Efficiently Solving Optimal Control Problems in CFD using Space-Time Multigrid Techniques

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Overview

- Introduction
- Optimal Control in Space and Time
- Design of a space-time One-Shot solver
- Numerical examples
- Outlook

Distributed Control of nonstationary flow

Distributed Control for the nonstationary Navier-Stokes equation with tracking-type functional for a given z:

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

on $Q = \Omega \times [0, T]$ such that

$$\begin{array}{rcll} y_t + (y\nabla)y - \nu\Delta y + \nabla p & = & u & \text{in } Q \\ -\nabla \cdot y & = & 0 & \text{in } Q \end{array} \quad + \text{BC}$$

No constraints on the control $u \in Q$.

Distributed Control of nonstationary flow

Corresponding KKT-System:

$$
\begin{aligned}
y_t + (y\nabla)y - \nu\Delta y + \nabla p &= u = -\tfrac{1}{\alpha}\lambda && \text{in } Q \\
-\nabla \cdot y &= 0 && \text{in } Q \\
-\lambda_t - \nu\Delta\lambda - (y\nabla)\lambda + (\nabla y)\lambda + \nabla\xi &= (y - z) && \text{in } Q \\
-\nabla \cdot \lambda &= 0 && \text{in } Q \\
\lambda(T) &= \gamma(y(T) - z(T)) && \text{in } \Omega
\end{aligned}
$$

+ boundary conditions

Design goals for a solver

Moderate performance measure; for C not too large:

$$\frac{\text{effort for optimization}}{\text{effort for simulation}} \leq C$$

Idea:

- One-shot approach $\rightarrow$ Newton + Multigrid in space–time.
- Efficient + accurate CFD-techniques: Multigrid + FEM methods for general configurations

Space–time discretisation

- Time discretisation:
  Backward Euler (later: Crank-Nicolson, FS-θ)

$$\frac{y_{i+1} - y_i}{\Delta t} - \Delta y_{i+1} + y_{i+1} \nabla y_{i+1} + \nabla p_{i+1} = \ldots$$

- Space discretisation:
  LBB-stable Finite Elements ($\tilde{Q}_1 / Q_0$, later $\tilde{Q}_2 / P_1$)
  on unstructured 2D meshes (later: 3D)

Space–time discretisation

$\Rightarrow$ Space–time system

$$A(x)x = b$$

Here (for n timesteps, $x_k = x(t_k)$):

$$x = (\underbrace{y_0, p_0, \lambda_0, \xi_0,}_{x_0} \; \ldots, \; \underbrace{y_n, p_n, \lambda_n, \xi_n}_{x_n})$$

Space–time discretisation

$A(x)$ has a very special structure! E.g. for 2 timesteps:

$$
\left(\begin{array}{c|c|c|c|c|c}
\begin{matrix} M & \\ & M \end{matrix} & & & & & \\
\hline
-M & \begin{matrix} \frac{M}{\Delta t} + N^* & -B \\ -B^T & \end{matrix} & & -\frac{M}{\Delta t} & & \\
\hline
-\frac{M}{\Delta t} & & \begin{matrix} \frac{M}{\Delta t} + N & -B \\ -B^T & \end{matrix} & \frac{1}{\alpha} M & & \\
\hline
& & -M & \begin{matrix} \frac{M}{\Delta t} + N^* & -B \\ -B^T & \end{matrix} & & -\frac{M}{\Delta t} \\
\hline
& & -\frac{M}{\Delta t} & & \begin{matrix} \frac{M}{\Delta t} + N & -B \\ -B^T & \end{matrix} & \frac{1}{\alpha} M \\
\hline
& & & & -\gamma M & \begin{matrix} \frac{M}{\Delta t} + N^* & -B \\ -B^T & \end{matrix}
\end{array}\right)
$$

$\rightarrow$ Sparse, (block) tridiagonal system

Design of a One-Shot solver

- Nonlinearity: Newton method.

$$x^{i+1} = x^i + A'^{-1}(x^i)(b - A(x^i)x^i)$$

$\longrightarrow$ Quadratic convergence

- Linear subproblems: space-time Multigrid solver

$\longrightarrow$ Convergence rates independent of refinement level of the space-time mesh

Space–time multigrid ingredients

Essential multigrid components:

- An efficient *smoother!*

  e.g. preconditioned defect correction loop
  (with $\tilde{A} := A'(x^i)$):

$$v^{j+1} = v^j + \omega P^{-1}(b - \tilde{A}v^j), \qquad j = 1, ..., \mathrm{NSM}$$

- Prolongation/Restriction
  - in space + time
  - only in time
  - mixed

Space–time discretisation

$\tilde{A}$ in compressed form (omitting B and B^T here):

$$\left(\begin{array}{cc|cc|cc|cc}
M & & & & & & & \\
-M & NST^* & & -\frac{M}{\Delta t} & & & & \\
\hline
-\frac{M}{\Delta t} & & NST & \frac{1}{\alpha}M & & & & \\
 & & -M & NST^* & & -\frac{M}{\Delta t} & & \\
\hline
 & & -\frac{M}{\Delta t} & & NST & \frac{1}{\alpha}M & & \\
 & & & & -M & NST^* & & -\frac{M}{\Delta t} \\
\hline
 & & & & & \cdots & & \cdots
\end{array}\right)$$

$\Rightarrow$ Block-Jacobi preconditioner:

$$P := P_{Jac} := \left(\begin{array}{cc|cc|cc|cc}
M & & & & & & & \\
-M & NST^* & & & & & & \\
\hline
 & & NST & \frac{1}{\alpha}M & & & & \\
 & & -M & NST^* & & & & \\
\hline
 & & & & NST & \frac{1}{\alpha}M & & \\
 & & & & -M & NST^* & & \\
\hline
 & & & & & & & \cdots
\end{array}\right)$$

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 & & -M & NST^* & & -\frac{M}{\Delta t} & & \\
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\hline
 & & & & & \dots & & \dots
\end{array}\right)
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& & & & -M & NST^* & & -\frac{M}{\Delta t} \\
\hline
& & & & & \dots & & \dots
\end{array}\right)$$

$\Rightarrow$ Gauß-Seidel-like preconditioner $P := P_{GS}$.

In every timestep:

$$\begin{pmatrix} -\frac{M}{\Delta t} & \\ & \end{pmatrix} v_{i-1} + {\color{red}\begin{pmatrix} NST & \frac{1}{\alpha}M \\ -M & NST^* \end{pmatrix}} v_i + \begin{pmatrix} & \\ & -\frac{M}{\Delta t} \end{pmatrix} v_{i+1} = \dots$$

$\rightarrow v_i$

Space–time preconditioner

Essential: To use $P^{-1}_{Jac/GS}$, separately apply

$$\begin{pmatrix} NST & \frac{1}{\alpha}M & B \\ -M & NST^* & B \\ B^T & B^T & \end{pmatrix}^{-1}$$

in every timestep!

Use:

$$\left.\begin{array}{l} \bullet \text{ Multigrid in space} \\ \quad \text{for coupled Nav.St.-problems} \\ \bullet \text{ Smoother: mod. LMPSC (VANKA-like)} \\ \quad \rightarrow \text{Primal and dual coupled!} \end{array}\right\} \textbf{FeatFlow!}$$

Numerical cost

- Assuming #NNL(Opt) = #NNL(Sim) per timestep
- NITT := #space-time MG iterations per nonlinear iteration
- NSM := #smoothing steps in space-time MG

A (pessimistic) upper bound is given by:

$$\frac{\text{effort for optimization}}{\text{effort for simulation}} \leq \text{NITT} \times \; 4 \times \text{NSM}$$

$\longrightarrow$ optimal case with 1 MG-step per nonlinear iteration

more...

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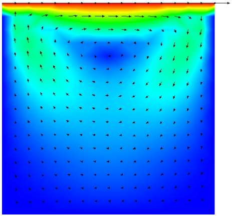
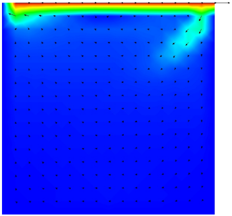
more...

Numerical example: Control of Driven Cavity

- Target flow z: Stokes flow, Re=1/400, $t \in [0, 1]$



Stokes, Re=1/400, $t = 1$



Nav.St., $Re = 400$, $t = 1$, uncontrolled

- Optimal control problem: Navier–Stokes, $Re = 400$.
- NSM=4, $\omega = 0.7$, fully implicit time discretisation.

Multigrid convergence

Time	Space	ρ
1..2 (10)	2..3	9.95E-04
	2..4	8.95E-04
	2..5	6.90E-04
1..3 (20)	2..3	8.80E-03
	2..4	8.00E-03
	2..5	6.51E-03
1..4 (40)	2..3	2.34E-02
	2..4	2.15E-02
	2..5	1.83E-02

Prol./Rest. only in time.

Time	Space	ρ
1..2 (10)	2..3	2.16E-03
1..3 (20)	2..4	7.72E-02
1..4 (40)	2..5	1.56E-01
1..5 (80)	2..6	9.83E-02

Prol./Rest. in space and time.

Level-independent convergence rates

Convergence of the Newton iteration

Step	Nonlinear defect
0	9.74E-04
1	6.86E-04
2	7.66E-06
3	1.94E-09
4	4.35E-16

Linear subproblems exact

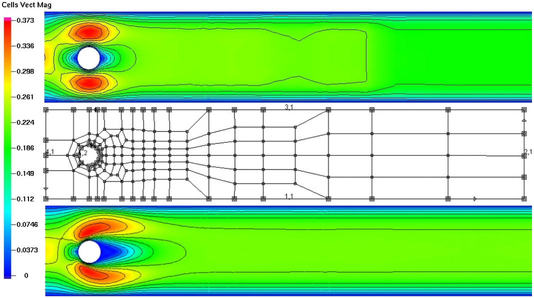
Step	Nonlinear defect
0	9.74E-04
1	6.86E-04
2	7.71E-06
3	4.61E-08
4	2.30E-11
5	2.07E-14
6	7.44E-16

Linear subproblems inexact (gain 2 digits)

Better: adaptive stopping criterion w.r.t. nonlinear damping

Numerical example: Benchmark configuration

- Target flow z: Stokes flow, $Re = 20$, $t \in [0, 1]$



Stokes at $t = 1$

Mesh

uncontrolled Nav.St.

- Optimal control problem: Navier–Stokes, $Re = 20$
- NSM=1, $\omega = 0.7$, fully implicit time discretisation
- 20 time steps (time level 3), 21216 unknowns in space (space level 3) $\Rightarrow$ 445536 unknowns total

Numerical example: Benchmark configuration

Convergence of the Newton solver

nonl. step	nonl. Res.	#MG-steps
0	1.51E-04	
1	2.40E-05	4
2	7.54E-07	4
3	5.43E-09	4
4	3.78E-11	6
	Total:	18

- Space-time MG gained 2 digits per step
- Space-preconditioner gained 2 digits per step

Numerical example: Benchmark configuration

A small calculation gives the performance measure; in this example:

$$\frac{\text{effort for optimization}}{\text{effort for simulation}} \leq 19$$

Upper bound of the performance measure was:

$$\frac{\text{effort for optimization}}{\text{effort for simulation}} \leq \text{NITT} \times 4 \times \text{NSM} = 18$$

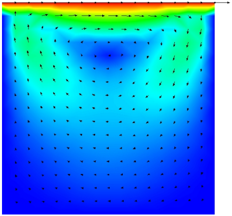
Roughly as estimated! Potential for improvement!

more...

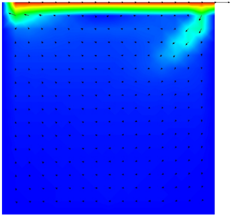
Current investigation

Again Driven Cavity

- Target flow z: Stokes flow, Re=1/400, $t = 0..1$:



Stokes, Re=1/400, $t = 1$



Nav.St., $Re = 400$, $t = 1$, uncontrolled

- Optimal control problem: Navier–Stokes, $Re = 400$.
- NSM=4, $\omega = 0.7$, fully implicit time discretisation.

Current investigation

Test of space-time multigrid.

- **Space level fixed to level 4.** Time level increasing.

Time	#It	ρ
1..3 (20)	4	4.15E-03
1..4 (40)	5	1.64E-02
1..5 (80)	6	2.96E-02
1..6 (160)	6	3.11E-02
1..7 (320)	6	2.91E-02

Prol./Rest. only in time.

Time	#It	ρ
1..3 (20)	6	3.79E-02
1..4 (40)	13	2.39E-01
1..5 (80)	36	5.84E-01
1..6 (160)	92	8.17E-01
1..7 (320)	>100	9.23E-01

Prol./Rest. in space and time.

Small timesteps $\Rightarrow$ Negative impact to the solver (Why?!?)

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Outlook

Further steps:

- $\tilde{Q}_2/P_1$ + Crank-Nicolson
  $\rightarrow$ higher accuracy, larger timesteps, fewer unknowns
- FEM-stabilisation $\rightarrow$ higher RE numbers, real nonst. flow
- **improved smoothers for the space-time problem**
- analyse implicit and semi-explicit time stepping schemes
- incorporate constraints
- include algorithms for memory management

Comparison: Implicit $\leftrightarrow$ semi-explicit

- Driven cavity, h=1/8, T=0..10
- Newton + 2-grid in time for preconditioning
- Semi-explicit time discretisation:

$$\frac{y_{i+1} - y_i}{\Delta t} - \Delta y_{i+1} + y_i \nabla y_i + \nabla p_{i+1} = \ldots$$

	implicit		semi-explicit	
Δt	#NL	#MG	#NL	#MG
10	4	4	1	1
10/2	5	43	3	23
10/4	5	40	4	32
10/8	4	25	4	25
10/16	4	23	4	21
10/32	4	22	4	22

$\Rightarrow$ semi-explicit method more stable for big timesteps

BUT well known: inaccurate!

Comparison: Implicit $\leftrightarrow$ semi-explicit

- Driven cavity, h=1/8, T=0..10
- Newton + 2-grid in time for preconditioning
- Semi-explicit time discretisation:

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Δt	#NL	#MG	#NL	#MG
10	4	4	1	1
10/2	5	43	3	23
10/4	5	40	4	32
10/8	4	25	4	25
10/16	4	23	4	21
10/32	4	22	4	22

$\Rightarrow$ semi-explicit method more stable for big timesteps

BUT well known: inaccurate!

Numerical cost (per nonlinear iteration)

- effort for 1 space-time smoothing step, highest level
  $\hat{=}$ 1$\times$ space-MG of coupled Nav.St. in each timestep
  $\hat{=}$ 2$\times$ space-MG of Nav.St. in each timestep, highest level
- 1 space time multigrid sweep, NSM smoothing-steps
  $\leq$ 2$\times$NSM smoothing steps on highest level
  $\leq$ 4$\times$NSM space-MG of Nav.St. in each timestep

With NITT := #MG-iterations per nonlinear step:

$$\frac{\text{effort for optimization}}{\text{effort for simulation}} \leq \text{NITT} \times 4 \times \text{NSM}$$

With exactly 1 MG step instead of P^{-1} exact:

$$\frac{\text{effort for optimization}}{\text{effort for simulation}} \leq 4 \times \text{NSM}$$

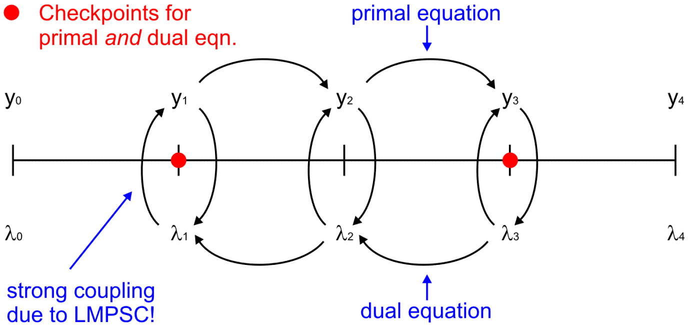
Numerical cost in the example

Our measure: *#Calls of the space-MG on finest mesh*

- Simulation: 20 timesteps, 6 nonlinear iteations each, 1 MG per nonlinear iteration.
  $\rightarrow$ $20 \times 6 = 120$ calls of the space MG
- Optimisation: 4 Newton steps, 4.5 MG iterations each, 2×21 space MG each. (Smoother performs 2 sweeps!)
  $\rightarrow$ $4 \times 4.5 \times 2 \times 21 = 756$ calls to space-MG
- Each space-Time-MG $1.5\times$ more expensive than space-time one-grid.
  Each space-time one-grid opt. control $2\times$ more expensive than simulation.

$$\frac{\text{effort for optimization}}{\text{effort for simulation}} \approx \frac{756 \times 1.5 \times 2}{120} \approx 19$$

Checkpointing in the One-shot approach



- Checkpoints $\longrightarrow$ nonlinear subproblems of the same kind.
- High computational costs necessary for recomputation $\longrightarrow$ due to strong coupling by LMPSC!