LECTURE 3

Optimal Flow Control

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3.0 Content

References

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3.1 Thoughts on adaptivity in optimization

General optimization problem (OPC) (u state, q control)

$$J(u,q) \to \min, \qquad \mathcal{A}(u,q) = 0$$

Notion of admissibility of states $u = u(q)$?

- Discretization introduces perturbation of state equation.
- Accuracy in discretization of PDEs is expensive.
- The efficient numerical solution of OPCs governed by PDEs requires work reduction by adaptive discretization.
- In PDEs the choice of error measures is a delicate matter.
- **Accuracy requirements should observe intrinsic problem sensitivities and is a modeling issue.**

Goals of adaptivity in optimal control:

- What are the relevant error control criteria?

$$|J(u_h, q_h) - J(u, q)| \leq \ TOL, \qquad \|q - q_h\|_? \leq \ TOL$$

  Alternative: **Monitoring of convergence behavior of the scalar quantity** $J(u_h, q_h)$

- Mesh adaptation criteria by local **error indicators**:

$$\eta_K \gg \delta \ \Rightarrow \ \text{refine}, \quad \eta_K \approx \delta \ \Rightarrow \ \text{keep}, \quad \eta_K \ll \delta \ \Rightarrow \ \text{coarsen}$$

Goal: Development of a universal approach for dimension reduction by weakening admissibility requirements, which can be applied for general systems of PDEs and general (Galerkin) discretization and does not rely on mostly unknown (or worst-case oriented) coercivity properties.

3.2 Theoretical framework (revisited)

Computation of stationary point $x \in X$ of diff. functional $L(\cdot)$ by Galerkin scheme in finite dim. subspace $X_h \subset X$:

$$L'(x)(y) = 0 \qquad \forall y \in X$$

$$L'(x_h)(y_h) = 0 \qquad \forall\, y_h \in X_h$$

Proposition 1 *There holds the error representation*

$$L(x) - L(x_h) = \tfrac{1}{2} \underbrace{L'(x_h)(x{-}y_h)}_{\textbf{weighted residual}} + \mathcal{R}_h, \quad y_h \in X_h,$$

where the remainder $\mathcal{R}_h$ *is* **cubic** *in* $x{-}x_h$.

Application to functional minimization

State variable $u \in V$, control variable $q \in Q$:

$$J(u,q) = \min! \qquad A(u,q)(\psi) = 0.$$

The state equation may be a stationary or nonstationary PDE.

Galerkin approximation in finite subspaces $V_h \times Q_h \subset V \times Q$

$$J(u_h,q_h) = \min! \qquad A(u_h,q_h)(\psi_h) = 0.$$

Lagrangian functional with adjoint variable λ:

$$\mathcal{L}(u,q,\lambda) := J(u,q) - A(u,q)(\lambda)$$

Continuous and discrete optimality systems (**KKT systems**):

$$\left\{ \begin{array}{l} J'_u(u,q)(\varphi) - A'_u(u,q)(\varphi,\lambda) \\ J'_q(u,q)(\chi) - A'_q(u,q)(\chi,\lambda) \\ -A(u,q)(\psi) \end{array} \right\} = 0$$

$$\left\{ \begin{array}{l} J'_u(u_h,q_h)(\varphi_h) - A'_u(u_h,q_h)(\varphi_h,\lambda_h) \\ J'_q(u_h,q_h)(\chi_h) - A'_q(u_h,q_h)(\chi_h,\lambda_h) \\ -A(u_h,q_h)(\psi_h) \end{array} \right\} = 0$$

Residuals:

$$\rho^*(\lambda_h)(\cdot) := J'_u(u_h,q_h)(\cdot) - A'_u(u_h,q_h)(\cdot,\lambda_h)$$

$$\rho^q(q_h)(\cdot) := J'_q(u_h,q_h)(\cdot) - A'_q(u_h,q_h)(\cdot,\lambda_h)$$

$$\rho(u_h)(\cdot) := -A(u_h)(\cdot)$$

a) Natural concept in optimal control:

Error control w.r.t. cost functional $J(\cdot,\cdot)$

Proposition 2 *There holds the error representation*

$$J(u,q)-J(u_h,q_h) = \frac{1}{2}\underbrace{\rho^*(\lambda_h)(u-I_hu)}_{\text{dual residual}} + \frac{1}{2}\underbrace{\rho^q(q_h)(q-I_hq)}_{\text{control residual}}$$
$$+\frac{1}{2}\underbrace{\rho(u_h)(\lambda-I_h\lambda)}_{\text{primal residual}} + \mathcal{R}_h$$

for arbitrary $I_hu, I_h\lambda \in V_h$ *and* $I_hq \in Q_h$. *The remainder* $\mathcal{R}_h$ *is cubic in the errors* $e^u := u-u_h$, $e^q := q-q_h$, $e^\lambda := \lambda-\lambda_h$.

b) Application in parameter identification

Model problem

$$-\Delta u + qu = f \;\text{ in } \Omega, \quad u_{|\partial\Omega} = 0$$

The goal is to determine the coefficient q by comparing the resulting observation $C(u)$ with given measurements $\bar{C}$

$$J(u,q) := \frac{1}{2}\|C(u)-\bar{C}\|_O^2 + \frac{1}{2}\alpha\|q\|^2 \;\rightarrow\; \text{min!} \quad (0 \le \alpha \ll 1)$$

First-order optimality system:

$$\begin{aligned}
\langle \varphi, C(u)-\bar{C}\rangle_O + (\nabla\varphi, \nabla\lambda) + (q\varphi, \lambda) &= 0 \quad \forall\varphi \\
\alpha(\chi, q) + (\chi u, \lambda) &= 0 \quad \forall\chi \\
(\nabla u, \nabla\psi) + (qu, \psi) &= (f, \psi) \quad \forall\psi
\end{aligned}$$

Adjoint equation for “identifiable” parameter $q > 0$:

$$-\Delta\lambda + q\lambda = u - \bar{u} = 0 \quad \Rightarrow \quad \lambda \equiv 0.$$

This may be achieved on coarse meshes.

- **Choice of (artificial) cost functional for a posteriori error control is questionable for mesh design.**
- An **energy-norm-type** a posteriori error estimate for $\|q - q_h\|_O$ can be derived based on a coercivity estimates for the saddle-point problem. However, the stability constant in this estimate is usually unknown and depends on α^{-1}.
- An a posteriori error estimate for a suitable expression of $q - q_h$ can be derived by an **“outer” duality argument**.

(i) Error estimation based on stability

KKT system for $U = (u, q, \lambda)$ and $\Phi = (\varphi^u, \varphi^q, \varphi^\lambda)$:

$$A(U)(\Phi) = 0$$

$$\begin{aligned} A(U)(\Phi) := \langle \varphi^u, C(u) - \bar{C} \rangle_O + (\nabla \varphi^\lambda, \nabla \lambda) + (q\varphi^\lambda, \lambda) \\ + \alpha(\varphi^q, q) + (\varphi^q u, \lambda) + (\nabla u, \nabla \varphi^u) + (qu, \varphi^u) - (f, \varphi^u) \end{aligned}$$

Stability assumption (worst-case oriented, with $\beta(\alpha) \sim \alpha$)

$$\sup_{\Psi \in X} \frac{A'(U)(\Phi, \Psi)}{\|\Psi\|_X} \geq \beta(\alpha) \|\Phi\|_X, \quad \Phi \in X$$

Resulting "worst case" a posteriori error estimate

$$\|U - U_h\|_X \leq \gamma(\alpha) \|R(U_h)\|_{X^*}, \quad \gamma(\alpha) \sim \frac{1}{\alpha}$$

(ii) Error estimation based on duality:

A posteriori error estimate (captures local features):

$$E(q) - E(q_h) = \eta + \mathcal{P}_h + \mathcal{R}_h$$

- Discretization error:

$$\eta = \frac{1}{2}\rho(u_h)(z - I_h z) + \frac{1}{2}\rho^q(q_h)(q - I_h q) + \frac{1}{2}\rho^*(z_h)(u - I_h u)$$

- Dual problem: $z \in V$

$$a'_u(u,q)(\varphi, z) = -\langle G(G^*G)^{-1}\nabla E(q), C'(u)(\varphi)\rangle_O \quad \forall \varphi \in V$$

(G derivative of solution operator $u = S(q)$ w.r.t. q)

- Remainder terms:
  - $\mathcal{R}_h$ is a cubic remainder term due to linearization
  - $|\mathcal{P}_h| \le c\,\|e\|_V\,\|C(u) - \bar{C}\|_O \ll \eta$

3.3 An illustrative model case

Neumann boundary control in the stationary diffusion problem

$$
\begin{aligned}
-\Delta u + s(u) &= f \quad \text{in } \Omega \subset \mathbb{R}^2 \quad (s(u) = u^3) \\
\partial_n u_{|\Gamma_N} &= 0, \quad \partial_n u_{|\Gamma_C} = q
\end{aligned}
$$

Control $q = q(x)$ such that

$$
J(u,q) = \frac{1}{2}\|u-\bar{u}\|^2_{\Gamma_O} + \frac{\alpha}{2}\|q\|^2_{\Gamma_C} \;\to\; \min! \qquad (\bar{u} \equiv 1,\ \alpha \geq 0)
$$

Variational formulation of state equation:

$$
(\nabla u, \nabla\psi)_\Omega + (s(u),\psi)_\Omega - (\mathbf{q},\psi)_{\mathbf{\Gamma_C}} = (f,\psi) \quad \forall \psi \in V
$$

KKT system in strong form:

$$\begin{cases} -\Delta\lambda + s'(u)\lambda = 0, \quad \text{in } \Omega \\ \partial_n \lambda_{|\Gamma_O} = u - u_0, \quad \partial_n \lambda_{|\Gamma_N \cup \Gamma_C} = 0 \end{cases}$$

$$\alpha q - \lambda_{|\Gamma_C} = 0$$

$$\begin{cases} -\Delta u + s(u) = f, \quad \text{in } \Omega \\ \partial_n u_{|\Gamma_N} = 0, \qquad \partial_n u_{|\Gamma_C} = q \end{cases}$$

Galerkin approximation: $\quad V_h = \{Q_1\text{-elements}\}, \quad Q_h := \{\partial_n V_{h|\Gamma_C}\}$

$$\begin{aligned} (\varphi_h, u_h - c_0)_{\Gamma_O} + (\nabla\varphi_h, \nabla\lambda_h)_\Omega + (s'(u_h)\varphi_h, \lambda_h)_\Omega &= 0 \quad \forall \varphi_h \in V_h, \\ \alpha(q_h, \chi_h)_{\Gamma_C} - (\lambda_h, \chi_h)_{\Gamma_C} &= 0 \quad \forall \chi_h \in Q_h, \\ (\nabla u_h, \nabla\psi_h)_\Omega + (s(u_h), \psi_h)_\Omega - (f, \psi_h)_\Omega - (q_h, \psi_h)_{\Gamma_C} &= 0 \quad \forall \psi_h \in V_h. \end{aligned}$$

A posteriori error estimate:

$$|J(u,q) - J(u_h,q_h)| \;\le\; \eta_\omega : \;=\; \sum_{K\in\mathbb{T}_h} \{ \underbrace{\rho_K^u\,\omega_K^\lambda + \rho_K^\lambda\,\omega_K^u + \rho_K^q\,\omega_K^q}_{\eta_K \text{ (refinement indicators)}} \},$$

cell-residuals and weights for $x_h = \{u_h, q_h, \lambda_h\}$ defined by

$$\rho_K^\lambda := \|R_h^\lambda\|_K + h_K^{-1/2}\|r_h^\lambda\|_{\partial K}, \quad \omega_K^u := \|u - I_h u\|_K + h_K^{1/2}\|u - I_h u\|_{\partial K},$$

$$\rho_K^q := h_K^{-1/2}\|r_h^q\|_{\partial K}, \qquad \omega_K^q := h_K^{1/2}\|q - I_h q\|_{\partial K},$$

$$\rho_K^u := \|R_h^u\|_K + h_K^{-1/2}\|r_h^u\|_{\partial K}, \quad \omega_K^\lambda := \|\lambda - I_h \lambda\|_K + h_K^{1/2}\|\lambda - I_h \lambda\|_{\partial K}.$$

with arbitrary $\{I_h u, I_h q, I_h\lambda\} \in V_h \times Q_h \times V_h$.

$$R^u_{h|K} := f + \Delta u_h - s(u_h), \qquad R^\lambda_{h|K} := \Delta\lambda_h - s'(u_h)\lambda_h$$

$$r^u_{h|\Gamma} := \begin{cases} \frac{1}{2}[\partial_n u_h], & \Gamma \not\subset \partial\Omega, \\ \partial_n u_h, & \Gamma \subset \partial\Omega \setminus \Gamma_C \\ \partial_n u_h - q_h, & \Gamma \subset \Gamma_C \end{cases}, \qquad r^\lambda_{h|\Gamma} := \begin{cases} \frac{1}{2}[\partial_n \lambda_h], & \Gamma \not\subset \partial\Omega \\ \partial_n \lambda_h, & \Gamma \subset \partial\Omega \setminus \Gamma_O \\ \partial_n \lambda_h + u_h - \bar{u}, & \Gamma \subset \Gamma_O \end{cases}$$

$$r^q_{h|\Gamma} := \lambda_h - \alpha q_h, \quad \Gamma \subset \Gamma_C, \qquad r^q_{h|\Gamma} = 0, \quad \Gamma \not\subset \Gamma_C$$

For comparison: "Energy norm" error indicators:

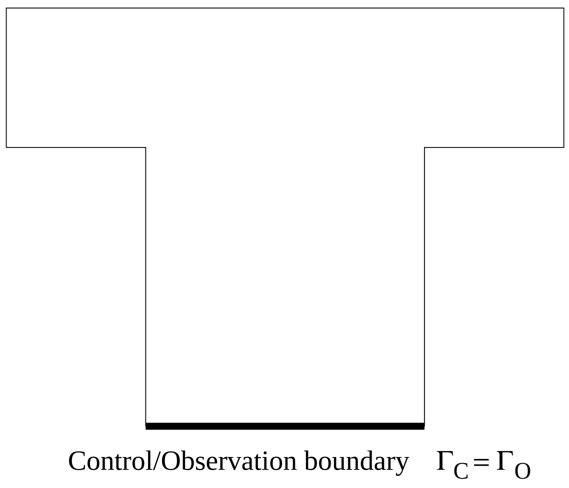
$$\eta_E^{(u)} := c_I \Big(\sum_{K \in \mathbb{T}_h} h_K^2 \, (\rho_K^u)^2 \Big)^{1/2}$$

$$\eta_E^{(u,\lambda)} := c_I \Big(\sum_{K \in \mathbb{T}_h} h_K^2 \, \big\{ (\rho_K^u)^2 + (\rho_K^\lambda)^2 \big\} \Big)^{1/2}$$

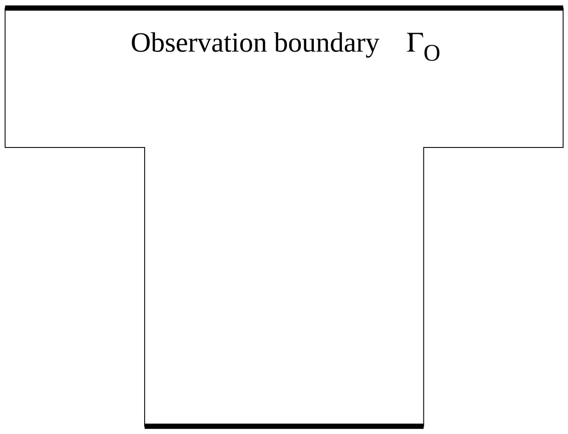
$$\eta_E^{(u,\lambda,q)} := c_I \Big(\sum_{K \in \mathbb{T}_h} h_K^2 \, \big\{ (\rho_K^u)^2 + (\rho_K^\lambda)^2 + (\rho_K^q)^2 \big\} \Big)^{1/2}$$

Testcases

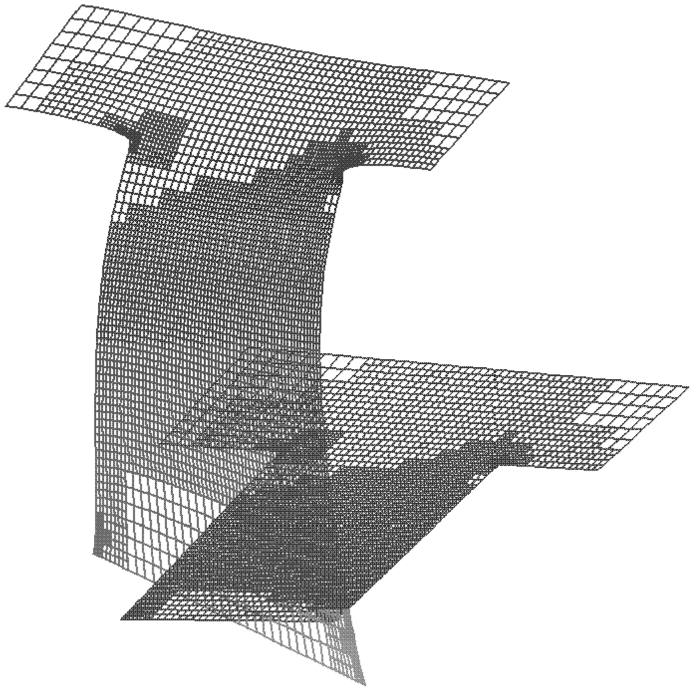
Configuration 1

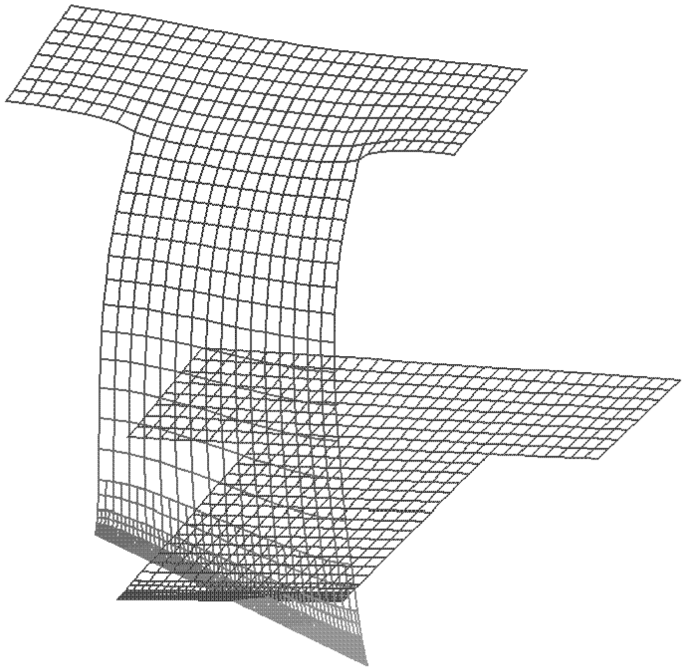


Configuration 2



Configuration 1

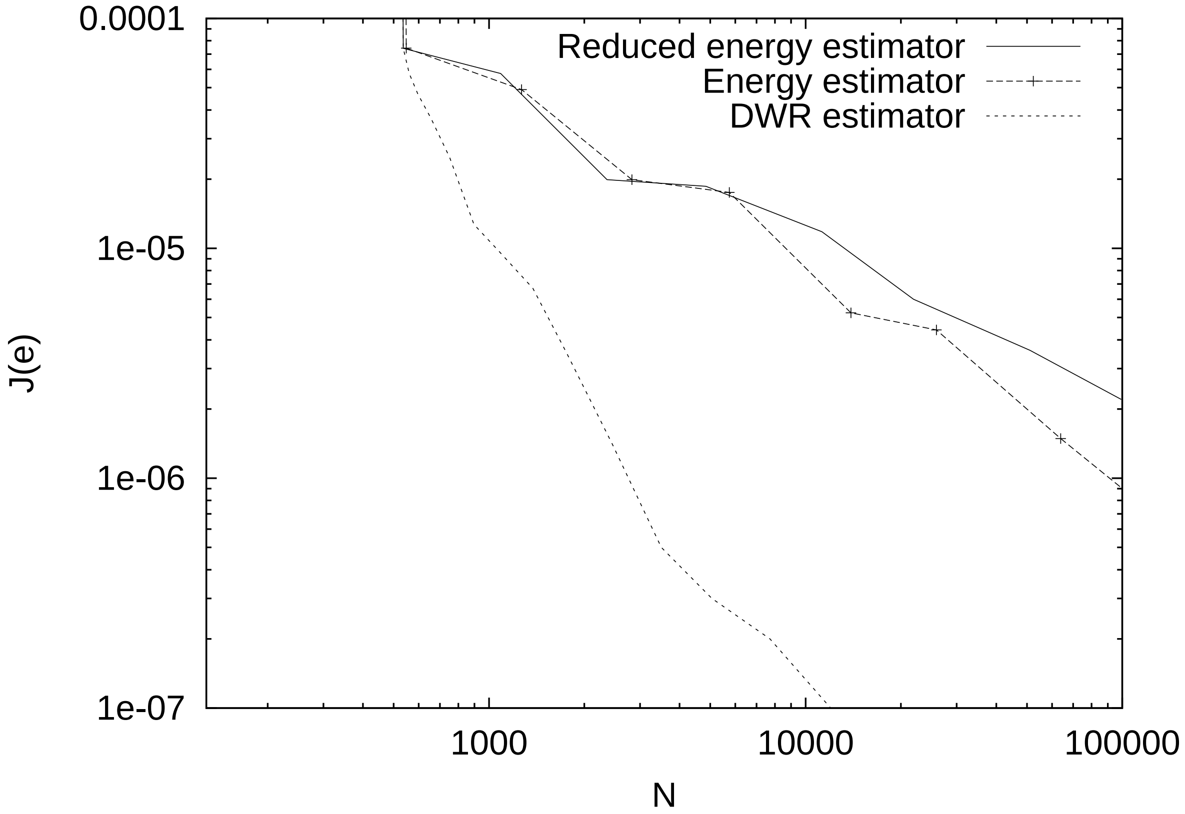




Solutions and meshes obtained by $\eta_{\mathbf{E}}$ (left) and η_ω (right)

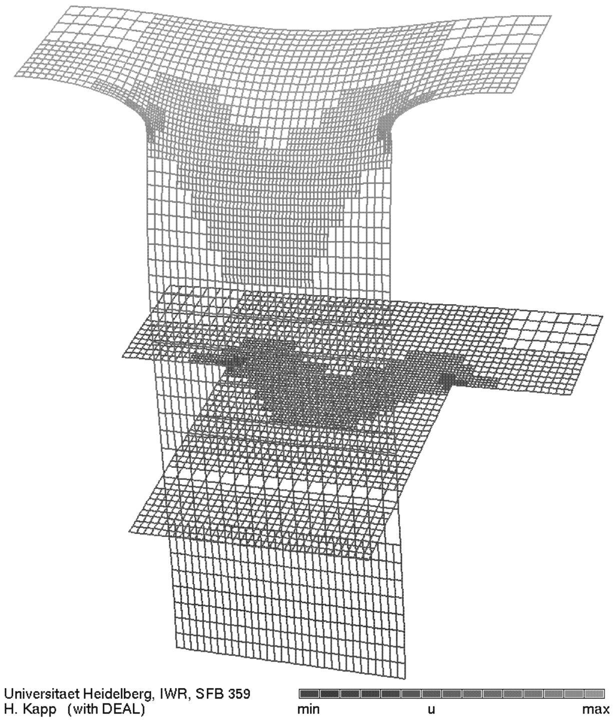
Configuration 1

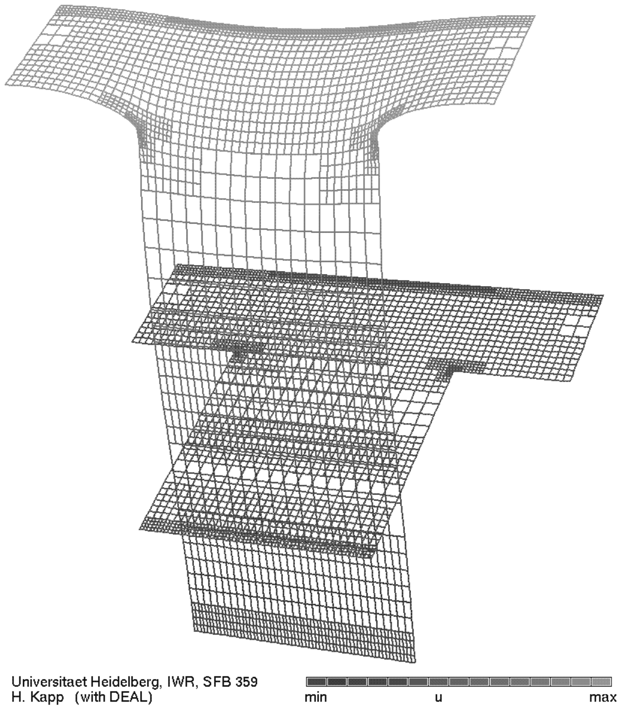
N	E_{rel}	I_{eff}
596	2.5e-4	0.34
1616	2.3e-4	0.81
5084	8.2e-5	0.46
8648	4.2e-5	0.29
15512	3.9e-5	0.43



Results for η_ω (left), and mesh efficiencies for $\eta_{\mathbf{E}}$ and η_ω (right)

Configuration 2

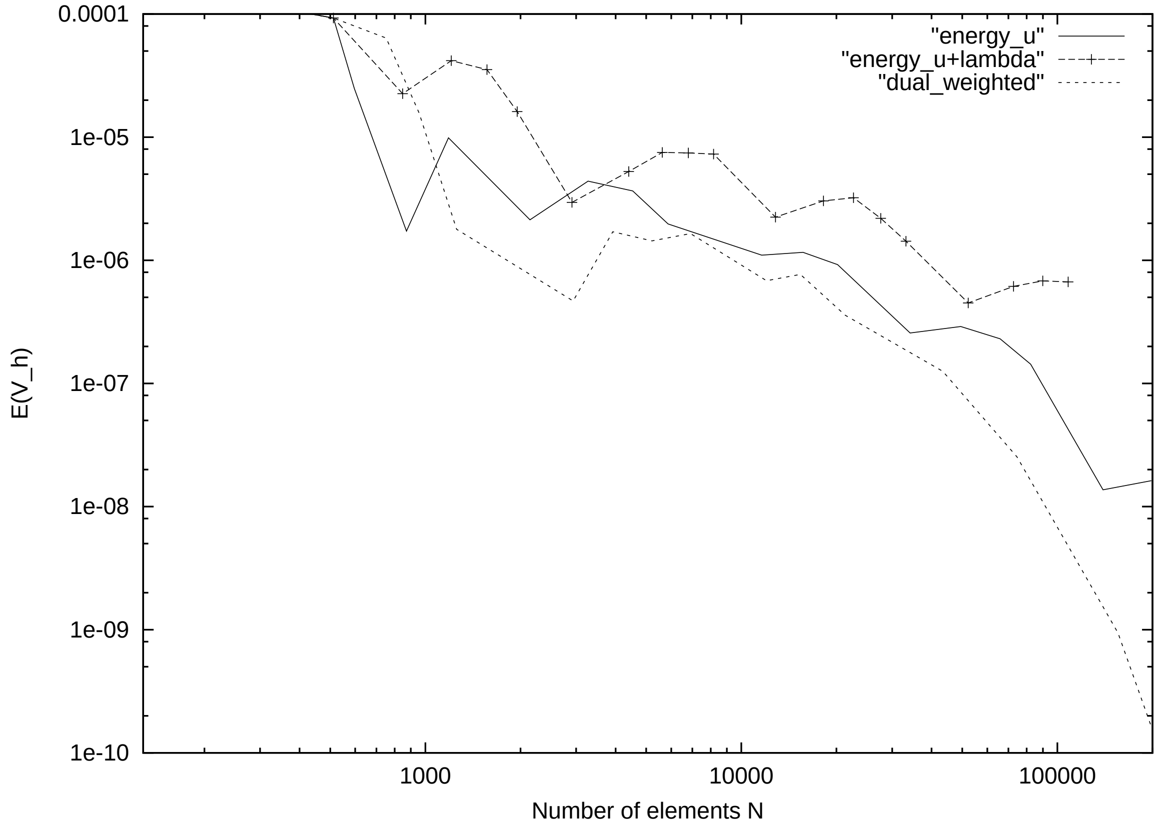




Solutions for $\eta_{\mathbf{E}}$ (left) and η_ω (right)

Configuration 2

N	E_{rel}	I_{eff}
512	9.3e-5	1.32
15368	8.1e-7	0.56
27800	4.9e-7	0.35
57632	2.3e-7	0.42
197408	4.6e-8	0.32



Results for η_ω (left), and mesh efficiencies for $\eta_{\mathbf{E}}$ and η_ω (right)

3.4 Some algorithmical issues

3.4.1 Direct versus indirect approach

a) Direct approach: Reformulation as unconstrained optimal control problem

$$j(q) := J(S(q), q) \to \min,$$

where $S : Q \to V$ is the solution operator of the state equation

$$A(S(q), q)(\psi) = 0 \quad \forall \psi \in V.$$

The local existence and sufficient regularity of S is assumed. First and second-order necessary conditions for an optimal q:

$$j'(q)(\delta q) = 0, \quad j''(q)(\delta q, \delta q) \geq 0 \quad \forall \delta q \in Q.$$

The derivatives of the reduced functional can be computed using the Lagrangian $\mathcal{L}(u, q, \lambda) = J(u, q) - a(u, q)(\lambda)$.

Computation of optimal control by **Newton-SQP method**

$$j''(q^n)(\delta q^n, \chi) = -j'(q^n)(\chi) \quad \forall \chi \in Q,$$

with update $q^{n+1} := q^n + \delta q^n$. Solution of Newton steps by Krylov-space methods requires evaluation of directional derivatives

$$j''(q^n)(\delta q^n, \chi), \quad j'(q^n)(\chi), \quad \chi \text{ fixed},$$

given by

$$\begin{aligned} j'(q)(\delta q) &= \mathcal{L}'_q(u, q, \lambda)(\delta q), \\ j''(q)(\delta q, \delta r) &= \mathcal{L}''_{qq}(u, q, \lambda)(\delta q, \delta r) + \mathcal{L}''_{uq}(u, q, \lambda)(\delta u, \delta r) \\ &\quad + \mathcal{L}''_{\lambda q}(u, q, \lambda)(\delta \lambda, \delta r) \end{aligned}$$

where for given $\delta q, \delta r$ the quantities $\delta u, \delta \lambda$ are obtained by solving certain auxiliary linear problems.

b) Indirect approach: Direct solution of the fully coupled discretized KKT system (e.g., by MG method)

$$\left\{\begin{array}{l} J'_u(u_h,q_h)(\varphi_h) - A'_u(u_h,q_h)(\varphi_h,\lambda_h) \\ J'_q(u_h,q_h)(\chi_h) - A'_q(u_h,q_h)(\chi_h,\lambda_h) \\ -A(u_h,q_h)(\psi_h) \end{array}\right\} = 0$$

There are various pros and cons, particularly in nonstationary situations!

NO FURTHER DETAILS, as this issues would deserve an extra lecture.

3.4.2 Balancing iteration and discretization error

We consider the linear-quadratic optimization problem

$$J(u,q) := \tfrac{1}{2}\|u-\bar{u}\|^2 + \tfrac{1}{2}\alpha\|q\|^2 \;\rightarrow\; \min,$$
$$-\Delta u = f + q \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega.$$

on $\Omega := (0,1)^2$ with force f, distribution $\bar{u}$, and $\alpha = 10^{-3}$.

The Euler-Lagrange approach uses the Lagrangian

$$\mathcal{L}(u,q,\lambda) := J(u,q) + (f+q,\lambda) - (\nabla u, \nabla\lambda),$$

with the adjoint variable $\lambda \in V$. Then, for any optimal solution $\{u,q\} \in V \times Q$ there exists an adjoint solution $\lambda \in V$ such that the triplet $\{u,q,\lambda\}$ is a stationary point of the Lagrangian, i.e., it solves the following (**linear**) saddle point system:

$$
\begin{aligned}
(\nabla\varphi, \nabla\lambda) - (u, \varphi) &= -(\bar{u}, \varphi) \quad \forall \varphi \in V, \\
(\chi, \lambda) + \alpha(\chi, q) &= 0 \quad \forall \chi \in Q, \\
(\nabla u, \nabla\psi) - (q, \psi) &= (f, \psi) \quad \forall \psi \in V.
\end{aligned}
$$

Using conforming bilinear Q_1 elements for discretizing all three variables $\{u, q, \lambda\}$ in associated finite element subspaces $V_h \subset V$ and $Q_h \subset Q$ leads to the discrete saddle point problems

$$
\begin{aligned}
(\nabla\varphi_h, \nabla\lambda_h) - (u_h, \varphi_h) &= -(\bar{u}, \varphi_h) \quad \forall \varphi_h \in V_h, \\
(\chi_h, \lambda_h) + \alpha(\chi_h, q_h) &= 0 \quad \forall \chi_h \in Q_h, \\
(\nabla u_h, \nabla\psi_h) - (q_h, \psi_h) &= (f, \psi_h) \quad \forall \psi_h \in V_h.
\end{aligned}
$$

These linear saddle point problems are solved by a MG method using a block ILU iteration as smoother.

Proposition. *Let* $\{u,q,\lambda\}\in V\times Q\times V$ *be the solution of the KKT system and* $\{\tilde u_h,\tilde q_h,\tilde\lambda_h\}\in V_h\times Q_h\times V_h$ *the approximative finite element solution of the discrete KKT system on the finest mesh* $\mathbb{T}_h$ *. Then, we have the following error representation:*

$$J(u,q)-J(\tilde u_h,\tilde q_h)=\tfrac12\rho^*(\tilde u_h,\tilde\lambda_h)(u-\tilde u_h)+\tfrac12\rho^q(\tilde q_h,\tilde\lambda_h)(q-\tilde q_h)$$
$$+\tfrac12\rho(\tilde u_h,\tilde q_h)(\lambda-\tilde\lambda_h)+\rho(\mathbf{\tilde u_h},\mathbf{\tilde q_h})(\tilde{\boldsymbol\lambda}_{\mathbf h})$$

with the residuals

$$\rho^*(\tilde u_h,\tilde\lambda_h)(\cdot):=(\tilde u_h-\bar u,\cdot)-(\nabla\cdot,\nabla\tilde\lambda_h),$$
$$\rho^q(\tilde q_h,\tilde\lambda_h)(\cdot):=\alpha(\cdot,\tilde q_h)+(\cdot,\tilde\lambda_h),$$
$$\rho(\tilde u_h,\tilde q_h)(\cdot):=(f+\tilde q_h,\cdot)-(\nabla\tilde u_h,\nabla\cdot).$$

Numerical example with smooth exact solution

The discretized KKT system solved by the adaptive multigrid method using the V-cycle and again $4 + 4$-block-ILU smoothing steps.

MG with block ILU smoothing, $\alpha = 10^{-3}$.

N	E	#It	E_h	η_h	I_{eff}^h	E_{it}	η_{it}	$I_{\text{eff}}^{\text{it}}$
81	1.64e-4	2	1.78e-4	2.19e-4	1.22	1.42e-5	1.68e-5	1.18
289	3.75e-5	2	4.16e-5	4.39e-5	1.05	4.13e-6	4.33e-6	1.04
1 089	1.05e-5	2	1.02e-5	1.03e-5	1.01	3.48e-7	3.52e-7	1.01
3 985	2.67e-6	2	2.54e-6	2.55e-6	1.00	1.28e-7	1.28e-7	1.00
13 321	6.65e-7	2	6.48e-7	6.49e-7	1.00	1.63e-8	1.63e-8	1.00
47 201	1.76e-7	2	1.70e-7	1.69e-7	0.99	6.76e-9	6.77e-9	1.00
163 361	4.89e-8	2	4.69e-8	4.68e-8	0.99	1.97e-9	1.97e-9	1.00

The discretized KKT system solved by the adaptive multigrid method using only one undamped block-Jacobi smoothing step.

MG II with block Jacobi smoothing, $\alpha = 10^{-3}$

N	E	#It	E_h	η_h	I_{eff}^h	E_{it}	η_{it}	$I_{\text{eff}}^{\text{it}}$
81	1.84e-4	5	2.20e-4	1.78e-4	1.23	7.59e-6	6.44e-6	1.18
289	4.36e-5	5	4.40e-5	4.16e-5	1.05	2.04e-6	1.96e-6	1.04
1 089	1.10e-5	4	1.03e-5	1.02e-5	1.01	8.53e-7	8.44e-7	1.01
3 985	2.69e-6	4	2.55e-6	2.56e-6	0.99	1.31e-7	1.30e-7	1.00
13 321	6.94e-7	4	6.47e-7	6.69e-7	0.96	2.51e-8	2.51e-8	1.00
47 201	1.95e-7	4	1.69e-7	1.90e-7	0.88	4.39e-9	4.40e-9	1.00
171 969	7.24e-8	3	4.42e-8	6.93e-8	0.63	3.07e-9	3.10e-9	0.99

3.5 Applications

3.5.1 Drag minimization

Example from optimal flow control

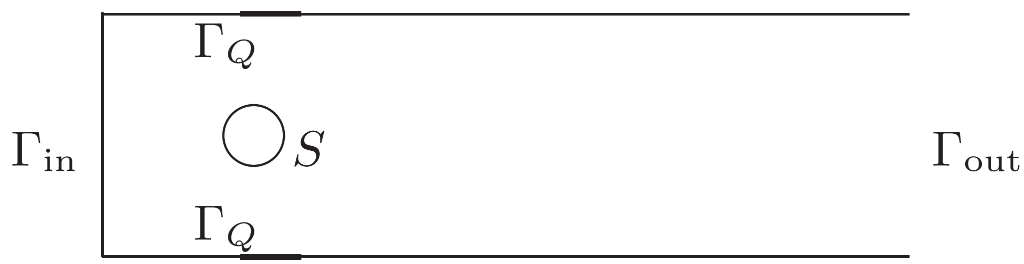
Stationary Navier-Stokes equations for $u := \{v, p\}$:

$$-\nu\Delta v + v \cdot \nabla v + \nabla p = 0 \qquad \nabla \cdot v = 0$$

$$v|_{\Gamma_{\text{rigid}}} = 0, \quad v|_{\Gamma_{\text{in}}} = v^{in}, \quad \nu\partial_n v - np|_{\Gamma_{\text{out}}} = 0$$

Goal: Minimize drag by Neumann control (pressure drop)

$$J_{\text{drag}} := \frac{2}{\bar{U}D} \int_S n^T \sigma(v,p) e_1 \, ds$$



Reynolds number $\quad \text{Re} = \bar{\text{U}}^2\text{D}/\nu = 40 \quad$ (initially stationary flow)

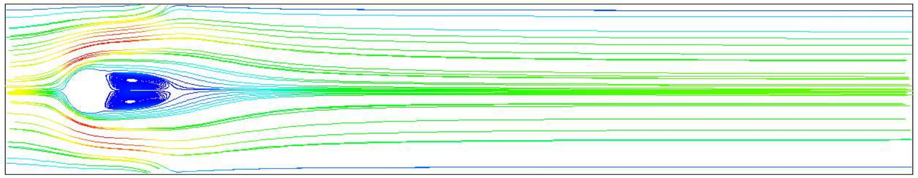
Variational formulation:

$$A(u,q)(\psi) = 0 \qquad \forall \psi \in V.$$

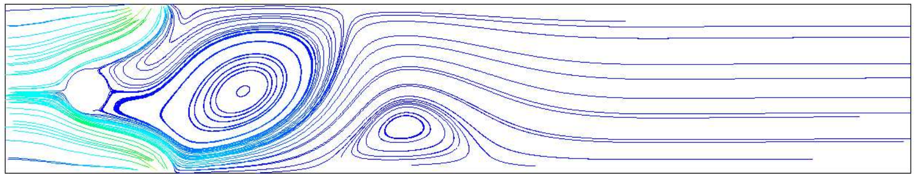
$$A(u,q)(\psi) := \nu(\nabla v, \nabla \psi) + (v \cdot \nabla v, \psi) - (\mathbf{q}, \mathbf{n} \cdot \psi)_{\mathbf{\Gamma_Q}} - (p, \nabla \cdot \psi) - (\chi, \nabla \cdot v)$$

---

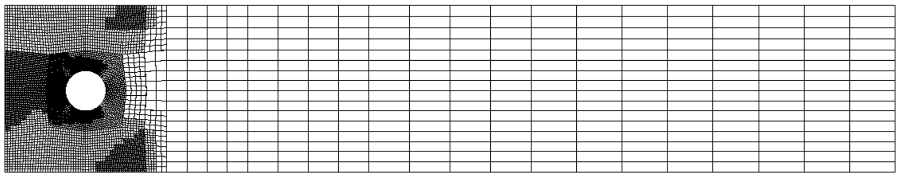
uncontrolled flow



controlled flow



optimally adapted mesh



Uniform refinement versus adaptive refinement for $\mathrm{Re} = 40$

Uniform refinement		**Adaptive** refinement	
N	J_{drag}	N	J_{drag}
10512	3.31321	1572	3.28625
41504	3.21096	4264	3.16723
164928	3.11800	11146	3.11972

Remarks.

- Optimization cycle for determining q_h^{opt}, u_h^{opt} on sparse meshes and recovery of admissible state $\tilde{u}_h^{opt}$ on fine mesh:

$$A(\tilde{u}_h^{opt}, q_h^{opt})(\psi_h) = 0 \quad \forall \psi_h \in \tilde{V}_h$$

- **Question:** Stability of stationary "optimal" state?

3.5.2 Estimation of reaction rates

Example from parameter estimation

Reaction-diffusion problem

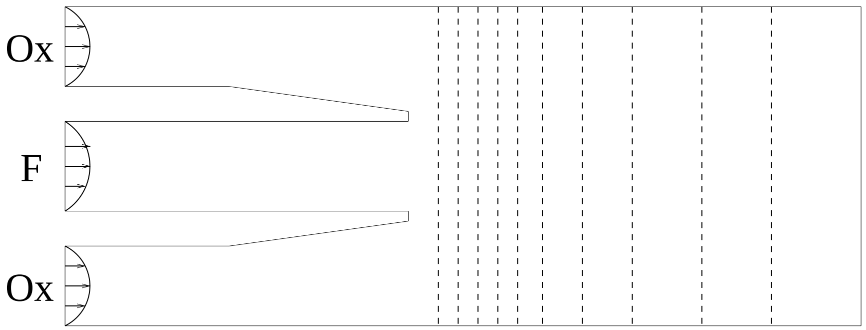
$$\beta \cdot \nabla u - \mu \Delta u = f(u) \quad \text{in } \Omega$$
$$u = \hat{u} \quad \text{on } \Gamma_{in}, \qquad \partial_n u = 0 \quad \text{on } \partial\Omega \setminus \Gamma_{in}$$

Arrhenius-type reaction law

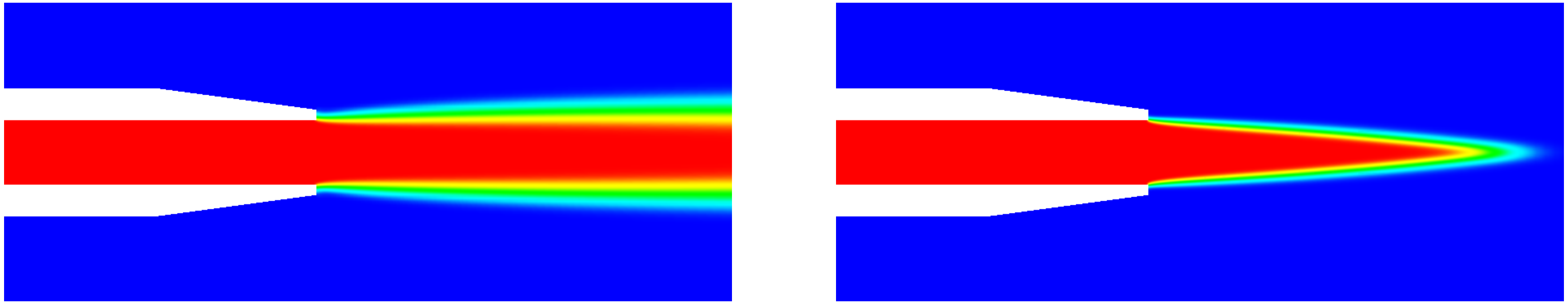
$$f(u) = A \exp\Big(- \frac{E}{1-u} \Big) u(1-u)$$

To determine are A and E from “measured” line averages

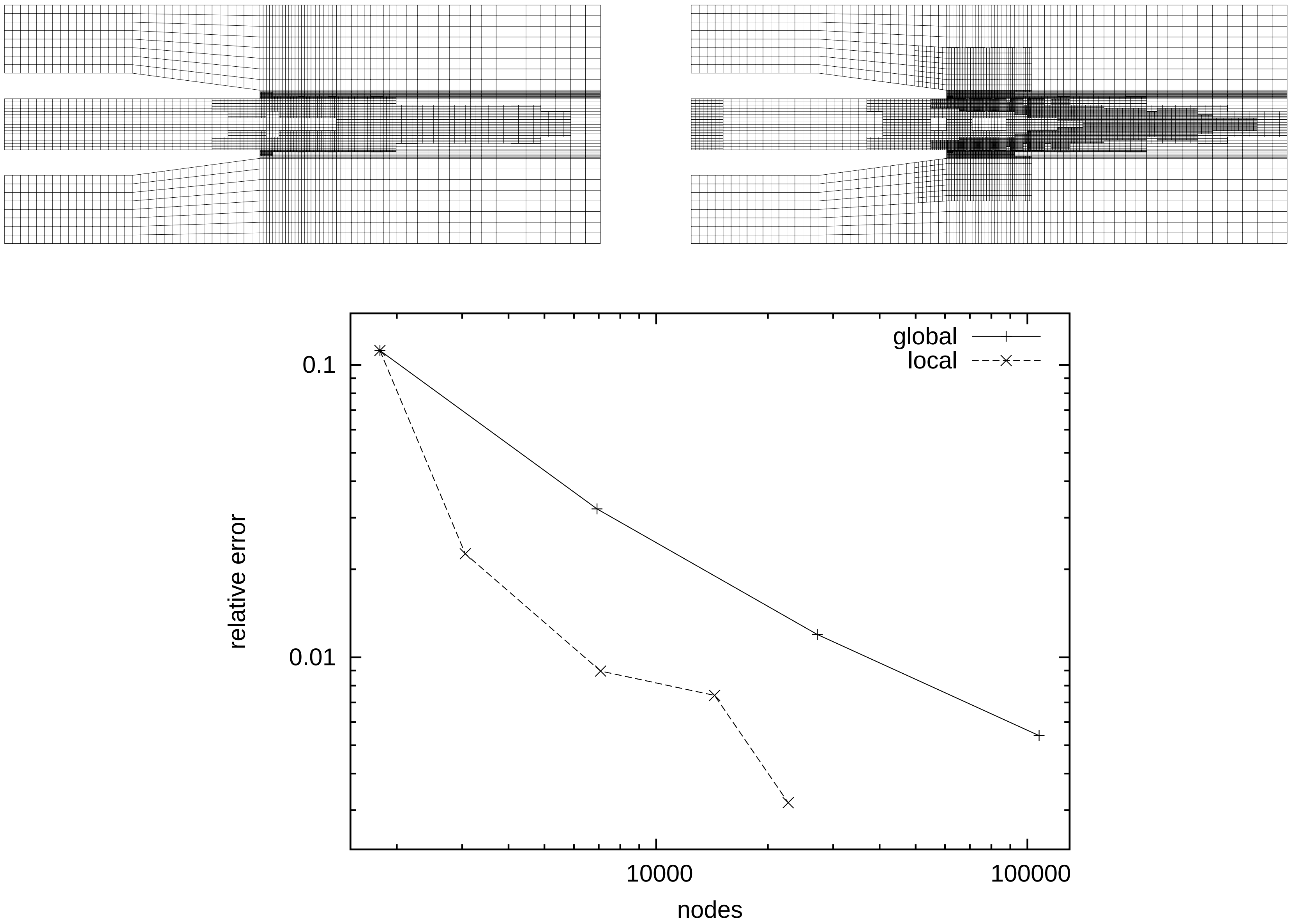
$$\int_{\Gamma_i} u\, ds, \quad i = 1, \ldots, 10.$$



Measurements:
vertical line-integrals of concentration



Initial solution for $A = 54.6$, $E = 0.15$ (left),
Estimated solution for $A = 992.3$, $E = 0.07$ (right)



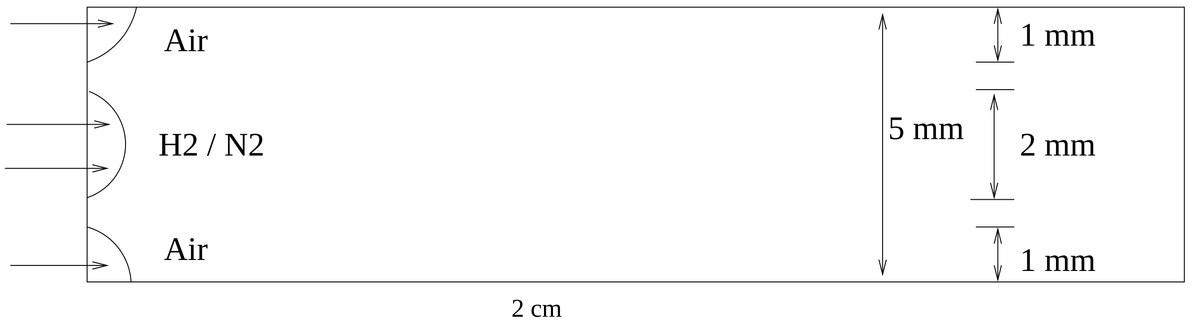
global
local
0.1
0.01
relative error
10000
100000
nodes

3.5.3 Application to model calibration

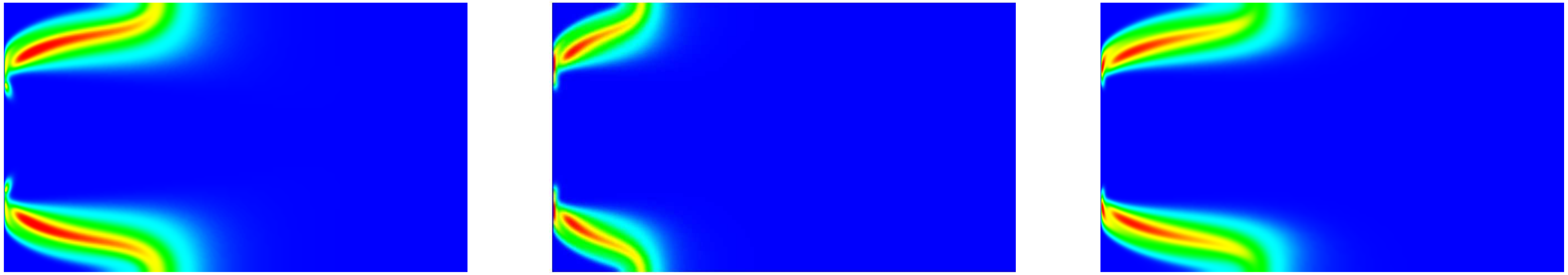
Example from diffusion model calibration

Reactive flow problem with diffusion model of Fick's type:

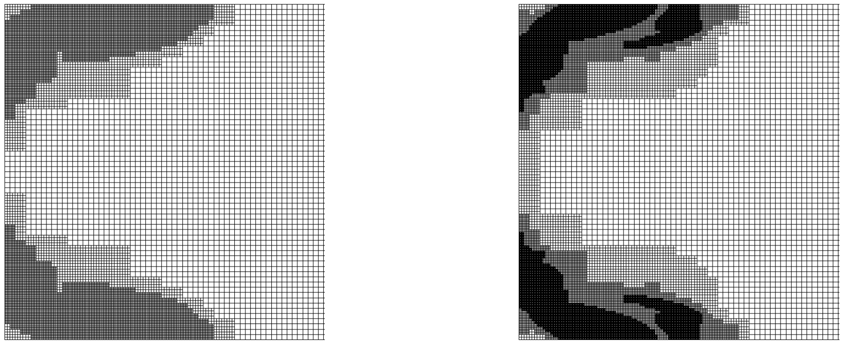
$$
\begin{aligned}
\operatorname{div}(\rho v) &= 0 \\
(\rho v \cdot \nabla) v + \operatorname{div} \pi + \nabla p &= 0 \\
\rho v \cdot \nabla T - c_p^{-1} \nabla \cdot \mathcal{Q} &= f_T \\
\rho v \cdot \nabla y_k + \nabla \cdot (q_k D_k^* \nabla y_k) &= f_k \quad k = 1, \ldots, 9
\end{aligned}
$$



Measurements: point-values of concentrations



Multicomponent diffusion (reference solution), Fick's law (initial parameters), Fitted Fick's law (estimated parameters)



Locally refined meshes (zooms)

3.6 Extensions

3.6.1 Nonstationary problems

"Initial control" in the nonstationary semi-linear diffusion problem

$$\begin{aligned}\partial_t u - \Delta u + s(u) &= f \quad \text{in } \; Q_T = \Omega\times(0,T],\\ \partial_n u = 0 \;\text{ on } \partial\Omega, &\quad u_{|t=0} = q.\end{aligned}$$

Control $q = q(x)$ such that

$$J(u,q) := \frac{1}{2}\|u(\cdot,T) - \bar{u}\|_\Omega^2 + \frac{\alpha}{2}\|q\|_\Omega^2 \;\rightarrow\; \min!$$

Variational formulation in space-time domain $Q_T = \Omega\times(0,T]$:

$$\begin{aligned}&(\partial_t u,\psi)_{Q_T} + (\nabla u,\nabla\psi)_{Q_T} + (s(u),\psi)_{Q_T}\\ &\qquad\qquad = (f,\psi)_{Q_T} + (q - u(0),\psi(0))_\Omega \quad \forall\psi\in V\end{aligned}$$

Lagrange formalism yields first-order necessary optimality condition in form of a saddle-point problem for $\{u, q, \lambda\}$:

$$
\begin{aligned}
-(\varphi, \partial_t\lambda)_{Q_T} + (\nabla\varphi, \nabla\lambda)_{Q_T} + (\varphi, s'(u)\lambda)_{Q_T} &= (\varphi(T), u(T) - \bar{u} - \lambda(T))_\Omega \\
(\lambda(0) + \alpha q, \chi)_\Omega &= 0 \\
(\partial_t u, \psi)_{Q_T} + (\nabla u, \nabla\psi)_{Q_T} + (s(u), \psi)_{Q_T} &= (q - u(0), \psi(0))_\Omega
\end{aligned}
$$

for all admissible test triplets $\{\psi, \chi, \varphi\}$. In strong form:

$$
\begin{aligned}
&-\partial_t\lambda - \Delta\lambda + s'(u)\lambda = 0 \quad \text{in } Q_T \\
&\lambda_{|t=T} = u(T) - \bar{u}, \quad \partial_n\lambda_{|\partial\Omega} = 0 \\
&\lambda_{|t=0} = -\alpha q \\
&\partial_t u - \Delta u + s(u) = 0 \quad \text{in } Q_T \\
&u_{|t=0} = q, \quad \partial_n u_{|\partial\Omega} = 0
\end{aligned}
$$

Discretization of the saddle-point problem by a space-time finite element Galerkin discretization using the so-called

"cG(1)" ("continuous Galerkin" = Crank-Nicolson scheme)

time discretization method. Time grid

$$0 = t_0 < ... < t_m < ... < t_M = T, \qquad k_m := t_m - t_{m-1},$$

with corresponding sequence of spatial meshes $\mathbb{T}_h^n$ and finite element spaces V_h^k consisting of spatially continuous functions which are cellwise bilinear in space and polynomial (constant or linear) in time.

Problem: Storing the primal solution over the whole time interval requires enormous storage space.

Efficient solution by **check-pointing** trading storage ("S") for work ("W"). Recursive ("multi-level") check-pointing results in (M time steps):

$$\mathbf{S}_{\min} = \mathbf{O}\big(\log_{\mathbf{2}}(\mathbf{M})\big), \qquad \mathbf{W}_{\min} = \mathbf{O}\big(\mathbf{M}\log_{\mathbf{2}}(\mathbf{M})\big).$$

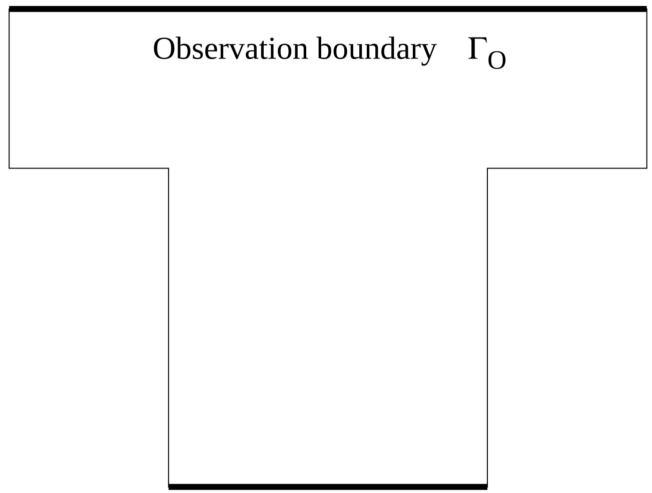
3.6.2 Control and state constraints

Distributed control of linear diffusion problem

$$J(u,q) := \tfrac{1}{2}\|u-\bar{u}\|^2_{\Gamma_O} + \tfrac{1}{2}\alpha\|q\|^2_{\Omega} \to \min$$

$$-\Delta u + s(u) = q \quad \text{in } \Omega, \qquad q_* \le q \le q^*$$

$$\partial_n u_{|\Gamma_N} = 0, \quad \partial_n u_{|\Gamma_C} = q$$



KKT system in strong form:

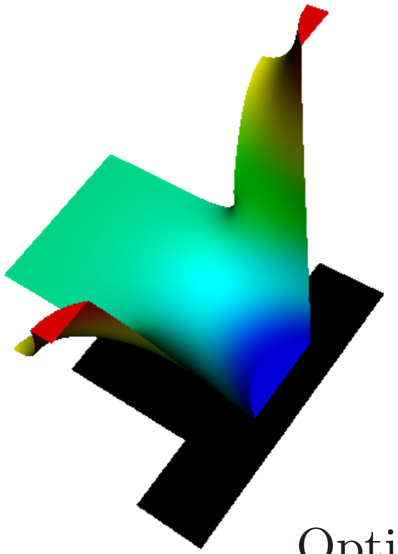
$$-\Delta\lambda + s'(u)\lambda = 0, \;\text{ in } \Omega, \quad \partial_n\lambda_{|\Gamma_O} = u_{|\Gamma_O} - \bar{u}, \;\; \partial_n\lambda_{|\Gamma_N\cup\Gamma_C} = 0$$

$$q = P_{[q_*,q^*]}(\alpha^{-1}\lambda)$$

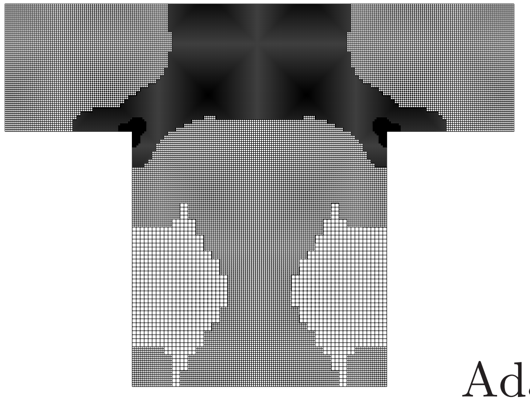
$$-\Delta u + s(u) = f, \;\text{ in } \Omega, \quad \partial_n u_{|\Gamma_N} = 0, \quad \partial_n u_{|\Gamma_C} = q$$

A posteriori error estimate: $\tilde{\rho}_K^q := \|\alpha q_h + \alpha P_{[q_*, q^*]}(\alpha^{-1}\lambda_h)\|_K$

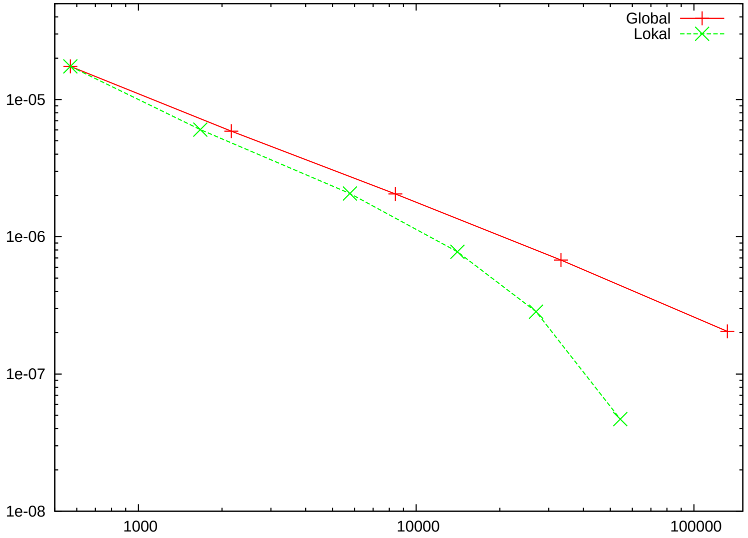
$$|J - J_h| \approx \eta_\omega := \sum_{K \in \mathcal{T}_h} \{\rho_K^u\, \omega_K^\lambda + \rho_K^\lambda\, \omega_K^u + \tilde{\rho}_K^q\, \omega_K^q\},$$



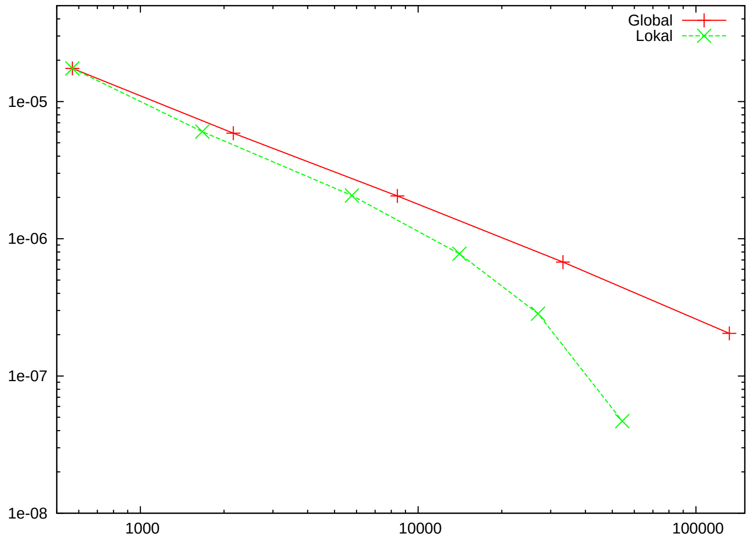
Optimal control



Adapted mesh



Local versus uniform mesh refinement



Local versus uniform mesh refinement

State constraints

Strategy: Penaltization of constraints and reduction to (singularly perturbed) unconstraint problem.

Problems: Solution method and error estimates robust w.r.t. penaltization parameter? (under work; W. Wollner)