A Numerical Study of Hierarchical Solution Concepts for Flow Control Problems

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Flow control model problem

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

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

subject to

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

+ BC, constraints, init. cond.

<u>Aim:</u> Solve with

$$\begin{cases} \text{costs for simulation} = O(N), \\ \text{costs for optimisation} = O(N), \\ \dfrac{\text{costs for optimisation}}{\text{costs for simulation}} \le C \approx 10 - 50 \end{cases}$$

Flow control model problem

KKT-System:

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

+ incompressibility, BC, constraints, ...

Ingredients:

- Newton + Space-time multigrid solvers
- Q_2/P_1^{disc}, IE + CN
- Distributed control, L_2+ $H^{\frac{1}{2}}$ boundary control
- Control constraints

Design of solution methods

General: Eliminate variables, apply Newton method

$$y_t - \nu\Delta y + \ldots = u$$
$$-\lambda_t - \nu\Delta\lambda + \ldots = y - z$$
$$\alpha u + \lambda = 0$$

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

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

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

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

Method 1: Newton approach in u

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Algorithm (Newton approach in u)

$$u_{n+1} = u_n + \bar{u}, \qquad F'(u_n)\bar{u} = -F(u_n)$$

Ingredients:

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

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

nonlinear simulation — linear simulation

Method 2: Newton approach in (y, λ, p, ξ)

Algorithm (Newton approach in $x = (y, \lambda, p, \xi)$)

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

Ingredients:

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

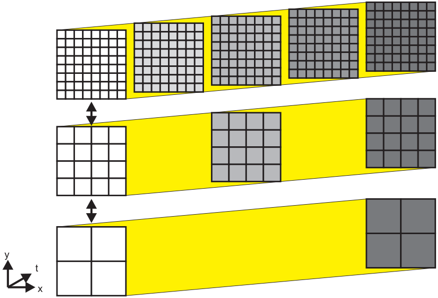
$$G'(x)\bar{x} := \begin{pmatrix} \bar{y}_t - \nu \Delta \bar{y} + ... + \frac{1}{\alpha}\bar{\lambda} \\ -\bar{\lambda}_t - \nu \Delta \bar{\lambda} + ... - \bar{y} \\ ... \end{pmatrix}$$

Multigrid solver methodology

Expensive parts:

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

Solve using multigrid on a (space-time) hierarchy:



On each level: CG, BiCGStab, GMRES,... (+ preconditioner?)

KKT-system

Idea 1: Apply optimal control methods

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

$$
\begin{aligned}
y_t - \nu \Delta y + (y \nabla) y + \nabla p &= u && \text{in } Q \\
-\lambda_t - \nu \Delta \lambda - (y \nabla) \lambda + (\nabla y)^t \lambda + \nabla \xi &= (y - z) && \text{in } Q \\
u &= -\frac{1}{\alpha} \lambda && \text{in } Q
\end{aligned}
$$

Idea 2: Exploit the ellipticity with MG methods

- Analysis $\Rightarrow$ elliptic charakter in space and time
  Problem equivalent to:

$$-y_{tt} + \Delta^2 y + \ldots = \ldots$$

- Monolithic Newton/MG in space + time

KKT-system

Idea 1: Apply optimal control methods

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

$$\begin{aligned} y_t + C(y)y \;\; + \nabla p &= -\frac{1}{\alpha}\lambda && \text{in } Q, && y(0) = y_0 \\ -\lambda_t + N^*(y)\lambda + \nabla\xi &= (y - z) && \text{in } Q, && \lambda(T) = 0 \end{aligned}$$

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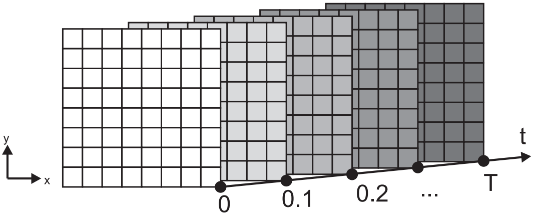
Space-time discretisation

Step 1: Space-time discretisation

- Unstructured mesh in space, $N \in \mathbb{N}$ timesteps



- Time discretisation: IE, CN, ..., timestep $k = 1/N$

$$
\begin{aligned}
(y_n - y_{n-1})/k + C(y_n)y_n \quad + \nabla p_n &= -\frac{1}{\alpha}\lambda_n \qquad \text{in } Q \\
(\lambda_n - \lambda_{n+1})/k + N^*(y_n)\lambda_n + \nabla \xi_n &= (y_n - z_n) \quad \text{in } Q
\end{aligned}
$$

- Space discretisation: FEM $(\tilde{Q}_1/Q_0,\ Q_2/P_1^{\text{disc}}, \ldots)$

Space-time system

Resultat: Nonlinear system in space and time

$$G(w)w = f$$

$$\left(\begin{array}{c|c|c|c|c} G_0 & \hat{M} & & & \\ \hline \check{M} & G_1 & \hat{M} & & \\ \hline & \check{M} & G_2 & \hat{M} & \\ \hline & & \ddots & \ddots & \ddots \\ \hline & & & \check{M} & G_N \end{array}\right) \begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_N \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix}$$

$\Rightarrow$ sparse block tridiagonal system

Space-time system

Resultat: Nonlinear system in space and time

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$$w_0 \to \begin{pmatrix} y_0 \\ \lambda_0 \\ p_0 \\ \xi_0 \\ \hline y_1 \\ \lambda_1 \\ p_1 \\ \xi_1 \\ \hline \vdots \end{pmatrix}$$

$\Rightarrow$ sparse block tridiagonal system

Space-time system

Resultat: Nonlinear system in space and time

$$G(w)w = f$$

$$\begin{pmatrix} G_0 & \hat{M} & & & \\ \check{M} & G_1 & \hat{M} & & \\ & \check{M} & G_2 & \hat{M} & \\ & & \ddots & \ddots & \ddots \\ & & & \check{M} & G_N \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_N \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix}$$

$$\check{M} = \begin{pmatrix} -\frac{I}{k} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$G_2 = \begin{pmatrix} \frac{I}{k} + C(y_2) & \frac{I}{\alpha} & \nabla & 0 \\ -I & \frac{I}{k} + N^*(y_2) & 0 & \nabla \\ \nabla\cdot & 0 & 0 & 0 \\ 0 & \nabla\cdot & 0 & 0 \end{pmatrix}$$

Space-time hierarchy and solver

Step 2: Space-time hierarchy

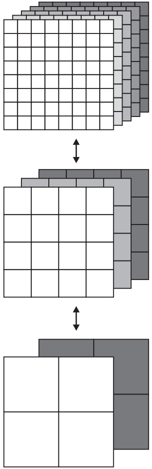
- Coarsening in space + time

Step 3: Space-time Newton-MG solver

- Newton solver on the fine mesh

$$w^{k+1} = w^k + G'(w^k)^{-1}(f - G(w^k)w^k)$$

- Space-time multigrid
  - To apply $G'(w^k)^{-1}$
  - Exploitation of the hierarchy
  - Needs smoother and prol./rest.



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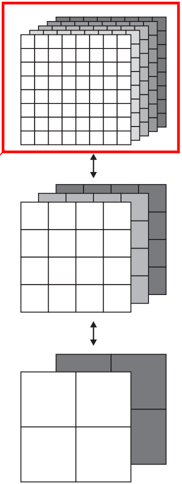

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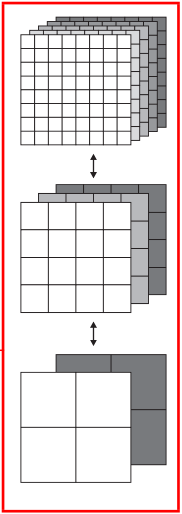

Construction of a smoother

- On every level: Linear subproblem

$$\begin{aligned} G'(w^k)x &= b \\ \Leftrightarrow \qquad Ax &= b \qquad \text{mit} \qquad A := G'(w^k) \end{aligned}$$

- Iterative smoother: Defect correction

$$x_{n+1} = x_n + P^{-1}(b - Ax_n)$$

- Typical preconditioner: Block methods

$$A = \left(\begin{array}{c|c|c|c|c} A_0 & \hat{M} & & & \\ \hline \check{M} & A_1 & \hat{M} & & \\ \hline & \check{M} & A_2 & \hat{M} & \\ \hline & & \ddots & \ddots & \ddots \\ \hline & & & \check{M} & A_N \end{array}\right)$$

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$$P_0 = \left(\begin{array}{c|c|c|c|c} A_0 & & & & \\ \hline & A_1 & & & \\ \hline & & A_2 & & \\ \hline & & & \ddots & \\ \hline & & & & A_N \end{array}\right) \quad \Rightarrow \quad \text{Block-Jacobi}$$

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$$\Leftrightarrow \quad Ax = b \quad \text{mit} \quad A := G'(w^k)$$

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$$P_1 = \begin{pmatrix} A_0 & & & & \\ \check{M} & A_1 & & & \\ & \check{M} & A_2 & & \\ & & \ddots & \ddots & \\ & & & \check{M} & A_N \end{pmatrix} \quad \Rightarrow \quad \text{Block-GS forward}$$

Construction of a smoother

- On every level: Linear subproblem

$$G'(w^k)x = b$$
$$\Leftrightarrow \qquad Ax = b \qquad \text{mit} \qquad A := G'(w^k)$$

- Iterative smoother: Defect correction

$$x_{n+1} = x_n + P^{-1}(b - Ax_n)$$

- Typical preconditioner: Block methods

$$P_2 = \left(\begin{array}{c|c|c|c|c} A_0 & \hat{M} & & & \\ \hline & A_1 & \hat{M} & & \\ \hline & & A_2 & \hat{M} & \\ \hline & & & \ddots & \ddots \\ \hline & & & & A_N \end{array}\right) \quad \Rightarrow \quad \text{Block-GS backward}$$

Forward-Backward block smoother

- robust+efficient: Forward-/Backward strategy
- Diagonal blocks A_i: Equation in space, Oseen type
- every "timestep": A_i^{-1} = monolithic MG, LPSC smoother

$$\begin{pmatrix} A_0 & & & \\ \check{M} & A_1 & & \\ & \check{M} & A_2 & \\ & & \ddots & \ddots \end{pmatrix}^{-1}$$

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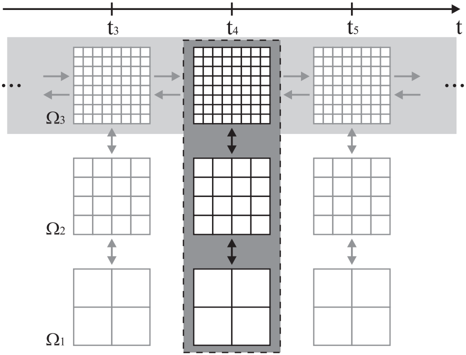
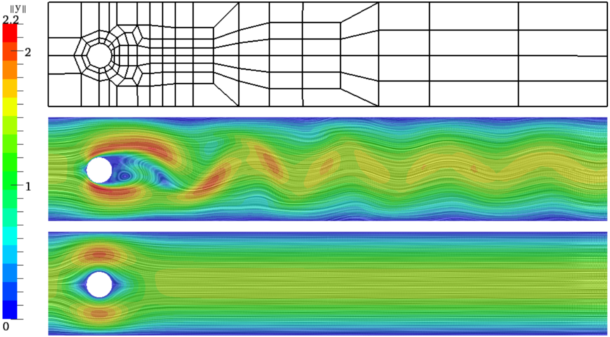


Numerical example

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



Mesh

Nav.St., periodic init. condition

Stokes, Target

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

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(u)	#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}
- Stopping crit. forward/backward in space 10^{-14}
- Residual reduction monolithic MG in space 10^{-2}

Test 1: Newton solver in u

Newton-solver in the control space was:

$$u_{n+1} = u_n - F'(u_n)^{-1} F(u_n), \qquad F(u) := \alpha u + \lambda$$

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

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 $F'(u_n)^{-1}$:

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

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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	$\frac{T_{\text{opt}}}{T_{\text{sim}}}$
2	20	9:05	0:40	5	25	13.8
3	40	1:53:48	6:38	6	31	17.2
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Comparison

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

	Newton in u	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	∅ →not necessary?	expensive → inexact √ → paralleliseable √
Space-time MG	√	√

General results

- Newton-solver in (y, λ, p, ξ) usually more efficient than in u
  $\rightarrow$ more freedom w.r.t. stopping criteria
  $\rightarrow$ more freedom w.r.t. preconditioners

- Newton-solver in u or (y, λ, p, ξ)?

Focus	Solver type
Black-box	Newton in u
Efficiency	Newton in (y, λ, p, ξ) $\rightarrow$ more freedom w.r.t. stopping criteria / preconditioners

$\Rightarrow$ use SQP-type solvers if possible

Disadvantage in Method 1:

$$u_{n+1} = u_n - F'(u_n)^{-1} F(u_n)$$

Defect $F(u_n)$ accurate $\Leftrightarrow$ Accurate nonlinear simulation!

Possible alternative:(Analogous to CFD solvers)

$$H(x,u) := \begin{pmatrix} y_t - \nu \Delta y + \ldots \\ -\lambda_t - \nu \Delta \lambda + \ldots \\ \alpha u + \lambda \end{pmatrix}$$

$$(x_{n+1}, u_{n+1}) := (x_n, u_n) - \text{"}F'(u_n)^{-1}\text{"} \; H(x_n, u_n)$$

$\Rightarrow$ Inexact solvers should not destroy the solution
$\Rightarrow$ No nonlinear systems in space
$\Rightarrow$ Black box applicable in subsystems

Efficiency comparison

	Newton in u	Newton in $x = (y, \lambda)$
$T_{\text{opt}}/T_{\text{sim}}$	≈ 50	≈ 20

Reason: Inexact subsolvers.

Method 1:

$$u_{n+1} = u_n - F'(u_n)^{-1} F(u_n), \qquad F(u) := \alpha u + \lambda$$

a) $F(u_n)$:

- Accurate $\Leftrightarrow$ Fw/bw simulation accurate! $\rightarrow$ expensive

b) $F'(u_n)$:

- Accurate $\Leftrightarrow$ Linear fw/bw simulation accurate! $\rightarrow$ expensive

Efficiency comparison

	Newton in u	Newton in $x = (y, \lambda)$
$T_{\mathrm{opt}} / T_{\mathrm{sim}}$	≈ 50	≈ 20

Reason: Inexact subsolvers.

Method 2:

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

a) $G(x_n)$:
- Accurate + cheap by construction (no simulation)

b) $G'(x_n)$:
- Applied for linear residual, cheap, accurate (no simulation)
- Internal solvers inexact $\rightarrow$ less expensive

but: Memory-intensive, no checkpointing, complicated.

Linear system for method 1

The Newton solver in u reads:

$$u_{n+1} = u_n + \bar{u}, \qquad F'(u_n)\bar{u} = \alpha\bar{u} + \bar{\lambda} \stackrel{!}{=} -F(u_n)$$

with

$$\left\{ \begin{array}{r} \bar{y}_t - \nu\Delta\bar{y} + (y\nabla)\bar{y} + (\bar{y}\nabla)y + \nabla\bar{p} = \bar{u} \\ -\bar{\lambda}_t - \nu\Delta\bar{\lambda} - (y\nabla)\bar{\lambda} - (\bar{y}\nabla)\lambda + (\nabla\bar{y})^T\lambda + (\nabla y)^T\bar{\lambda} + \nabla\bar{\xi} = \bar{y} \\ + \text{incompressibility, BC, constraints, ...} \end{array} \right\}$$

Simple defect correction solver for the linear system, $\omega \in (0,1]$:

$$\bar{u}^{\text{new}} = \bar{u} + \omega\Big(- F(u_n) - \underbrace{(\alpha\bar{u} + \bar{\lambda})}_{=F'(u_n)\bar{u}}\Big)$$

$\Rightarrow$ One linear fw/bw solve per iteration, but no preconditioning.

Similar: CG, GMRES,...

Linear system for method 2

The Newton solver in x reads:

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

$$G'(x)\bar{x} = \begin{pmatrix} \bar{y}_t - \nu\Delta\bar{y} + (y\nabla)\bar{y} + (\bar{y}\nabla)y + \nabla\bar{p} + \frac{1}{\alpha}\bar{\lambda} \\ -\bar{\lambda}_t - \nu\Delta\bar{\lambda} - (y\nabla)\bar{\lambda} - (\bar{y}\nabla)\lambda + (\nabla\bar{y})^T\lambda + (\nabla y)^T\bar{\lambda} + \nabla\bar{\xi} - \bar{y} \\ + \text{incompressibility, BC, constraints, ...} \end{pmatrix}$$

Simple defect correction solver for the linear system:

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

$\Rightarrow$ $C \approx G'(x_n)$ preconditioner.

Similar: CG, GMRES,...

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

Summary

Two solution methods analysed:

- Newton in u $\quad + \quad$ Newton in (y, λ, p, ξ)
- Space-time Multigrid for linear subproblems
- Distributed/boundary control, Control constraints

Main achivements:

- "Optimal" complexity
- $T_{\text{opt}} / T_{\text{sim}} \approx 20 - 50 \quad \rightarrow \quad$ for 'optimal' sim.
- Newton in (y, λ, p, ξ) usually more efficient than in $u \rightarrow$ due to inexact inner solvers + strong preconditioning

Outlook

Possible challenges for the future:

- Combination of both solvers in a ”Reduced SQP” approach.
- Detailed analysis concerning stopping criteria
- Higher RE-numbers
- 3D
- Non-isothermal, Non-Newtonian flow
- Fluid-Structure interaction?