Hierarchical Solution Concepts for Flow Control Problems

Michael Hinze, Stefan Turek

Part of the SPP1253: Optimization with PDE's

Michael Köster

Institute for Applied Mathematics
TU Dortmund

ASIM 2013, 28.02. – 01.03.2013

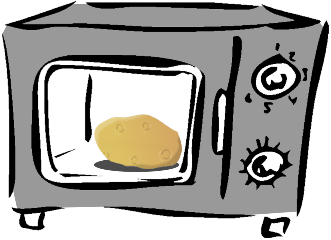
Overview

- Introduction
- Solution methods for optimal flow control
- Numerical example
- Summary

Heating of a potato in a microwave oven

Description of the heating process via the heat equation:

$$\partial_t u - \Delta u = f \qquad \text{in} \quad \mathcal{Q} := (0, T) \times \Omega$$



Heating of a potato in a microwave oven

Description of the heating process via the heat equation:

$$\partial_t u - \Delta u = f \qquad \text{in} \quad \mathcal{Q} := (0, T) \times \Omega$$

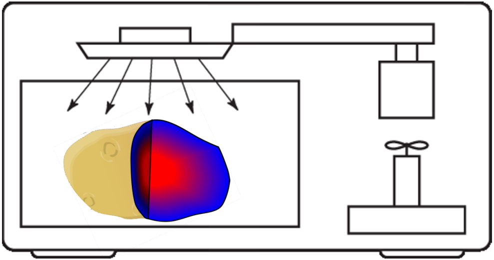
What is the optimal microwave field?

$\rightarrow$ Find best RHS f such that $u \approx z$ (given temp.)!

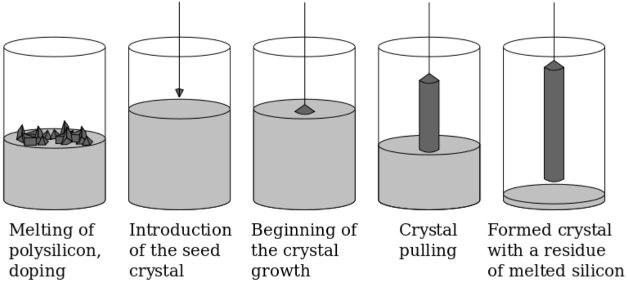
Minimisation with the heat equation as side condition:

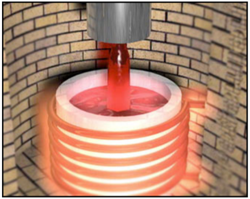
$$J(u,f) := \frac{1}{2}||u-z||_{\mathcal{Q}}^2 + \frac{\alpha}{2}||f||_{\mathcal{Q}}^2 \quad \longrightarrow \quad \text{min!}$$

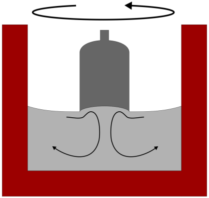
$$\text{with} \qquad \partial_t u - \Delta u = f \qquad \text{in} \quad \mathcal{Q} := (0,T)\times\Omega$$

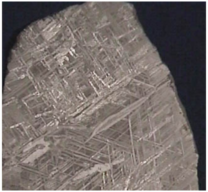


Czochralski method for crystal growth









Turbulence on the interface $\Rightarrow$ Structural defects

Simplified model problem

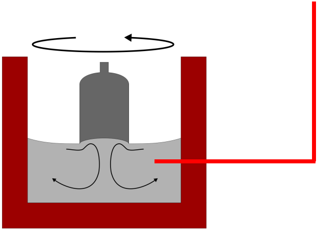
Distributed Control for the nonstationary Navier-Stokes equation
of tracking-type for a given z on $Q = \Omega \times (0, T)$:

$$J(u, f) = \frac{1}{2}||u - z||_Q^2 + \frac{\alpha}{2}||f||_Q^2 \quad \rightarrow \quad \text{min!}$$

subject to

$$\begin{aligned} u_t - \nu\Delta u + (u\nabla)u + \nabla p &= f \quad \text{in } Q \\ -\nabla \cdot u &= 0 \quad \text{in } Q \end{aligned}$$

+ BC, constraints, ...

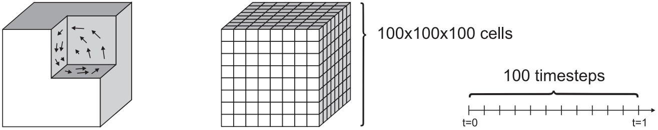


$u \approx z$

Challenges

Difficulty 1: Very high number of degrees of freedom

u, f:



- Distributed control $\Rightarrow$ f „lives” in the domain
- 4D, fully coupled, lin. FEM $\approx$ 500.000.000 DOFs $\approx$ 4 GB
- here prototypically: 2D + time $\Rightarrow$ 3D

Difficulty 2: fine meshes $\Rightarrow$ bad condition

- Eqn. contains $-\Delta$ + convection
- conventional solvers degenerate

Consequence: Conventional optimisation not applicable

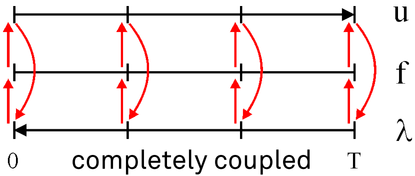
Idea 1: **Use methods from optimal control**

Lagrange approach on $\mathcal{Q} = (0, T) \times \Omega \quad \Rightarrow \quad$ KKT system

$$
\begin{aligned}
u_t - \nu \Delta u + (u\nabla)u + \nabla p &= f \\
-\lambda_t - \nu \Delta \lambda - (u\nabla)\lambda + (\nabla u)^T \lambda + \nabla \xi &= u - z \\
\alpha f + \lambda &= 0
\end{aligned}
$$

$$u(0) = u_0, \quad \lambda(T) = 0$$

+ incompressibility, BC, constraints, ...



Design of solution methods

Idea 2: **Eliminate variables, apply Newton.**

$$u_t - \nu \Delta u + \ldots = f$$
$$-\lambda_t - \nu \Delta \lambda + \ldots = u - z$$
$$\alpha f + \lambda = 0$$

Method 1: With $\lambda = \lambda(u(f))$, apply Newton solver to

$$F(f) := \alpha f + \lambda \overset{!}{=} 0$$

Method 2: With $x = (u, \lambda, p, \xi)$, apply Newton solver to

$$G(x) := \begin{pmatrix} u_t - \nu \Delta u + \ldots + \frac{1}{\alpha}\lambda \\ -\lambda_t - \nu \Delta \lambda + \ldots - u + z \\ \text{incompressibility, BC, constraints, ...} \end{pmatrix} \overset{!}{=} 0$$

Method 1: Newton approach in u

Algorithm (Newton applied to RHS space)

$$f_{n+1} := f_n + \bar{f}, \qquad F'(f_n)\bar{f} = -F(f_n)$$

Ingredients:

$$F(f) := \alpha f + \lambda \stackrel{!}{=} 0 \qquad\qquad F'(f)\bar{f} = \alpha\bar{f} + \bar{\lambda}$$

$$\left\{ \begin{array}{c} u_t - \nu\Delta u + ... = f \\ -\lambda_t - \nu\Delta\lambda + ... = u - z \end{array} \right\}, \qquad \left\{ \begin{array}{c} \bar{u}_t - \nu\Delta\bar{u} + ... = \bar{f} \\ -\bar{\lambda}_t - \nu\Delta\bar{\lambda} + ... = \bar{u} \end{array} \right\}$$

nonlinear simulation black box — linear simulation black box

+ CG for linear equation

Method 1: Newton approach in u

Algorithm (Newton applied to RHS space)

$$f_{n+1} := f_n + \bar{f}, \qquad F'(f_n)\bar{f} = -F(f_n)$$

$$\text{"}Ax = b\text{"}$$

Ingredients:

$$F(f) := \alpha f + \lambda \stackrel{!}{=} 0 \qquad\qquad F'(f)\bar{f} = \alpha\bar{f} + \bar{\lambda}$$

$$\left\{ \begin{array}{c} u_t - \nu\Delta u + \ldots = f \\ -\lambda_t - \nu\Delta\lambda + \ldots = u - z \end{array} \right\}, \qquad \left\{ \begin{array}{c} \bar{u}_t - \nu\Delta\bar{u} + \ldots = \bar{f} \\ -\bar{\lambda}_t - \nu\Delta\bar{\lambda} + \ldots = \bar{u} \end{array} \right\}$$

nonlinear simulation black box — linear simulation black box

+ CG for linear equation

Method 2: Newton approach in $x = (u, \lambda, p, \xi)$

Algorithm (Newton applied to primal/dual system)

$$x_{n+1} = x_n + \bar{x}, \qquad G'(x_n)\bar{x} = -G(x_n)$$

Ingredients:

$$G(x) := \begin{pmatrix} u_t - \nu\Delta u + ... + \frac{1}{\alpha}\lambda \\ -\lambda_t - \nu\Delta\lambda + ... - u + z \\ ... \end{pmatrix} \stackrel{!}{=} 0$$

$$G'(x)\bar{x} := \begin{pmatrix} \bar{u}_t - \nu\Delta\bar{u} + ... + \frac{1}{\alpha}\bar{\lambda} \\ -\bar{\lambda}_t - \nu\Delta\bar{\lambda} + ... - \bar{u} \\ ... \end{pmatrix}$$

+ preconditioned BiCGStab, GMRES,... for linear equation.

Method 2: Newton approach in $x = (u, \lambda, p, \xi)$

Algorithm (Newton applied to primal/dual system)

$$x_{n+1} = x_n + \bar{x}, \qquad G'(x_n)\bar{x} = -G(x_n)$$

$$\boxed{\text{"}Ax = b\text{"}}$$

Ingredients:

$$G(x) := \begin{pmatrix} u_t - \nu\Delta u + \ldots + \frac{1}{\alpha}\lambda \\ -\lambda_t - \nu\Delta\lambda + \ldots - u + z \\ \ldots \end{pmatrix} \stackrel{!}{=} 0$$

$$G'(x)\bar{x} := \begin{pmatrix} \bar{u}_t - \nu\Delta\bar{u} + \ldots + \frac{1}{\alpha}\bar{\lambda} \\ -\bar{\lambda}_t - \nu\Delta\bar{\lambda} + \ldots - \bar{u} \\ \ldots \end{pmatrix}$$

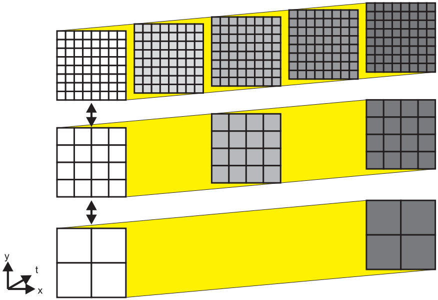
+ preconditioned BiCGStab, GMRES,... for linear equation.

Multigrid solver methodology

Expensive parts:

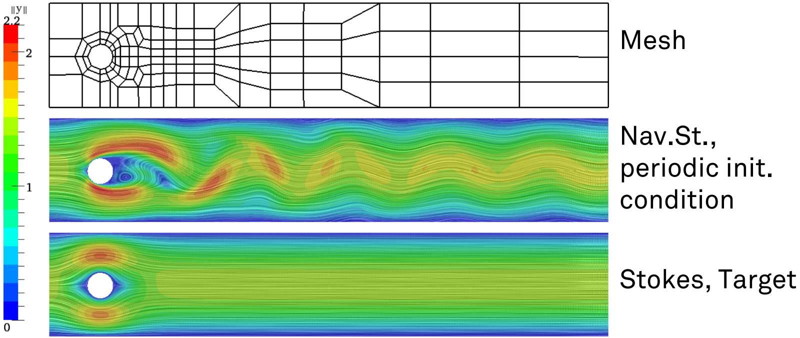
- $F'(f_n)\bar{f} = -F(f_n)$ $\Rightarrow$ space-time linear system in f.
- $G'(x_n)\bar{x} = -G(x_n)$ $\Rightarrow$ space-time linear system in x.

Solve using multigrid on a space-time hierarchy:



On each level: CG, BiCGStab, GMRES,...

Flow-around-cylinder (based on DFG benchmark BENCH2)



- Problem/Init. Cond.: Navier–Stokes, $Re = 100$, $t \in [0, 0.35]$
- Target flow z: Stationary Stokes flow
- Coarse mesh: Standard DFG benchmark

Numerical example

Discretisation:

- Q_2/P_1^{disc} in space, IE in time
- Coarse mesh: 520 elements, 20 timesteps, $\times 8$ per level

SLv.	#int.	#DOF(f)	#DOF(x)
2	20	87 360	237 120
3	40	682 240	1 863 680
4	80	5 391 360	14 776 320
5	160	42 864 640	117 678 080

Solver configuration (method 1+2):

- Residual reduction Newton 10^{-6}
- Residual reduction space-time MG 10^{-2}

Test 1: Newton solver in f

Newton-solver in the control space was:

$$f_{n+1} = f_n - F'(f_n)^{-1} F(f_n), \qquad F(f) := \alpha f + \lambda$$

CG solver for $F'(f_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	20:33	0:40	5	32	31.1
3	40	4:12:29	6:38	5	35	38.1
4	80	36:54:08	52:19	5	43	42.3

MG solver for $F'(f_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	coarse mesh				
3	40	5:40:00	6:38	4	8	51.3
4	80	46:03:22	52:19	5	9	52.7
5	160	297:26:50	6:13:18	5	8	47.8

Test 1: Newton solver in f

Newton-solver in the control space was:

$$f_{n+1} = f_n - F'(f_n)^{-1} F(f_n), \qquad F(f) := \alpha f + \lambda$$

CG solver for $F'(f_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	20:33	0:40	5	32	31.1
3	40	4:12:29	6:38	5	35	38.1
4	80	36:54:08	52:19	5	43	42.3

MG solver for $F'(f_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	coarse mesh				
3	40	5:40:00	6:38	4	8	51.3
4	80	46:03:22	52:19	5	9	52.7
5	160	297:26:50	6:13:18	5	8	47.8

Test 1: Newton solver in f

Newton-solver in the control space was:

$$f_{n+1} = f_n - F'(f_n)^{-1} F(f_n), \qquad F(f) := \alpha f + \lambda$$

CG solver for $F'(f_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{\text{opt}}}{T_{\text{sim}}}$
2	20	20:33	0:40	5	32	31.1
3	40	4:12:29	6:38	5	35	38.1
4	80	36:54:08	52:19	5	43	42.3

MG solver for $F'(f_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{\text{opt}}}{T_{\text{sim}}}$
2	20	coarse mesh				
3	40	5:40:00	6:38	4	8	51.3
4	80	46:03:22	52:19	5	9	52.7
5	160	297:26:50	6:13:18	5	8	47.8

Test 2: Newton solver in x

Newton-solver in the primal/dual space was:

$$x_{n+1} = x_n - G'(x_n)^{-1} G(x_n), \qquad G(x) := \begin{pmatrix} y_t - \nu \Delta y + \dots \\ -\lambda_t - \nu \Delta y + \dots \end{pmatrix}$$

BiCGStab solver for $G'(x_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	9:05	0:40	5	25	13.8
3	40	1:53:48	6:38	6	31	17.2
4	80	12:09:20	52:19	6	34	13.9

MG-solver for $G'(x_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	coarse mesh				
3	40	2:22:30	6:38	6	9	21.5
4	80	16:41:27	52:19	6	10	19.1

Test 2: Newton solver in x

Newton-solver in the primal/dual space was:

$$x_{n+1} = x_n - G'(x_n)^{-1} G(x_n), \qquad G(x) := \begin{pmatrix} y_t - \nu \Delta y + \dots \\ -\lambda_t - \nu \Delta y + \dots \end{pmatrix}$$

BiCGStab solver for $G'(x_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	9:05	0:40	5	25	13.8
3	40	1:53:48	6:38	6	31	17.2
4	80	12:09:20	52:19	6	34	13.9

MG-solver for $G'(x_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	coarse mesh				
3	40	2:22:30	6:38	6	9	21.5
4	80	16:41:27	52:19	6	10	19.1

Test 2: Newton solver in x

Newton-solver in the primal/dual space was:

$$x_{n+1} = x_n - G'(x_n)^{-1} G(x_n), \qquad G(x) := \begin{pmatrix} y_t - \nu \Delta y + \ldots \\ -\lambda_t - \nu \Delta y + \ldots \end{pmatrix}$$

BiCGStab solver for $G'(x_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	9:05	0:40	5	25	13.8
3	40	1:53:48	6:38	6	31	17.2
4	80	12:09:20	52:19	6	34	13.9

MG-solver for $G'(x_n)^{-1}$:

SLv.	#int	T_{opt}	T_{sim}	NL	$\sum$LIN	$\frac{T_{opt}}{T_{sim}}$
2	20	coarse mesh				
3	40	2:22:30	6:38	6	9	21.5
4	80	16:41:27	52:19	6	10	19.1

Comparison

- Newton in f: $f_{n+1} = f_n + \bar{f}$, $F'(f_n)\bar{u} = -F(f_n)$
- Newton in x: $x_{n+1} = x_n + \bar{x}$, $G'(x_n)\bar{x} = -G(x_n)$

	Newton in f	Newton in x
alg. complexity	low...medium → black-box applicable	high
$-F(u)$, $-G(x)$	simulation (nl.) → stopping criteria? robustness?	MatVec
apply $F'(u)$, $G'(x)$	simulation (lin.) → stopping criteria? robustness?	MatVec
preconditioner	Ø →not necessary?	expensive → inexact $\surd$ → paralleliseable $\surd$
Space-time MG	$\surd$	$\surd$

Summary

Two solution methods analysed:

- Newton in f $\leftrightarrow$ Newton in (u, λ, p, ξ)
- Space-time MG for linear subproblems

Main achievements:

- ”Optimal” complexity
- $T_{\text{opt}} / T_{\text{sim}} \approx 20 - 50$ $\rightarrow$ for ’optimal’ sim.
- Newton in (u, λ, p, ξ) usually more efficient than in f

Extensions: Combination of the methods? (Reduced-SQP)

Method 2: Construction of preconditioners

Algorithm (Defect correction loop)

$$\bar{x}_{new} = \bar{x} + C^{-1}(-G(x_n) - G'(x_n)\bar{x})$$

Discrete counterparts of $G'(x_n)$ and C (e.g., Block Jacobi):

$$G'_h(x_n) = \begin{pmatrix} A_{11} & M_{12} & & \\ M_{22} & A_{22} & M_{23} & \\ & M_{32} & A_{33} & \ddots \\ & & \ddots & \ddots \end{pmatrix}, \qquad C_h = \begin{pmatrix} A_{11} & & & \\ & A_{22} & & \\ & & A_{33} & \\ & & & \ddots \end{pmatrix}$$

$\Rightarrow \quad C^{-1}$ = solve coupled Nav.St. (A_{ii}^{-1}) in each timestep