

Adaptive finite element methods for PDE-constrained optimization problems

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- 2 Examples
- 3 Adaptive algorithm
- 4 Optimization problems governed by parabolic equations
- 5 Space-time finite element discretization
- 6 A posteriori error estimation
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- Applications from engineering and natural sciences
- mathematical models with partial differential equations (PDEs)
- Goals:
 - Numerical simulation of the process
 - Calibration of the mathematical model
 - Optimization / Optimal control of the underlying process

Optimization problem (infinite dimensional)

$$\text{Minimize } J(q, u), \quad q \in Q_{\text{ad}}, \quad u \in V_{\text{ad}}$$

subject to

$$A(q, u) = 0$$

Discretized optimization problem

$$\text{Minimize } J(q_h, u_h), \quad q_h \in Q_h \cap Q_{\text{ad}}, \quad u_h \in V_h \cap V_{\text{ad}}$$

subject to

$$A_h(q_h, u_h) = 0$$

- $\dim V_h, \dim Q_h < \infty$
- Discretization error between (q, u) and (q_h, u_h)
- Numerical effort depends on $\dim V_h$ and $\dim Q_h$



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→ Goal:

- “Discretization error” \leq tolerance
- Numerical effort \rightarrow min!

→ Questions:

- What kind of error is important?
 - Quantity of interest: $J(q, u)$
- How to measure/estimate this error?
 - A posteriori error estimation: $J(q, u) - J(q_h, u_h) \approx \eta_h$
- How to construct an appropriate discretization?
 - Adaptive choice of discretizations: \rightarrow locally refined meshes



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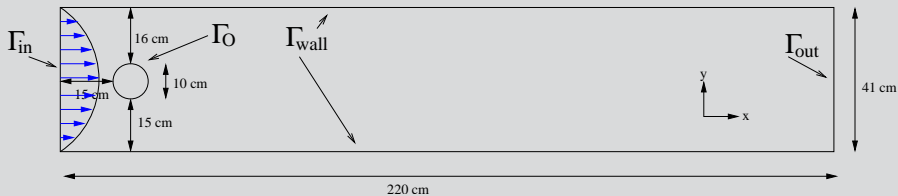
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- Becker, Kapp, Rannacher
- Liu et al.
- Hoppe, Kieweg, Hintermüller
- Vexler, Benedix, Wollner
- Günther, Hinze, Schiela
- Meidner, Vexler
- ...

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Flow around a cylinder



Optimization problem

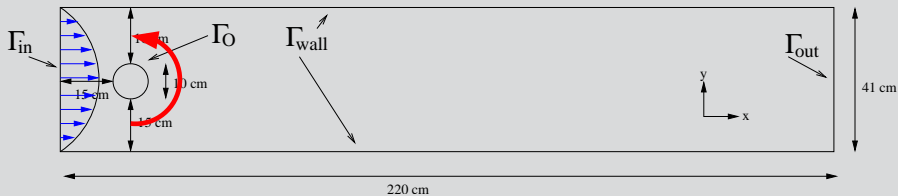
$$\text{Minimize } J(u) = c_0 \int_{\Gamma_O} n \cdot \sigma(u) \cdot d \, ds, \quad \sigma(u) = \frac{\nu}{2} (\nabla v + \nabla v^T) - pl, \quad u = (v, p)$$

$$-\nu \Delta v + v \cdot \nabla v + \nabla p = 0, \quad \nabla \cdot v = 0 \text{ in } \Omega$$

$$v = v_{in} \text{ on } \Gamma_{in}, \quad v = 0 \text{ on } \Gamma_w, \quad \nu \partial_n v - p \cdot n = 0 \text{ on } \Gamma_{out}$$

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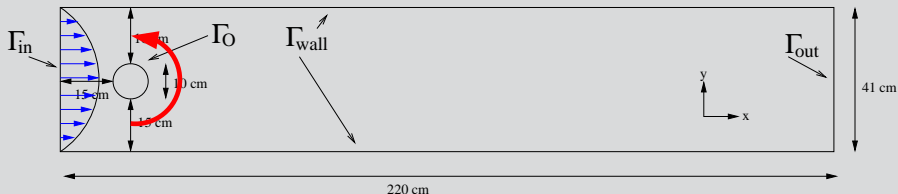
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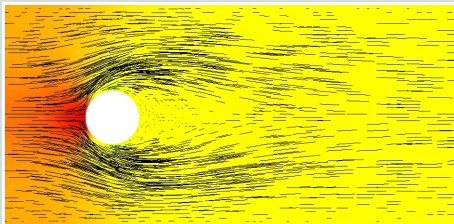
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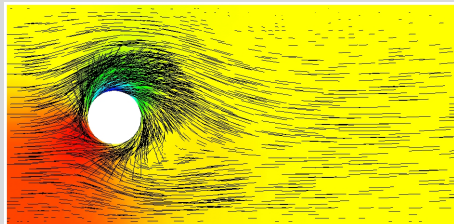
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uncontrolled flow, $J(u) \approx 5.58$

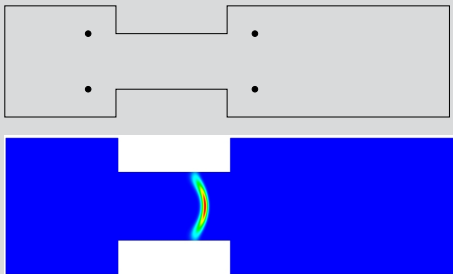


controlled flow, $J(u) \approx 5.04$



- Quantity of interest $I(q, u) = J(u)$ (QI = Cost functional)
- Discretization of the state variable $u = (v, p)$ in space
- Error estimation $J(u) - J(u_h)$

Configuration



Mathematical model

$$\partial_t \theta - \Delta \theta = \omega \quad \text{in } (0, T) \times \Omega$$

$$\partial_t y - \frac{1}{L} \Delta y = -\omega \quad \text{in } (0, T) \times \Omega$$

$$\omega = \frac{\beta^2}{2\gamma} y \exp\left(\frac{\beta(\theta - 1)}{1 + \alpha(\theta - 1)}\right)$$

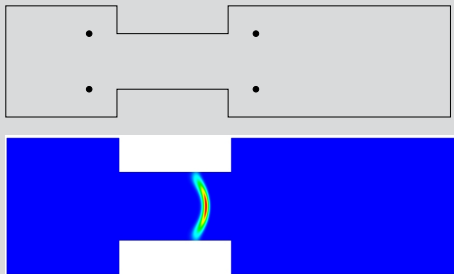
+ Initial and boundary conditions

- The state $u = (\theta, y)$ consists of temperature and concentration of the fuel
- The parameter $q = \alpha$ has to be estimated

State equation

$$A(q, u) = 0$$

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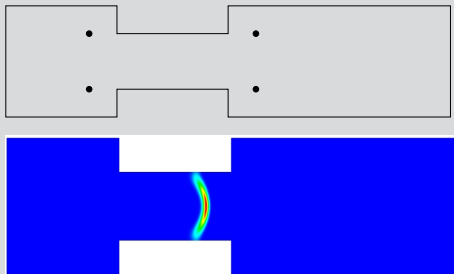
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State equation

$$A(q, u) = 0$$

- Comparison of an experiment and the simulation
- Observation \bar{C} vs. $C(u)$

Optimization problem

$$\text{Minimize } J(q, u) = \frac{1}{2} \|C(u) - \bar{C}\|_Z^2, \quad q \in Q, u \in V$$

subject to

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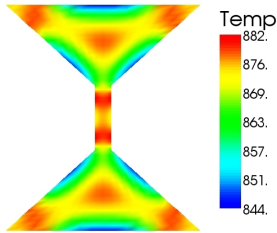
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$$\partial_t \theta - k \Delta \theta = \frac{1}{3\kappa} \Delta \rho \quad \text{in } (0, T) \times \Omega$$

$$-\frac{\varepsilon^2}{3\kappa} \Delta \rho + \kappa \rho = 4\kappa \pi a \theta^4 \quad \text{in } (0, T) \times \Omega$$

$$\frac{1}{\varepsilon k} \theta + n \cdot \nabla \theta = \frac{1}{\varepsilon k} q \quad \text{auf } (0, T) \times \partial \Omega$$

$$\frac{3\kappa}{2\varepsilon} \rho + n \cdot \nabla \rho = \frac{3\kappa}{2\varepsilon} 4\pi a q^4 \quad \text{auf } (0, T) \times \partial \Omega$$

- The state $u = (\theta, \rho)$ consist of the temperature and the radiation transfer
- Die control q is the ambient temperature

State equation

$$A(q, u) = 0$$

Optimization problem

$$\text{Minimize } J(q, u) = \int_0^T \int_{\Omega} (\theta - \theta_d)^2 dx dt + \frac{\alpha}{2} \int_0^T q^2 dt, \quad q \in Q_{\text{ad}}, u \in V_{\text{ad}}$$

subject to

$$A(q, u) = 0$$

- Control constraints

$$q \in Q_{\text{ad}} = \{ q \in L^2(0, T) \mid q_a \leq q(t) \leq q_b \text{ a.e. in } (0, T) \}$$

- State constraints

$$\theta_a \leq \theta(t, x) \leq \theta_b \quad \text{and/or} \quad |\nabla \theta(t, x)| \leq c_b$$

- Discretization of the state variable in space and time
- Discretization of the control variable in time

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Degrees of freedom for the choice of discretization

- Temporal discretization
 - Choice of the time steps
- Spatial discretization
 - Choice of spatial meshes for each time step
- Control discretization
 - Choice of the discretization of the control space

Goal: Error estimators

$$l(q, u) - l(q_\sigma, u_\sigma) \approx \eta_k + \eta_h + \eta_l$$



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- 2 Compute (q_σ, u_σ)
- 3 Evaluate $\eta_{k_n}, \eta_{h_n}, \eta_{l_n}$
- 4 if $\eta_{k_n} + \eta_{h_n} + \eta_{l_n} \leq TOL$ break;
- 5 else
 - $\eta_k \gg \eta_h, \eta_k \gg \eta_l \Rightarrow$ Refine time discr.
 - $\eta_k \approx \eta_h \gg \eta_l \Rightarrow$ Refine time & space discr.
 - $\eta_k \approx \eta_h \approx \eta_l \Rightarrow$ Refine time, space & control discr.
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- 6 $n = n + 1$, go to 2

→ Refinement is based on local information from η_k, η_h, η_l

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→ State equation: $u_t + A(q, u) = f$, $u(0) = u_0$

Weak formulation

$$u \in X = W(0, T; V, V^*) : a(q, u)(\phi) = f(\phi) \quad \forall \phi \in X$$

with

$$a(q, u)(\phi) = \int_0^T \left(\langle \partial_t u(t), \phi(t) \rangle_{V^*, V} + a_s(q, u(t))(\phi(t)) \right) dt + (u(0) - u_0, \phi(0))$$

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- Lagrange functional

$$\mathcal{L}(q, u, z) = J(q, u) + f(z) - a(q, u)(z)$$

- Necessary optimality conditions:

$$\mathcal{L}'(q, u, z)(\delta q, \delta u, \delta z) = 0 \quad \forall \delta q \in Q, \forall \delta u, \delta z \in X$$

Optimality system

$$a(q, u)(v) = f(v) \quad \forall v \in X \quad (\text{state equation})$$

$$a'_u(q, u)(v, z) = J'_u(q, u)(v) \quad \forall v \in X \quad (\text{adjoint equation})$$

$$a'_q(q, u)(\delta q, z) = J'_q(q, u)(\delta q) \quad \forall \delta q \in Q \quad (\text{gradient equation})$$

$$\rightarrow J'_q(q, u)(\delta q - q) - a'_q(q, u)(\delta q - q, z) \geq 0 \quad \forall \delta q \in Q_{ad}$$



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Optimize-then-Discretize versus Discretize-then-Optimize

→ Optimize-then-Discretize

- Build up the optimality system on the continuous level
- Discretize the state, the adjoint and the gradient equations
- Appropriate and stable discretizations of all involved equations

→ Discretize-then-Optimize

- Discretize the state equation
- Build up the optimality system for the discrete optimization problem
- Preserving problem structure (symmetry of the optimality system)

→ For a pure Galerkin discretization:

Optimize-then-Discretize = Discretize-then-Optimize

→ Exact discrete derivatives



- Use finite elements for spatial and temporal discretization
 - Optimize-then-Discretize = Discretize-then-Optimize
 - Systematic a priori error analysis
 - Systematic a posteriori error estimation
 - Dynamic meshes

- Temporal discretization: Discontinuous Galerkin methods
 - Time partitioning: $\bar{T} = \{0\} \cup I_1 \cup I_2 \dots \cup I_M$ with

$$I_m = (t_{m-1}, t_m] \text{ and } 0 = t_0 < t_1 < \dots < t_{M-1} < t_M = T$$

- Semidiscretized state space

$$X_k^r = \{v_k \in L^2(I, V) \mid v_k|_{I_m} \in P_r(I_m, V) \text{ and } v_k(0) \in H\}$$

- Use finite elements for spatial and temporal discretization

- Optimize-then-Discretize = Discretize-then-Optimize
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Semi-discretization in time

$$u_k \in X_k^r : a_k(q_k, u_k)(\phi_k) = f(\phi_k) \quad \forall \phi_k \in X_k^r$$

with

$$a_k(q_k, u_k)(\phi_k) := a(q_k, u_k)(\phi) + \sum_{m=1}^{M-1} ([u_k]_m, \phi_m^+)$$

Spatial discretization

$$u_{kh} \in X_{kh}^{r,s} : a_k(q_{kh}, u_{kh})(\phi_{kh}) = f(\phi_{kh}) \quad \forall \phi_{kh} \in X_{kh}^{r,s}$$

with the discrete state space:

$$X_{kh}^{r,s} = \{v_{kh} \in X_k^r : v_{kh}|_{I_m} \in P_r(I_m, V_{h,m}^s) \text{ and } v_k(0) \in V_{h,0}^s\}$$

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→ Reinterpret Galerkin methods as time stepping schemes

- $dG(0) \implies$ (variant of) implicit Euler scheme
- $dG(r) \implies$ A-stable scheme of order $r + 1$

Discrete optimization problem

$$\text{Minimize } J(q_\sigma, u_\sigma), \quad q_\sigma \in Q_I, u_\sigma \in X_{kh}^{r,s}$$

subject to

$$a_k(q_\sigma, u_\sigma)(\phi_{kh}) = f(\phi_{kh}) \quad \forall \phi_{kh} \in X_{kh}^{r,s}$$

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→ Goal: $I(q, u) - I(q_\sigma, u_\sigma) \approx \eta_k + \eta_h + \eta_l$

→ Lagrange functional: $\mathcal{L}(q, u, z) = J(q, u) + f(z) - a_k(q, u)(z)$

$$\xi = (q, u, z) \quad \in \quad Q \times X \times X \quad \mathcal{L}'(\xi)(\delta\xi) \quad = 0$$

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$$\xi_{kh} = (q_{kh}, u_{kh}, z_{kh}) \quad \in \quad Q \times X_{kh} \times X_{kh} \quad \mathcal{L}'(\xi_{kh})(\delta\xi_{kh}) \quad = 0$$

$$\xi_\sigma = (q_\sigma, u_\sigma, z_\sigma) \quad \in \quad Q_l \times X_{kh} \times X_{kh} \quad \mathcal{L}'(\xi_\sigma)(\delta\xi_\sigma) \quad = 0$$

Error splitting

$$\begin{aligned} I(q, u) - I(q_\sigma, u_\sigma) &= I(q, u) - I(q_k, u_k) \\ &\quad + I(q_k, u_k) - I(q_{kh}, u_{kh}) \\ &\quad + I(q_{kh}, u_{kh}) - I(q_\sigma, u_\sigma) \end{aligned}$$

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Error estimation w.r.t the cost functional

$$J(q, u) - J(q_k, u_k) = \frac{1}{2} \rho_u(x_\sigma)(u - \tilde{u}_k) + \frac{1}{2} \rho_z(x_\sigma)(z - \tilde{z}_k) + R_k$$

$$J(q_k, u_k) - J(q_{kh}, u_{kh}) = \frac{1}{2} \rho_u(x_\sigma)(u_k - \tilde{u}_{kh}) + \frac{1}{2} \rho_z(x_\sigma)(z_k - \tilde{z}_{kh}) + R_{kh}$$

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$$\rho_u(x_\sigma)(\phi) = J'_u(q_\sigma, u_\sigma)(\phi) - a'_{k,u}(q_\sigma, u_\sigma)(\phi, z_\sigma)$$

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- Remainder terms: $R_k, R_{kh}, R_\sigma \rightarrow \mathcal{O}(\|\text{error}\|^3)$

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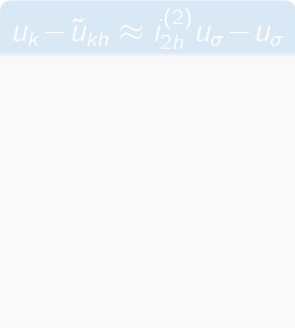
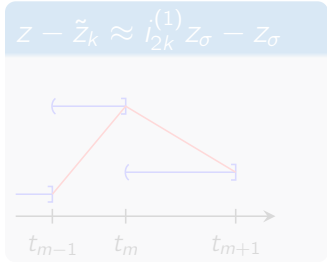
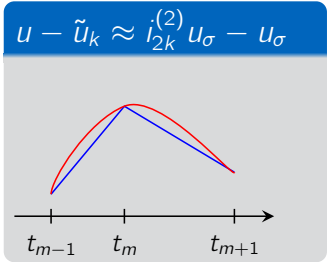
- Residuals:

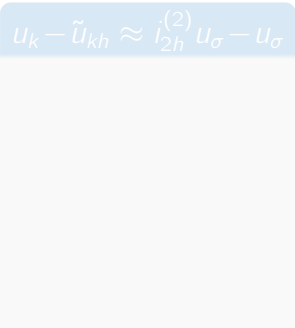
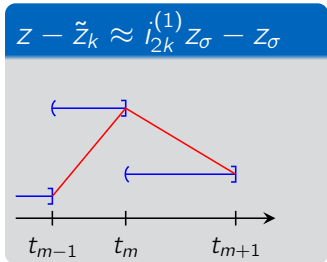
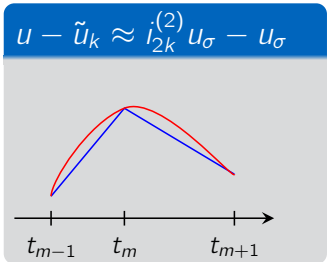
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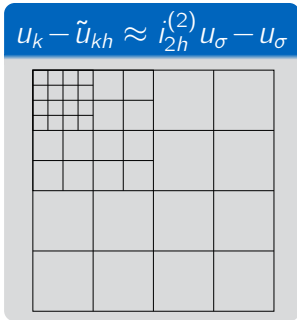
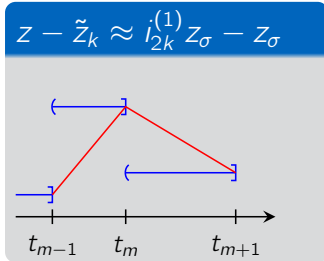
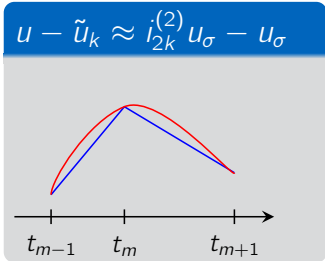
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- Error estimation w.r.t the cost functional
 - Evaluation of residuals
 - Approximation of weights

- Error estimation w.r.t a quantity of interest

- Solution of a linear problem (\sim Newton step)

$$\chi = (p, v, y) : \mathcal{L}''(q, u, z)\chi = -l'_q(q, u) - l'_u(q, u)$$

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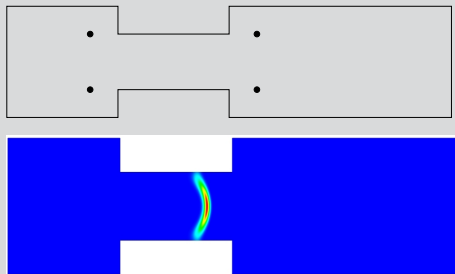
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Configuration



Mathematical model

$$\begin{aligned} \partial_t \theta - \Delta \theta &= \omega & \text{in } (0, T) \times \Omega \\ \partial_t y - \frac{1}{L} \Delta y &= -\omega & \text{in } (0, T) \times \Omega \end{aligned}$$

$$\omega = \frac{\beta^2}{2\gamma} y \exp\left(\frac{\beta(\theta - 1)}{1 + \alpha(\theta - 1)}\right)$$

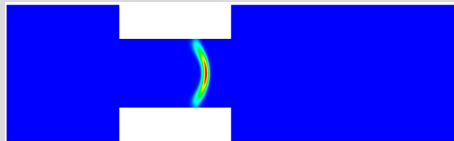
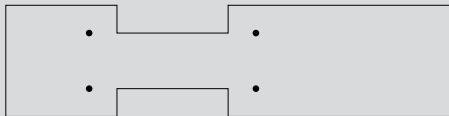
+ Initial and boundary conditions

Goal:

Estimation of Arrhenius parameters α using measurements $\theta(T, \xi_i)$ and $Y(T, \xi_i)$

→ Quantity of interest: $I(\alpha) = \alpha$

Configuration



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$$\partial_t \theta - \Delta \theta = \omega \quad \text{in } (0, T) \times \Omega$$

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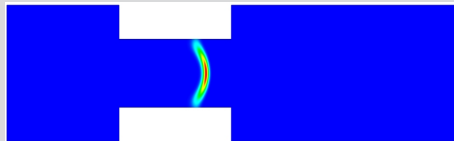
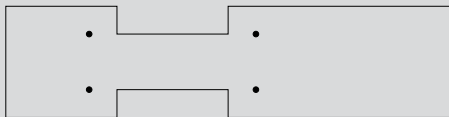
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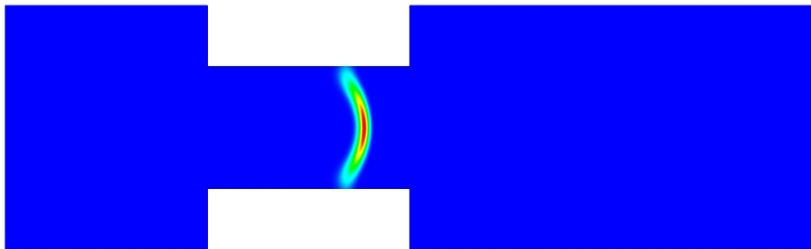
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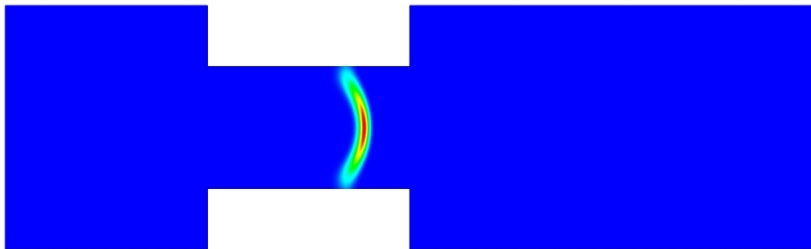
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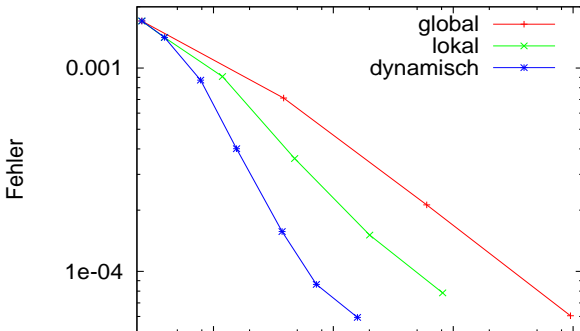
Simulation:



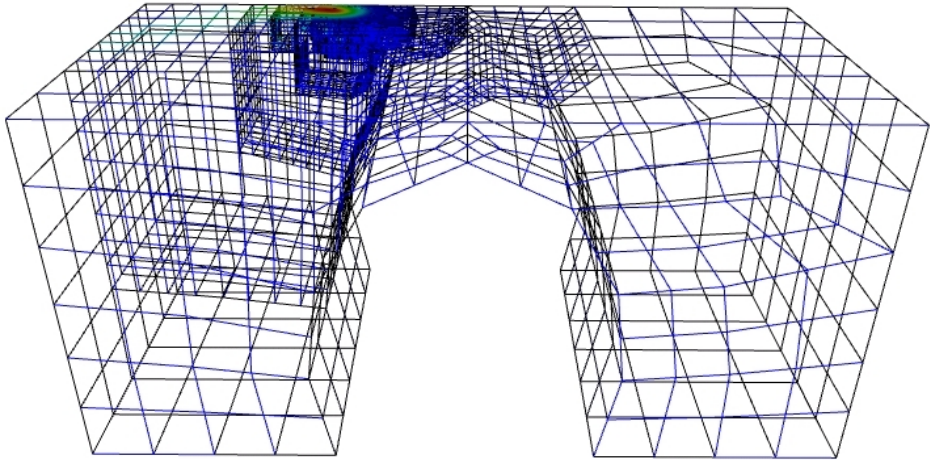
Optimization (Parameter identification):



M	N_{\max}	η_k	η_h	$\eta_k + \eta_h$	$J(u) - J(u_{kh})$	l_{eff}
256	985	$-7.8 \cdot 10^{-04}$	$4.1 \cdot 10^{-05}$	$-7.4 \cdot 10^{-04}$	$-1.7 \cdot 10^{-03}$	2.29
396	985	$-7.4 \cdot 10^{-04}$	$2.0 \cdot 10^{-04}$	$-5.4 \cdot 10^{-04}$	$-1.4 \cdot 10^{-03}$	2.63
616	1427	$-2.5 \cdot 10^{-04}$	$-3.3 \cdot 10^{-04}$	$-5.8 \cdot 10^{-04}$	$-8.7 \cdot 10^{-04}$	1.51
872	2309	$-1.0 \cdot 10^{-04}$	$-1.4 \cdot 10^{-04}$	$-2.4 \cdot 10^{-04}$	$-4.0 \cdot 10^{-04}$	1.64
1370	3927	$-5.0 \cdot 10^{-05}$	$-6.8 \cdot 10^{-05}$	$-1.2 \cdot 10^{-04}$	$-1.6 \cdot 10^{-04}$	1.33
1528	6927	$-4.6 \cdot 10^{-05}$	$-2.8 \cdot 10^{-05}$	$-7.4 \cdot 10^{-05}$	$-8.6 \cdot 10^{-05}$	1.17
1772	14683	$-4.0 \cdot 10^{-05}$	$-1.1 \cdot 10^{-06}$	$-5.2 \cdot 10^{-05}$	$-5.9 \cdot 10^{-05}$	1.15



3D – laser surface hardening of steel



- Space-time finite elements methods
 - optimize-then-discretize = discretize-then-optimize
 - exact derivatives on the discrete level

- Error estimation w.r.t. to a given **quantity of interest**
 - separation of time, space, control error
 - dynamic meshes

- Extensions: problems with inequality constraints
 - control constraints
 - state constraints