An Interior-Point Algorithm with Inexact Step Computations for Large-scale Optimization

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Outline

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Introduction

Interior-Point with Inexact Steps

Numerical Results

Summary and Future Work

Large-scale constrained optimization

Consider large-scale problems of the form

$$\begin{aligned} \min\ & f(x) \\ \text{s.t.}\ & c^{\mathcal{E}}(x) = 0 \\ & c^{\mathcal{I}}(x) \geq 0 \end{aligned}$$

Large-scale constrained optimization

Consider large-scale problems of the form

$$\begin{aligned} &\min\ f(x) \\ &\text{s.t. } c^{\mathcal{E}}(x) = 0 \\ &\qquad c^{\mathcal{I}}(x) \geq 0 \end{aligned}$$

- True problem of interest is infinite-dimensional
- Equality constraints include a discretized PDE
- $x = (y, u)$ is composed of states y and controls u
- Inequality constraints include control (and state?) bounds

Strengths

We propose an algorithm for large-scale nonlinear optimization:

- It can handle ill-conditioned/rank-deficient problems
- It can handle nonconvex problems
- Inexactness is allowed and controlled with loose conditions
- The conditions are implementable (in fact, implemented)
- The algorithm is globally convergent
- It can handle problems with control and state constraints
- Numerical results are very encouraging so far

Weaknesses

Aim to have an algorithm for PDE-constrained optimization, but so far:

- We solve for a single discretization
- We use finite-dimensional norms
- Our implementation does not exploit structure
- We need further experimentation on interesting problems

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Aim to have an algorithm for PDE-constrained optimization, but so far:

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- Our implementation does not exploit structure
- We need further experimentation on interesting problems

I'll close the talk with questions; you might have the answers!

Interior-point methods

- Add slacks to form the logarithmic-barrier subproblem

$$\begin{aligned} \min \ & f(x) - \mu \sum_{i \in \mathcal{I}} \ln s^i \\ \text{s.t. } & c^{\mathcal{E}}(x) = 0 \\ & c^{\mathcal{I}}(x) = s \end{aligned}$$

- The first-order optimality conditions are

$$\begin{aligned} \nabla f(x) + \nabla c^{\mathcal{E}}(x)\lambda^{\mathcal{E}} + \nabla c^{\mathcal{I}}(x)\lambda^{\mathcal{I}} &= 0 \\ -\mu S^{-1} e - \lambda^{\mathcal{I}} &= 0 \\ c^{\mathcal{E}}(x) &= 0 \\ c^{\mathcal{I}}(x) - s &= 0 \end{aligned}$$

along with $s > 0$

Newton's method

- Newton iteration involves the linear system

$$\begin{bmatrix} H_k & 0 & \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & \mu S_k^{-2} & 0 & -I \\ {\nabla c_k^{\mathcal{E}}}^T & 0 & 0 & 0 \\ {\nabla c_k^{\mathcal{I}}}^T & -I & 0 & 0 \end{bmatrix} \begin{bmatrix} d_k^x \\ d_k^s \\ \delta_k^{\mathcal{E}} \\ \delta_k^{\mathcal{I}} \end{bmatrix} = - \begin{bmatrix} \nabla f_k + \nabla c_k^{\mathcal{E}} \lambda_k^{\mathcal{E}} + \nabla c_k^{\mathcal{I}} \lambda_k^{\mathcal{I}} \\ -\mu S_k^{-1} e - \lambda_k^{\mathcal{I}} \\ c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix}$$

- Search direction computation followed by a line search

Usual questions

- How do we ensure global convergence?
- How do we solve ill-conditioned problems?
- How do we handle nonconvexity?

Usual answers

- How do we ensure global convergence?
  - KKT conditions (convex case)
  - Merit/penalty function
  - Filter
- How do we solve ill-conditioned problems?
  - Matrix modifications
  - Trust regions
- How do we handle nonconvexity?
  - Matrix modifications
  - Trust regions

More questions

For large-scale problems:

- What if the derivative matrices cannot be stored?
- What if the derivative matrices cannot be factored?

We can use iterative in place of direct methods:

- Can we allow inexactness?
- How do we ensure global convergence, handle ill-conditioning, and handle nonconvexity if solutions are inexact?

Outline

Scaling and slack reset

- We begin by scaling the Newton system

$$\begin{bmatrix} H_k & 0 & \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & \Omega_k & 0 & -S_k \\ \nabla c_k^{\mathcal{E}\,T} & 0 & 0 & 0 \\ \nabla c_k^{\mathcal{I}\,T} & -S_k & 0 & 0 \end{bmatrix} \begin{bmatrix} d_k^x \\ \tilde{d}_k^s \\ \delta_k^{\mathcal{E}} \\ \delta_k^{\mathcal{I}} \end{bmatrix} = - \begin{bmatrix} \nabla f_k + \nabla c_k^{\mathcal{E}} \lambda_k^{\mathcal{E}} + \nabla c_k^{\mathcal{I}} \lambda_k^{\mathcal{I}} \\ -\mu e - S_k \lambda_k^{\mathcal{I}} \\ c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix}$$

- Primal-dual matrix now has nicer properties
- The use of a slack reset

$$s_k \geq \max\{0, c^{\mathcal{I}}(x_k)\}$$

allows easier infeasibility detection

Rank deficiency

$$\begin{bmatrix} H_k & 0 & \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & \Omega_k & 0 & -S_k \\ \nabla c_k^{\mathcal{E}\,T} & 0 & 0 & 0 \\ \nabla c_k^{\mathcal{I}\,T} & -S_k & 0 & 0 \end{bmatrix} \begin{bmatrix} d_k^x \\ \tilde{d}_k^s \\ \delta_k^{\mathcal{E}} \\ \delta_k^{\mathcal{I}} \end{bmatrix} = - \begin{bmatrix} \nabla f_k + \nabla c_k^{\mathcal{E}} \lambda_k^{\mathcal{E}} + \nabla c_k^{\mathcal{I}} \lambda_k^{\mathcal{I}} \\ -\mu e - S_k \lambda_k^{\mathcal{I}} \\ c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix}$$

If the constraint Jacobian is singular or ill-conditioned

- The system may be inconsistent
- The search directions $(d_k^x, \tilde{d}_k^s, \delta_k^{\mathcal{E}}, \delta_k^{\mathcal{I}})$ may blow up
- The line search may break down

Matrix modifications

$$\begin{bmatrix} H_k & 0 & \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & \Omega_k & 0 & -S_k \\ {\nabla c_k^{\mathcal{E}}}^T & 0 & -\xi I & 0 \\ {\nabla c_k^{\mathcal{I}}}^T & -S_k & 0 & -\xi I \end{bmatrix} \begin{bmatrix} d_k^x \\ \tilde{d}_k^s \\ \delta_k^{\mathcal{E}} \\ \delta_k^{\mathcal{I}} \end{bmatrix} = - \begin{bmatrix} \nabla f_k + \nabla c_k^{\mathcal{E}} \lambda_k^{\mathcal{E}} + \nabla c_k^{\mathcal{I}} \lambda_k^{\mathcal{I}} \\ -\mu e - S_k \lambda_k^{\mathcal{I}} \\ c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix}$$

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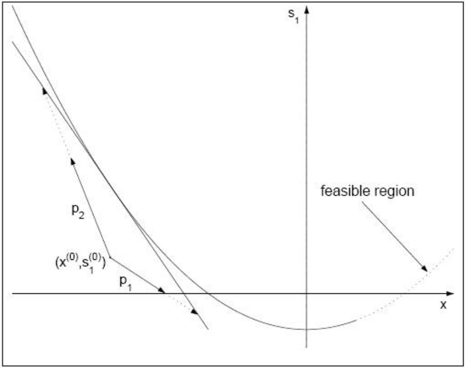
However, without matrix factorizations (i.e., no idea of the inertia)

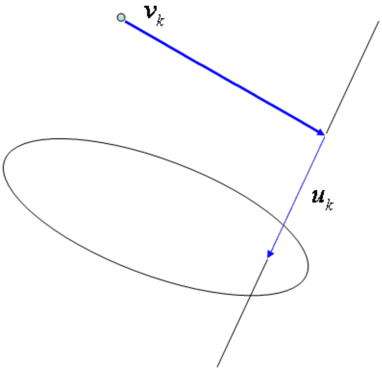
- When should this modification be performed?
- What value should ξ take? How large?
- How do we ensure that in the end we solve the right problem?

Failure of line search methods

- Recall the counter-example of Wächter and Biegler (2000)



Step decomposition

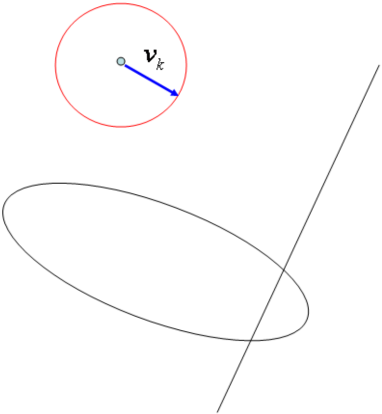


Normal step

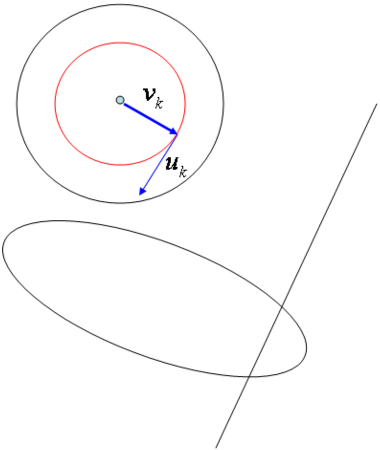
$$\min \frac{1}{2} \left\| \begin{bmatrix} c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix} + \begin{bmatrix} \nabla c_k^{\mathcal{E}\,T} & 0 \\ \nabla c_k^{\mathcal{I}\,T} & -S_k \end{bmatrix} \begin{bmatrix} v_k^x \\ \tilde{v}_k^s \end{bmatrix} \right\|^2$$

$$\text{s.t.} \left\| \begin{bmatrix} v_k^x \\ \tilde{v}_k^s \end{bmatrix} \right\| \leq \omega \left\| \begin{bmatrix} \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & -S_k \end{bmatrix} \begin{bmatrix} c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix} \right\|$$

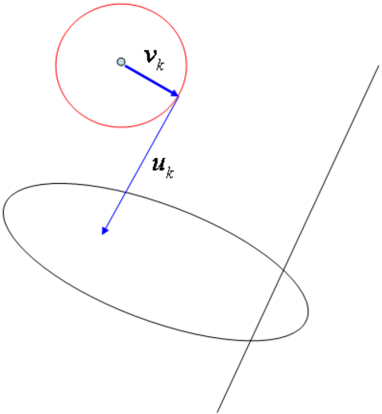
- QP w/ trust region constraint
- Trust region radius is zero at first-order minimizers of infeasibility
- Radius updates automatically
- Solve w/ CG or inexact dogleg



Tangential step



Tangential step



Nonconvexity

- During primal-dual step computation, convexify the Hessian

$$\begin{bmatrix} H_k + \xi I & 0 & \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & \Omega_k + \xi I & 0 & -S_k \\ \nabla c_k^{\mathcal{E}\,T} & 0 & 0 & 0 \\ \nabla c_k^{\mathcal{I}\,T} & -S_k & 0 & 0 \end{bmatrix}$$

(i.e. increase ξ) whenever

$$\left\| \begin{bmatrix} u_k^x \\ \tilde{u}_k^s \end{bmatrix} \right\| > \psi \left\| \begin{bmatrix} v_k^x \\ \tilde{v}_k^s \end{bmatrix} \right\|$$

$$\begin{bmatrix} u_k^x \\ \tilde{u}_k^s \end{bmatrix}^T \begin{bmatrix} H_k + \xi I & 0 \\ 0 & \Omega + \xi I \end{bmatrix} \begin{bmatrix} u_k^x \\ \tilde{u}_k^s \end{bmatrix} < \theta \left\| \begin{bmatrix} u_k^x \\ \tilde{u}_k^s \end{bmatrix} \right\|^2$$

for some $\psi, \theta > 0$

- In our tests, modifications are few and early
- We avoid having to develop conditions for inexact projections

Primal-dual step computation

We can be brave and approach the full system (avoid normal step)

$$\begin{bmatrix} H_k & 0 & \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & \Omega_k & 0 & -S_k \\ \nabla c_k^{\mathcal{E}\,T} & 0 & 0 & 0 \\ \nabla c_k^{\mathcal{I}\,T} & -S_k & 0 & 0 \end{bmatrix} \begin{bmatrix} d_k^x \\ \tilde{d}_k^s \\ \delta_k^{\mathcal{E}} \\ \delta_k^{\mathcal{I}} \end{bmatrix} = - \begin{bmatrix} \nabla f_k + \nabla c_k^{\mathcal{E}} \lambda_k^{\mathcal{E}} + \nabla c_k^{\mathcal{I}} \lambda_k^{\mathcal{I}} \\ -\mu e - S_k \lambda_k^{\mathcal{I}} \\ c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix}$$

... or compute a normal step, then approach the perturbed system

$$\begin{bmatrix} H_k & 0 & \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & \Omega_k & 0 & -S_k \\ \nabla c_k^{\mathcal{E}\,T} & 0 & 0 & 0 \\ \nabla c_k^{\mathcal{I}\,T} & -S_k & 0 & 0 \end{bmatrix} \begin{bmatrix} d_k^x \\ \tilde{d}_k^s \\ \delta_k^{\mathcal{E}} \\ \delta_k^{\mathcal{I}} \end{bmatrix} = - \begin{bmatrix} \nabla f_k + \nabla c_k^{\mathcal{E}} \lambda_k^{\mathcal{E}} + \nabla c_k^{\mathcal{I}} \lambda_k^{\mathcal{I}} \\ -\mu e - S_k \lambda_k^{\mathcal{I}} \\ -\nabla c_k^{\mathcal{E}\,T} v_k^x \\ -\nabla c_k^{\mathcal{I}\,T} v_k^x + d_k^s \end{bmatrix}$$

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How do we allow inexact solutions?

Consistency between the direction and the merit function

- In unconstrained optimization and nonlinear equations, there is always consistency (even w/ inexact steps) between the step computation and the function that measures progress
- In constrained optimization, however, our search direction is based on optimality conditions

$$\begin{bmatrix} \nabla f(x) + \nabla c^{\mathcal{E}}(x)\lambda^{\mathcal{E}} + \nabla c^{\mathcal{I}}(x)\lambda^{\mathcal{I}} \\ -\mu S^{-1}e - \lambda^{\mathcal{I}} \\ c^{\mathcal{E}}(x) \\ c^{\mathcal{I}}(x) - s \end{bmatrix} = 0$$

  but we judge progress by a merit function

$$\phi(x, s; \pi) \triangleq f(x) - \mu \sum_{i \in \mathcal{I}} \ln s^i + \pi \left\| \begin{bmatrix} c^{\mathcal{E}}(x) \\ c^{\mathcal{I}}(x) - s \end{bmatrix} \right\|$$

- Consistency is not automatic! A direction that may reduce the KKT error may not be a direction of descent for the merit function

Model reductions

- We ensure consistency by requiring model reductions
- Define the model of $\phi(x, s; \pi)$ at (x_k, s_k):

$$m_k(d^x, \tilde{d}^s; \pi) \triangleq f_k + \nabla f_k^T d^x - \mu \sum_{i \in \mathcal{I}} \ln s_k^i - \mu \tilde{d}^s + \pi \left(\left\| \begin{bmatrix} c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix} + \begin{bmatrix} \nabla c_k^{\mathcal{E}\,T} & 0 \\ \nabla c_k^{\mathcal{I}\,T} & -S_k \end{bmatrix} \begin{bmatrix} d^x \\ \tilde{d}^s \end{bmatrix} \right\| \right)$$

- d_k is acceptable if

$$\Delta m_k(d_k^x, \tilde{d}_k^s; \pi) \triangleq m_k(0, 0; \pi_k) - m_k(d_k^x, \tilde{d}_k^s; \pi) \gg 0$$

- This ensures descent (and more)

Termination tests

$$\begin{bmatrix} H_k & 0 & \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & \Omega_k & 0 & -S_k \\ \nabla c_k^{\mathcal{E}\,T} & 0 & 0 & 0 \\ \nabla c_k^{\mathcal{I}\,T} & -S_k & 0 & 0 \end{bmatrix} \begin{bmatrix} d_k^x \\ \tilde{d}_k^s \\ \delta_k^{\mathcal{E}} \\ \delta_k^{\mathcal{I}} \end{bmatrix} = - \begin{bmatrix} \nabla f_k + \nabla c_k^{\mathcal{E}} \lambda_k^{\mathcal{E}} + \nabla c_k^{\mathcal{I}} \lambda_k^{\mathcal{I}} \\ -\mu e - S_k \lambda_k^{\mathcal{I}} \\ c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix} + \begin{bmatrix} \rho_k^x \\ \rho_k^s \\ \rho_k^{\mathcal{E}} \\ \rho_k^{\mathcal{I}} \end{bmatrix}$$

Search direction is acceptable if

- (TT1) dual residual is sufficiently small, tangential component is bounded by normal component or by sufficient convexity, and model reduction is sufficiently large for current penalty parameter
- (TT2) dual residual is sufficiently small, tangential component is bounded by normal component or by sufficient convexity, and sufficient progress in linearized feasibility (model reduction obtained with increase in penalty parameter)
- (TT3) sufficient progress in reducing dual infeasibility

Interior-point algorithm with inexact step computations

(C., Schenk, and Wächter (2009))
for $k = 0, 1, 2, \ldots$

- Approximately solve for a normal step (optional?)
- Iteratively solve the primal-dual equations until TT1, TT2, or TT3 is satisfied, modifying the Hessian matrix when appropriate
- If only termination test 2 is satisfied, then increase π
- Backtrack from $\alpha_k \leftarrow 1$ to satisfy fraction-to-the-boundary and sufficient decrease conditions for the merit function ϕ
- Update the iterate
- Reset the slacks

Convergence (inner iteration)

Assumption

The sequence $\{(x_k, s_k, \lambda_k^{\mathcal{E}}, \lambda_k^{\mathcal{I}})\}$ *is contained in a convex set* Ω *over which* f, $c^{\mathcal{E}}$, $c^{\mathcal{I}}$, *and their first derivatives are bounded and Lipschitz continuous*

Theorem

If all limit points of the constraint Jacobians have full row rank, then

$$\lim_{k\to\infty} \left\| \begin{bmatrix} \nabla f_k + \nabla c_k^{\mathcal{E}} \lambda_k^{\mathcal{E}} + \nabla c_k^{\mathcal{I}} \lambda_k^{\mathcal{I}} \\ -\mu e - S_k \lambda_k^{\mathcal{I}} \\ c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix} \right\| = 0.$$

Otherwise,

$$\lim_{k\to\infty} \left\| \begin{bmatrix} \nabla c_k^{\mathcal{E}} & \nabla c_k^{\mathcal{I}} \\ 0 & -S_k \end{bmatrix} \begin{bmatrix} c_k^{\mathcal{E}} \\ c_k^{\mathcal{I}} - s_k \end{bmatrix} \right\| = 0$$

and if $\{\pi_k\}$ *is bounded, then*

$$\lim_{k\to\infty} \left\| \begin{bmatrix} \nabla f_k + \nabla c_k^{\mathcal{E}} \lambda_k^{\mathcal{E}} + \nabla c_k^{\mathcal{I}} \lambda_k^{\mathcal{I}} \\ -\mu e - S_k \lambda_k^{\mathcal{I}} \end{bmatrix} \right\| = 0$$

Convergence (outer iteration)

Theorem

If the algorithm yields a sufficiently accurate solution to the barrier subproblem for each $\{\mu_j\} \to 0$ *and if the linear independence constraint qualification (LICQ) holds at a limit point* $\bar{x}$ *of* $\{x_j\}$*, then there exist Lagrange multipliers* $\bar{\lambda}$ *such that the first-order optimality conditions of the nonlinear program are satisfied*

Outline

Implementation details

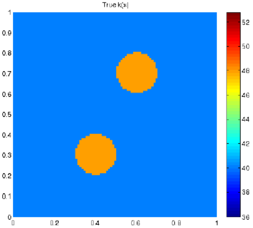
- Incorporated in `IPOPT` software package (Wächter)
  - `inexact_algorithm yes`
- Linear systems solved with `PARDISO` (Schenk)
  - SQMR (Freund (1994))
- Preconditioning in `PARDISO`
  - incomplete multilevel factorization with inverse-based pivoting
  - stabilized by symmetric-weighted matchings
- Optimality tolerance: 1e-8

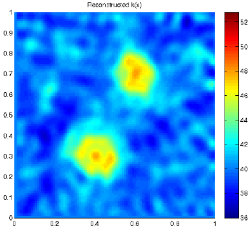
CUTEr and COPS collections

- 684 problems written in AMPL
- 580 solved successfully
- Robustness: $\sim$85%
- Original `IPOPT`: $\sim$94%

Parameter estimation for Helmholtz equation

Recover parameter k based on data collected from propagating waves





N	n	p	q	# iter	CPU sec (per iter)
32	14724	13824	1800	37	807.823 (21.833)
64	56860	53016	7688	25	3741.42 (149.66)
128	227940	212064	31752	20	54581.8 (2729.1)

Boundary control

$$\min \frac{1}{2}\int_\Omega (y(x) - y_t(x))^2 dx$$

$$\text{s.t.} \begin{cases} -\nabla \cdot (e^{y(x)} \cdot \nabla y(x)) & = & 20 & \text{in } \Omega \\ y(x) & = & u(x) & \text{on } \partial\Omega \\ 2.5 \leq u(x) & \leq & 3.5 & \text{on } \partial\Omega \end{cases}$$

where

$$y_t(x) = 3 + 10x_1(x_1 - 1)x_2(x_2 - 1)\sin(2\pi x_3)$$

N	n	p	q	# iter	CPU sec (per iter)
16	4096	2744	2704	13	2.8144 (0.2165)
32	32768	27000	11536	13	103.65 (7.9731)
64	262144	238328	47632	14	5332.3 (380.88)

Original `IPOPT` with $N = 32$ requires 238 seconds per iteration

Hyperthermia treatment planning

$$\min \frac{1}{2}\int_{\Omega}(y(x)-y_t(x))^2 dx$$

$$\text{s.t.} \left\{ \begin{array}{rcl} -\Delta y(x) - 10(y(x)-37) & = & u^* M(x) u \quad \text{in } \Omega \\ 37.0 \leq y(x) & \leq & 37.5 \quad \text{on } \partial\Omega \\ 42.0 \leq y(x) & \leq & 44.0 \quad \text{in } \Omega_0 \end{array} \right.$$

where

$$u_j = a_j e^{i\phi_j}, \quad M_{jk}(x) = < E_j(x), E_k(x) >, \quad E_j = \sin(j x_1 x_2 x_3 \pi)$$

N	n	p	q	# iter	CPU sec (per iter)
16	4116	2744	2994	68	22.893 (0.3367)
32	32788	27000	13034	51	3055.9 (59.920)

Original `IPOPT` with $N = 32$ requires 408 seconds per iteration

Groundwater modeling

$$\min \frac{1}{2}\int_\Omega (y(x)-y_t(x))^2 dx + \frac{1}{2}\alpha\int_\Omega [\beta(u(x)-u_t(x))^2 + |\nabla(u(x)-u_t(x))|^2] dx$$

$$\text{s.t.} \left\{ \begin{array}{rcll} -\nabla\cdot(e^{u(x)}\cdot\nabla y_i(x)) & = & q_i(x) & \text{in } \Omega, \quad i=1,\ldots,6 \\ \nabla y_i(x)\cdot n & = & 0 & \text{on } \partial\Omega \\ \int_\Omega y_i(x)dx & = & 0, & i=1,\ldots,6 \\ -1 \leq u(x) & \leq & 2 & \text{in } \Omega \end{array} \right.$$

where

$$q_i = 100\sin(2\pi x_1)\sin(2\pi x_2)\sin(2\pi x_3)$$

N	n	p	q	# iter	CPU sec (per iter)
16	28672	24576	8192	18	206.416 (11.4676)
32	229376	196608	65536	20	1963.64 (98.1820)
64	1835008	1572864	524288	21	134418. (6400.85)

Original IPOPT with $N = 32$ requires approx. 20 hours for the first iteration

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Interior-Point with Inexact Steps

Numerical Results

Summary and Future Work

Summary

We proposed an algorithm for large-scale nonlinear optimization:

- It can handle ill-conditioned/rank-deficient problems
- It can handle nonconvex problems
- Inexactness is allowed and controlled with loose conditions
- The conditions are implementable (in fact, implemented)
- The algorithm is globally convergent
- It can handle problems with control and state constraints
- Numerical results are very encouraging so far

Future work and questions

What are we missing (to *really* solve PDE-constrained problems)?

- PDE-specific preconditioners
- Use of appropriate norms
- Mesh refinement, error estimators

What does it take to transform an algorithm for finite-dimensional optimization into one for solving infinite-dimensional problems?

- Can the finite-dimensional solver be a black-box?
- If not, to what extent do the outer and inner algorithms need to be coupled? (Do *all* components of the finite-dimensional solver need to be checked for their effect on the infinite-dimensional problem?)

What interesting problems may be solved with our approach?

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