PDE-constrained Optimization and Beyond

Youngsoo Choi, Walter Murray, Philip Avery,
and hopefully (Charbel Farhat)

Institute for Computational and Mathematical Engineering,
Stanford University

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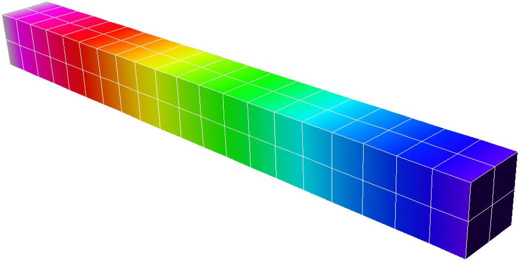
Outline

Outline

Thermal Conduction



Given boundary condition and temperature distribution

- Where and how much heat source do you need to apply?
- What if you are only allowed to supply heat source on the top surface?
- What if the number of heat source supplier is limited?

Forward PDE problem

continuous

$$-\Delta y = f$$
$$y = y_c \qquad \text{on } \Gamma$$

discretized (Finite Element)

$$Ky + K_{uc} y_c = f$$

Optimal Control

discretized

$$\begin{aligned} \underset{y,f}{\text{minimize}} \quad & J(y,f) := \frac{1}{2}\|y - \bar{y}\|_M^2 + \frac{\phi}{2}\|f\|_G^2 \\ \text{subject to} \quad & Ky - f = -K_{uc}y_c. \end{aligned}$$

- It is a strictly convex quadratic programming!
- No inequality constraints!

Outline

Optimality Condition

Lagrangian Function

$$L(y, f, \lambda) = \frac{1}{2}\|y - \bar{y}\|_M^2 + \frac{\phi}{2}\|f\|_G^2 + \lambda^T(Ky - f + K_{uc}y_c)$$

$$\downarrow$$

Optimality Condition

$$\begin{aligned}
\frac{\partial L}{\partial y} &= M(y - \bar{y}) + K^T\lambda = 0, \\
\frac{\partial L}{\partial f} &= \phi G f - \lambda = 0, \\
\frac{\partial L}{\partial \lambda} &= Ky - f = -K_{uc}y_c.
\end{aligned}$$

1. Dual Method

Dual function $g(\lambda)$ is defined as

$$g(\lambda) = \inf_{y,f} L(y, f, \lambda)$$

Dual solution λ^* is obtained by

$$\lambda^* = \arg\max_{\lambda} g(\lambda)$$

Dual Solution

$$(KM^{-1}K^T + \frac{1}{\phi}G^{-1})\lambda = K\bar{y} + K_{uc}y_c$$

Primal Solution

$$y^* = \bar{y} - M^{-1}K^T\lambda^*$$

$$f^* = \frac{1}{\phi}G^{-1}\lambda^*.$$

2. Primal-Dual Method

Primal-Dual Solution

$$\begin{bmatrix} M & & K^T \\ & \phi G & -I \\ K & -I & \end{bmatrix} \begin{bmatrix} y \\ f \\ \lambda \end{bmatrix} = \begin{bmatrix} M\bar{y} \\ 0 \\ -K_{uc}y_c \end{bmatrix}$$

Preconditioner

$$P = \begin{bmatrix} M & & \\ & \phi G & \\ & & KM^{-1}K^T + \frac{1}{\phi}G^{-1} \end{bmatrix}.$$

- Malcolm F. Murphy, Gene H. Golub, and Andrew J. Wathen. A note on preconditioning for indefinite linear systems, 1999.

3. Unconstrained Method

Optimal Control

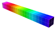
$$\begin{aligned} \underset{y,f}{\text{minimize}} \quad & J(y,f) := \frac{1}{2}\|y-\bar{y}\|_M^2 + \frac{\phi}{2}\|f\|_G^2 \\ \text{subject to} \quad & Ky + K_{uc}y_c = f. \end{aligned}$$

Variable Reduction

$$\underset{y}{\text{minimize}} \quad \bar{J}(y) := \frac{1}{2}y^T(M+\phi K^T G K)y - (\bar{y}^T M - \phi y_c^T K_{uc}^T G K)y$$

Solutions

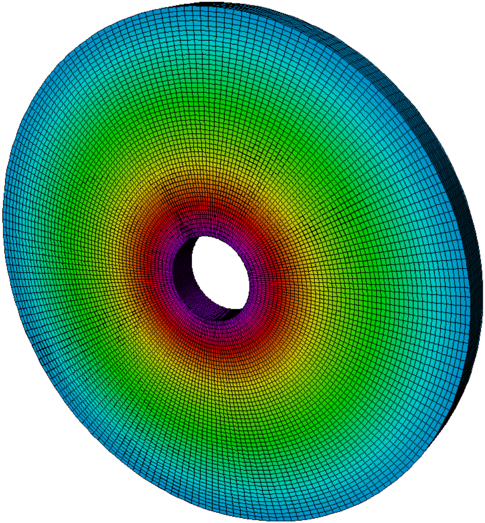
$$\begin{aligned} y^* &= (M+\phi K^T G K)^{-1}(M\bar{y} - \phi K^T G K_{uc} y_c), \\ f^* &= Ky^* + K_{uc}y_c. \end{aligned}$$

Computational Results 

comparison of various methods of solving linear thermal optimal control on metal bar.

# of dof : 180				
method	ϕ	comput. time(sec)	# of iter.	difference with target
dual	0.00001	0.01	3	1.74855693e-08
(minres)	0.0001	0.01	3	1.74853013e-07
	0.001	0.01	3	1.74826218e-06
	0.01	0.01	4	1.74558828e-05
primal & dual	0.00001	0.02(0.01)	34(6)	6.72648805e-08(1.81436529e-08)
(minres)	0.0001	0.02(0.01)	34(4)	1.91104769e-07(1.82765295e-07)
	0.001	0.02(0.01)	34(6)	1.75505860e-06(1.74823793e-06)
	0.01	0.02(0.01)	34(5)	1.74635852e-05(1.74559038e-05)
unconstrained	0.00001	0.01	8	1.71522833e-08
(minres)	0.0001	0.01	10	1.74855476e-07
	0.001	0.01	11	1.74822134e-06
	0.01	0.01	14	1.74558774e-05

Convection Boundary Condition



Computational Results 

comparison of various methods of solving linear thermal optimal control on donut.

# of dof : 96900				
method	ϕ	comput. time(sec)	# of iter.	difference with target
dual	0.00001	3.14	2	1.82738070e-13
(minres)	0.0001	3.15	2	1.81193236e-12
	0.001	3.19	2	1.81167574e-11
	0.01	3.18	2	1.81166632e-10
primal & dual	0.00001	10.59(3.72)	52(3)	9.33730206e-05(1.34913699e-05)
(minres)	0.0001	10.35(8.99)	52(16)	9.33730206e-05(1.16234951e-03)
	0.001	10.62(9.29)	52(16)	9.33730206e-05(2.77568592e-04)
	0.01	10.63(9.01)	52(16)	9.33730206e-05(5.06289542e-04)
unconstrained	0.00001	7.59	52	9.35276895e-05
(gmres)	0.0001	7.79	53	4.81800609e-05
	0.001	7.79	53	4.68677512e-05
	0.01	8.48	56	3.65794083e-05

- For primal-dual method, if no preconditioner is applied, although minres has converged, constraints violation was considerable.
- For primal-dual method, if preconditioner is applied, minres has stagnated except the case of $\phi = 1.0e^{-5}$.

Questions

Given boundary condition and temperature distribution

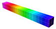
- Where and how much heat source do you need to apply?
- What if you are only allowed to supply heat source on the top surface?
- What if the number of heat source supplier is limited?

Restricted Optimal Control

Restricted Optimal Control

$$\begin{aligned} \underset{y, f_r}{\text{minimize}} \quad & J(y, f_r) := \frac{1}{2}\|y - \bar{y}\|_M^2 + \frac{\phi}{2}\|f_r\|_G^2 \\ \text{subject to} \quad & Ky + K_{uc} y_c = Bf_r. \end{aligned}$$

- Dual and primal-dual methods are applicable, but not unconstrained method.

Computational Results 

comparison of various methods of solving restricted optimal control on metal bar.

# of dof : 180				
method	ϕ	comput. time(sec)	# of iter.	difference with target
dual	0.00001	0.02	85	3.88274489e-02
(minres)	0.0001	0.02	84	3.88274604e-02
	0.001	0.01	83	3.88275760e-02
	0.01	0.01	82	3.88287308e-02
primal-dual	0.00001	0.05(0.1)	201(6)	3.88277111e-02(3.88274487e-02)
(minres)	0.0001	0.04(0.1)	201(6)	3.88277226e-02(3.88274605e-02)
	0.001	0.05(0.1)	200(8)	3.88278379e-02(3.88275760e-02)
	0.01	0.04(0.12)	200(9)	3.88289877e-02(3.88287301e-02)

Questions

Given boundary condition and temperature distribution

- Where and how much heat source do you need to apply?
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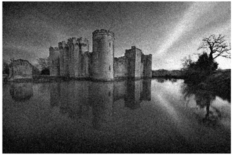
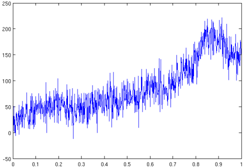
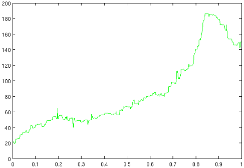
Outline

ℓ_1-regularization

- ℓ_1-regularization tends to give sparser solution.
- It is used a lot in compressed sensing.
- Below is a simple example of denoising (using subgradient method)







ℓ_1-regularization

ℓ_1-regularization

$$\begin{aligned} \underset{y,f}{\text{minimize}} \quad & J_1(y,f) := \frac{1}{2}\|y-\bar{y}\|_M^2 + \phi\|f\|_1 \\ \text{subject to} \quad & Ky + K_{uc}y_c = f. \end{aligned}$$

- It is not quadratic programming anymore.
- It is still strictly convex.
- No inequality constraints.
- Two numerical methods: (1)subgradient and (2)transformation to LP

Transformation to LP

Let $f = f_u - f_v$, where $f_u \geq 0$ and $f_v \geq 0$

Linear Programming in control variables

$$\begin{aligned} \underset{y, f_u, f_v}{\text{minimize}} \quad & J_L(y, f_u, f_v) := \frac{1}{2}\|y - \bar{y}\|_M^2 + \phi \sum_{i=1}^{m} (f_{u,i} + f_{v,i}) \\ \text{subject to} \quad & Ky + K_{uc} y_c = f_u - f_v, \\ & f_u \geq 0, \\ & f_v \geq 0. \end{aligned}$$

- Inequality Constraints have appeared
- Interior point method is applied

Interior Point Method

Logarithmic Barrier Formulation

$$\underset{y, f_u, f_v}{\text{minimize}} \quad J_L(y, f_u, f_v; t) := \frac{t}{2}\|y - \bar{y}\|_M^2 + t\phi \sum_{i=1}^{m} (f_{u,i} + f_{v,i}) - \sum_{i=1}^{m} \log f_{u,i} - \sum_{i=1}^{m} \log f_{v,i}$$

$$\text{subject to} \quad Ky + K_{uc} y_c = f_u - f_v.$$

- Inequality Constraints have disappeared
- Increase t gradually $\rightarrow$ continuation method
- It is easy to get gradient and hessian

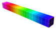
Gradient and Hessian

Gradient

$$g = \begin{bmatrix} tM(y - \bar{y}) \\ t\phi e - \begin{bmatrix} \frac{1}{f_{u,1}} \\ \vdots \\ \frac{1}{f_{u,m}} \end{bmatrix} \\ t\phi e - \begin{bmatrix} \frac{1}{f_{v,1}} \\ \vdots \\ \frac{1}{f_{v,m}} \end{bmatrix} \end{bmatrix}.$$

Hessian

$$H = \begin{bmatrix} tM & & \\ & \begin{bmatrix} \frac{1}{f_{u,1}^2} & & \\ & \ddots & \\ & & \frac{1}{f_{u,m}^2} \end{bmatrix} & \\ & & \begin{bmatrix} \frac{1}{f_{v,1}^2} & & \\ & \ddots & \\ & & \frac{1}{f_{v,m}^2} \end{bmatrix} \end{bmatrix}.$$

Computational Results 

ℓ_2-regularization

6.15291e-08 3.46168e-08 6.15291e-08 3.46381e-08 -1.51674e-07 3.46381e-08 6.15296e-08 3.46177e-08 6.1529e-08 -62.5 -125 -62.5 -125 -250 -125 -62.5 -125 -62.5

$\downarrow$

ℓ_1-regularization

0 0 0 0 0 0 0 0 0 -62.4865 -124.881 -62.4338 -124.779 -249.977 -124.761 -62.4165 -124.845 -62.4626

Outline

Nonlinear PDE-based Optimal Control

Nonlinear Constraint

$$\begin{aligned} \underset{y,f}{\text{minimize}} \quad & J(y,f) := \frac{1}{2}\|y-\bar{y}\|_M^2 + \frac{\phi}{2}\|f\|_G^2 \\ \text{subject to} \quad & F(y,f) = 0, \end{aligned}$$

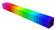
- Radiation makes heat conduction problem nonlinear
- SQP method is used

Sequential Quadratic Programming

Quadratic Subproblem

$$\begin{aligned} \underset{\Delta y, \Delta f}{\text{minimize}} \quad & J_s(\Delta y, \Delta f) := \frac{1}{2}\|y + \Delta y - \bar{y}\|_M^2 + \frac{\phi}{2}\|f + \Delta f\|_G^2 \\ \text{subject to} \quad & F(y, f) + K\Delta y - \Delta f = 0, \end{aligned}$$

- Any three methods introduced earlier is applicable.
- Δy^*, Δf^* are served as search direction.
- Augmented Lagrangian function is used in line search

Computational Results 

On metal bar

# of dof : 6561				
method	ϕ	comput. time(sec)	# of iter.	difference with target
SQP	0.000001	6.62	3	5.10127915e-11
	0.00001	6.67	3	5.10127711e-10
	0.0001	6.6	3	5.10126484e-09
	0.001	6.62	3	5.10113886e-08

Outline

1. An application of PDE-based Optimal Control
2. Three Numerical Methods
3. ℓ_1-regularization
4. Nonlinear PDE-based Optimal Control
5. Parallel Implementation of Optimal Control
6. Summary

Parallel Implementation of Optimal Control

FETI

$$K_s y_s = f_s + {B_s}^T \lambda \qquad \text{for } s = 1, \ldots, N_s,$$

$$\sum_{s=1}^{N_s} B_s y_s = 0,$$

- KKT system of equations from optimization problem
- λ can be interpreted as action-reaction force between interfaces
- A straight forward implementation of Optimal Control exists

FETIOP

- Consider $N_s = 2$ for simplicity
- Generalization to N_s case is straightforward

FETIOP

$$\begin{aligned}
\underset{y,f,\lambda}{\text{minimize}} \quad & J(y,f,\lambda) := \frac{1}{2}\sum_{s=1}^{2} \|y_s - \bar{y}_s\|_{M_s}^2 + \frac{1}{2}\sum_{s=1}^{2} \phi_s \|f_s\|_G^2 + \frac{\phi_\lambda}{2}\|\lambda\|_G^2 \\
\text{subject to} \quad & K_s y_s = f_s + {B_s}^T \lambda \qquad \text{for } s = 1, 2, \\
& \sum_{s=1}^{2} B_s y_s = 0.
\end{aligned}$$

- λ does not have to be included
- However, it is nice to include it

FETIOP

Lagrangian function

$$L(y, f, \lambda, \mu, \gamma) = J(y, f, \lambda) + \sum_{s=1}^{2} \mu_s^T (K_s y_s - f_s - {B_s}^T \lambda) + \gamma^T \sum_{s=1}^{2} B_s y_s.$$

- Note that there are two kinds of Lagrange multipliers: μ_s and γ.

FETIOP

KKT optimality condition

$$
\begin{aligned}
\frac{\partial L}{\partial y_s} &= M_s(y_s - \bar{y}_s) + K_s{}^T \mu^s + B_s{}^T \gamma = 0, \\
\frac{\partial L}{\partial f_s} &= \phi_s G f_s - \mu_s = 0, \\
\frac{\partial L}{\partial \lambda} &= -\sum_{s=1}^{2} B_s \mu_s + \phi_\lambda G \lambda = 0, \\
\frac{\partial L}{\partial \mu_s} &= K_s y_s - f_s - B_s{}^T \lambda = 0, \\
\frac{\partial L}{\partial \gamma} &= \sum_{s=1}^{2} B_s y_s = 0.
\end{aligned} \tag{1}
$$

- Solve dual problem

FETIOP

Dual Problem

$$Ax = b,$$

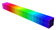
where

$$A = \begin{bmatrix} K^1 {M_1}^{-1} {K_1}^T + \frac{1}{\phi_1} G^{-1} + \frac{1}{\phi_\lambda} {B_1}^T B^1 & \frac{1}{\phi_\lambda} {B_1}^T B_2 & K_1 {M_1}^{-1} {B_1}^T \\ \frac{1}{\phi_\lambda} {B_2}^T B_1 & K_2 {M_2}^{-1} {K_2}^T + \frac{1}{\phi_2} G^{-1} + \frac{1}{\phi_\lambda} {B_2}^T B_2 & K_2 {M_2}^{-1} {B_2}^T \\ B_1 {M_1}^{-1} {K_1}^T & B_2 {M_2}^{-1} {K_2}^T & \sum_{s=1}^{N_s} B_s {M_s}^{-1} {B_s}^T \end{bmatrix}$$

$$x = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \gamma \end{bmatrix}$$

$$b = \begin{bmatrix} K_1 \bar{y}_1 \\ K_2 \bar{y}_2 \\ 0 \end{bmatrix}$$

- Then update primal solutions

Computational Results 

On metal bar

# of dof : 189				
method	ϕ	comput. time(sec)	# of iter.	difference with target
DAE	$1.0e^{-9}$	0.01	2	2.13539170e-12
	$1.0e^{-8}$	0.01	2	2.13639672e-11
	$1.0e^{-7}$	0.02	2	2.13650113e-10
	$1.0e^{-6}$	0.01	4	2.13651127e-09

Outline

Summary

- Three methods to solve QP, which arises in solving linear PDE-based optimal control, are presented.
- ℓ_1 regularization is introduced to invoke sparser control solution.
- Nonlinear PDE-based optimal control has been solved
- Straightforward parallel implementation of optimal control, using FETI, has been introduced.
- All the methods and problems introduced and solved above are promising for two reasons:
  1. They are ready to attack bigger and practical problems.
  2. They will base the dynamic optimal control problems.

Thank you