactive set.

- Similar preconditioning ideas can be applied: need a coarse space $V_{2h}^{\mathcal{I}} \subset V_h^{\mathcal{I}}$ then preconditioner is

$$\mathbf{M}_h = \beta(\mathbf{I} - \pi_{2h}^{\mathcal{I}}) + \mathbf{G}_h^{\mathcal{I}} \pi_{2h}^{\mathcal{I}}$$

Coarse space



Analysis

Theorem (A.D., 2011)

$$\rho(I - M_h^{-1}G_h) \leq C\beta^{-1} \left(h^2 + \sqrt{\mu_h^{\text{in}}} \right), \quad (8)$$

where μ_h^{in} is the Lebesgue measure of $\partial_n \Omega_h^{\text{in}}$

- Preconditioner is expected to be of suboptimal quality:

$$\rho(I - M_h^{-1}G_h) \leq Ch^{\frac{1}{2}}.$$

Outline

- 1 Model problems
- 2 Unconstrained problems with linear PDE constraints
- 3 **Nonlinear constraints, control constraints**
 - A semilinear elliptic constrained problem
 - Control-constrained problems
 - **Optimal control problems constrained by the Stokes equations**

Stokes control (with Ana Maria Soane)

- Model optimal control problem:

$$\begin{aligned} \text{minimize} \quad & \frac{\gamma_u}{2} \|\vec{u} - \vec{u}_d\|^2 + \frac{\gamma_p}{2} \|\boldsymbol{p} - \boldsymbol{p}_d\|^2 + \frac{\beta}{2} \|\vec{f} - \vec{f}_0\|^2 \\ \text{subj to:} \quad & -\nu \Delta \vec{u} + \nabla \boldsymbol{p} = \vec{f}, \\ & \operatorname{div} \vec{u} = 0, \quad \vec{u}|_{\Omega} = \vec{0} \end{aligned}$$

- Identify force \vec{f} closest to reference force \vec{f}_0 leading to given velocity and/or pressure “measurements” $\vec{u}_d, \boldsymbol{p}_d$

The Hessian

- The Hessian:

$$\mathbf{G}_h = \beta \mathbf{I} + \gamma_u \mathbf{U}_h^* \mathbf{U}_h + \gamma_p \mathbf{P}_h^* \mathbf{P}_h$$

- The proposed two-grid preconditioner:

$$\mathbf{M}_h = \beta \rho + \mathbf{G}_{2h} \pi$$

$$\mathbf{L}_h = (\mathbf{M}_h)^{-1} = \beta^{-1} \rho + (\mathbf{G}_{2h})^{-1} \pi$$

Two-grid preconditioner: Analysis

Theorem (A.D., A. Soane 2011)

With a Taylor-Hood $Q_2 - Q_1$ discretization and under regularity assumptions allowing for

$$\|(U - U_h)(f)\| \leq Ch^2 \|f\|, \quad \|(P - P_h)(f)\| \leq Ch \|f\|$$

we have

$$d_\sigma(G_h, M_h) \leq \frac{C}{\beta} (\gamma_u h^2 + \gamma_p h),$$

C independent of h , β , provided the coarsest grid is sufficiently fine.

Numerical Experiments – Pressure control

Table: Pressure measured only ($\gamma_u = 0$, $\gamma_p = 1$)

N	16			32			64			128			256	
no. levels	1	2	3	1	2	3	1	2	3	1	2	3	1	4
$\beta = 10^{-2}$	29	15	-	29	12	16	29	10	12	30	-	10	30	15
$\beta = 10^{-3}$	59	35	-	62	21	-	66	14	22	71	-	16	70	21

Time comparison at $n = 256$, number of state variables (velocity and pressure): 588290, number of control variables: 261121

no. levels	1	4
$\beta = 10^{-2}$	3460 s	2156 s
$\beta = 10^{-3}$	8457 s	2866 s

Matlab on 2x Intel (Nehalem) Xeon E5540 Quad Core (8M Cache, 2.53 GHz) CPUs with 24Gig RAM

Numerical Experiments – Velocity control

Table: Velocity measured only ($\gamma_u = 1$, $\gamma_p = 0$)

N	32			64			128			256		
no. levels	1	2	3	1	2	3	1	2	3	1	2	4
$\beta = 10^{-4}$	11	3	3	11	3	3	-	-	-	-	-	-
$\beta = 10^{-5}$	20	4	4	20	3	3	21	-	3	22	-	2
$\beta = 10^{-6}$	42	6	8	44	4	4	45	-	3	45	-	3

Time comparison at $n = 256$, number of state variables (velocity and pressure): 588290, number of control variables: 261121

no. levels	1	4
$\beta = 10^{-5}$	2622 s	393 s
$\beta = 10^{-6}$	5303 s	599 s

Conclusions

- Multigrid techniques open the possibility of solving an increasing class of large-scale PDE constrained optimal control problems at a reasonable cost.
- Main ingredients: a fast and reliable outer iteration (Newton, IPM, semismooth Newton), fast methods for the linear systems involved.
- Current techniques do not work as well for control-constrained problems (require special formulation, linear elements).

Future work and open problems

- Good preliminary results for steady-state Navier-Stokes controlled problems.
- Space-time PDEs and controls.
- Hyperbolic PDE constrained problems.
- Control-constrained problems: reconcile multigrid preconditioners for IPM and SSNM; handle higher order elements.
- State-constrained problems: will any of this work?