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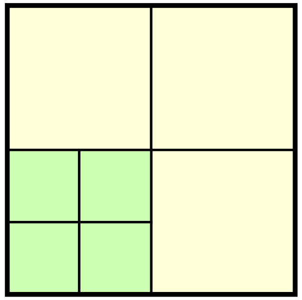
ADAPTIVE FINITE ELEMENT METHODS FOR PARTIAL DIFFERENTIAL EQUATIONS



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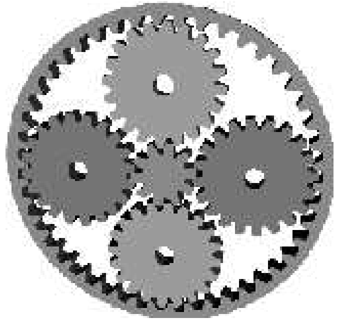

With contributions by

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V. Heuveline, Th. Richter, R. Hartmann, Th. Dunne, B. Vexler, D. Meidner, ...

Contents

Literature (reference texts suggested for reading)

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- R. Becker, D. Meidner, R. Rannacher, and B. Vexler: *Adaptive finite element methods for PDE-constrained optimal control problems*, in Reactive Flow, Diffusion and Transport (W. Jäger et al., eds), Springer, Berlin-Heidelberg, 2007.

1. Basic concepts of adaptivity

Goal of simulation: Computation of a "discrete" approximation u_h to the solution u of a continuous model with accuracy TOL, by using a discrete model of dimension N:

$$\mathcal{A}(u) = 0, \qquad \mathcal{A}_h(u_h) = 0,$$

- to gain an overall picture of the solution,
- to evaluate a certain functional quantity $J(u)$.

Goal of adaptivity: "Optimal" use of computing resources:

- $N \to \min, \quad TOL$ given.
- $TOL \to \min, \quad N$ given.

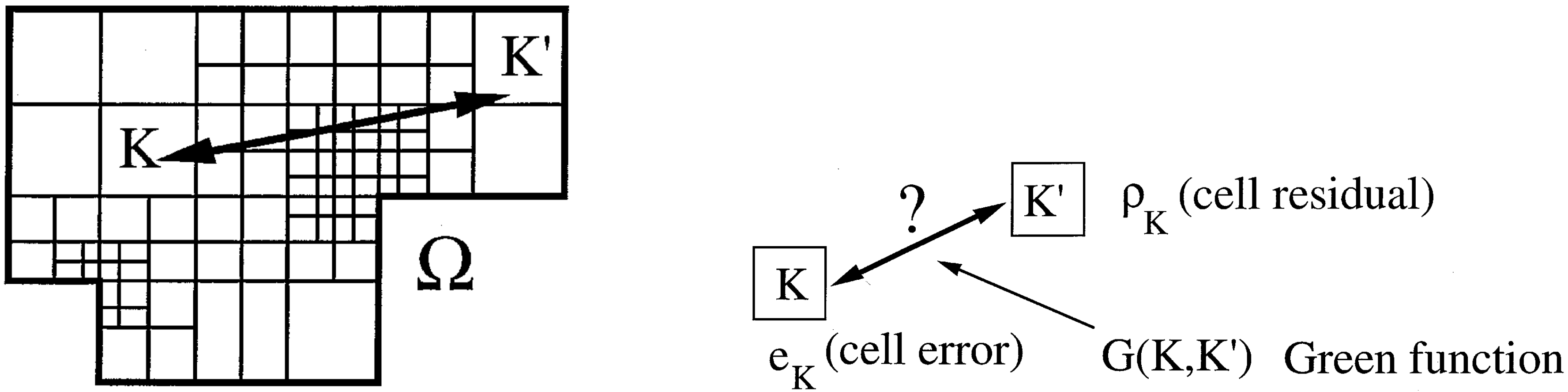
Theoretical framework:

- Variational problem: $u \in V$ (Hilbert space),

$$A(u)(\varphi) = F(\varphi) \quad \forall \varphi \in V.$$

- Galerkin (finite Element) approximation: $u_h \in V_h \subset V$,

$$A(u_h)(\varphi_h) = F(\varphi_h) \quad \forall \varphi_h \in V_h.$$



Finite element mesh and scheme of error propagation

Approaches: $\mathbb{T}_h = \{K\}$ discretization mesh

- Mesh adaptation based on local "smoothness indicators":

$$\eta_K^i := c h_K^2 \omega_K^i \|D_h^2 u_h^i\|_K, \quad D_h^2 u_h^i \text{ difference quotient.}$$

- Mesh adaptation based on local "residual indicators":

$$\eta_K^i := c h_K^2 \omega_K^i \|R_i(u_h)\|_K, \quad R_i(u_h) \text{ cell residuals.}$$

What is the appropriate weighting ω_K^i of refinement indicators based on "smoothness" or "residual" information?

- Local error sensitivity: interplay of solution components.
- Global error sensitivity: global error transport (pollution effect).

$\Rightarrow$ **Dual Weighted Residual (DWR) Method**

General concepts of error estimation

Regular matrices $A,\ A_h \in \mathbb{R}^{n\times n}$ and vectors $b,\ b_h \in \mathbb{R}^n$

$$Ax = b, \quad A_h x_h = b_h, \qquad e := x - x_h ?$$

- "truncation error" $\tau := A_h x - b_h$, "residual" $\rho := b - Ax_h$

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a) Truncation-error based error estimation ("a priori" error):

$$A_h e = A_h x - A_h x_h = A_h x - b_h = \tau$$

$$\|e\| \le \|A_h^{-1}\|\,\|\tau\|, \qquad c_{S,h} := \|A_h^{-1}\|$$

b) Residual-error based error estimation ("a posteriori" error):

$$Ae = Ax - Ax_h = b - Ax_h = \rho$$

$$\|e\| \le \|A^{-1}\|\,\|\rho\|, \qquad c_S := \|A^{-1}\|$$

c) Estimation of error moments:

$$J(e) := \langle e, j \rangle, \quad j \in \mathbb{R}^n.$$

Dual problem $\quad z \in \mathbb{R}^n : \quad A^* z = j$

Error representation

$$J(e) = \langle e, j \rangle = \langle e, A^* z \rangle = \langle Ae, z \rangle = \langle \rho, z \rangle$$

"Weighted" a posteriori error estimate

$$|J(e)| \leq \sum_{i=1}^{n} |z_i| \, |\rho_i|$$

The evaluation of the weights $|z_i|$ requires the solution of an auxiliary problem, i.e., "goal oriented" error estimation has its cost.

d) Extension to nonlinear problems

Diff' mappings $A(\cdot),\, A_h(\cdot) : \mathbb{R}^n \to \mathbb{R}^n$ and vectors $b,\, b_h \in \mathbb{R}^n$

$$A(x) = b, \quad A_h(x_h) = b_h, \qquad e := x - x_h?$$

residual $\rho := b - A(x_h)$, Jacobi matrix $A'(x)$,

$$\langle \rho, y\rangle = \langle A(x) - A(x_h), y\rangle = \int_0^1 \frac{d}{ds}\langle A(x_h + se), y\rangle\, ds$$

$$= \int_0^1 \langle A'(x_h + se)e, y\rangle\, ds = \langle Be, y\rangle$$

$$B := B(x, x_h) := \int_0^1 A'(x_h + se)\, ds$$

Error functional $J(e) = \langle e, j\rangle$ and dual problem $\quad B^* z = j$

Error identity

$$J(e) = \langle e, j \rangle = \langle e, B^* z \rangle = \langle Be, z \rangle = \langle \rho, z \rangle$$

$$|J(e)| \le \eta := \sum_{i=1}^{n} |z_i| \, |\rho_i|$$

Evaluation of weights:

$$B \approx \tilde{B} := B(x_h, x_h) = \int_0^1 A'(x_h) \, ds = A'(x_h)$$

$$A'(x_h)^* \tilde{z} = j, \qquad A'_h(x_h)^* \tilde{z}_h = j$$

Approximate a posteriori error estimate

$$|J(e)| \approx \tilde{\eta} := |(\rho, \tilde{z}_h)| = \sum_{i=1}^{n} \tilde{\omega}_i |\rho|, \qquad \tilde{\omega}_i := |\tilde{z}_{h,i}|$$

Estimation of approximation error:

$$
\begin{aligned}
J(e) = \langle e, j \rangle = \langle e, \tilde{B}^* \tilde{z} \rangle &= \langle \tilde{B} e, \tilde{z} \rangle \\
&= \langle (\tilde{B} - B) e, \tilde{z} \rangle + \langle B e, \tilde{z} \rangle \\
&= ((\tilde{B} - B) e, \tilde{z} \rangle + \langle \rho, \tilde{z} \rangle \\
&= \langle (\tilde{B} - B) e, \tilde{z} \rangle + \langle \rho, \tilde{z} - \tilde{z}_h \rangle + \langle \rho, \tilde{z}_h \rangle
\end{aligned}
$$

$$
\|\tilde{B} - B\| = \left\| \int_0^1 \{A'(x_h) - A'(x_h + se)\} \, ds \right\| \leq \tfrac{1}{2} L' \|e\|
$$

$$
|J(e)| \leq \tfrac{1}{2} L' \|\tilde{z}\| \|e\|^2 + \|\rho\| \|\tilde{z} - \tilde{z}_h\| + \tilde{\eta}
$$

The approximate error estimator $\tilde{\eta}$ is the dominant error term.

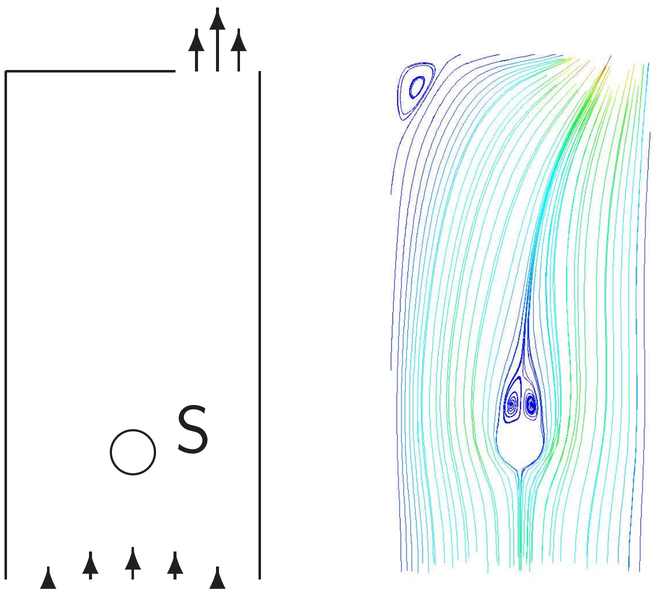
Examples of "goal-oriented" simulation

1. Drag of a body in a viscous fluid (flow direction d)

"Incompressible" Navier-Stokes equations:

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

$$J(p,v) := \kappa \int_S (n^T\tau - pn^T)d\,do$$

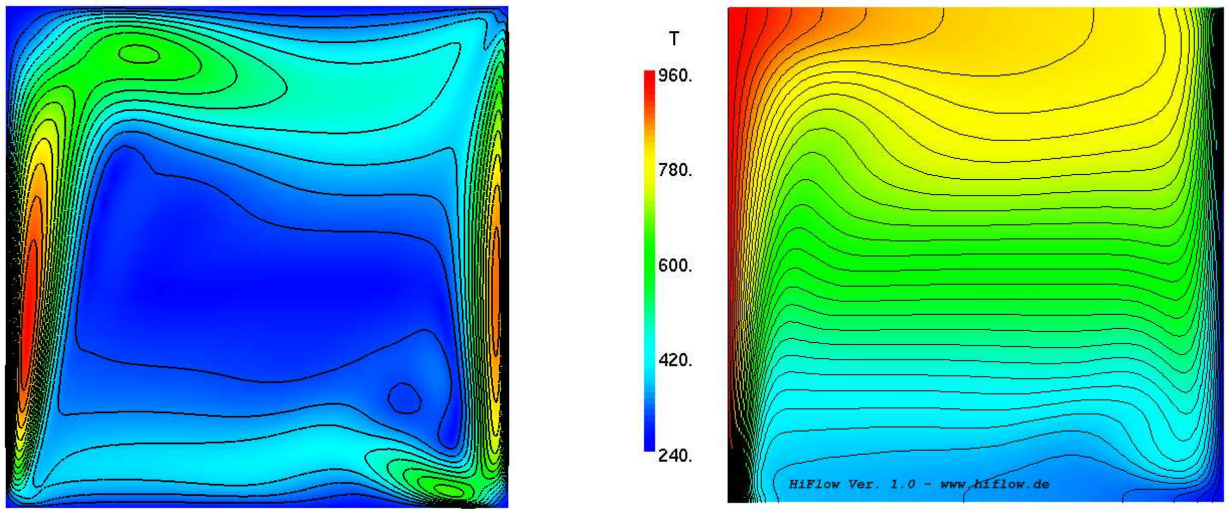


2. Nusselt number in a heat exchanger flow

"Compressible" Navier-Stokes equations + energy equation:

$$c_p \rho \partial_t \theta + \rho v \cdot \nabla \theta - \nabla(\kappa \nabla \theta) = h$$

$$J(p, v, \theta) := \kappa \int_{\Gamma_{\mathrm{cold}}} \partial_n \theta \, do$$



Velocity norm isolines (left) and temperature isolines (right)

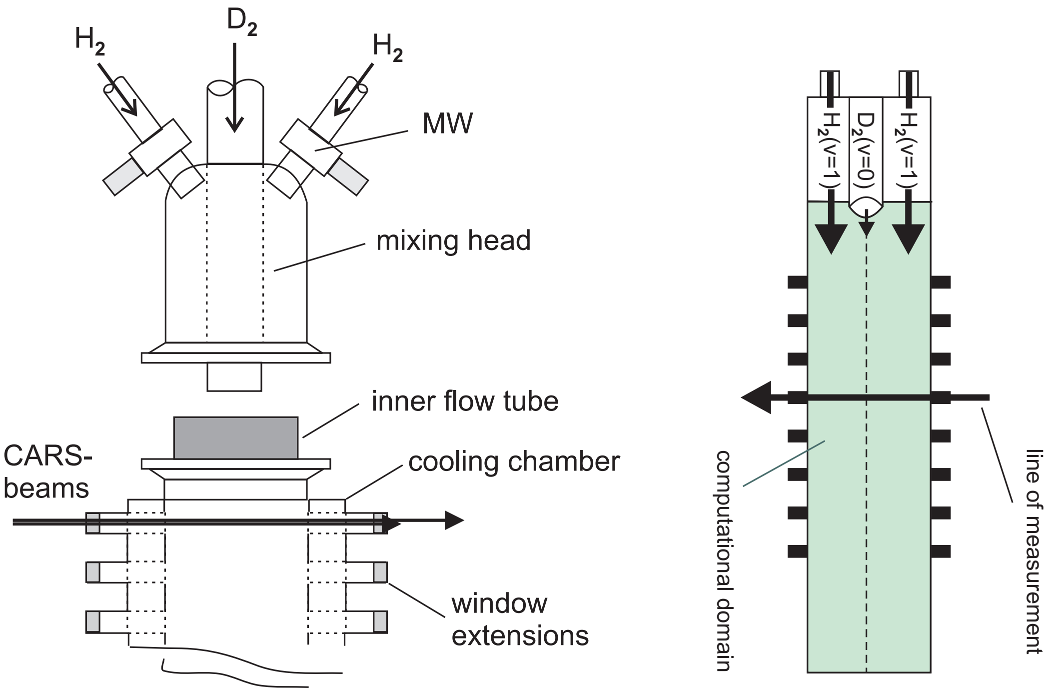
3. CARS signal in a flow reactor

"Compressible" Navier-Stokes equations + chemistry equations:

$$c_p \partial_t w_i + \rho v \cdot \nabla w_i - \nabla(\rho D_i \nabla w_i) = f_i(\theta, w)$$

$$J(p, v, \theta, w) := \kappa \int_{\Gamma_{\mathrm{CARS}}} w_i^2 \, \sigma \, do$$

Configuration of the low-temperature flow reactor (CARS experiment): experimental setting (left) and computational domain (right)



4. Boundary mean stress of an elasto-plastic body

Lamé-Navier equations with constraint:

$$-\nabla\cdot\sigma = f, \quad \sigma = C\epsilon(u), \quad \epsilon = \tfrac{1}{2}(\nabla u + \nabla u^T), \quad |\sigma| \le \sigma_0$$

$$J(u,\sigma) := \int_{\Gamma_D} n\cdot\sigma\cdot n\, do$$

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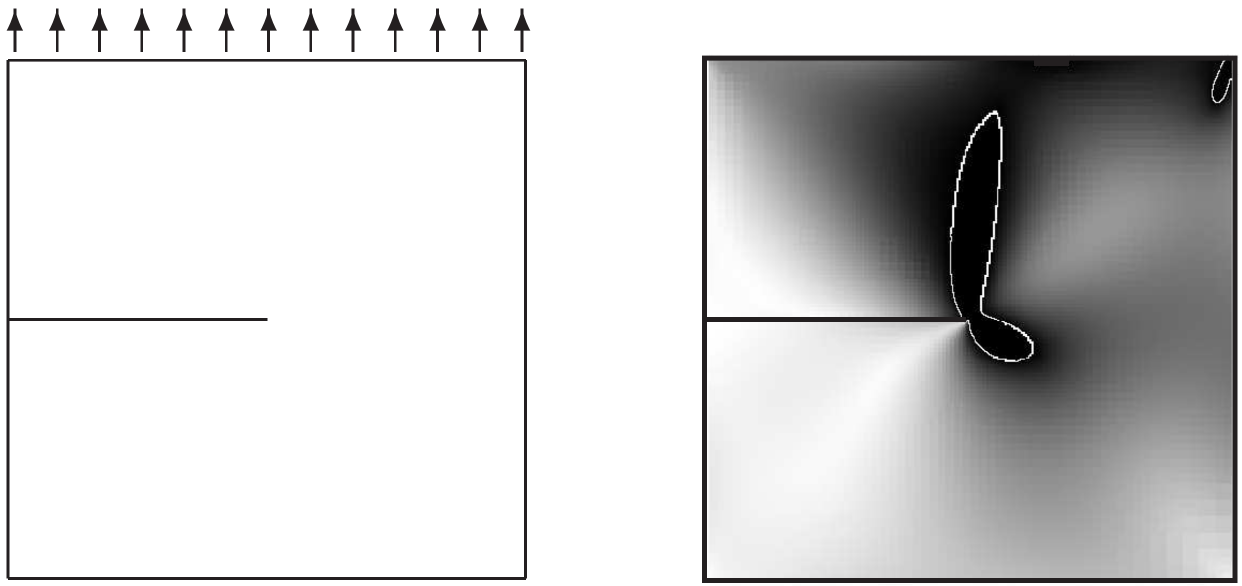
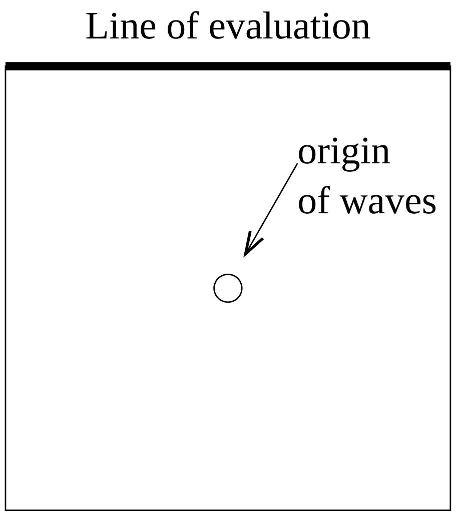


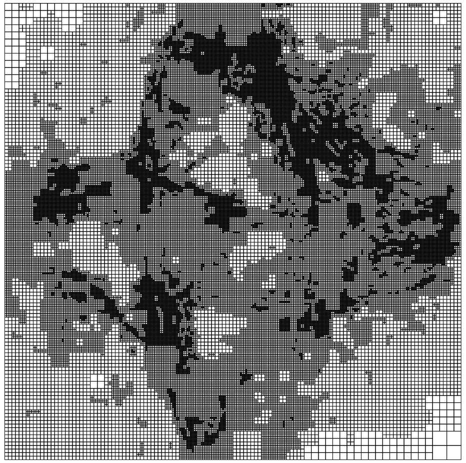
5. Local intensity measurement of a seismic signal

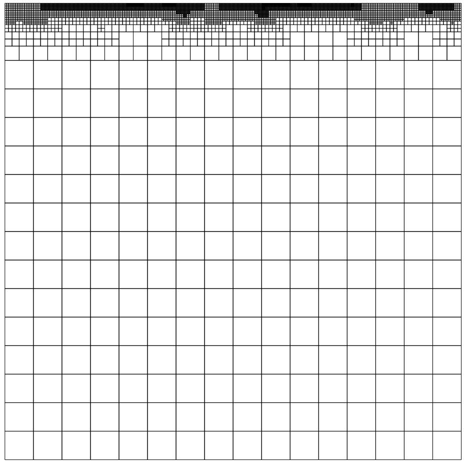
Acoustic/elastic wave equation:

$$\rho \partial_t^2 u - \nabla(a \nabla u) = 0$$

$$J(u) := \int_{T-\delta}^{T+\delta} \int_\Gamma u(x_{\text{obs}}, t)\omega(\xi, t)\, d\xi\, dt$$





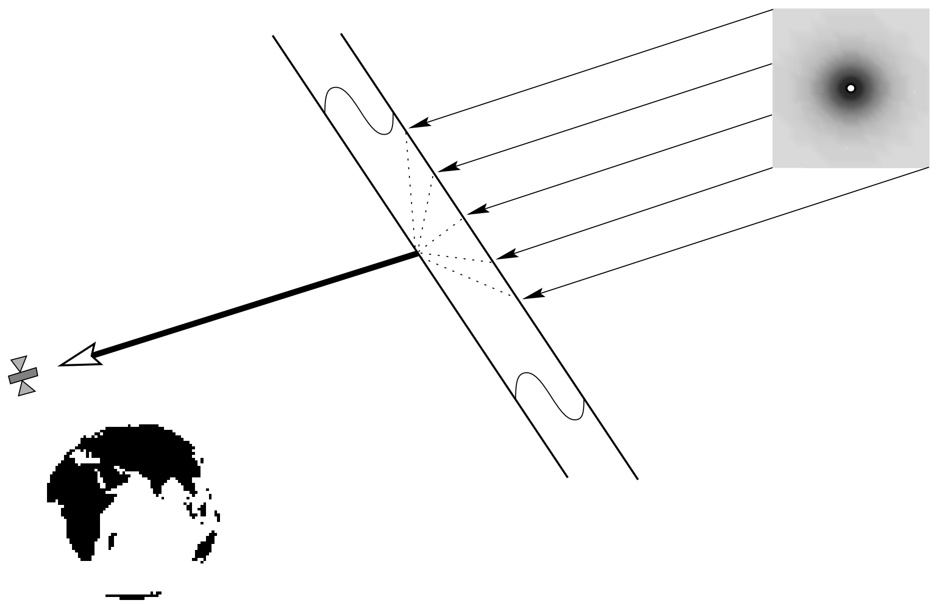


6. Observed light emission of a proto-stellar dust cloud

Radiative transfer equation for intensity $u = u(x, \theta, \lambda_0)$:

$$r_\theta \cdot \nabla u + (\kappa + \mu) u = B - \int_{S^d} R(\theta, \theta') u \, d\theta'$$

$$J(u) := \int_{n \cdot \theta_{\mathrm{obs}} \geq 0} u(x, \theta, \lambda_0) \, do$$

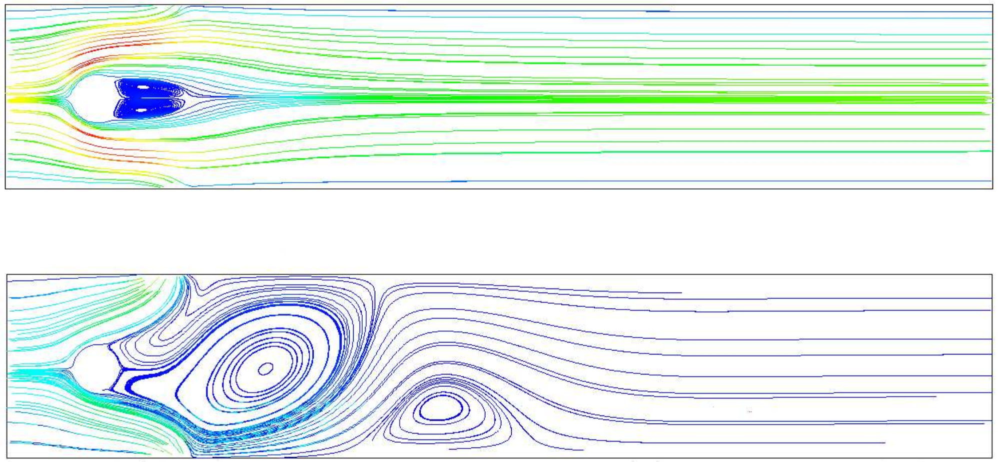


7. Cost functional in an optimization problem

State equation with cost functional:

$$J_{\mathrm{cost}}(u,q) \to \min, \quad \mathcal{A}(u,q) = 0$$

$$J(u,q) := J_{\mathrm{cost}}(u,q) = \text{“drag coefficient”}$$



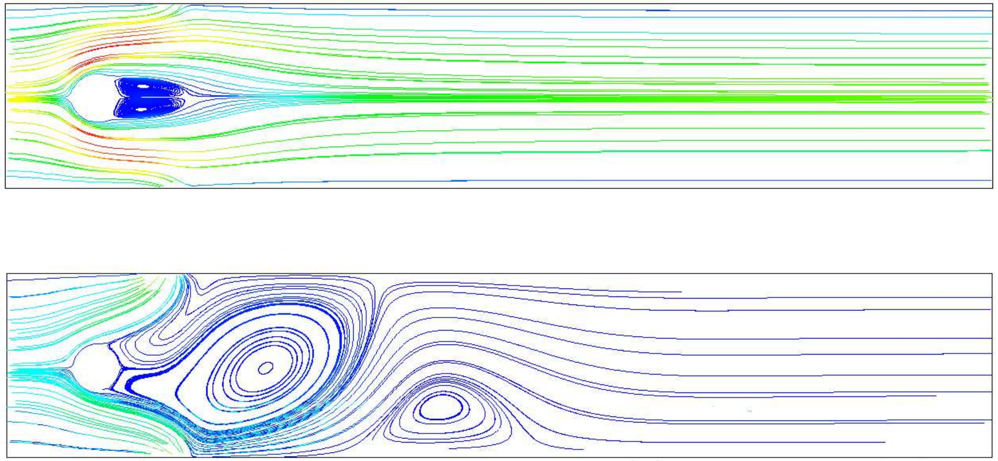
Uncontrolled flow and optimally controlled flow

8. Critical eigenvalue in stability analysis

Linearized (stationary) Navier-Stokes equations:

$$-\nu\Delta v + \hat{v}\cdot\nabla v + v\cdot\nabla\hat{v} + \nabla p = \lambda v, \quad \nabla\cdot v = 0$$

$$J(p,v,\lambda) := \lambda^{\mathrm{crit}}$$



Uncontrolled flow and (stationary) controlled flow: stable ?

2. Galerkin finite element method (short introduction)

Standard notation

$$\Omega \subset \mathbb{R}^d \; (d = 2, 3) \text{ bounded domain,} \quad \partial\Omega \text{ boundary}$$

Function spaces $L^2(\Omega)$, $H^1(\Omega)$, and $H_0^1(\Omega)$ as usual
L^2 scalar product and norm:

$$(v, w) = (v, w)_{L^2} = \int_\Omega v(x) w(x) \, dx, \quad \|v\| = \|v\|_{L^2} = (v, v)^{1/2}$$

L^2 scalar product and norm over subset S (boundary, cell, etc.):

$$(v, w)_S, \quad \|v\|_S$$

Differential operators:

∇ gradient, $\Delta = \nabla \cdot \nabla$ Laplacian, $\partial_n = n \cdot \nabla$ normal derivative

Elliptic model problem: Poisson equation on $\Omega \subset \mathbb{R}^2$

$$-\Delta u = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega.$$

Discretization by Galerkin finite element (FE) method

$$u \in V := H_0^1(\Omega): \qquad a(u,\varphi) := (\nabla u, \nabla\varphi)_{L^2} = (f,\varphi)_{L^2} \quad \forall \varphi \in V$$

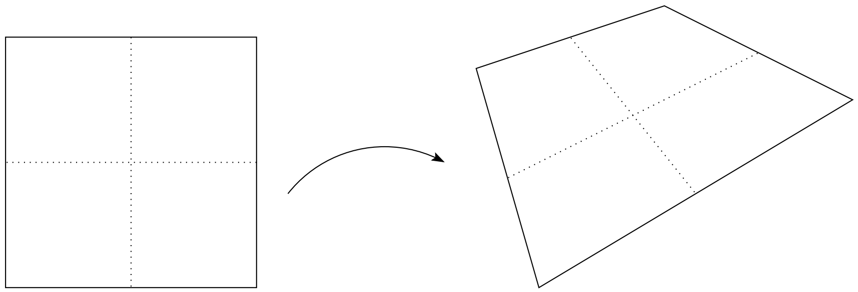
$$u_h \in V_h \subset V: \qquad a(u_h,\varphi_h) = (f,\varphi_h)_{L^2} \quad \forall \varphi_h \in V_h$$

Finite element subspaces on family of "regular" meshes $\mathbb{T}_h = \{K\}$,
K triangles/tetrahedra or (convex) quadrilaterals/hexahedra,
$h := \max_{K\in\mathbb{T}_h}\{h_K\},\ h_K := \mathrm{diam} K$:

$$V_h := \{\varphi \in V,\ \varphi|_K \in P(K),\ K \in \mathbb{T}_h\}$$

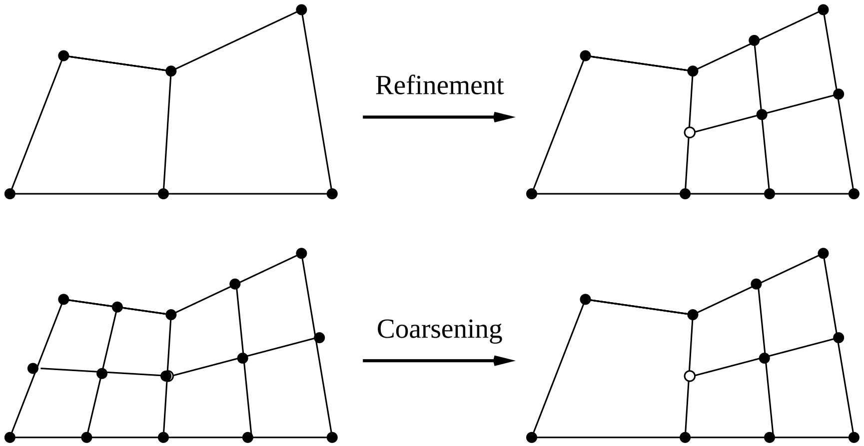
$P(K) \supseteq P_p$ polynom space ($p \in \mathbb{N}_0$ polynomial degree)

“Isoparametric quadrilateral finite elements

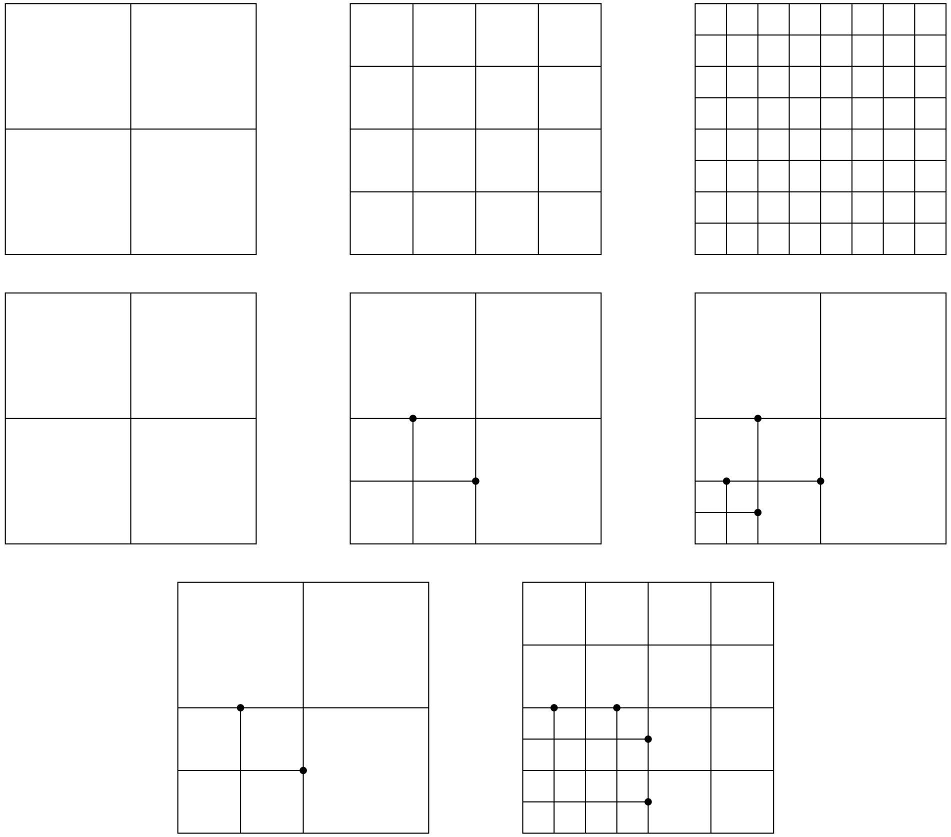


Reference mapping $\sigma_K : \hat{K} \to K$

Mesh adaptation (refinement and coarsening) with hanging nodes:



Quadrilateral meshes



Uniform refinement, local refinement (using hanging nodes),

and “patchwise” refinement

Algebraic system: $\{\varphi_h^{(i)},\, i = 1, \dots, N := \dim V_h\}$ "nodal basis"

$$u_h = \sum_{i=1}^{N} u_h(a_i)\varphi_h^{(i)}, \quad x_h = (u_h(a_i))_{i=1}^{N} \in \mathbb{R}^N$$

$$A_h = a(\varphi_h^{(j)}, \varphi_h^{(i)})_{i,j=1}^{N} \in \mathbb{R}^{N\times N}, \quad b_h = (f, \varphi_h^{(j)})_{j=1}^{N} \in \mathbb{R}^N$$

$$\mathbf{A_h x_h = b_h}$$

The "system matrices" ("stiffness matrices") A_h share the essential properties of the bilinear ("energy") form $a(\cdot,\cdot)$:

1. symmetric
2. positive definite
3. stable (in the right norms)

(I) A priori error anlysis (special case $p = 1$ linear/d-linear)

$I_h v \in V_h$ nodal interpolant ($I_h v(a_i) = v(a_i)$, $i = 1, \dots, N$)

$$\|v - I_h v\|_K + h_K \|\nabla(v - I_h v)\|_K \le c h_K^2 \|\nabla^2 v\|_K, \quad v \in H^2(K).$$

"Galerkin orthogonality" for error $e := u - u_h$

$$a(e, \varphi_h) = 0, \quad \varphi_h \in V_h$$

Best-approximation property

$$\|\nabla e\|_{L^2} = \min_{\varphi_h \in V_h} \|\nabla(u - \varphi_h)\|_{L^2}.$$

"Energy-norm" error estimate

$$\|\nabla e\|_{L^2} \le c h \|\nabla^2 u\|_{L^2}.$$

L^2-norm error estimate via (Aubin-Nitsche) duality argument

$$\|e\|_{L^2} \le c h \|\nabla(u - u_h)\| \le c h^2 \|\nabla^2 u\|_{L^2}.$$

Proof. Let $z \in V$ be the solution of the "dual" ("adjoint') problem

$$a(\varphi, z) = J(\varphi) := \|e\|_{L^2}^{-1}(e,\varphi)_{L^2} \quad \forall \varphi \in$$

A priori estimate (on convex domain): $\|\nabla^2 z\|_{L^2} \le 1$

Error representation (via "Galerkin orthogonality")

$$\begin{aligned}\|e\|_{L^2} = J(e) = a(e,z) = a(e, z - I_h z) &\le \|\nabla e\|_{L^2}\|\nabla(z - I_h z)\|_{L^2} \\ &\le ch\|\nabla e\|_{L^2}\|\nabla^2 z\|_{L^2} \le ch\|\nabla e\|_{L^2}\end{aligned}$$

L^∞-norm (pointwise) error estimate

$$\|e\|_{L^\infty} + h\ln(1/h)\,\|\nabla e\|_{L^\infty} \le ch^2\ln(1/h)\,\|\nabla^2 u\|_{L^\infty}$$

Proof via duality argument with functionals $J(\cdot) \approx \delta_\epsilon(\cdot)$ and $J(\cdot) \approx \partial\delta_\epsilon(\cdot)$ (regularized Green functions)

(II) A posteriori error estimation and mesh adaptation

Error control w.r.t. some (linear) "output functional" $J(\cdot)$:

$$|J(u-u_h)| \le TOL\,!$$

Let $z \in V$ be the solution of the "dual" ("adjoint") problem

$$a(\varphi, z) = J(\varphi) \quad \forall \varphi \in V$$

$z_h \in V_h$ finite element approximation

$$a(\varphi_h, z_h) = J(\varphi_h) \quad \forall \varphi_h \in V_h$$

A posteriori error representation (via "Galerkin orthogonality")

$$\begin{aligned} J(e) &= a(e, z) = a(e, z-\psi_h), \quad \psi_h \in V_h \\ &= (f, z-\psi_h) - a(u_h, z-\psi_h) =: \underbrace{\rho(u_h)(z-\psi_h)}_{\textbf{residual}} \end{aligned}$$

Evaluation of residual

Cell-wise integration by parts (Ω polygonal domain):

$$\rho(u_h)(z-\varphi_h) = \sum_{K\in\mathbb{T}_h} \{(f+\Delta u_h, z-\psi_h)_K - (\partial_n u_h, z-\psi_h)_{\partial K}\}$$

$$= \sum_{K\in\mathbb{T}_h} \{(\underbrace{f+\Delta u_h}_{=:\,R(u_h)}, z-\psi_h)_K + (\underbrace{-\tfrac{1}{2}[\partial_n u_h]}_{=:\,r(u_h)}, z-\psi_h)_{\partial K\setminus\partial\Omega}\}$$

$[\nabla u_h]$ the jump of ∇u_h across the inter-element edges Γ,
cell and edge residuals $R(u_h)$ and $r(u_h)$:

$$R(u_h)_{|K} := f+\Delta u_h$$

$$r(u_h)_{|\Gamma} := \left\{ \begin{array}{rl} -\tfrac{1}{2}n\cdot[\nabla u_h], & \text{if } \Gamma\subset\partial K\setminus\partial\Omega \\ 0, & \text{if } \Gamma\subset\partial\Omega \end{array} \right\}$$

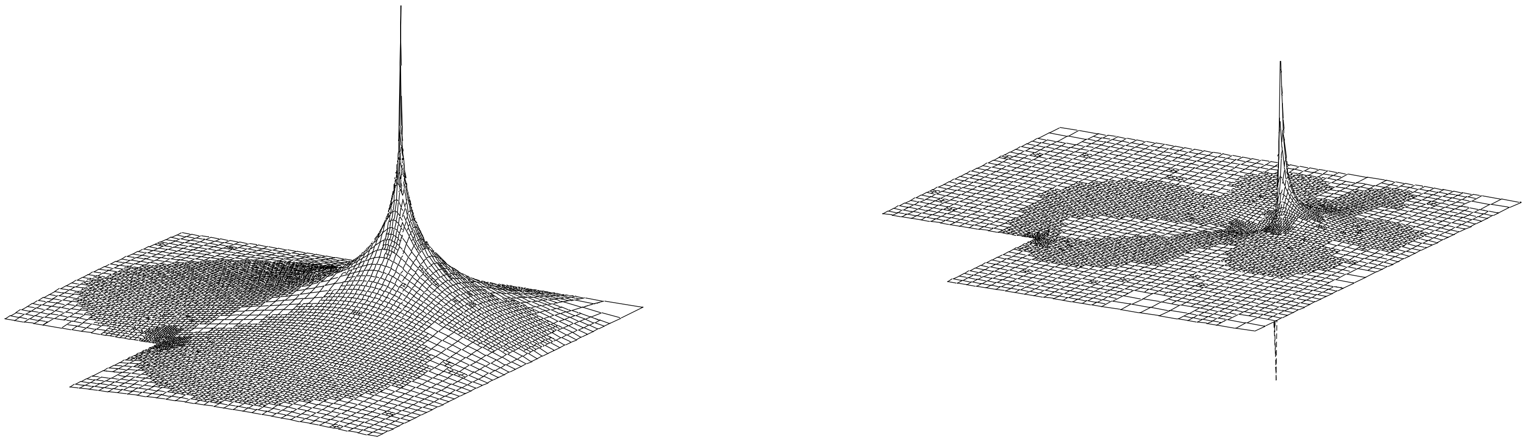
$\Rightarrow$ a posteriori error estimator η (stopping criterion)

$$J(e) = \eta := \sum_{K\in\mathbb{T}_h} \{(R(u_h), z-\psi_h)_K + (r(u_h), z-\psi_h)_{\partial K}\},$$

will be approximated without further estimation.

$\Rightarrow$ local error indicators η_K (refinement indicators)

$$|J(e)| \le \sum_{K\in\mathbb{T}_h} \underbrace{|(R(u_h), z-\psi_h)_K + (r(u_h), z-\psi_h)_{\partial K}|}_{:=\eta_\mathbf{K}}.$$



Examples of computed dual solutions for $u(a)$ and $\partial_1 u(a)$

Application to L^2-norm error bound

$$J(\varphi) := \|e\|^{-1}(e,\varphi), \qquad J(e) = \|e\|$$

The dual solution $z \in V \cap H^2(\Omega)$ satisfies

$$c_S := \|\nabla^2 z\| \leq 1.$$

Using Hölder inequality in the error representation yields

$$\|e\| \leq \sum_{K\in\mathbb{T}_h} \rho_K\,\omega_K \leq \Big(\sum_{K\in\mathbb{T}_h} h_K^4\rho_K^2\Big)^{1/2}\Big(\sum_{K\in\mathbb{T}_h} h_K^{-4}\omega_K^2\Big)^{1/2}$$

with residuals and weights ($\psi_h := I_h z$ the nodal interpolant)

$$\rho_K^2 := \|R(u_h)\|_K^2 + h_K^{-1}\|r(u_h)\|_{\partial K}^2$$
$$\omega_K^2 := \|z - I_h z\|_K^2 + h_K\|z - I_h z\|_{\partial K}^2$$

Strong interpolation estimate (à la Bramble/Hilbert):

$$\Big(\sum_{K\in\mathbb{T}_h} h_K^{-4}\big\{\|z-I_hz\|_K^2+h_K\|z-I_hz\|_{\partial K}^2\big\}\Big)^{1/2}\le c_I\,\|\nabla^2 z\|$$

L^2-error estimator (with $c_S=1$)

$$\|e\|\le c_I\Big(\sum_{K\in\mathbb{T}_h} h_K^4\rho_K^2\Big)^{1/2}\|\nabla^2 z\|\le \underbrace{c_Ic_S\Big(\sum_{K\in\mathbb{T}_h} h_K^4\rho_K^2\Big)^{1/2}}_{=:\,\eta_{\mathbf{L^2}}(\mathbf{u_h})}.$$

Exercise: By similar arguments derive the H^1-norm (energy-norm) a posteriori error estimate (with $c_S=1$)

$$\|\nabla e\|\le\eta_E(u_h):=c_Ic_S\Big(\sum_{K\in\mathbb{T}_h} h_K^2\rho_K^2\Big)^{1/2}.$$

An illustrative example : Mean normal-flux error

$$J(u) = \int_{\partial\Omega} \partial_n u \, ds, \qquad \Omega = B_1(0)$$

Question: What is an "efficient" mesh-size distribution for computing $J(u)$?

Remark:

$$J(u) = \int_\Omega \Delta u \, dx = -\int_\Omega f \, dx$$

The corresponding dual problem

$$a(\varphi, z) = (1, \partial_n \varphi)_{\partial\Omega} \quad \forall \varphi \in V \cap C^1(\bar{\Omega})$$

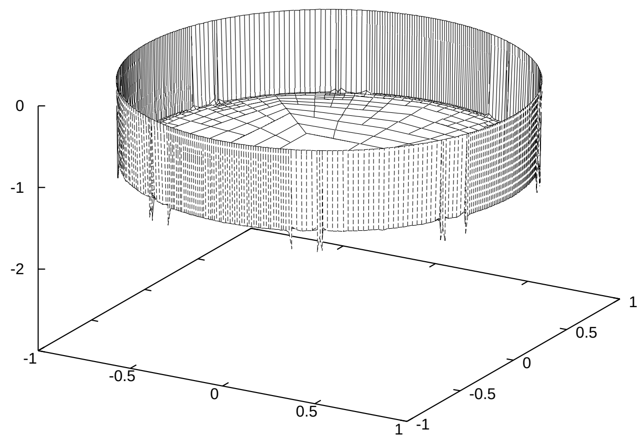
has a measure solution "$z \equiv -1$" in Ω, "$z = 0$" on $\partial\Omega$. To avoid dealing with measures, we use regularization.

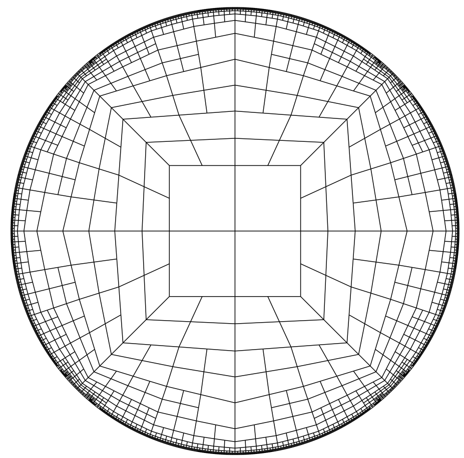
Regularized output functional

$$J_\epsilon(\varphi) = \frac{1}{|S_\epsilon|}\int_{S_\epsilon} \partial_n \varphi \, dx = \int_{\partial\Omega} \partial_n \varphi \, ds + \mathcal{O}(\epsilon),$$

where $S_\epsilon = \{x \in \Omega : \text{dist}\{x, \partial\Omega\} < \epsilon\}$ and $\epsilon := TOL$. The corresponding dual solution is

$$z_\epsilon = \begin{cases} -1 & \text{in } \Omega \setminus S_\epsilon, \\ -\epsilon^{-1}\text{dist}\{x, \partial\Omega\} & \text{in } S_\epsilon. \end{cases}$$





On cells $K \subset \Omega \backslash S_\epsilon$ there holds $z - I_h z \equiv 0$:

$$J_\epsilon(e) \leq \eta = \sum_{K \in \mathbb{T}_h, \mathbf{K} \cap \mathbf{S}_\epsilon \neq \emptyset} \rho_K \omega_K.$$

Conclusion: *There is no contribution to the error from cells in the interior of Ω.* Hence, whatever right-hand side f, the optimal strategy is to refine the elements adjacent to the boundary and to leave the others unchanged. In practice, due to hanging nodes, this may also lead to some refinement in the interior.

Remark. Normally the dual solution z corresponding to a user-chosen functional $J(\cdot)$ is not known explicitly. It rather has to be computed numerically. In some cases the possible "singularities" of z may be known, for example the singularity of the Green function in the case of point evaluations.

Requirements on a posteriori error estimators

- Reliability (safe upper bound):

$$|J(e)| \le \eta(u_h)$$

- Efficiency (in terms of "effectivity index"):

$$I_{\text{eff}} := \left|\frac{\eta(u_h)}{J(e)}\right| \to 1 \quad (TOL \to 0)$$

- Economical: The costs of evaluating the estimator and organizing the mesh adaptation should not make up for much more than 50% of the total solution cost.

Goal: The adaptive solution process should not only provide a reasonably efficient and reliable error bound but should also guide the generation of economical meshes on which the total solution costs are much lower than on ad-hoc meshes.

"Energy-norm" versus "goal-oriented" error estimation

The "energy-norm" $\|\nabla \cdot\|$ is the natural measure for the discretization error of the finite element Galerkin approximation of the Poisson equation as it is directly linked to the variational setting of the problem. However, "energy-norm error" is essentially the "error in energy",

$$\begin{aligned}\|\nabla e\|^2 &= \|\nabla e\|^2 - 2(\nabla u, \nabla u_h) + \|\nabla u_h\|^2 \\ &= \|\nabla u\|^2 - 2(\nabla u_h, \nabla u_h) + \|\nabla u_h\|^2 = \|\nabla u\|^2 - \|\nabla u_h\|^2,\end{aligned}$$

which may not be of much practical interest. Hence, the concept of "goal-oriented error estimation" is much more versatile in treating practically relevant questions.

Warning: "Goal-oriented" error estimation is only asymptotically (for $TOL \to 0$) reliable and may not be efficient in certain cases.

Convergence of adaptive mesh refinement algorithm (Is "adaptivity" provably superior over "heuristics"?

There are strong results for low-order FEM for the Poisson equation (elliptic, symmetric, positive definite). Let $u_i \in V_i$ be the discrete solutions computed on a sequence of adapted meshes $\mathbb{T}_i$, $i \in \mathbb{N}_0$.

Theorem. (Convergence of adaptive method: Dörfler 1996) *For a certain refinement strategy there exists a $\rho \in (0,1)$ such that*

$$\|\nabla e_i\| \leq \rho \|\nabla e_{i-1}\|, \quad i \in \mathbb{N}.$$

Theorem. (Optimality of adaptive method: Stevenson 2005) *The error level is reached with minimal complexity, i.e.,*

$$\|\nabla e_i\| \approx \min \big\{ \|\nabla(u - \varphi_h)\|, \, \varphi_h \in V_h, \, \mathrm{dim} V_h \leq N_i := \mathrm{dim} V_i \big\}.$$

This result has recently been extended to "goal-oriented" adaptivity.

Warning. These results do not really predict the behavior of an adaptive mesh refinement algorithm for a particular problem since they are of asymptotic character only.

Example. Computation of derivative point value $\partial_k u(a)$ in the Poisson equation in $\mathbb{R}^2$. A priori analysis gives the error estimate (for a smooth solution) on quasi-uniform meshes,

$$|\partial_k e(a)| = \mathcal{O}(h) = \mathcal{O}(\mathsf{N}^{-1/2}),$$

but on uniform meshes (by super-approximation),

$$|\partial_k e(a)| = \mathcal{O}(h^2) = \mathcal{O}(\mathsf{N}^{-1}),$$

Numerical tests show that an adptive algorithm can also achieve

$$|\partial_k e(a)| = \mathcal{O}(\mathsf{N}^{-1}),$$

which is also "optimal". But here the $\mathcal{O}$ is much smaller.

2.20

3. Goal-oriented error estimation (DWR method)

Preliminaries

Primal and dual Galerkin approximations of linear problems:

$$A(u,\varphi) = F(\varphi) \quad \forall \varphi \in V, \qquad A(u_h,\varphi_h) = F(\varphi_h) \quad \forall \varphi_h \in V_h$$
$$A(\psi,z) = J(\psi) \quad \forall \psi \in V, \qquad A(\psi_h,z_h) = J(\psi_h) \quad \forall \psi_h \in V_h$$

Primal solution u, dual solution z:

$$J(u) = A(u,z) = F(z)$$

Primal error $e := u - u_h$, dual error $e^* := z - z_h$
(by Galerkin orthogonality):

$$J(e) = A(e,z) = A(e,e^*) = A(u,e^*) = F(e^*)$$

$$J(e) = A(e, z - \psi_h) = \underbrace{F(z - \psi_h) - A(u_h, z - \psi_h)}_{=: \rho(u_h)(z - \psi_h)} \quad \psi_h \in V_h$$

$$F(e^*) = A(u - \varphi_h, e^*) = \underbrace{J(u - \varphi_h) - A(u - \varphi_h, z_h)}_{=: \rho^*(z_h)(u - \varphi_h)} \quad \varphi_h \in V_h$$

$$\Rightarrow \qquad J(e) = \tfrac{1}{2}\rho(u_h)(z - \psi_h) + \tfrac{1}{2}\rho^*(z_h)(u - \varphi_h), \quad \varphi_h, \psi_h \in V_h$$

This error representation provides the basis of simultaneous control of the errors in approximationg the primal as well the dual solution.

Recall the identity (only valid in the linear case)

$$J(e) = \rho(u_h)(z - \psi_h) = \rho^*(z_h)(u - \varphi_h) = F(e^*)$$

Galerkin approximation of nonlinear variational equations

Variational equation in function space V :

$$A(u)(\cdot) = F(\cdot), \qquad \text{target quantity } J(u)$$

Galerkin approximation in finite dimensional subspaces $V_h \subset V$:

$$A_h(u_h)(\cdot) = F(\cdot), \qquad \text{error measure } J(u) - J(u_h)$$

Idea for a posteriori error estimation: Interpretation as a constrained optimization problem (with "trival" admissible set):

$$J(u) \to \min, \qquad A(u)(\cdot) = F(\cdot).$$

Example: Nonlinear convection-diffusion equation (Burgers eq.)

$$-\nu\Delta u + u \cdot \nabla u = f, \quad V = H_0^1(\Omega)^d,$$

$$A(u)(\varphi) := \nu(\nabla u \nabla\varphi) + (u \cdot \nabla u, \varphi), \quad F(\varphi) := (f, \varphi)$$

Formal Euler-Lagrange approach:

"Dual" (or "adjoint") variable z ("Lagrangian multiplier")

Lagrangian functional $\quad \mathcal{L}(u,z) := J(u) + F(z) - A(u)(z)$

The solutions of the constrained optimization problem are among the stationary points, $\mathcal{L}'(u,z) = 0$ (KKT system).

(P) Stationary point $\{u,z\} \in V \times V$:

$$
\begin{aligned}
J'(u)(\varphi) - A'(u)(\varphi, z) &= 0 \quad \varphi \in V,\\
F(\psi) - A(u)(\psi) &= 0 \quad \forall \psi \in V.
\end{aligned}
$$

(P_h) Galerkin approximation $\{u_h, z_h\} \in V_h \times V_h$:

$$
\begin{aligned}
J'(u_h)(\varphi_h) - A'(u_h)(\varphi_h, z_h) &= 0, \quad \forall \varphi_h \in V_h,\\
F(\psi_h) - A(u_h)(\psi_h) &= 0 \quad \forall \psi_h \in V_h.
\end{aligned}
$$

Goal: Estimation of error $J(u) - J(u_h)$ in terms of "primal" and "dual" residuals:

$$\rho(u_h)(\cdot) := F(\cdot) - A(u_h)(\cdot)$$
$$\rho^*(u_h, z_h)(\cdot) := J'(u_h)(\cdot) - A'(u_h)(\cdot, z_h)$$

Proposition. *Let the nonlinear form $A(\cdot)(\cdot)$ and the functional $J(\cdot)$ be three times Gâteaux differentiable. Then, there holds*

$$J(u) - J(u_h) = \tfrac{1}{2} \underbrace{\rho(u_h)(z - \psi_h)}_{\text{primal}} + \tfrac{1}{2} \underbrace{\rho^*(u_h, z_h)(u - \varphi_h)}_{\text{dual}} + R_h^{(3)},$$

with arbitrary approximations $\varphi_h, \psi_h \in V_h$ and a remainder $R_h^{(3)}$ which is cubic in the primal and dual errors $e := u - u_h$ and $e^* := z - z_h$.

Proof. Set $x := \{u, z\}$, $x_h := \{u_h, z_h\}$, $e := x - x_h$, and $L(x) := \mathcal{L}(u, z)$. By elementary calculus:

$$J(u) - J(u_h) = L(x) - L(x_h) - \underbrace{F(z) + A(u)(z)}_{=0} + \underbrace{F(z_h) - A_h(u_h)(z_h)}_{=0}$$

$$= \int_0^1 L'(x_h + se)(e)\, ds$$

Applying the trapezoidal rule

$$\int_0^1 f(t)\, dt = \tfrac{1}{2}\{f(0) + f(1)\} + \tfrac{1}{2}\int_0^1 f''(s)s(s-1)\, ds,$$

$$J(u) - J(u_h) = \tfrac{1}{2}\{L'(x_h)(e) + \underbrace{L'(x)(e)}_{=0}\} + R_h^{(3)}$$

$$R_h^{(3)} = \tfrac{1}{2}\int_0^1 L'''(x_h + se)(e, e, e)\, s(s-1)\, ds$$

Observing

$$
\begin{aligned}
L'''(x_h+se)(e,e,e) = J'''(u_h+se)(e,e,e) \\
&- A'''(u_h+se)(e,e,e,z_h+se^*) \\
&- 3A''(u_h+se)(e,e,e^*)
\end{aligned}
$$

and, by Galerkin orthogonality,

$$
\begin{aligned}
L'(x_h)(e) &= L'(x_h)(x-y_h) + \underbrace{L'(x_h)(y_h-x_h)}_{=0}, \quad y_h \in V_h \times V_h \\
&= J'(u_h)(u-\varphi_h) - A'(u_h)(u-\varphi_h, z_h) \\
&\quad + F(z-\psi_h) - A(u_h)(z-\psi_h) \\
&= \rho^*(u_h, z_h)(u-\varphi_h) + \rho(u_h)(z-\psi_h), \quad \varphi_h,\, \psi_h \in V_h.
\end{aligned}
$$

completes the proof.

Remarks:

1. The derivation of the error representation does not require the uniqueness of solutions (important for application to eigenvalue problems). The a priori assumption $x_h \to x\ (h \to 0)$ makes the result meaningful for cases with non-unique solutions.

2. The error representation contains the unknown primal and dual solutions u and z, which need to be approximated.

3. The cubic remainder term $R_h^{(3)}$ is usually neglected.

4. The solution of the discrete dual problem takes only a "linear" work unit.

Proposition. *There holds the simplified error representation:*

$$J(u) - J(u_h) = \rho(u_h)(z - \varphi_h) + R_h^{(2)},$$

for arbitrary $\varphi_h \in V_h$ *, with the quadratic remainder*

$$R_h^{(2)} := \int_0^1 \big\{ A''(u_h + se)(e, e, z) - J''(u_h + se)(e, e) \big\} s \, ds.$$

Proof. By integration by parts,

$$\begin{aligned} R_h^{(2)} &= - \int_0^1 \big\{ A'(u_h + se)(e, z) - J'(u_h + se)(e) \big\} \, ds \\ &\qquad + \underbrace{A'(u)(e, z) - J'(u)(e)}_{= 0} \\ &= F(z) - A(u)(z) - F(z) + A(u_h)(z) + J(u) - J(u_h) \\ &= -\rho(u_h)(z - \varphi_h) + J(u) - J(u_h). \end{aligned}$$

Remark: Application of the abstract theory to the Galerkin approximation of the nonlinear diffusion-convection problem with the quadratic nonlinearity $(u \cdot \nabla u, \cdot)_{L^2}$ yields the remainder terms

$$R_h^{(2)} = 2(e^u \cdot \nabla e^u, z), \qquad R_h^{(3)} = -\frac{1}{2}(e^u \cdot \nabla e^u, e^z)$$

The DWR method:

- *Linarization:* Neglect the remainder terms.
- *Approximation:* For evaluating the weights use approximations of primal and dual solutions u and z as described below.
- On the current mesh refine according to one of the strategies described below.
- Embed the mesh adaptation into a nested multilevel solution process as described below.

Nested Solution Approach

For solving the nonlinear problems by a Galerkin finite element method, we employ the following iterative scheme. Starting from a coarse initial mesh $\mathbb{T}_0$, a hierarchy of refined meshes

$$\mathbb{T}_0 \subset \mathbb{T}_1 \subset \cdots \subset \mathbb{T}_l \subset \cdots \subset \mathbb{T}_L$$

and corresponding finite element spaces $V_l,\, l = 1, ..., L,$ is generated by a nested solution process.

1. *Initialization:* For $j = 0$, compute the solution $u_0 \in V_0$ on the coarsest mesh $\mathbb{T}_0$.
2. *Defect correction:* For $l \geq 1$, start with $u_l^{(0)} = u_{l-1} \in V_l$.
3. *Iteration step:* For computed iterate $u_l^{(j)}$ evaluate the defect

$$(d_l^{(j)}, \varphi) = F(\varphi) - A(u_l^{(j)})(\varphi), \quad \varphi \in V_l$$

and solve the correction equation

$$\tilde{A}'(u_l^{(j)})(v_l^{(j)},\varphi) = (d_l^{(j)},\varphi) \quad \forall \varphi \in V_l$$

by Krylov-space-multigrid iterations on the hierarchy of already constructed meshes $\{\mathbb{T}_l, ..., \mathbb{T}_0\}$. Update $u_l^{(j+1)} = u_l^{(j)} + v_l^{(j)}$, set $j = j+1$ and go back to (2). This process is repeated until a limit $u_l \in V_l$ is reached within a certain prescribed accuracy.

4. *Error estimation:* Solve the (linearized) discrete dual problem

$$z_l \in V_l : \quad A'(u_l)(\varphi, z_l) = J(\varphi) \quad \forall \varphi \in V_l,$$

and evaluate the a posteriori error representation and refinement indicators, $J(e_l) \approx \tilde{\eta}(u_l), \quad \eta_K,\ K \in \mathbb{T}_h$.
If $|\tilde{E}(u_l)| \leq TOL$, or $N_l \geq N_{max}$, then stop. Otherwise cell-wise mesh adaptation yields the new mesh $\mathbb{T}_{l+1}$. Then, set $l = l+1$ and go back to (1).

Application of the DWR method (guideline)

Example: Dual mixed formulation of the Poisson equation

$$-\Delta u = f \ \text{ in } \Omega, \quad u|_{\partial\Omega} = 0.$$

The pair $\{u, v := \nabla u\}$ satisfies the system

$$v - \nabla u = 0, \quad -\nabla \cdot v = f \quad \text{in } \Omega, \quad u|_{\partial\Omega} = 0.$$

Using the space $W := L^2(\Omega) \times H_{\mathrm{div}}(\Omega)$ this can be written in variational form for $U := \{u, v\} \in W$ as follows:

$$A(U, \Phi) = F(\Phi) \quad \forall \Phi = \{\varphi^u, \varphi^v\} \in W,$$

$$A(U, \Phi) := (v, \varphi^v) + (u, \nabla \cdot \varphi^v) - (\nabla \cdot v, \varphi^u), \quad F(\Phi) := (f, \varphi^u).$$

This formulation contains the two state equations and the Dirichlet boundary condition for u in weak form. It is well-posed.

For the Galerkin finite element approximation choose appropriate (conforming or nonconforming) finite element subspaces $L_h \subset L^2(\Omega)$ and $H_h \subset H_{\rm div}(\Omega)$, e.g., the $H_{\rm div}$-conforming lowest-order Raviart-Thomas element:

$$L_h := \{\varphi_h^u,\, \varphi_h^u|_K \in P_0\}, \quad H_h := \{\varphi_h^v,\, \varphi_h^v|_K \in (P_0)^2 \oplus xP_0\}$$

Then, compute $U_h = \{u_h, v_h\} \in W_h = L_h \times H_h$ from

$$A(U_h, \Phi_h) = F(\Phi_h) \quad \forall \Phi_h \in W_h,$$

or, equivalently, from the saddle point system

$$\begin{aligned} (v_h, \varphi_h^v) + (u_h, \nabla\cdot\varphi_h^v) &= 0 \quad \forall \varphi_h^v \in H_h, \\ -(\nabla\cdot v_h, \varphi_h^u) &= (f, \varphi_h^u) \quad \forall \varphi_h^u \in L_h. \end{aligned}$$

This discretization is stable for $h \to 0$ with first-order convergence

$$\|u - u_h\|_{L^2} + \|v - v_h\|_{H_{\rm div}} = \mathcal{O}(h).$$

A posteriori error analysis by DWR method

For a given (linear) target functional $J(\cdot) = \{j_u, j_v\}$ the corresponding "dual problem" has to be set up with care. Starting from the saddle point formulation for the pair $\{u, v\}$ may easily lead to mistakes (though not in this simple situation). One rather should simply use the formal adjoint of the coupled bilinear form $A(\cdot,\cdot)$, which automatically leads to the correct dual formulation for $Z = \{z^u, z^v\} \in W$:

$$A(\Phi, Z) = J(\Phi) \quad \forall \Phi \in W.$$

This is equivalent to the "dual" saddle point problem

$$\begin{aligned} (\varphi^v, z^v) - (\nabla\cdot\varphi^v, z^u) &= j_v(\varphi^v) \quad \forall \varphi^v \in H, \\ (\varphi^u, \nabla\cdot z^v) &= j_u(\varphi^u) \quad \forall \varphi^u \in L. \end{aligned}$$

The general result underlying the DWR method yields the following representation for the error $E = \{e^u, e^v\}$:

$$J(E) = \rho(U_h, Z - I_h Z)$$

where

$$\rho(U_h, Z - I_h Z) = \sum_{K \in \mathbb{T}_h} \Big\{ (v_h - \nabla u_h, z^v - I_h z^v)_K + \tfrac{1}{2}([u_h]n, z^v - I_h z^v)_{\partial K} + (f + \nabla \cdot v_h, z^u - I_h z^u)_K \Big\}$$

By the special choice of the target functional $J(\cdot)$, we can focus the computational effort on certain properties of the gradient variable $v = \nabla u$, which may be of higher interest than the displacement u itself.

4. Practical aspects

Questions to be considered:

- Evaluation of error estimators
- Mesh refinement strategies
- Control of linearization
- Balancing of iteration and discretization error

- Use of error identities for postprocessing
- Anisotropic mesh adaptation
- Adaptive h/p FEM
- Theoretical justification
- ...

4.1 Evaluation of error estimators

- The cell and edge residuals $R(u_h)$ and $r(u_h)$ can be obtained directly from computed solution u_h .
- The weights ω_K need to be approximated since the dual solution z is unknown.

A posteriori error estimate

$$|J(e)| \leq |E(u_h)| \leq \eta(u_h) := \sum_{K \in \mathbb{T}_h} \eta_K$$

with the local "error indicators"

$$\eta_K = \Big| (R(u_h), z - I_h z)_K + (r(u_h), z - I_h z)_{\partial K} \Big|$$

Remark. Already by this localization the asymptotic sharpness of the error estimate may get lost. One should use an approximation to the error representation $E(u_h)$, avoiding any localization.

Aspects of relevance:

- sharpness of the global error bound $\eta(u_h)$
- effectivity of local error indicators η_K for mesh refinement

Quality measure for error estimation: "Effectivity index"

$$I_{\text{eff}} := \frac{\eta(u_h)}{|J(u-u_h)|}$$

1. *Approximation by* global *higher order methods:* The dual problem is solved by using *biquadratic* finite elements on the current mesh yielding an approximation $z_h^{(2)}$ to z:

$$\eta_K^{(1)} = \left|(R(u_h), z_h^{(2)} - I_h z_h^{(2)})_K + (r(u_h), z_h^{(2)} - I_h z_h^{(2)})_{\partial K}\right|$$

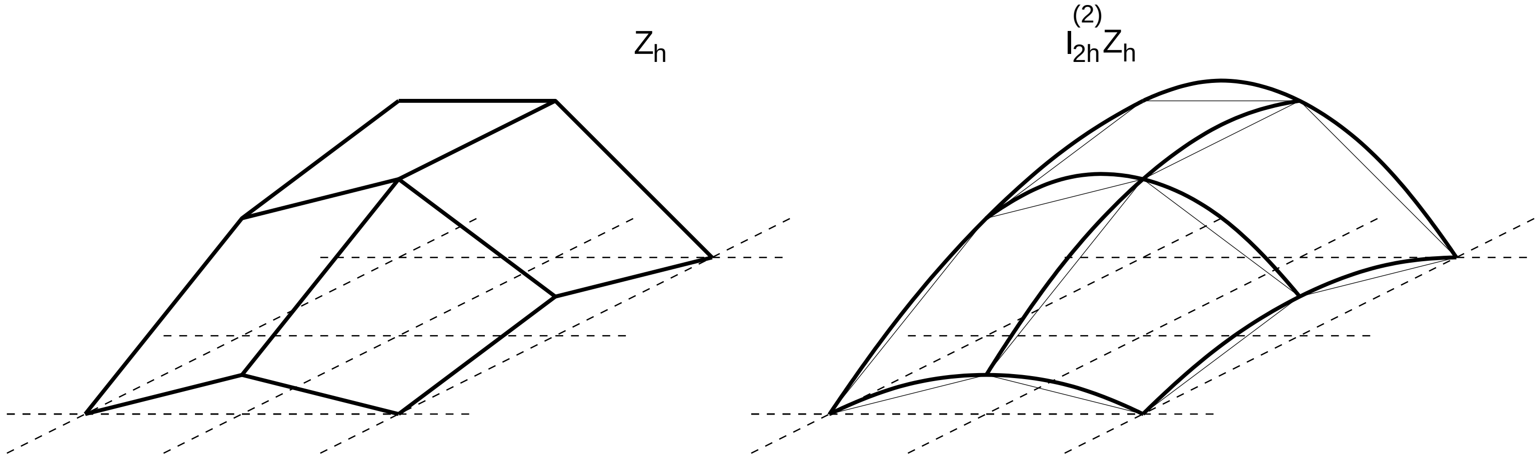
$$\Rightarrow \qquad \lim_{TOL \to 0} I_{\text{eff}} = 1$$

---

2. *Approximation by* local *higher order interpolation:* Patchwise *biquadratic* interpolation of the bilinear approximation $z_h^{(1)}$ on the current mesh yields an approximation $I_{2h}^{(2)} z_h^{(1)}$ to z:

$$\eta_K^{(2)} = \left|(R(u_h), I_{2h}^{(2)} z_h^{(1)} - z_h^{(1)})_K + (r(u_h), I_{2h}^{(2)} z_h^{(1)} - z_h^{(1)})_{\partial K}\right|$$

$$\Rightarrow \qquad \lim\inf_{TOL \to 0} I_{\text{eff}} \sim 1 - 2$$



3. *Approximation by (local) difference quotients:*
Interpolation estimate à la Bramble/Hilbert yields

$$\|z - I_h z\|_K + h_K^{1/2} \|z - I_h z\|_{\partial K} \le c_I h_K^2 \|\nabla^2 z\|_K$$

The second derivative $\nabla^2 z$ is replaced by a suitable second-order difference quotient $\nabla_h^2 z_h^{(1)}$ of the approximate dual solution:

$$\eta_K^{(3)} = c_I h_K^{-1/2} \rho_K \|n \cdot [\nabla z_h^{(1)}]\|_{\partial K}$$

$$\Rightarrow \qquad \liminf_{TOL \to 0} I_{\text{eff}} \sim 5 - 10$$

L	N	$I_{\text{eff}}^{(1)}$	$I_{\text{eff}}^{(2)}$	$I_{\text{eff}}^{(3)}$
2	4^4	1.253	13.51	45.45
3	4^5	1.052	3.105	9.345
4	4^6	1.007	2.053	7.042
5	4^7	1.003	1.886	6.667

Efficiency of *weighted* error indicators for controlling the point-error $J(e) \approx e(0)$

Idea: "patchwise bi-quadratic" defect correction

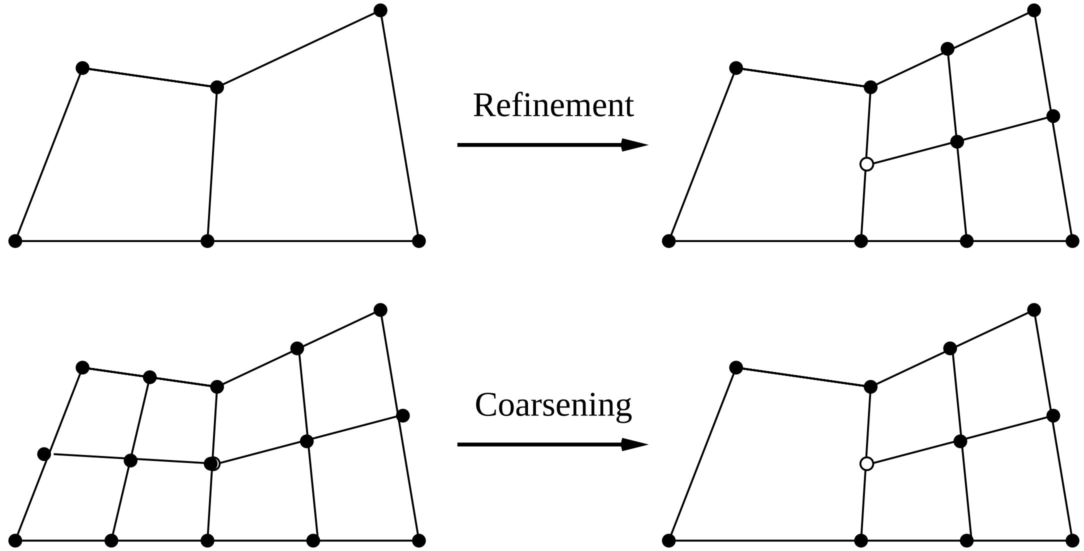
$$u_h \in V_h : \quad a(u_h, \varphi) = (f, \varphi) \quad \forall \varphi \in V_h$$

$$v_h \in V_h : \quad a(v_h, \varphi) = a(I_{2h}^{(2)} u_h, \varphi) - (f, \varphi) \quad \forall \varphi \in Vh$$

Correction: $\tilde{u}_h := u_h + v_h$

Exercise: Prove or disprove (by numerical experiment) that $\tilde{u}_h$ is an improved approximation to u.

4.2 Mesh refinement strategies



A posteriori error indicators

$$|J(e)| \approx \eta := \sum_{K \in \mathbb{T}_h} \eta_K, \quad N := \#\{K \in \mathbb{T}_h\}$$

- “Error balancing” strategy: Equilibrate by iteration

$$\eta_K \approx TOL/N \quad \Rightarrow \quad \eta \approx TOL$$

“optimal” mesh characterized by equilibrated error indicators.

- “Fixed error reduction” strategy: Order cells according to

$$\eta_{K,1} \geq \cdots \geq \eta_{K,i} \geq \cdots \geq \eta_{K,N}$$

For prescribed fractions $0 \leq X, Y \leq 1$, $X + Y \leq 1$ form

$$\sum\nolimits_{i=1}^{N_*} \eta_{K,i} \approx X\,\eta, \qquad \sum\nolimits_{i=N^*+1}^{N} \eta_{K,i} \approx Y\,\eta$$

Cells $K_1, \ldots, K_{N_*}$ are refined and $K_{N^*}, \ldots, K_N$ coarsened.

Alternatively, refine $X\,N$ and coarsen $Y\,N$ of those cells with largest and smalles error indicator (“Fixed fraction” strategy).

- "Mesh optimization" strategy:

$$\eta = \sum_{K\in\mathbb{T}_h} \eta_K \approx \int_\Omega h(x)^2 \Phi(x)\, dx \;\to\; min, \qquad N_{\max} \text{ given}$$

with $\Phi(u(x), z(x))$ a mesh-independent weighting function.
Calculus of variations yields "optimal" mesh-distribution function

$$h_{\text{opt}}(x) = \Big(\frac{W}{N_{\max}}\Big)^{1/2} \Phi(x)^{-1/4}, \qquad W := \int_\Omega \Phi(x)^{1/2}\, \mathrm{dx}$$

- "Look-ahead" strategy (2D): $\eta_{K,1} \ge \cdots \ge \eta_{K,i} \ge \cdots \ge \eta_{K,N}$

Determine $m \in \{1, \dots N\}$ and refine all cells K_i, $1 \le i \le m$.
The new mesh has $N_m = N + 3m$ cells. The resulting error estimator is extrapolated to be $\eta_m = \eta - \frac{3}{4}\sum_{i=1}^m \eta_{K,i}$.

$$m := \arg \min_{1\le m\le N} \eta_m N_m$$

Analysis of "mesh optimization" strategy for the model problem:

$$\eta = \sum_{K\in\mathbb{T}_h} \big\{(f+\Delta u_h, z-I_hz)_K - \tfrac{1}{2}([\partial_n u_h], z-I_hz)_{\partial K}\big\}$$

for estimating the error with respect to functional $J(\cdot)$.

- Convergence of residuals

$$f(x)+\Delta u_h(x_K) \to \Phi_1(x_K), \qquad -\tfrac{1}{2}h_K^{-1}[\partial_n u_h](x_K) \to \Phi_2(x_K)$$

- Convergence of weights $\quad h_K^{-2}(z-I_hz)(x_K) \to \Phi_3(x_K)$
- Error representation formula with $\Phi := (\Phi_1+\Phi_2)\Phi_3$:

$$\eta \approx \sum_{K\in\mathbb{T}_h} h_T^4\{\Phi_1+\Phi_2\}\Phi_3(x_K) \approx \int_\Omega h(x)^2\Phi(x)\,dx =: E(h)$$

with a distributed mesh-size function $h(x)$.

- Mesh complexity formula:

$$N(h) = \sum_{K \in \mathbb{T}_h} h_K^d h_K^{-d} \approx \int_\Omega h(x)^{-d}\, dx$$

Mesh optimization problems:

$$\begin{aligned} &(I) \quad E(h) \to \min, \quad N(h) \le N_{max}, \\ &(II) \quad N(h) \to \min, \quad E(h) \le TOL \end{aligned}$$

Solutions:

$$h_{opt}^{(I)}(x) = \Big(\frac{W}{N_{\max}}\Big)^{1/d} \Phi(x)^{-1/(2+d)},$$

$$h_{opt}^{(II)}(x) = \Big(\frac{TOL}{W}\Big)^{1/d} \Phi(x)^{-1/(2+d)}$$

$$W = \int_\Omega \Phi(x)^{d/(2+d)}\, dx < \infty \quad (!)$$

Proof for Problem (I): Classical Lagrange approach:

$$L(h,\lambda) = E(h) + \lambda\{N(h) - N_{max}\}$$

with Lagrangian multiplier $\lambda \in \mathbb{R}$. First-order optimality condition

$$\frac{d}{dt} L(h + t\varphi, \lambda + t\mu)_{|t=0} = 0$$

for all admissible variations φ and μ,

$$2h(x)\Phi(x) - d\lambda h(x)^{-d-1} = 0, \qquad \int_\Omega h(x)^{-d}\,dx - N_{\max} = 0$$

and, consequently,

$$h(x) = \Big(\frac{2}{d\lambda}\Phi(x)\Big)^{-1/(2+d)}, \quad \Big(\frac{2}{d\lambda}\Big)^{d/(2+d)} \int_\Omega \Phi(x)^{d/(2+d)}\,dx = N_{\max}$$

From this, we deduce the desired relations

$$\lambda \equiv \frac{2}{d}\, h(x)^{2+d}\Phi(x)\,, \qquad h_{opt}(x) = \Big(\frac{W}{N_{\max}}\Big)^{1/d}\Phi(x)^{-1/(2+d)}$$

Remarks.

- The mesh-optimization problem (II) can be treated in an analogous way.
- The first identity implies that an optimal mesh-size distribution with local cell-widths h_T is characterized by the equilibration of the cell-indicators η_T as assumed by the *error balancing strategy*.

- Even for rather *irregular* functionals $J(\cdot)$ the quantity W is bounded. For example, the evaluation of $J(u) = \partial_i u(P)$ for smooth u in $\mathbb{R}^2$ leads to $\Phi(x) \approx |x_P|^{-3}$ and, consequently,

$$W \approx \int_\Omega |x - P|^{-3/2}\, dx < \infty$$

- The explicit formulas for $h_{opt}(x)$ have to be used with care in designing a mesh as their derivation implicitly assumes that they actually correspond to *scalar* mesh-size functions of *isotropic* meshes, a condition however which is not incorporated into the formulation of the mesh-optimization problems.

- A strong objection against the practical value of this formula is the need of approximating the weighting function $\Phi(x)$ on the current mesh for steering the refinement process which seems a contradiction in itself.

4.3 Control of linearization

Remainder terms in nonlinear error representation formula:

$$R_h^{(3)} = \tfrac{1}{2}\int_0^1 \Big\{ J'''(u_h{+}se)(e,e,e) - A'''(u_h{+}se)(e,e,e,z_h{+}se^*)$$
$$- 3A''(u_h{+}se)(e,e,e^*)\Big\}\, s(s{-}1)\,ds$$
$$R_h^{(2)} = \int_0^1 \{A''(u_h{+}se)(e,e,z) - J''(u_h{+}se)(e,e)\}\,ds.$$

For quadratic nonlinearities such as $(u\cdot\nabla u,\cdot)_{L^2}$ the remainder terms take the form

$$R_h^{(2)} = 2(e^u\cdot\nabla e^u, z), \qquad R_h^{(3)} = -\tfrac{1}{2}(e^u\cdot\nabla e^u, e^z)$$

which could be controlled by “global” energy-norm error estimates.

4.4. Balancing of iteration and discretization error

In practice the "exact" discrete solution $u_h \in V_h$ on the current mesh $\mathbb{T}_h$ is not known but rather an approximation $\tilde{u}_h \in V_h$ to it obtained by some iterative process such as a simple fixed point method (Newton, Gauß-Seidel method), a preconditioned Krylov space method (CG method), or multigrid method (MG method). Hence, in the a posteriori error representation

$$J(u) - J(u_h) = \eta := \rho(u_h)(z - \psi_h)$$

we have to use this approximation $\tilde{u}_h$,

$$J(u) - J(u_h) \approx \tilde{\eta} := \rho(\tilde{u}_h)(z - \psi_h).$$

We would like to balance the "iteration error" against the unavoidable "discretization error" in order to having a useful stopping criterion for the iteration.

Proposition (linear case). *Let $\tilde{u}_L \in V_L$ be any approximation to the exact discrete solution $u_L \in V_L$ on the finest mesh $\mathbb{T}_L$. Then, for the error $\tilde{e}_L := u - \tilde{u}_L$ there holds the error representation*

$$J(\tilde{e}_L) = \rho(\tilde{u}_L)(z - \hat{z}_L) + \rho(\tilde{u}_L)(\hat{z}_L).$$

If the multigrid method has been used with natural components the following refined representation holds for the iteration residual:

$$\rho(\tilde{u}_L)(\hat{z}_L) = \sum_{j=1}^{L} \big(R_j(\tilde{v}_j), \hat{z}_j - \hat{z}_{j-1}\big).$$

Here, $\hat{z}_j \in V_j$ can be chosen arbitrarily, $R_j(\tilde{v}_j)$ is the iteration residual on mesh level j, and $\rho(\tilde{u}_L)(\cdot)$ is as defined above.

Error balancing criterion: (observe: $\rho(u_L)(\hat{z}_L) = 0$)

$$|\rho(\tilde{u}_L)(\hat{z}_L)| \leq |\rho(\tilde{u}_L)(z - \hat{z}_L)|$$

Proof. There holds

$$\begin{aligned} J(e) = a(e,z) &= a(e, z-\hat{z}_L) + a(e,\hat{z}_L) \\ &= (f, z-\hat{z}_L) - a(\tilde{u}_L, z-\hat{z}_L) + (f,\hat{z}_L) - a(\tilde{u}_L,\hat{z}_L) \\ &= \rho(\tilde{u}_L)(z-\hat{z}_L) + \rho(\tilde{u}_L)(\hat{z}_L). \end{aligned}$$

In the multigrid case the second term can be rewritten by using the particular structure (projection properties) of the MG algorithm.

- The first error representation can be used for approximative solutions $\tilde{u}_L$ obtained by any solution process.
- The second error representation holds for V-, W- or F-cycles and for any type of smoothing. It allows not only to balance the iteration against the discretization error but also to tune the smoothing iteration separately on the different mesh levels.

Exercise: Prove for the general situation with semilinear "energy form" $a(\cdot)(\cdot)$ and nonlinear functional $J(\cdot)$ (both three times Gateaux differentiable) the following error representation:

Proposition (nonlinear case). *Let $\tilde{u}_L,\, \tilde{z}_h \in V_L$ be any approximations to the primal and dual discrete solutions $u_L,\, z_L \in V_L$ on the finest mesh $\mathbb{T}_L$. Then, there holds the error representation*

$$J(u)-J(\tilde{u}_L) = \tfrac{1}{2}\rho(\tilde{u}_L)(z-\hat{z}_L) + \tfrac{1}{2}\rho^*(\tilde{z}_L)(u-\hat{u}_L) + \tilde{R}_L^{(3)}$$
$$+ \tfrac{1}{2}\big\{J'(\tilde{u}_L) - a'(\tilde{u}_L)(\hat{u}_L-\tilde{u}_K, \hat{z}_L-\tilde{z}_L) + a(\tilde{u}_L)(\tilde{z}_L)\big\}$$

where the remainder $\tilde{R}_H^{(3)}$ is cubic in the errors $u-\tilde{u}_L$ and $z-\tilde{z}_L$

This error representation can also be used to control the accuracy in a Newton or in a simple fixed point iteration for dealing with the nonlinearity.

5. Eigenvalue problems

- The *symmetric* eigenvalue problem of the Laplace operator:

$$-\Delta u = \lambda u \quad + \ B.C.$$

- The *nonsymmetric* eigenvalue problem of a convection-diffusion operator:

$$-\Delta u + b \cdot \nabla u = \lambda u \quad + \ B.C.$$

- The *stability* eigenvalue problem governed by the linearized Navier-Stokes operator:

$$-\nu \Delta v + \hat{v} \cdot \nabla v + v \cdot \nabla \hat{v} + \nabla p = \lambda v, \quad \nabla \cdot v = 0 \quad + \ B.C.$$

where $\hat{v}$ is some "base solution" the stability of which is to be investigated.

Eigenvalue problem in (complex) function space V
($m(\cdot,\cdot)$ semi-scalar product):

$$a(u,\varphi) = \lambda\, m(u,\varphi) \quad \forall \varphi \in V, \quad \lambda \in \mathbb{C}, \quad m(u,u) = 1$$

Galerkin approximation in finite dimensional subspaces $V_h \subset V$:

$$a(u_h,\varphi_h) = \lambda_h\, m(u_h \varphi_h) \quad \forall \varphi_h \in V_h, \quad \lambda_h \in \mathbb{C}, \quad m(u_h,u_h) = 1$$

Goal: *Control of error in eigenvalues* $\lambda - \lambda_h$ *in terms of the residual*

$$\rho(u_h,\lambda_h)(\cdot) := \lambda_h\, m(u_h,\cdot) - a(u_h,\cdot)$$

A posteriori error analysis

Embedding into the general framework of variational equations

$$U := \{u, \lambda\} \in \mathcal{V} := V \times \mathbb{C}, \qquad U_h := \{u_h, \lambda_h\} \in \mathcal{V}_h := V_h \times \mathbb{C}$$

Semilinear form for $\Phi = \{\varphi, \mu\} \in \mathcal{V}$:

$$A(U)(\Phi) := \lambda\, m(u, \varphi) - a(u, \varphi) + \overline{\mu}\, \underbrace{\{m(u, u) - 1\}}_{\text{normalization}}$$

Compact variational formulation of eigenvalue problems

$$A(U)(\Phi) = 0 \quad \forall \Phi \in \mathcal{V}$$
$$A(U_h)(\Phi_h) = 0 \quad \forall \Phi_h \in \mathcal{V}_h$$

Error control functional: $\quad J(\Phi) := \mu\, m(\varphi, \varphi), \ \ \Phi = \{\varphi, \mu\}$

$$m(u, u) = 1 \quad \Rightarrow \quad J(U) = \lambda$$

Dual solutions $Z=\{z,\pi\}\in\mathcal{V}$, $Z_h=\{z_h,\pi_h\}\in\mathcal{V}_h$:

$$A'(U)(\Phi,Z)=J'(U)(\Phi)\qquad \forall\Phi\in\mathcal{V}$$

$$A'(U_h)(\Phi_h,Z_h)=J'(U_h)(\Phi_h)\quad \forall\Phi_h\in\mathcal{V}_h$$

Detailed form of adjoint equations:

$U=\{u,\lambda\},\ \Phi=\{\varphi,\mu\},\ Z=\{z,\pi\}$

$$\begin{aligned} A'(U)(\Phi,Z) \;&=\; \lambda\, m(\varphi,z)-a(\varphi,z)+\mu\, m(u,z)+2\bar\pi\mathrm{Re}\, m(\varphi,u)\\ &\quad + \mu\{m(u,u)-1\} \end{aligned}$$

$$J'(U)(\Phi) \;=\; \mu\, m(u,u)+2\lambda\mathrm{Re}\, m(\varphi,u)$$

Observing that $m(u,u)=1$, the dual problem takes the form

$$\bar\lambda\, m(z,\varphi)-a(\varphi,z)+\mu\,\{m(u,z)-1\}+2\{\bar\pi-\lambda\}\mathrm{Re}\, m(\varphi,u) \;=\; 0$$

for all $\Phi=\{\varphi,\mu\}$.

This system is equivalent to the "dual" eigenvalue problem

$$a(\varphi, z) = \bar{\pi}\, m(\varphi, z) \quad \forall \varphi \in V, \quad \bar{\pi} = \lambda, \quad m(u, z) = 1$$

or identifying $z = u^*$ and $\pi = \lambda^*$,

$$a(\varphi, u^*) = \bar{\lambda}^*\, m(\varphi, u^*) \quad \forall \varphi \in V, \quad m(u, u^*) = 1$$

The discrete adjoint problem is equivalent to

$$a(\varphi_h, u_h^*) = \bar{\lambda}_h^*\, m(\varphi_h, u_h^*) \quad \forall \varphi_h \in V_h, \quad m(u_h, u_h^*) = 1$$

Associated dual residual:

$$\rho^*(u_h^*, \lambda_h^*)(\cdot) := \bar{\lambda}_h^*\, m(\cdot, u_h^*) - a(\cdot, u_h^*)$$

Proposition. *There holds the error representation*

$$\lambda-\lambda_h \;=\; \tfrac{1}{2}\rho(u_h,\lambda_h)(u^*-\psi_h)+\tfrac{1}{2}\rho^*(u_h^*,\lambda_h^*)(u-\varphi_h)+\; R_h^{(3)}$$

for arbitrary $\psi_h,\,\varphi_h\in V_h$*, with the cubic remainder term*

$$R_h^{(3)} \;=\; \tfrac{1}{2}(\lambda-\lambda_h)\,m(u-u_h,u^*-u_h^*).$$

Proof: Setting $E:=\{u-u_h,\lambda-\lambda_h\}$ and $E^*:=\{u^*-u_h^*,\lambda^*-\lambda_h^*\}$, the general remainder term from the abstract theory has the form

$$\begin{aligned} R_h^{(3)} = \tfrac{1}{2}\int_0^1 \Big\{ & J'''(U_h+sE)(E,E,E) \\ & - A'''(U_h+sE)(E,E,E,Z_h+sE^*) \\ & - 3A''(U_h+sE)(E,E,E^*)\Big\}\, s(s-1)\,ds \end{aligned}$$

In the present case, by a simple calculation, we have

$$
\begin{aligned}
J'''(U_h+sE)(E,E,E) &= 6(\lambda-\lambda_h)m(u-u_h,u-u_h),\\
A'''(U_h+sE)(E,E,E,Z_h+sE^*) &= 0\\
-3A''(U_h+sE)(E,E,E^*) &= -6(\lambda-\lambda_h)\,m(u-u_h,u^*-u_h^*)\\
&\quad -6(\overline{\lambda^*-\lambda_h^*})\,m(u-u_h,u-u_h)
\end{aligned}
$$

Consequently, noting that $\lambda-\lambda_h = \overline{\lambda^*-\lambda_h^*}$, it follows that

$$
\begin{aligned}
R_h^{(3)} &= -3\int_0^1 (\lambda-\lambda_h)\,m(u-u_h,u^*-u_h^*)s(s-1)\,ds\\
&= \tfrac{1}{2}(\lambda-\lambda_h)\,m(u-u_h,u^*-u_h^*)
\end{aligned}
$$

which completes the proof.

Remarks:

- Simultaneous solution of **primal and adjoint** eigenvalues problems is necessary within an optimal multigrid solver of nonsymmetric eigenvalue problems. Here, a complex Arnoldi method with solving the inner linear subproblems by multigrid has been used.
- Case of **multiple** eigenvalues can easily be treated.
- The case of a **degenerate** eigenvalue can also be handled.
- Error estimates for **functionals** $j(u)$ of eigenfunctions.
- Case of additional **approximation in operator** $\mathcal{A} = \mathcal{A}(\hat{u})$ (stability eigenvalue problem).

Evaluation of eigenvalue residuals

On a polygonal/hedrahedral domain $\Omega \subset \mathbb{R}^d$ consider the nonsymmetric eigenvalue problem

$$\mathcal{A}v := -\Delta v + b \cdot \nabla v \; = \; \lambda v \quad \text{in } \Omega, \quad \text{v} = 0 \quad \text{on} \;\; \partial\Omega.$$

with a smooth (or even constant) transport coefficient b, and $\mathcal{M} := \mathrm{id}$. This eigenvalue problem is approximated by the Galerkin method using piecewise linear or d-linear finite elements on meshes $\mathbb{T}_h = \{K\}$.

Within this setting, we can proceed analogously as before, obtaining

$$
\begin{aligned}
\rho(u_h,\lambda_h)(\psi) &= \lambda_h\, m(u_h,\psi) - a(u_h,\psi) \\
&= \sum_{K\in\mathbb{T}_h} \big\{(\lambda_h\mathcal{M}u_h - \mathcal{A}u_h,\psi)_K - (\partial_n^{\mathcal{A}}u_h,\psi)_{\partial K}\big\} \\
&= \sum_{K\in\mathbb{T}_h} \big\{(\lambda_h\mathcal{M}u_h - \mathcal{A}u_h,\psi)_K - \tfrac{1}{2}([\partial_n^{\mathcal{A}}u_h],\psi)_{\partial K}\big\}
\end{aligned}
$$

$$
\begin{aligned}
\rho^*(u_h^*,\lambda_h^*)(\varphi) &= \lambda_h^*\, m(\varphi,z_h) - a(\psi,z_h) \\
&= \sum_{K\in\mathbb{T}_h} \big\{(\varphi,\lambda_h^*\mathcal{M}z_h - \mathcal{A}^*z_h)_K - (\varphi,\partial_n^{\mathcal{A}^*}z_h)_{\partial K}\big\} \\
&= \sum_{K\in\mathbb{T}_h} \big\{(\varphi,\lambda_h^*\mathcal{M}z_h - \mathcal{A}^*z_h)_K - \tfrac{1}{2}(\varphi,[\partial_n^{\mathcal{A}^*}z_h])_{\partial K}\big\}
\end{aligned}
$$

Hence, using again the notation of "equation" and "jump residuals", the primal residual admits the estimate

$$|\rho(u_h,\lambda_h)(u^*-i_hu^*)| \le \sum_{K\in\mathbb{T}_h} \rho_K\omega_K^*$$

$$\rho_K := \big(\|R(u_h,\lambda_h)\|_K^2 + h_K^{-1/2}\|r(u_h)\|_{\partial K}^2\big)^{1/2}$$

$$\omega_K^* := \big(\|u^*-I_hu^*\|_K^2 + h_K^{1/2}\|u^*-I_hu^*\|_{\partial K}^2\big)^{1/2}$$

Correspondingly, for the dual residual:

$$|\rho^*(u_h^*,\lambda_h^*)(u-i_hu)| \le \sum_{K\in\mathbb{T}_h} \rho_K^*\omega_K$$

$$\rho_K^* := \big(\|R^*(u_h^*,\lambda_h^*)\|_K^2 + h_K^{-1/2}\|r^*(u_h^*)\|_{\partial K}^2\big)^{1/2}$$

$$\omega_K := \big(\|u-I_hu\|_K^2 + \tfrac{1}{2}h_K^{1/2}\|u-I_hu\|_{\partial K}^2\big)^{1/2}$$

Proposition. *Within the above setting, assuming that*

$$|m(u-u_h, u^*-u_h^*)| \le 1,$$

there holds the a posteriori error estimate

$$|\lambda-\lambda_h| \;\le\; \eta_\lambda^\omega := \sum_{K\in\mathbb{T}_h} \left\{\rho_K\omega_K^* + \rho_K^*\omega_K\right\}$$

Proof: By the above estimates,

$$|\lambda-\lambda_h| \le \tfrac{1}{2} \sum_{K\in\mathbb{T}_h} \left\{\rho_K\omega_K^* + \rho_K^*\omega_K\right\} + R_h^{(3)}$$

Since, by the assumption,

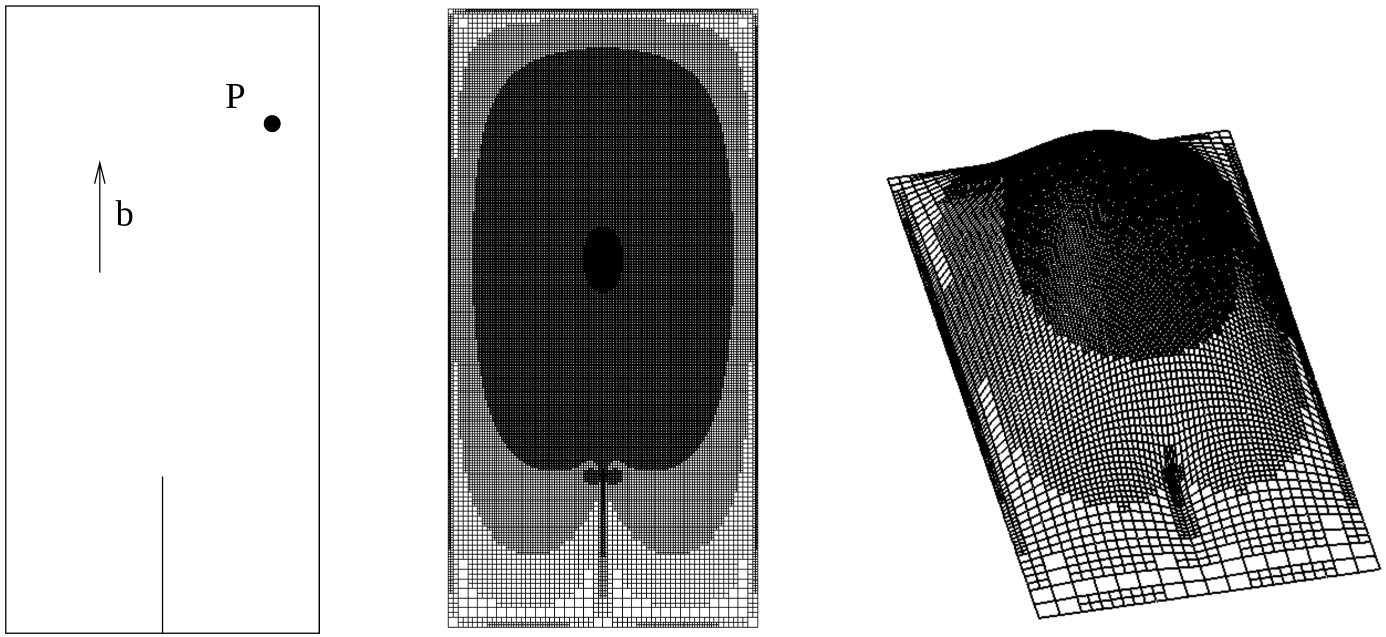
$$|R_h^{(3)}| = \tfrac{1}{2}|(\lambda-\lambda_h)\, m(u-u_h, u^*-u_h^*)| \le \tfrac{1}{2}\,|\lambda-\lambda_h|$$

the asserted estimate follows.

Numerical example

Convection-diffusion problem: $b = (0, b_y)^T$, $\Omega = (-1,1)\times(-1,3)$

$$-\Delta v + b\cdot\nabla v \;=\; \lambda v \quad \text{in } \Omega, \qquad \text{v} = 0 \;\text{ on } \partial\Omega$$



Configuration for $b \equiv 0$ (left), adapted mesh with $12,000$ cells (middle), normlized eigenfunctions (right)

Different refinement indicators:

a) Weight-free error estimates:

$$\eta_\lambda^{(1)} := \sum_{K\in\mathbb{T}_h} h_K^2 \big\{\rho_K^2 + \rho_K^{*2}\big\}$$

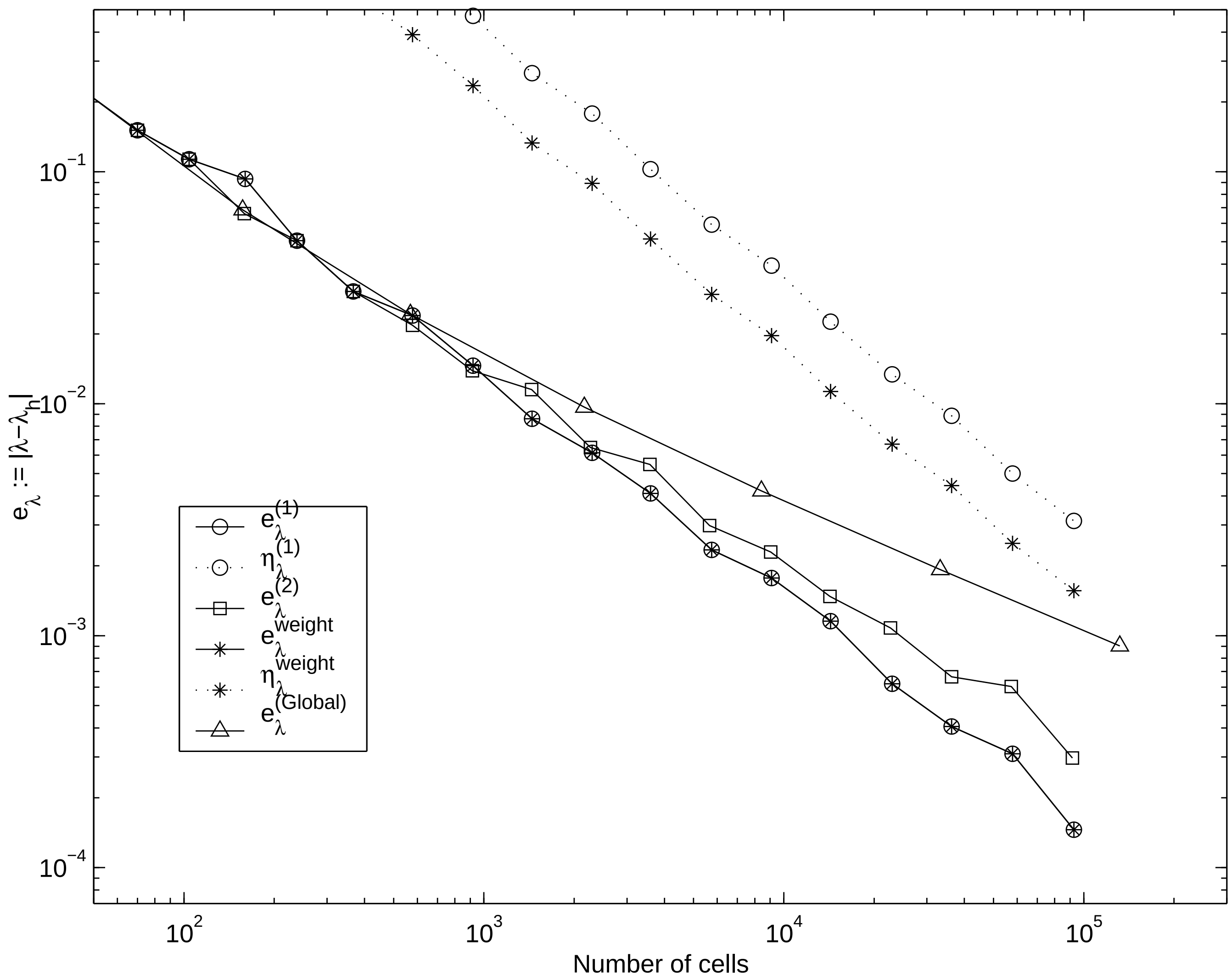
$$\eta_\lambda^{\mathrm{red}} := \sum_{K\in\mathbb{T}_h} h_K^2 \rho_K^2$$

$$\eta_\lambda^{(2)} := \Big(\sum_{K\in\mathbb{T}_h} h_K^4 \big\{\rho_K^2 + \rho_K^{*2}\big\}\Big)^{1/2}$$

b) Weighted error estimate:

$$\eta_\lambda^{\omega} := \sum_{K\in\mathbb{T}_h} h_K^2 \big\{\rho_K \tilde{\omega}_K^* + \rho_K^* \tilde{\omega}_K\big\}$$

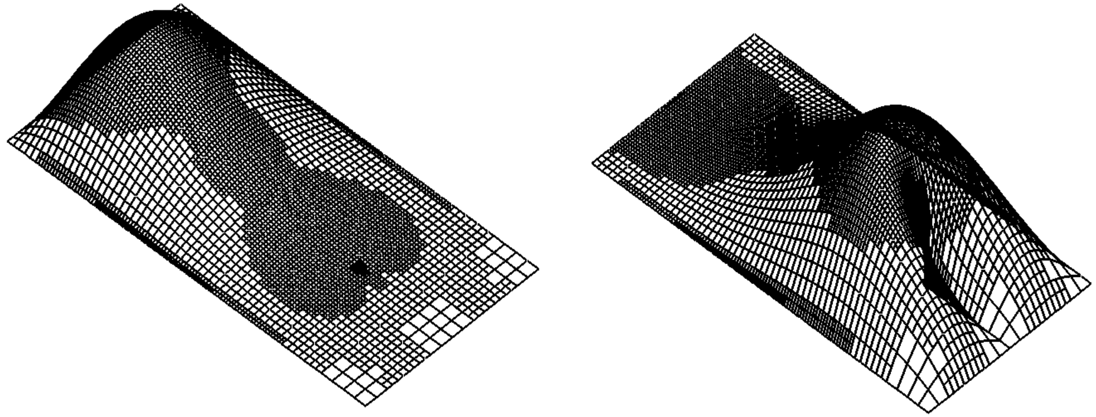
Test case 1: Symmetric problem

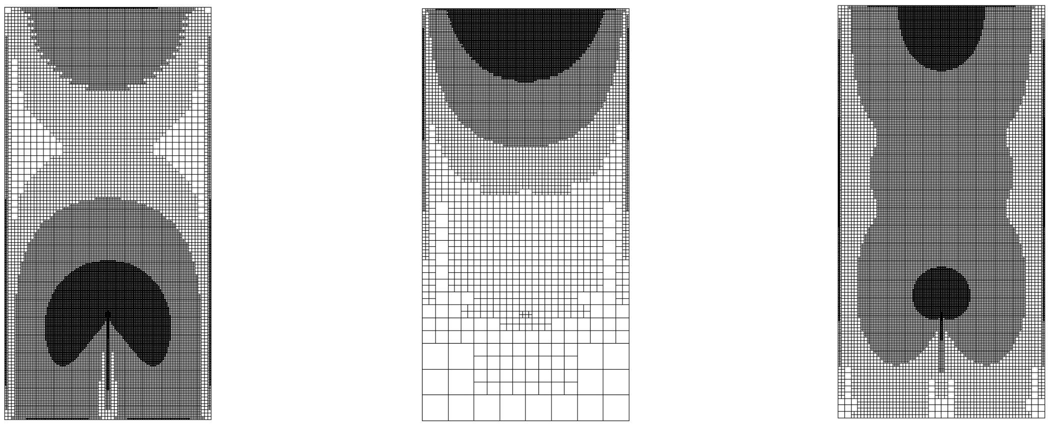


$\eta_\lambda^{(1)}$ (O), $\eta_\lambda^{(2)}$ ($\square$), $\eta_\lambda^{\mathrm{weight}}$ ($*$), uniform ($\triangle$)

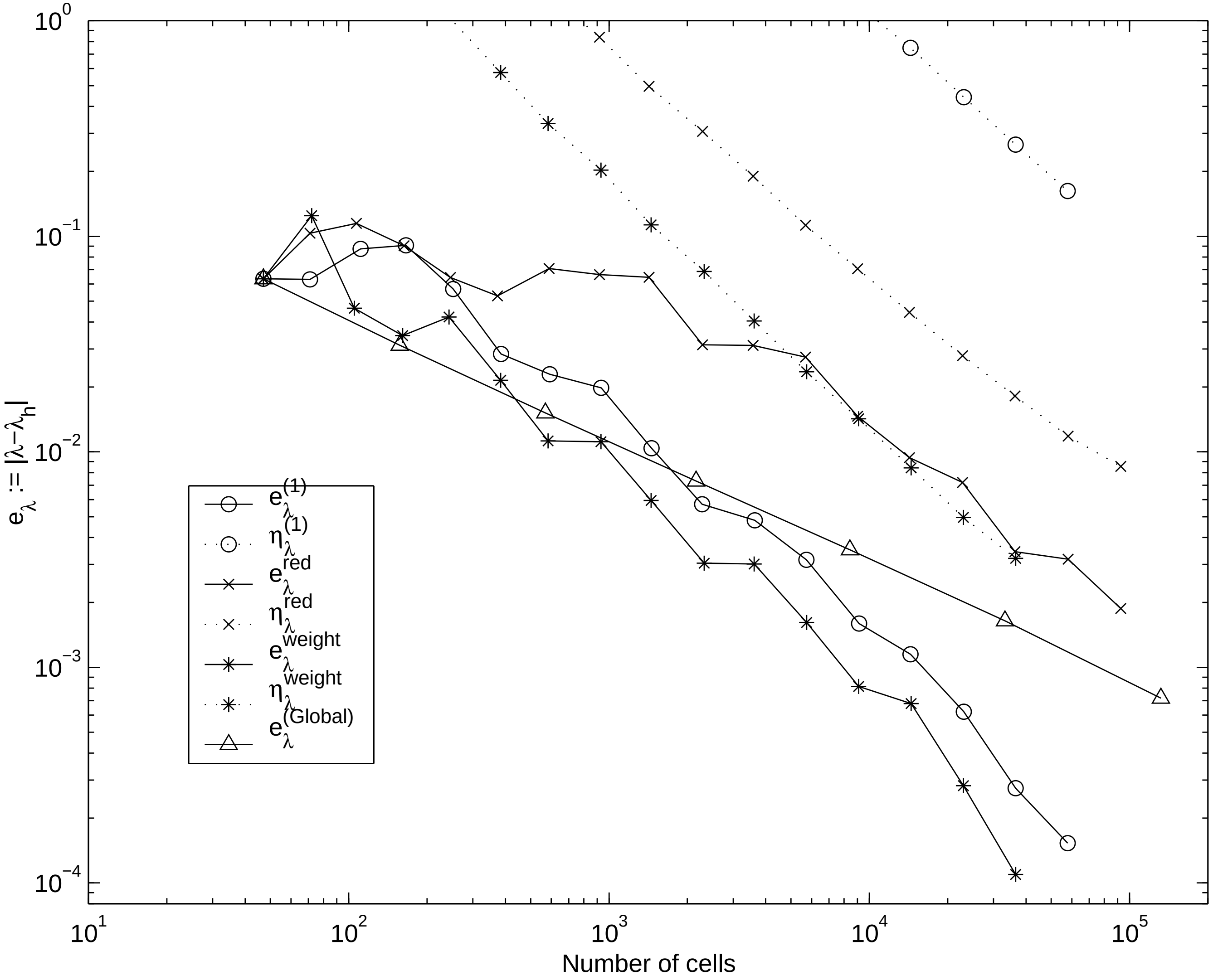
Test case 2: Vertical transport $b_y = 3$

Primal (left) and dual eigenfunction (right)





Adapted mesh with $10,000$ cells by $\eta_\lambda^{(1)}$ (left), $\eta_\lambda^{\text{red}}$ (middle), $\eta_\lambda^{\text{weight}}$ (right) (fixed-rate strategy with $X = 20\%, Y = 0\%$)



$\eta_\lambda^{(1)}$ (O), $\eta_\lambda^{\mathrm{red}}$ ($\times$), $\eta_\lambda^{\mathrm{weight}}$ ($*$), uniform ($\triangle$)

Perturbed eigenvalue problems (stability analysis)

Stability of base solution $\hat{u} = \{\hat{v}, \hat{q}\}$

a) Linear stability theory ("spectral argument"):

Non-sym. eigenvalue problem for $u := \{v, p\} \in V$ and $\lambda \in \mathbb{C}$:

$$-\nu\Delta v + \hat{v}\cdot\nabla v + v\cdot\nabla\hat{v} + \nabla p = \lambda v, \qquad \nabla\cdot v = 0.$$

$$\mathrm{Re}\,\lambda \geq \mathbf{0} \quad \Rightarrow \quad \hat{\mathbf{u}}\ \textbf{stable}\ (?)$$

b) Nonlinear stability theory ("energy argument"):

Symmetric eigenvalue problem for $u := \{v, p\} \in V$ and $\lambda \in \mathbb{R}$:

$$-\nu\Delta v + \tfrac{1}{2}(\nabla\hat{v} + \nabla\hat{u}^T)v + \nabla p = \lambda\, v, \qquad \nabla\cdot v = 0.$$

$$\mathrm{Re}\,\lambda \geq \mathbf{0} \quad \Rightarrow \quad \hat{\mathbf{u}}\ \textbf{stable}\ (!)$$

Variational formulation of stability eigenvalue problem:

$$a'(\hat{u})(\psi,\varphi) := \nu(\nabla\psi^v,\nabla\varphi^v) + (\hat{v}\cdot\nabla\psi^v,\varphi^v) + (\psi^v\cdot\nabla\hat{v},\varphi^v)$$
$$- (\psi^p,\nabla\cdot\varphi^v) + (\varphi^p,\nabla\cdot\psi^v),$$
$$m(\psi,\varphi) := (\psi^v,\varphi^v).$$

Primal and dual eigenvalue problems: $u,\, u^* \in V:$

$$a'(\hat{u})(u,\varphi) = \lambda\, m(u,\varphi) \qquad \forall\varphi\in V$$
$$a'(\hat{u})(\varphi,u^*) = \lambda\, m(\varphi,u^*) \qquad \forall\varphi\in V$$

Normalization: $m(u,u) = m(u,u^*) = 1\,.$

If $m(u,u^*) = 0$, the boundary value problem

$$a'(\hat{u})(\tilde{u},\varphi) - \lambda\, m(\tilde{u},\varphi) = m(u,\varphi) \qquad \forall\varphi\in V$$

has a solution $\tilde{u}\in V$ ("gener. eigenf.") $\Rightarrow$ $\text{defect}(\lambda) > \mathbf{0}$

Discretization

Stabilized sesquilinear form

$$a'_\delta(\hat{v}_h)(u_h, \varphi_h) := a'(\hat{u})(u_h, \varphi) + (\mathcal{A}'(\hat{u})u - \lambda_h v, \mathcal{S}(\hat{u})\varphi)_\delta$$

Discrete primal and dual eigenvalue problems $u_h,\ u_h^* \in V_h,\ \lambda_h \in \mathbb{C}$:

$$a'_\delta(\hat{u}_h)(u_h, \varphi_h) = \lambda_h\, m(u_h, \varphi_h) \qquad \forall \varphi_h \in V_h$$

$$a'_\delta(\hat{u}_h)(\varphi_h, u_h^*) = \lambda_h\, m(\varphi_h, u_h^*) \qquad \forall \varphi_h \in V_h$$

Stabilization $\quad m(u_h, u_h) = m(u_h, u_h^*) = 1$

Blow-up criterion ("pseudo-spectrum")

$$m(v_h^*, v_h^*) \to \infty \quad (h \to 0) \quad \Rightarrow \quad \mathrm{defect}(\lambda) > 0$$

A posteriori error estimation

Embedding into the general framework of variational equations:

$$\mathcal{V} := V \times V \times \mathbb{C}, \quad \mathcal{V}_h := V_h \times V_h \times \mathbb{C}$$

$$U := \{\hat{u}, u, \lambda\}, \quad U_h := \{\hat{u}_h, u_h, \lambda_h\}, \quad \Phi = \{\hat{\varphi}, \varphi, \mu\} \in \mathcal{V}$$

$$A(U)(\Phi) := \underbrace{f(\hat{\varphi}) - a_\delta(\hat{u})(\hat{\varphi})}_{\text{base solution}} + \underbrace{\lambda\, m(u,\varphi) - a'_\delta(\hat{u})(u,\varphi)}_{\text{eigenvalue problem}}$$
$$+ \underbrace{\overline{\mu}\{m(u,u) - 1\}}_{\text{normalization}}$$

Compact variational formulation:

$$A(U)(\Phi) = 0 \qquad \forall \Phi \in \mathcal{V}$$
$$A(U_h)(\Phi_h) = 0 \qquad \forall \Phi_h \in \mathcal{V}_h$$

Error functional:

$$J(\Phi) := \mu\, m(\varphi,\varphi) \quad \Rightarrow \quad J(U) = \lambda m(u,u) = \lambda.$$

Dual solutions $Z = \{\hat z, z, \pi\} \in \mathcal{V}$, $Z_h = \{\hat z_h, z_h, \pi_h\} \in \mathcal{V}_h$:

$$A'(U)(\Phi, Z) = J'(U)(\Phi) \qquad \forall \Phi \in \mathcal{V}$$

$$A'(U_h)(\Phi_h, z_h) = J'(U_h)(\Phi_h) \qquad \forall \Phi_h \in \mathcal{V}_h$$

Observation: $z = u^*,\ \pi = \lambda,\ \hat z = \hat u^*$,

$$a'(\hat u)(\psi, \hat u^*) = -a''(\hat u)(\psi, u, u^*) \qquad \forall \psi \in V.$$

Residuals:

$$\rho(\hat u_h)(\cdot) := (f,\cdot) - a_\delta(\hat u_h)(\cdot)$$

$$\rho^*(\hat u_h^*)(\cdot) := -a''_\delta(\hat u)(\cdot, u_h, u_h^*) - a'_\delta(\hat u_h)(\cdot, \hat u_h^*)$$

$$\rho(\{u_h, \lambda_h\})(\cdot) := \lambda_h\, m(u_h, \cdot) - a'_\delta(\hat u_h)(u_h, \cdot)$$

$$\rho^*(\{u_h^*, \lambda_h\})(\cdot) := \lambda_h\, m(\cdot, u_h^*) - a'_\delta(\hat u_h)(\cdot, u_h^*)$$

Application of Proposition 1:

Proposition 3. *There holds the error representation*

$$\lambda - \lambda_h = \underbrace{\tfrac{1}{2}\rho(\hat{u}_h)(\hat{u}^* - I_h\hat{u}^*) + \tfrac{1}{2}\rho^*(\hat{u}_h^*)(\hat{u} - I_h\hat{u})}_{\textit{base solution residuals}}$$

$$+ \underbrace{\tfrac{1}{2}\rho(\{u_h, \lambda_h\})(u^* - I_h u^*) + \tfrac{1}{2}\rho^*(\{u_h^*, \lambda_h\})(u - I_h u)}_{\textit{eigenvalue residuals}} + \mathcal{R}_h^{(3)},$$

for arbitrary $I_h\hat{u}^*, I_h\hat{u}, I_h u^*, I_h u \in V_h$*. The remainder* $R_h^{(3)}$ *is cubic in the errors* $\hat{e}_h^v := \hat{v} - \hat{v}_h$, $\hat{e}_h^{v*} := \hat{v}^* - \hat{v}_h^*$ *and* $e_h^\lambda := \lambda - \lambda_h$, $e_h^v := v - v_h$, $e_h^{v*} := v^* - v_h^*$.

Numerical test (hydrodynamic stability analysis)

Stability of base solution $\hat{u} = \{\hat{v}, \hat{p}\}$ by **linear stability theory**:

Non-symmetric eigenvalue problem for $u := \{v, p\} \in V$, $\lambda \in \mathbb{C}$

$$\mathcal{A}'(\hat{\mathbf{u}})u := -\nu\Delta v + \hat{\mathbf{u}} \cdot \nabla v + (\nabla \hat{\mathbf{u}})^T v + \nabla p = \lambda v, \quad \nabla \cdot v = 0$$

$$\operatorname{Re}\lambda \geq \mathbf{0} \quad \Rightarrow \quad \hat{\mathbf{u}} \ \text{stable (?)}$$

Error estimator and **balancing criterion**:

$$|\lambda - \lambda_h| \approx \sum_{K \in \mathbb{T}_h} \{\hat{\eta}_K + \eta_K^\lambda\}, \qquad \sum_{\mathbf{K} \in \mathbb{T}_\mathbf{h}} \hat{\eta}_\mathbf{K} \leq \sum_{\mathbf{K} \in \mathbb{T}_\mathbf{h}} \eta_\mathbf{K}^\lambda \ !$$

An application will be presented below.

6. Optimization problems

Abstract optimal control problem

$$J(u,q) = \min! \qquad A(u,q)(\psi) = F(\psi) \quad \forall \psi \in V$$

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

$$J(u_h,q_h) = \min! \qquad A(u_h,q_h)(\psi_h) = F(\psi_h) \quad \forall \psi_h \in V_h$$

Preliminary thoughts:

- **Notion of admissible states $u = u(q)$?**
  Accuracy in discretization of PDEs is expensive.
  To what extent is "admissibility" relevant for the optimization?
- **How to "measure" admissibility:**
  In PDE context the choice of error measures is not clear:
  "energy" norm, L^2-norm, local max-norm, ... ?

Euler-Lagrange approach and Galerkin approximation:

Lagrangian functional $\mathcal{L}(u,q,z) := J(u,q) + F(z) - A(u,q)(z)$

(P) Determine stationary point $x := \{u,q,z\} \in X := V\times Q\times V$:

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

(P_h) Galerkin approx. $x_h := \{u_h,q_h,z_h\} \in X_h := V_h\times Q_h\times V_h$:

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

Idea: Measure accuracy in terms of cost functional $J(u)-J(u_h)$ depending on residuals of $x_h := (u_h, q_h, z_h)$:

$$\rho^*(x_h)(\cdot) := J_u'(u_h,q_h)(\cdot) - A_u'(u_h,q_h)(\cdot,z_h) \qquad \text{(dual)}$$

$$\rho^q(x_h)(\cdot) := J_q'(u_h,q_h)(\cdot) - A_q'(u_h,q_h)(\cdot,z_h) \qquad \text{(control)}$$

$$\rho(x_h)(\cdot) := F(\cdot) - A(u_h)(\cdot) \qquad \text{(primal)}$$

Proposition. *We have the a posteriori error representation*

$$J(u,q)-J(u_h,q_h) = \frac{1}{2}\underbrace{\rho^*(z_h)(u-\varphi_h)}_{\text{dual residual}} + \frac{1}{2}\underbrace{\rho^q(q_h)(q-\chi_h)}_{\text{control residual}} + \frac{1}{2}\underbrace{\rho(u_h)(z-\psi_h)}_{\text{primal residual}} + \underbrace{R_h^{(3)}(e^u,e^q,e^z)}_{\text{cubic}}$$

for arbitrary $\varphi_h,\ \psi_h \in V_h$ and $\chi_h \in Q_h$.

Proof. Embedding into the general framework:

$$x := \{u, q, z\} \in X = V \times Q \times V, \qquad L(x) := \mathcal{L}(u, q, z)$$

Variational equation: $\qquad L'(x)(y) = 0 \quad \forall y \in X$

$$x_h := \{u_h, q_h, z_h\} \in X_h = V_h \times Q_h \times V_h$$

Galerkin approximation: $\qquad L'(x_h)(y_h) = 0 \quad \forall\, y_h \in X_h.$

Observing that $J(u) - J(u_h) = L(x) - L(x_h)$ the general error representation for functionals

$$L(x) - L(x_h) = \frac{1}{2} \underbrace{L'(x_h)(x - y_h)}_{\text{Residual}} + \frac{1}{2} \int_0^1 L'''(x_h + se)(e, e, e)\, s(s-1)\, \mathrm{ds}$$

yields the desired result.

Remarks.

- The evaluation of the residual terms requires reliable guesses for the unknown solution $\{u, q, z\}$ as described above.
- This error estimation only uses available information (no extra dual problem has to solve).
- Practical solution process by nesting outer Newton iteration with mesh adaptation (successive "model enrichment").
- **Problem:** Method results in **"nonadmissible"** solution q_h^{opt}, u_h^{opt}.
  Solution: Recover an admissible state $\tilde{u}_h^{opt}$ from q_h^{opt} by solving the state equation on a finer mesh $\mathbb{T}_{h'}$:

$$A(\tilde{u}_h^{opt}, q_h^{opt})(\psi_{h'}) = F(\psi_{h'}) \quad \forall \psi_{h'} \in V_{h'}$$

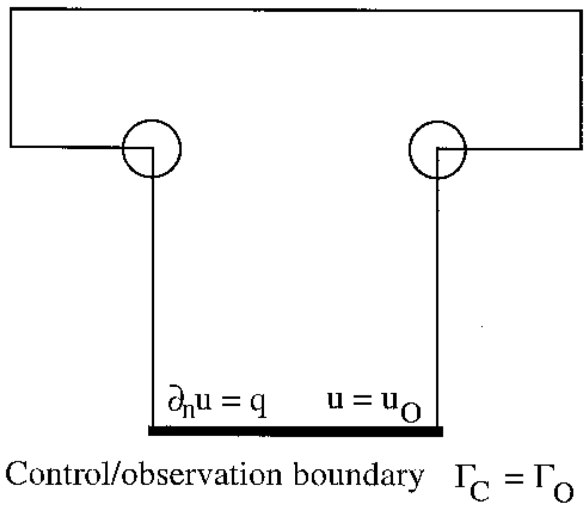
An example of boundary control (H. Kapp 1999)

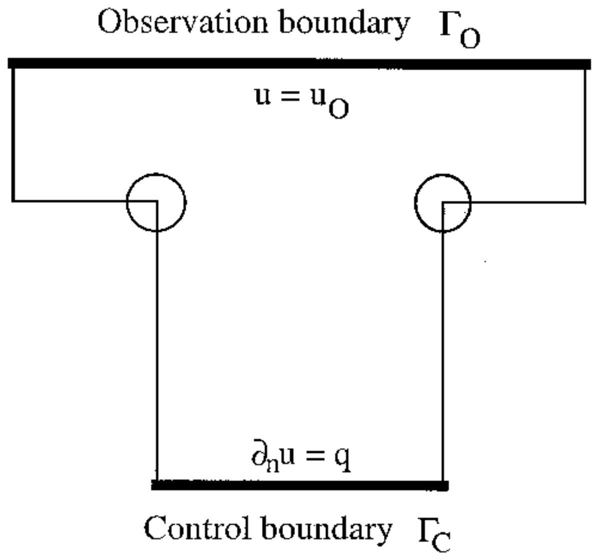
$$-\Delta u + s(u) = f \quad \text{in } \Omega \subset \mathbb{R}^2, \quad s(u) = u^3 - u$$

$$\partial_n u = 0 \;\; \text{on } \Gamma_N, \quad \partial_n u = q \;\; \text{on } \Gamma_C \;\; \text{(control)}$$

$$J(u,q) = \tfrac{1}{2}\|u - c_0\|^2_{\Gamma_O} + \tfrac{\alpha}{2}\|q\|^2_{\Gamma_C} \qquad (c_0 \equiv 1,\; \alpha = 1)$$

state space $V = H^1(\Omega)$, control space $Q = L^2(\Gamma_C)$





Configuration 1 (left) and Configuration 2 (right)

Necessary optimality conditions (KKT system):

$$
\begin{aligned}
(u - c_0, \psi)_{\Gamma_O} + (\nabla\psi, \nabla z)_\Omega + (\psi, z)_\Omega &= 0 \quad \forall \psi \in V \\
\alpha(q, \chi)_{\Gamma_C} - (z, \chi)_{\Gamma_C} &= 0 \quad \forall \chi \in Q \\
(\nabla u, \nabla\varphi)_\Omega + (u, \varphi)_\Omega - (f, \varphi)_\Omega - (q, \varphi)_{\Gamma_C} &= 0 \quad \forall \varphi \in V
\end{aligned}
$$

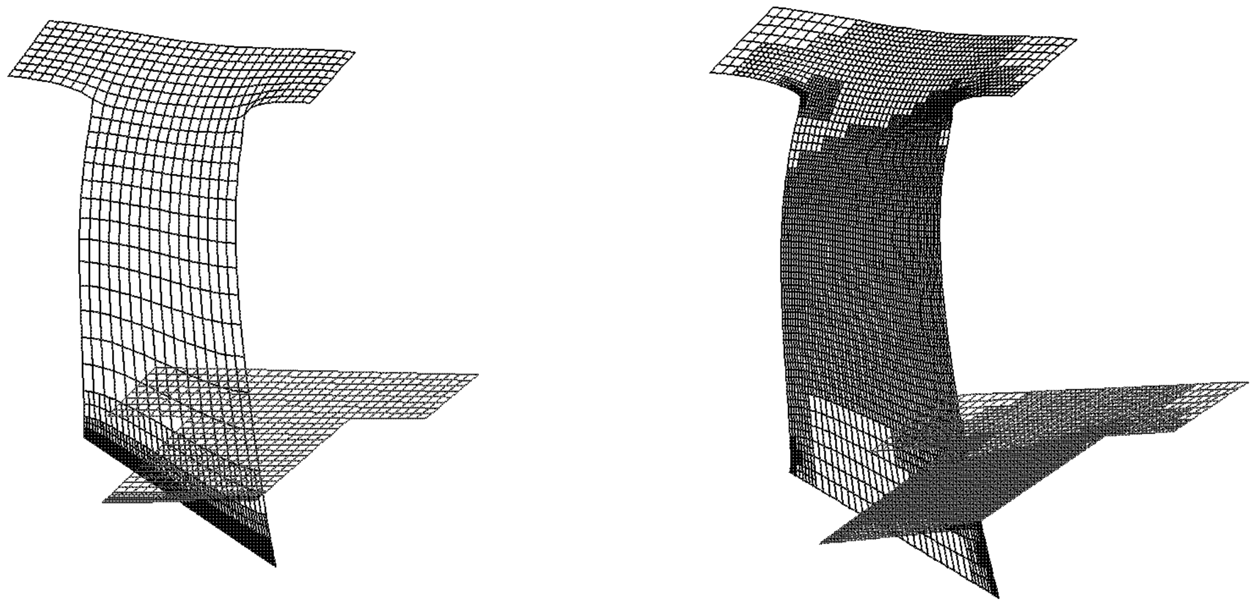
Galerkin approximation in $V_h = Q_1$ elements, $Q_h := \partial_n V_{h|\Gamma_C}$

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

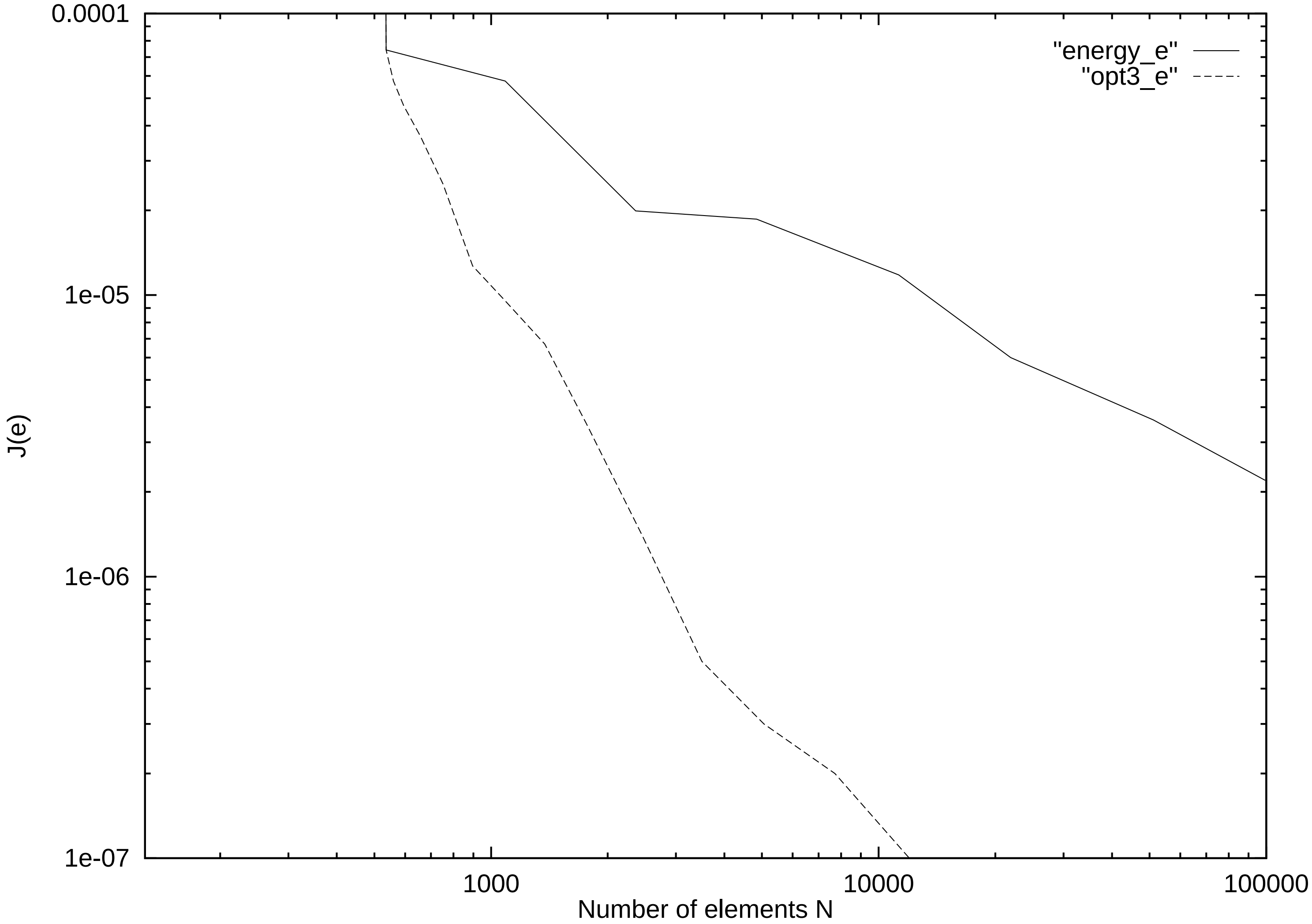
Test case 1:

N	596	1616	5084	8648	15512
E_h	2.56e-04	2.38e-04	8.22e-05	4.21e-05	3.99e-05
I_{eff}	0.34	0.81	0.46	0.29	0.43

Efficiency of the weighted error estimator for Configuration 1



Optimal state and adapted mesh for Configuration 1 obtained by the weighted error estimator (left) and the "energy norm" estimator (right)

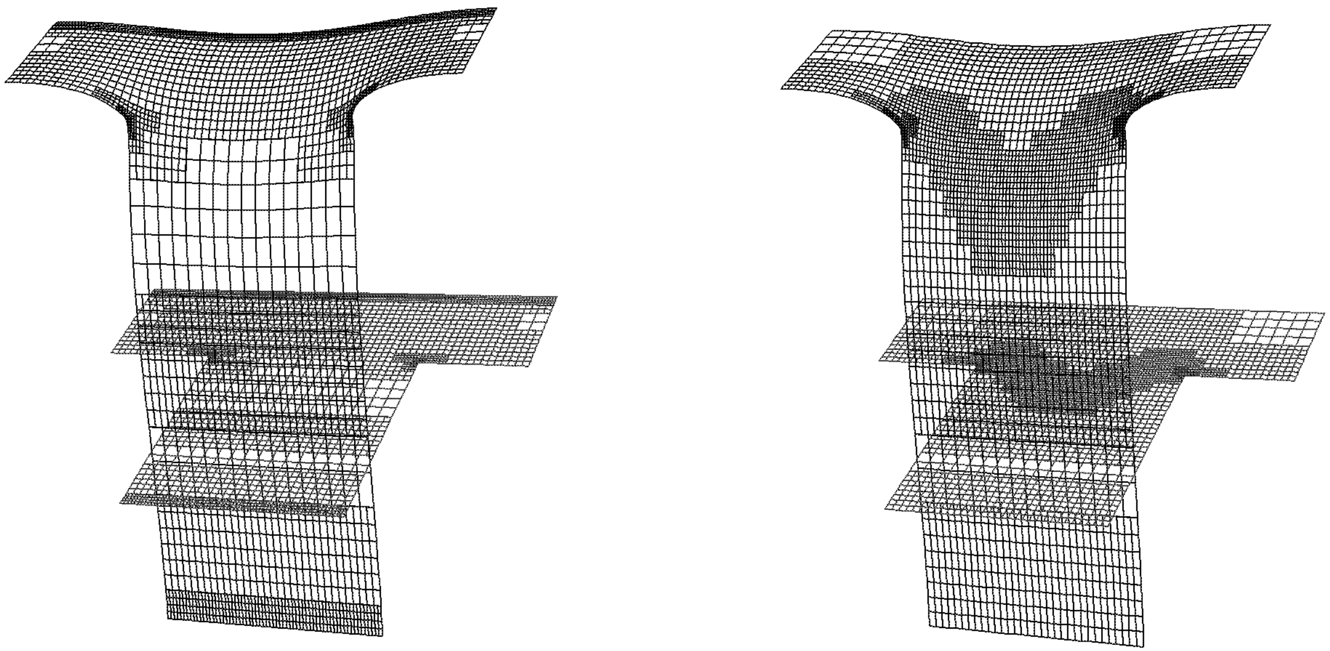


Efficiency of the meshes generated by the weighted error estimator ($\square$) and the energy-error estimator ($\times$) in $\log/\log$ *scale*

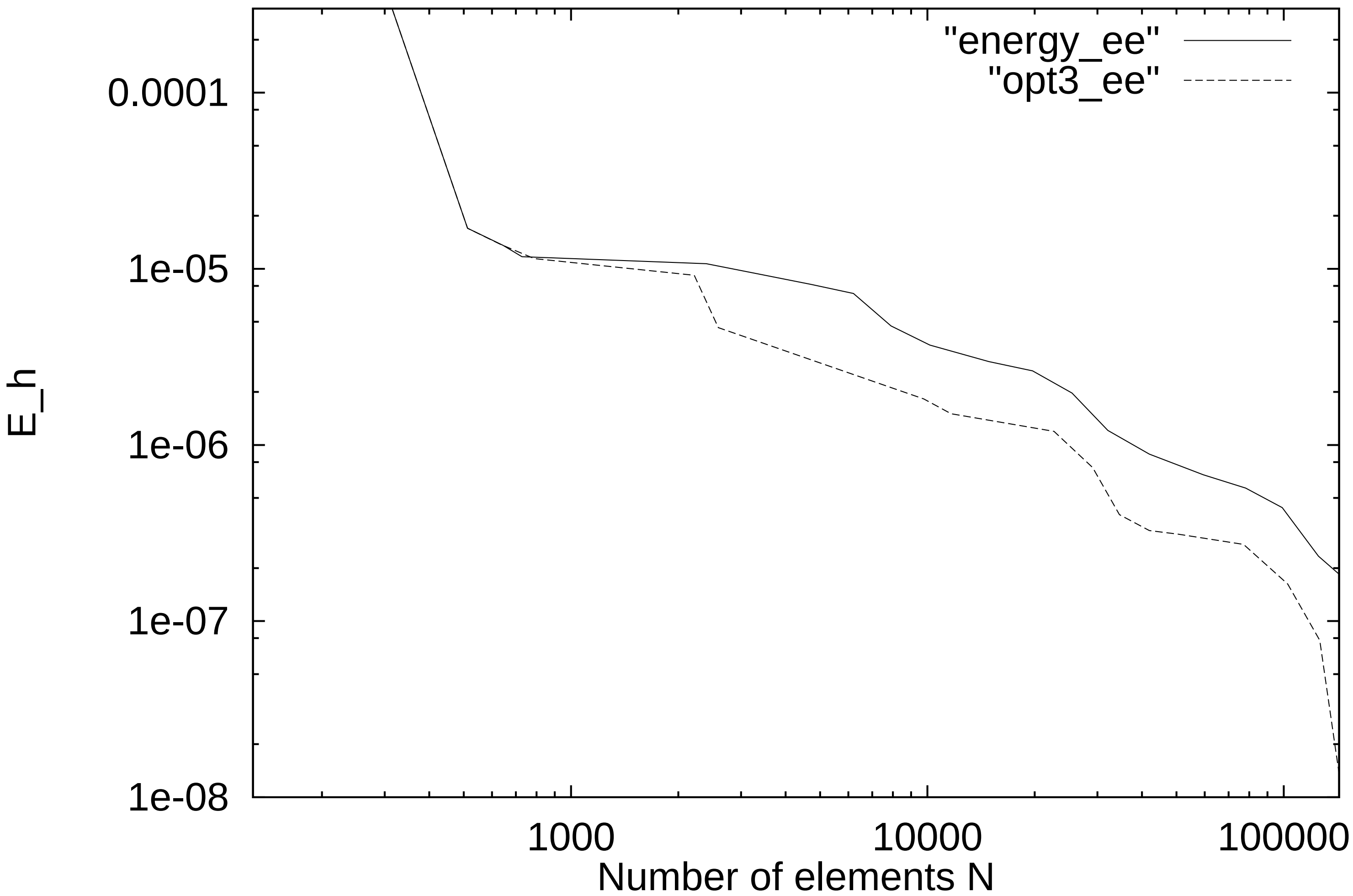
Test case 2:

N	512	15368	27800	57632	197408
E_h	9.29e-05	8.14e-07	4.86e-07	2.31e-07	4.58e-08
I_{eff}	1.32	0.56	0.35	0.42	0.32

Efficiency of the weighted error estimator for Configuration 2



Optimal state and adapted mesh for Configuration 2 obtained by the weighted error estimator (left) and the "energy norm" estimator (right)



Efficiency of the meshes generated by the weighted error estimator ($\square$) *and the energy-error estimator* ($\times$) *in* $\log / \log$ *scale*

6.11

Special case parameter estimation: Model problem

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

Determine the coefficient q by comparison with given data

$$J(u,q) := \tfrac{1}{2}\|u^q - \bar{u}\|^2 + \tfrac{1}{2}\epsilon\|q\|^2 \to \min \qquad (0 \le \epsilon \ll 1)$$

Reformulating the problem within the Euler-Lagrange approach, we seek a stationary point $\{u,q,z\}$ of the Lagrangian functional,

$$L(u,q,z) := J(u,q) + (f,z) - (\nabla u, \nabla z) - (qu, z),$$

determined by

$$\begin{aligned}
L'_u(u,q,z)(\varphi) &= (u - \bar{u}, \varphi) - (\nabla\varphi, \nabla z) - (q\varphi, z) = 0 \quad \forall\varphi, \\
L'_q(u,q,z)(\chi) &= (\chi q, z) = 0 \quad \forall\chi, \\
L'_z(u,q,z)(\psi) &= (f,\psi) - (\nabla u, \nabla\psi) - (qu, \psi) = 0 \quad \forall\psi
\end{aligned}$$

Discretization of this saddle-point problem by the usual Galerkin finite element method yields approximations $\{u_h, q_h, z_h\}$. For these the general a posteriori error analysis yields the error identity

$$J(u,q) - J(u_h,q_h) = \tfrac{1}{2}\underbrace{\rho^*(z_h)(u-\varphi_h)}_{\text{dual residual}} + \tfrac{1}{2}\underbrace{\rho^q(q_h)(q-\chi_h)}_{\text{control residual}} + \tfrac{1}{2}\underbrace{\rho(u_h)(z-\psi_h)}_{\text{primal residual}} + R_h^{(3)}.$$

The error identity based on the artificial "cost functional" $J(u,q)$ may be useless for steering the mesh adaptation. For an identifiable parameter $q \geq 0$ the adjoint variable z vanishes:

$$-\Delta z + qz = \bar{u} - u = 0 \quad \Rightarrow \quad z \equiv 0$$

Remedy.

- A posteriori error estimate for $\epsilon\|q-q_h\|$ based on a coercivity estimate for the saddle-point problem.
- A posteriori error estimate for $\|q-q_h\|$ using an extra "outer" duality argument.

A posteriori error estimate:

$$\|q - q_h\| \approx \eta := \dots$$

Realization and numerical examples by R. Becker, M. Braack, and B. Vexler 2001ff)

Example 1: Fitting of reaction parameters

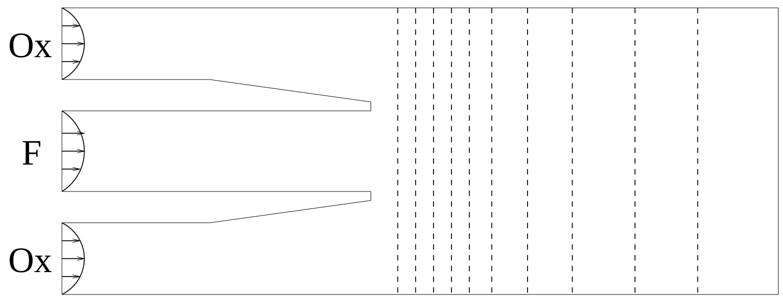
Reaction-diffusion problem

$$\beta \cdot \nabla u - \mu \Delta u + f(u) = 0 \quad \text{in} \;\; \Omega$$

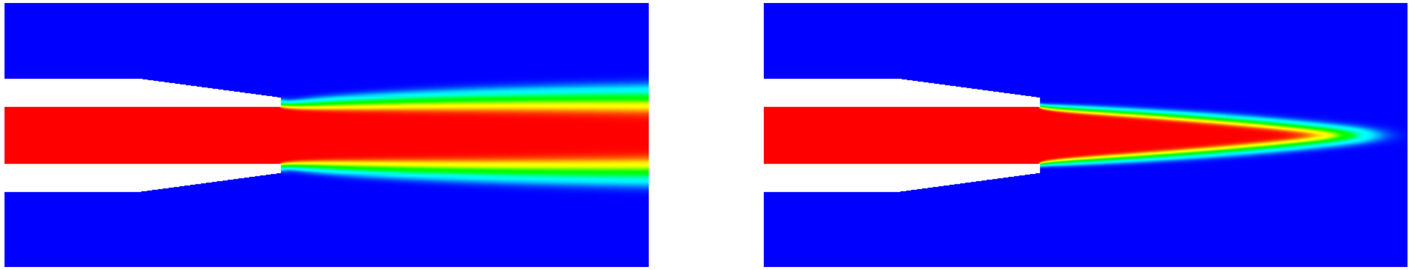
$$u = \hat{u} \quad \text{on} \;\; \Gamma_{in}, \qquad \partial_n u = 0 \quad \text{on} \;\; \partial\Omega \setminus \Gamma_{in}$$

Arrhenius-type reaction law

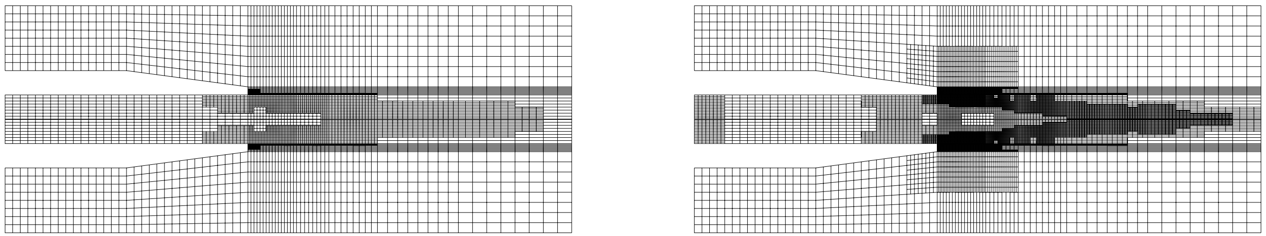
$$f(u) = A \exp\Big(- \frac{E}{1-y} \Big) y(c-y)$$



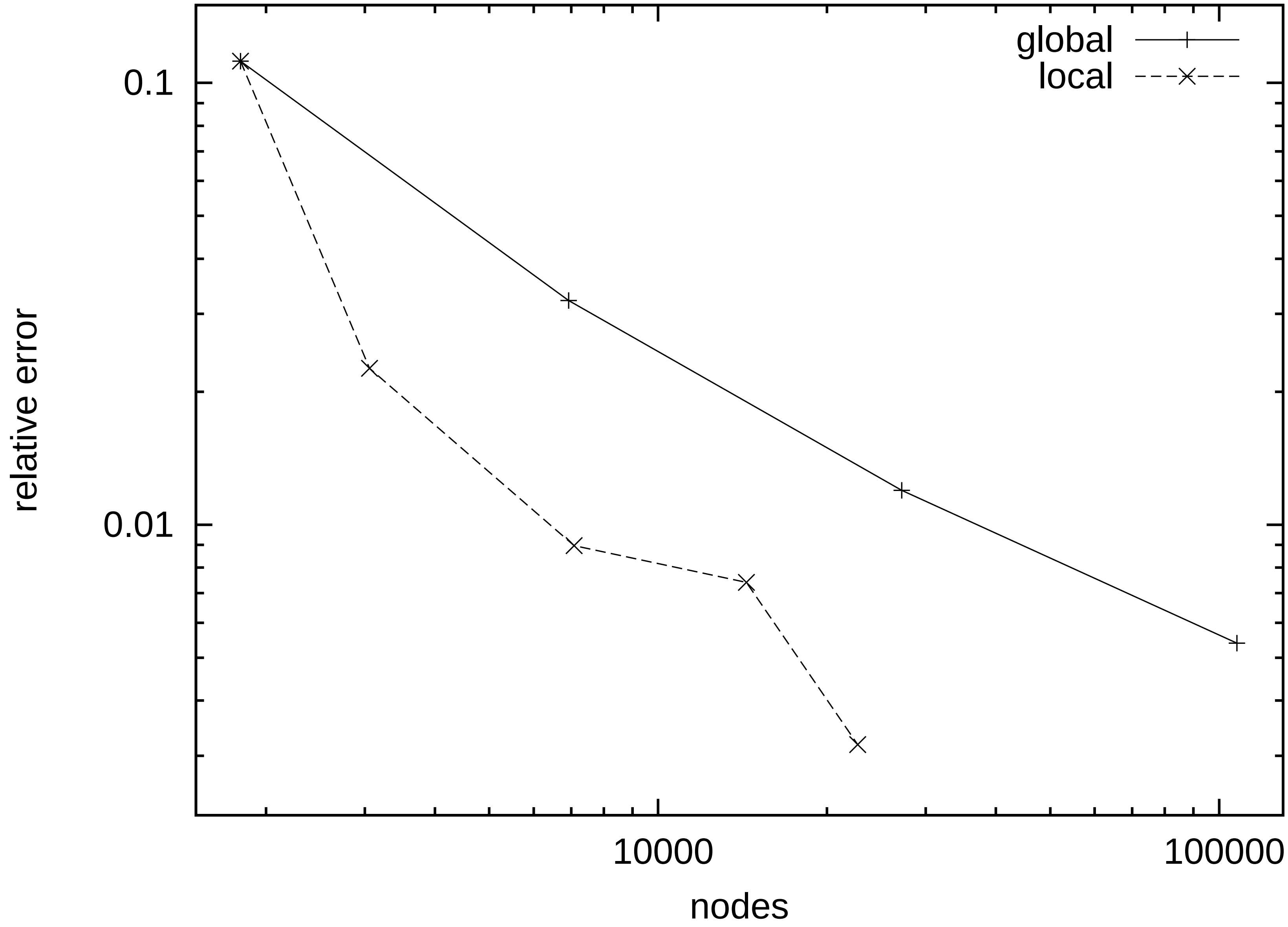
Measurements:
vertical line-integrals
of concentration



Left: initial solution $(A = 54.6,\ E = 0.15)$*, right: estimated solution* $(A = 992.3,\ E = 0.07)$



Locally refined meshes



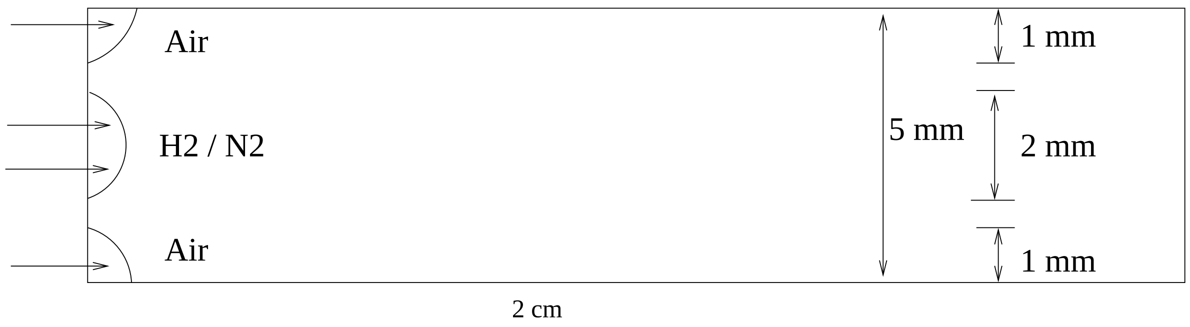
Quality of generated meshes

6.17

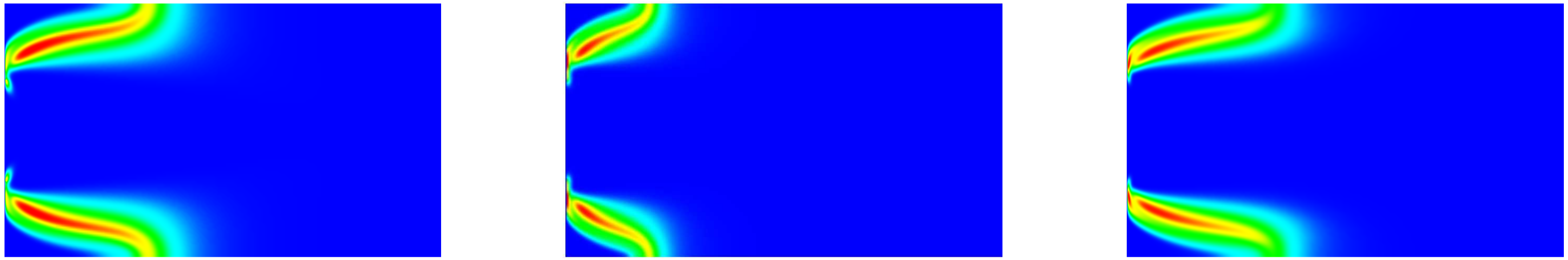
Example 2: Fitting of diffusion parameters

Reactive flow problem

$$
\begin{aligned}
\operatorname{div}(\rho v) &= 0 \\
(\rho v \cdot \nabla) v + \operatorname{div} \pi + \nabla p &= 0 \\
\rho v \cdot \nabla T - \frac{1}{c_p} \operatorname{div} \mathcal{Q} &= - \sum_{i \in \mathcal{S}} h_i f_i \\
\rho v \cdot \nabla y_k + \operatorname{div} \mathcal{F}_k &= f_k \quad k \in \mathcal{S},\ \#S = 9 \\
\mathcal{F}_k &= q_k D_k^* \nabla y_k \\
D_k^* &= (1 - y_k) \Big(\sum_{l \neq k} \frac{x_l}{D_{kl}^{bin}} \Big)^{-1}
\end{aligned}
$$

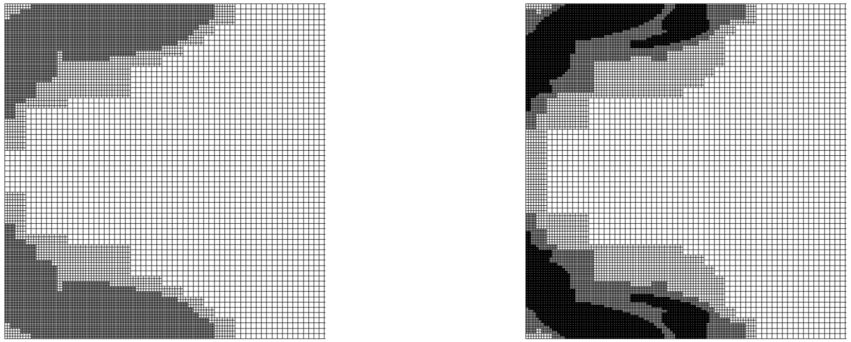


Measurements: point-values of concentrations



Left: Multicomponent diffusion (reference solution),

middle: Fick's law (initial parameters), right: Fitted Fick's law (estimated parameters)



Example 3: Fitting of outflow boundary condition

Navier-Stokes equations (bypass simulation)

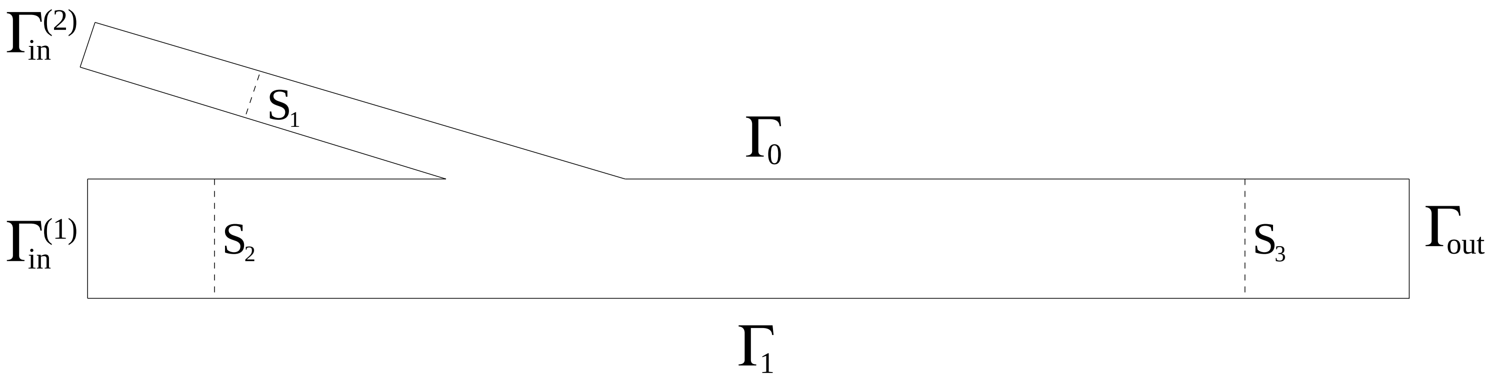
$$-\nu\Delta v + v\cdot\nabla v + \nabla p = 0, \quad \nabla\cdot v = 0 \quad \text{in} \;\; \Omega$$

$$v = \hat{u} \;\; \text{on} \;\; \Gamma_{\mathrm{in}}, \quad \partial_n u = 0 \;\; \mathrm{on} \;\; \partial\Omega\setminus\Gamma_{in}, \quad v = 0 \;\; \text{on} \;\; \Gamma_0$$

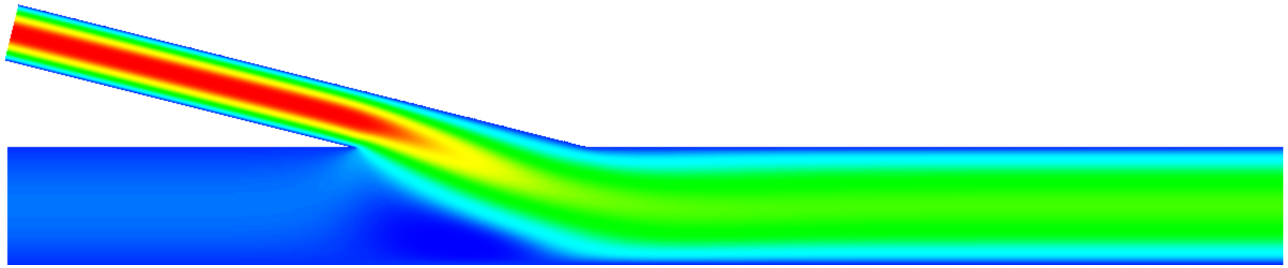
$$\nu\partial_n v - p\cdot n = q_1\cdot n \mathrm{on} \Gamma_{\mathrm{in}}^{(1)}$$

$$\nu\partial_n v - p\cdot n = q_2\cdot n \mathrm{on} \Gamma_{\mathrm{in}}^{(2)}$$

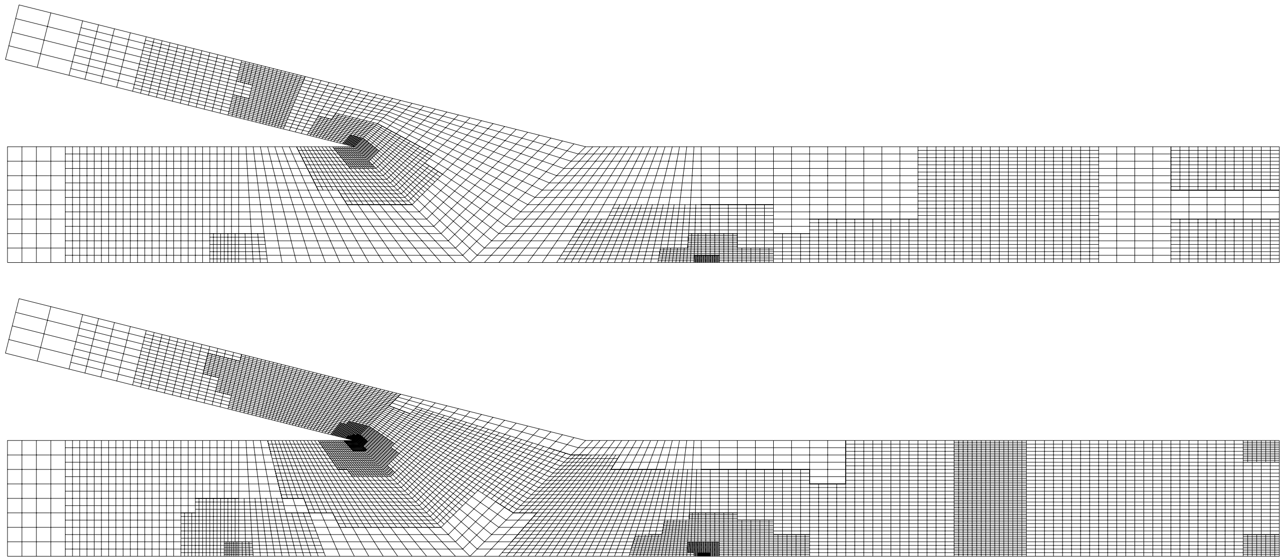
$$\nu\partial_n v - p\cdot n = 0 \mathrm{on} \Gamma_{out}$$



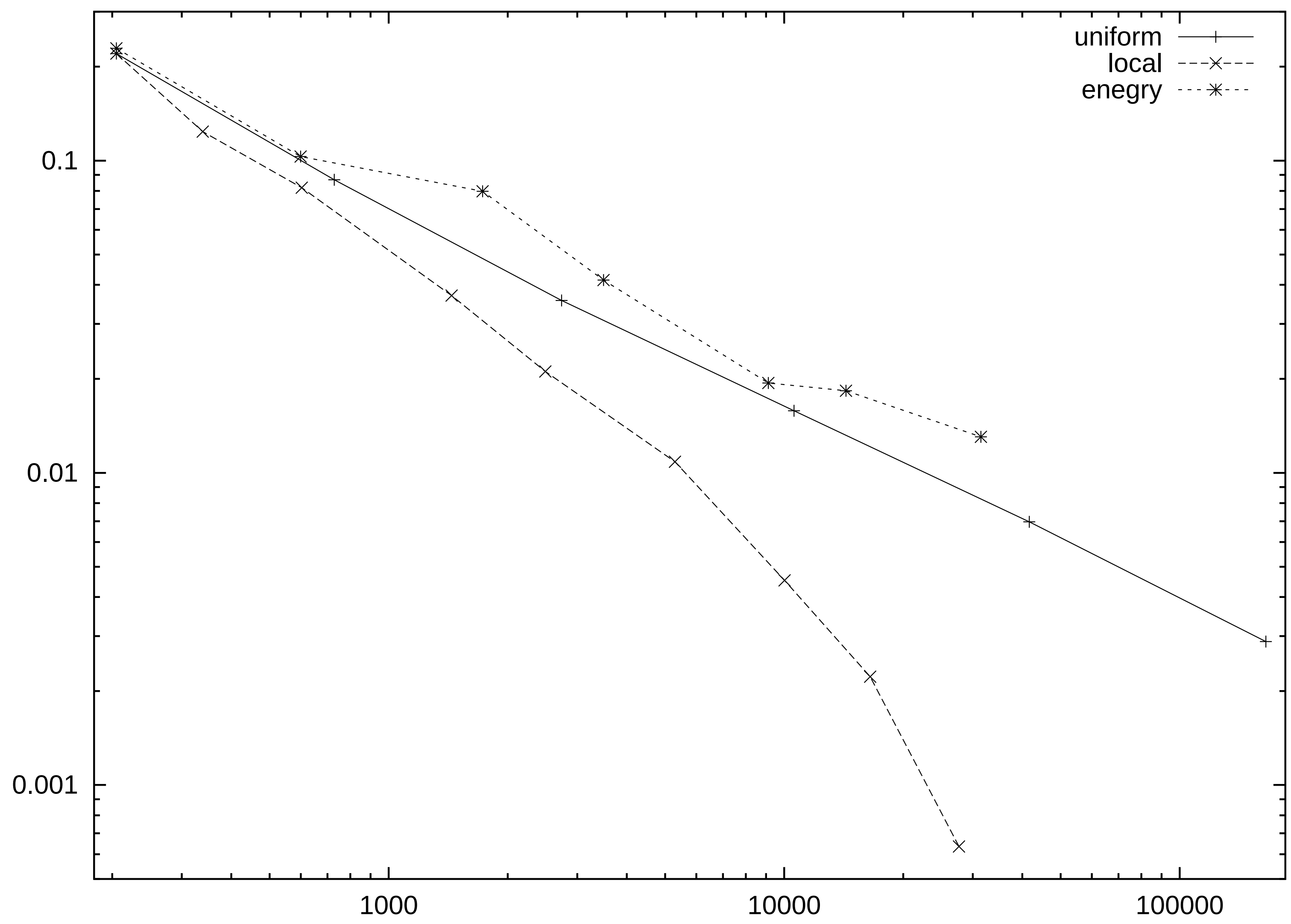
Measurements: point-values of pressure



Estimated solution



Locally refined meshes



Quality of generated meshes

6.24

7. Time-dependent problems

(I) A parabolic model problem: Heat equation

Heat-conduction problem

$$\partial_t u - \Delta u = f \quad \text{in } \ Q_T := \Omega \times I,$$

$$u_{|t=0} = u^0 \quad \text{in } \Omega, \qquad u_{|\partial\Omega} = 0 \ \text{ on } I,$$

where $\Omega \subset \mathbb{R}^2$ and $I = [0, T]$. This model is used to describe diffusive transport of energy or certain species concentrations. For its discretization, we consider the first-order dG(0) method in time ($\approx$ backward Euler scheme) combined with a conforming FE method with bilinear elements in space.

We split the time interval $[0, T]$ into subintervals $I_n = (t_{n-1}, t_n]$,

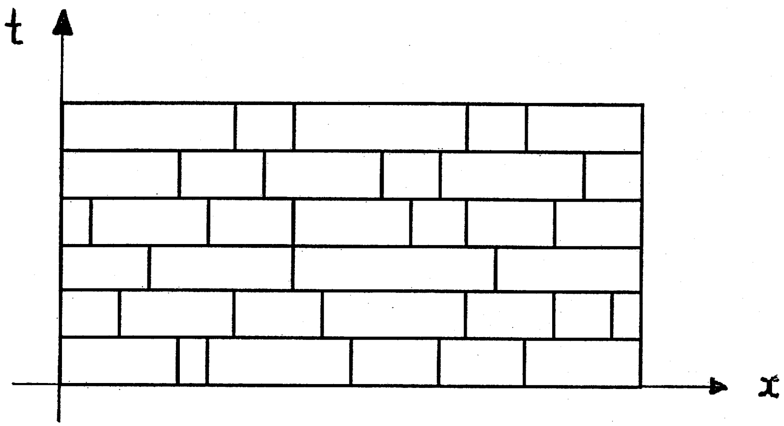
$$0 = t_0 < ... < t_n < ... < t_N = T, \qquad k_n := t_n - t_{n-1}.$$

At each time level t_n, let $V_h^n \subset V$ be appropriate finite dimensional subspaces. Then, we use

$$V_h^k := \{v : I \to V,\ v_{|I_n} \in V_h^n \times P_0(I_n)\} \ \subset\ V \quad \text{(trialspace)}$$
$$W_h^k := \{w : I \to V,\ w_{|I_n} \in V_h^n \times P_0(I_n)\} \ \subset\ W \quad \text{(testspace)}.$$

For functions in these spaces and their continuous analogues, we set

$$v^{n+} = \lim_{t \to t_n + 0} v(t), \quad v^{n-} = \lim_{t \to t_n - 0} v(t), \quad [v]^n = v^{n+} - v^{n-}.$$



Sketch of a space-time mesh with hanging nodes

Any sufficiently smooth solution u of the (general semilinear) "continuous" problem satisfies the variational relation (initial conditions imposed in variational form)

$$A(u)(\varphi) = (u^0, \varphi^{0+}) \quad \forall \varphi \in W_h^k,$$

$$A(u)(\varphi) := \sum_{n=1}^{N} \int_{I_n} \left\{ (\partial_t u, \varphi) + a(u)(\varphi) - (f, \varphi) \right\} dt$$
$$+ \sum_{n=2}^{N} ([u]^{n-1}, \varphi^{n-1+}) + (u^{0+}, \varphi^{0+}).$$

The "space-time" Galerkin method seeks $U \in V_h^k$, satisfying

$$A(U)(\varphi) = (u^0, \varphi^{0+}) \quad \forall \varphi \in W_h^k.$$

By construction, the error $e := u - U$ satisfies Galerkin orthogonality,

$$A(u)(\varphi) - A(U)(\varphi) = 0, \quad \varphi \in W_h^k.$$

Due to the time-discontinuity of the test functions, the dG(0) scheme reduces to a sequence of time steps,

$$\int_{I_n} \{a(U)(\varphi_h) - (f, \varphi_h)\}\, dt + (U^{n+} - U^{n-}, \varphi_h) = 0 \quad \forall \varphi_h \in V_h^n$$

or, setting $U^n := U^{n-} \in V_h^n$ (backward Euler scheme),

$$(U^n, \varphi_h) + k_n a(U^n)(\varphi_h) = (U^{n-1}, \varphi_h) + \int_{I_n} (f, \varphi_h)\, dt \quad \forall \varphi_h \in V_h^n$$

Remark. We note that in a similar way one defines the so-called $cG(1)$ method ("continuous" Galerkin method) in time, which is closely related to the second-order Crank-Nicolson scheme.

Suppose that the error is to be estimated in terms of some functional $J(\cdot)$ (for simplicity assumed to be linear). Let z be the solution of the corresponding linearized dual problem

$$A'(U)(\psi, z) = J'(U)(\psi) \quad \forall \psi \in V.$$

Then, by the general theory, we have the following error identity:

$$J(u) - J(U) = (u^0, (z-\varphi)^{0+}) - A(U)(z-\varphi) + R_h^{(2)}, \quad \varphi \in V_h^k,$$

$$R_h^{(2)} = \int_0^1 \big\{A''(U+se)(e,e,z) - J'(U+se)(e,z)\big\} s\, ds.$$

From this abstract result, we can derive concrete error estimates.

We shall consider only the linear model problem (heat equation) for which the remainder term is zero and the residual simplifies a bit.

We consider control of the error with respect two functionals.

- Space-time L^2 error: $\|e\|_{Q_T}$

$$J(\varphi) := \|e\|_{Q_T}^{-1} \int_I (\varphi, e)\, dt$$

  with the associated dual problem

$$-\partial_t z - \Delta z = \|e\|_{Q_T}^{-1} e \quad \text{in } \Omega \times I,$$
$$z_{|t=T} = 0 \ \text{ in } \Omega, \quad z_{|\partial\Omega} = 0 \ \text{ on } I,$$

  or in variational form

$$A(\varphi, z) = \|e\|_{Q_T}^{-1} (\varphi, e)_{Q_T} \qquad \forall \varphi \in W.$$

- Spatial L^2 error at the end time $T = t_N$: $\|e^{N-}\|_\Omega$

$$J(\varphi) := \|e^{N-}\|_\Omega^{-1} (e^{N-}, \varphi^{N-})_\Omega,$$

with the associated dual problem

$$-\partial_t z - \Delta z = 0 \quad \text{in } \Omega \times I,$$
$$z_{|t=T} = \|e^{N-}\|_\Omega^{-1} e^{N-} \ \text{ in } \Omega, \quad z_{|\partial\Omega} = 0 \ \text{ on } I,$$

or in variational form

$$A(\varphi, z) = \|e^{N-}\|_\Omega^{-1} (\varphi^{N-}, e^{N-})_\Omega \qquad \forall \varphi \in W.$$

Then, the general approach yields the error representation

$$J(e) = \sum_{n=1}^{N} \sum_{K \in \mathbb{T}_h^n} \Big\{ (R(U), z - I_h^k z)_{K \times I_n} + (r(U), z - I_h^k z)_{\partial K \times I_n}$$
$$- ([U]^{n-1}, (z - I_h^k z)^{(n-1)+})_K \Big\}, \quad I_h^k z \in V_h^k.$$

with the local residuals

$$R(U)_{|K} := f + \Delta U - \partial_t U,$$

$$r(U)_{|\Gamma} := \begin{cases} -\frac{1}{2}[\partial_n U], & \text{if } \Gamma \subset \partial T \backslash \partial\Omega, \\ 0, & \text{if } \Gamma \subset \partial\Omega. \end{cases}$$

In order to separate the time and spatial errors, we introduce the time-averages

$$\bar{f}(x) := k_n^{-1} \int_{I_n} f(x,t)\, dt, \qquad \bar{z}(x) := k_n^{-1} \int_{I_n} z(x,t)\, dt.$$

Since the averaged equation residual $\overline{R(U)} = \bar{f} + \Delta U - \partial_t U$ as well as the jump-residual $r(U)$ are constant in time, the a posteriori error identity can be rewritten in the form

$$
\begin{aligned}
|J(e)| = \Big| \sum_{n=1}^{N} \sum_{K \in \mathbb{T}_h^n} \Big\{ & \underbrace{(f - \bar{f}, z - I_h^k z)_{K \times I_n}}_{\text{time error}} + \underbrace{(\overline{R(U)}, \bar{z} - I_h^k z)_{K \times I_n}}_{\text{spatial error}} \\
& + \underbrace{(r(U), \bar{z} - I_h^k z)_{\partial K \times I_n}}_{\text{spatial error}} - \underbrace{([U]^{n-1}, (z - I_h^k z)^{(n-1)+})_K}_{\text{time error}} \Big\} \Big| \\
\le \eta := \sum_{n=1}^{N} \eta_k^n + \sum_{n=1}^{N} \sum_{K \in \mathbb{T}_h^n} \eta_{h,K}^n
\end{aligned}
$$

Remark. The use of this a posteriori error estimate requires the evaluation of the various weighting terms $\omega_K^{n,i}$. In principle, this is done analogously as in the stationary case by local post-processing the discrete approximation $Z \in V_h^k$ to the dual solution z.

Numerical test (R. Hartmann 1998)

The results of space and time step adaptation for the dG(0) method is illustrated by a test with a (given) exact solution representing a smooth rotating bump on the unit square.

Adaptation strategy $N := \#$ time steps, $N_n := \#$ cells of $\mathbb{T}_h^n$

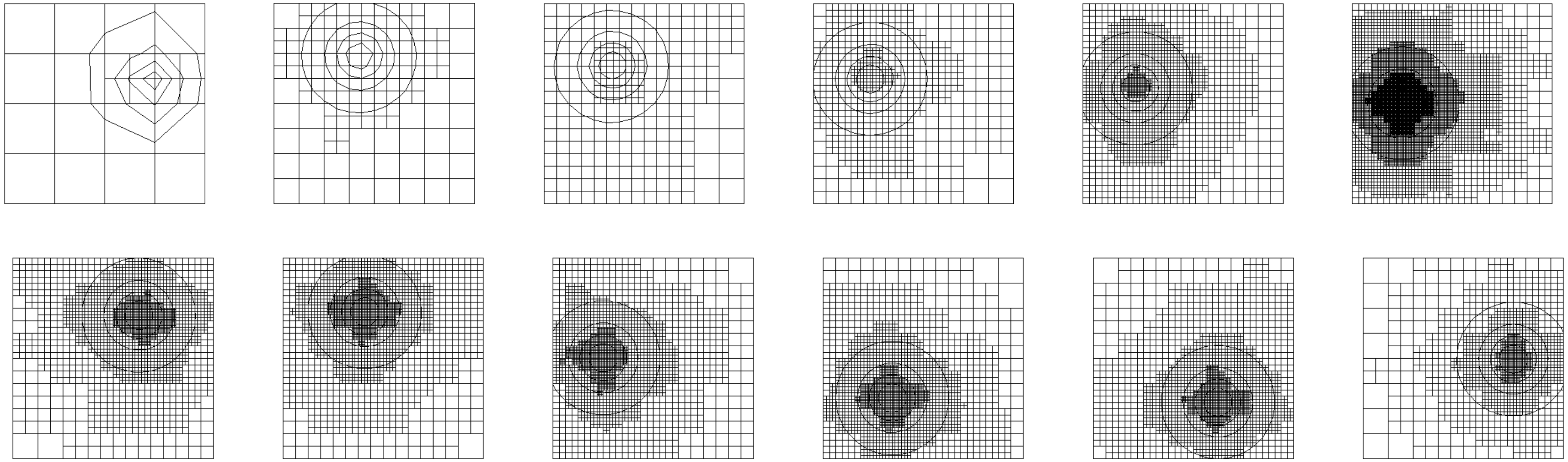
- Time adaptation: time step k_n uniform on mesh T_h^n

$$\alpha \frac{\mathrm{TOL}}{2N} \le \eta_k^n \le \frac{\mathrm{TOL}}{2N} \qquad (\alpha \approx \tfrac{1}{4}).$$

- Space adaptation:

$$\beta \frac{k_n}{T} \frac{\mathrm{TOL}}{2N_n} \le \eta_{h,K}^n \le \frac{k_n}{T} \frac{\mathrm{TOL}}{2N_n} \qquad (\beta \approx \tfrac{1}{4}).$$

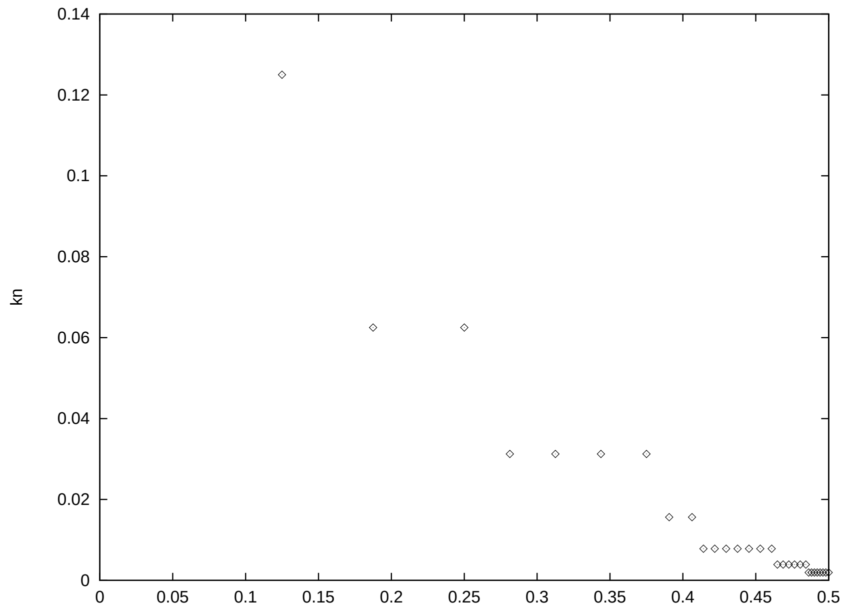
$$
\begin{aligned}
|J(e)| = \eta := \sum_{n=1}^{N} \eta_k^n + \sum_{n=1}^{N} \sum_{K \in \mathbb{T}_h^n} \eta_{h,K}^n \\
\leq \sum_{n=1}^{N} \frac{TOL}{2N} + \sum_{n=1}^{N} \sum_{K \in \mathbb{T}_h^n} \frac{k_n}{T} \frac{\mathrm{TOL}}{2N_n} \\
\leq \frac{TOL}{2} \sum_{n=1}^{N} \frac{1}{N} + \frac{TOL}{2} \sum_{n=1}^{N} \frac{k_n}{T} \sum_{K \in \mathbb{T}_h^n} \frac{1}{N_n} \\
\leq TOL
\end{aligned}
$$

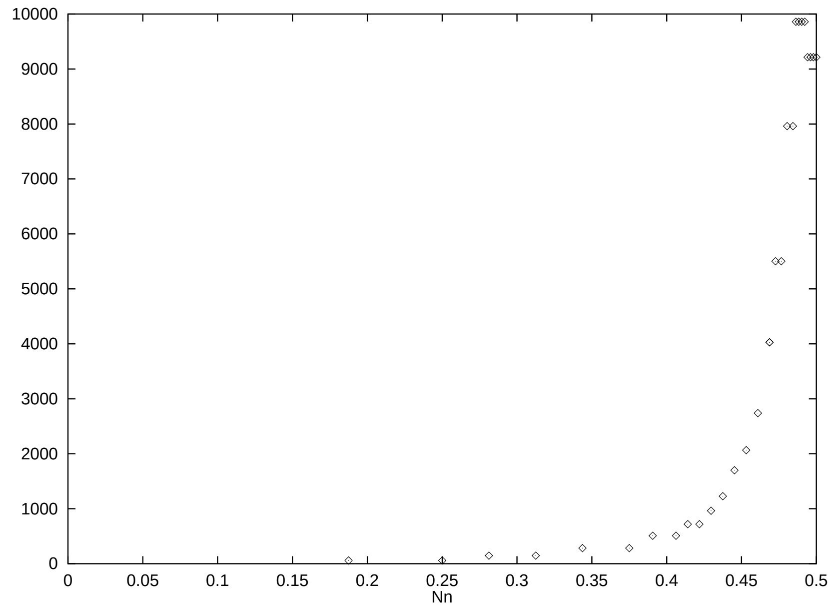


Refined meshes for the end-time L^2-error at times $t_n = 0.125, \ldots, 0.5$, and the global L^2-error at times $t_n = 0.16, \ldots, 1$

N	N_{max}	$J(e)$	$\eta_\omega(u_h)$	I_{eff}
46	760	2.91e-3	6.60e-3	2.27
81	3472	7.92e-4	1.08e-3	1.36
119	9919	3.99e-4	6.64e-4	1.67

Simultaneous adaptation of spatial and time mesh size ($N = \#$ time-steps, $N_{max} = max \, \#$ mesh-cells).





Development of the time-step size (left) and the number N_n of mesh cells (right) over the time interval $I = [0, 0.5]$.

(II) A hyperbolic model problem: Acoustic wave equation

We consider the acoustic wave equation

$$\begin{aligned} \partial_t^2 w - \nabla\cdot\{a\nabla w\} &= 0 \qquad \text{in } \; Q_T := \Omega\times I, \\ w_{|t=0} = w^0, \quad \partial_t w_{|t=0} &= v^0 \qquad \text{on } \; \Omega, \\ n\cdot a\nabla w_{|\partial\Omega} &= 0 \qquad \text{on } \; I, \end{aligned}$$

where $\Omega\subset\mathbb{R}^d$, $d\geq 1$, and $I=(0,T)$; the elastic coefficient a may vary in space. This equation occurs in the simulation of acoustic waves in gaseous or fluid media. We consider approximation by a "velocity-displacement" formulation which is obtained by introducing a new velocity variable $v:=\partial_t w$. Then, the pair $u=\{w,v\}$ satisfies the system

$$\partial_t w - v = 0,$$
$$\partial_t v - \nabla\cdot\{a\nabla w\} = 0,$$

with the natural solution space

$$V := [H^1(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega))] \times H^1(0,T;L^2(\Omega)).$$

This system is discretized by a cG(1) method in space and time corresponding to the splitting

$$0 = t_0 < \ldots < t_n < \ldots < t_N = T, \qquad k_n := t_n - t_{n-1}.$$

On the corresponding function spaces, we introduce the bilinear form

$$\begin{aligned} A(u,\varphi) \;:=\; & (\partial_t w, \xi)_{Q_T} - (v,\xi)_{Q_T} + (w(0),\xi(0)) \\ & + (\partial_t v, \psi)_{Q_T} + (a\nabla w, \nabla\psi)_{Q_T} + (v(0),\psi(0)). \end{aligned}$$

The Galerkin approximation seeks $u_h = \{w_h, v_h\} \in V_{h,k}$ satisfying

$$A(u_h, \varphi_h) = (w^0, \xi(0)) + (v^0, \psi(0)) \quad \forall \varphi_h = \{\psi_h, \xi_h\} \in W_{h,k}.$$

This "cG(1)" ($continuous$ Galerkin) method is a "Petrov-Galerkin" method. Since the solution $u = \{w, v\}$ also satisfies the Galerkin equation, we again have Galerkin orthogonality for $e := \{e^w, e^v\}$:

$$A(e, \varphi_h) = (w^0, \xi(0)) + (v^0, \psi(0)), \quad \varphi_h \in V_{h,k}.$$

This scheme is closely related to the standard Crank-Nicolson scheme in time (combined with a spatial finite element method):

$$\begin{aligned} (w^n - w^{n-1}, \varphi) - \tfrac{1}{2} k_n (v^n + v^{n-1}, \varphi) &= 0, \\ (v^n - v^{n-1}, \psi) + \tfrac{1}{2} k_n (a \nabla (w^n + w^{n-1}), \nabla \psi) &= 0. \end{aligned}$$

This system splits into two equations, a discrete Helmholtz equation and a discrete L^2-projection.

We want to control the error in terms of a functional of the form

$$J(e) := (j, e^w)_{Q_T},$$

with some density function $j(x,t)$. To this end, we again use a duality argument in space-time employing the time-reversed wave equation

$$\begin{aligned} \partial_t^2 z^w - \nabla\cdot\{a\nabla z^w\} &= j \quad \text{in } \; Q_T, \\ {z^w}_{|t=T} = 0, \quad -\partial_t {z^w}_{|t=T} &= 0 \quad \text{on } \; \Omega, \\ n\cdot a\nabla {z^w}_{|\partial\Omega} &= 0 \quad \text{on } \; I. \end{aligned}$$

Its strong solution $z = \{-\partial_t z^w, z^w\} \in \hat{W}$ satisfies the variational equation

$$A(\varphi, z) = J(\varphi) \quad \forall \varphi \in \hat{V}.$$

Then, by the general approach, we obtain the a posteriori error estimate

$$|(j, w)_{Q_T}| \le \sum_{n=1}^{N} \sum_{K \in \mathbb{T}_h^n} \Big| (R^u(u_h), \partial_t z^w - \varphi_h^v)_{K \times I_n} \\ - (R^v(u_h), z^w - \varphi_h^w)_{K \times I_n} - (r(u_h), z^w - \varphi_h^w)_{(\partial K \setminus \partial\Omega) \times I_n} \Big|,$$

with the cell residuals

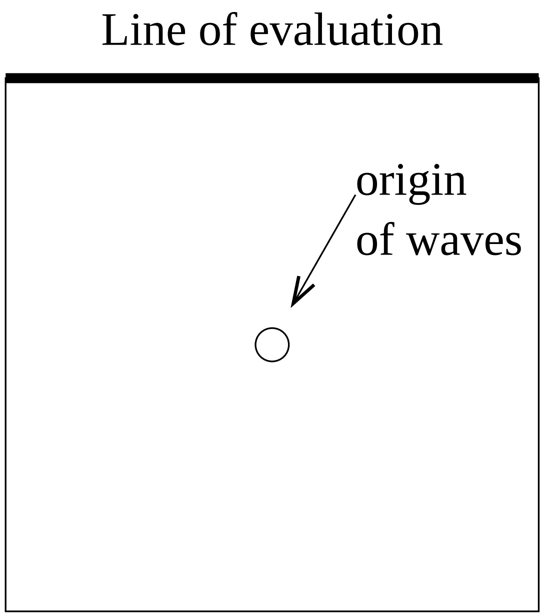
$$R^w(u_h)_{|K} := \partial_t w_h - v_h, \qquad R^v(u_h)_{|K} := \partial_t v_h - \nabla\cdot\{a \nabla w_h\}$$

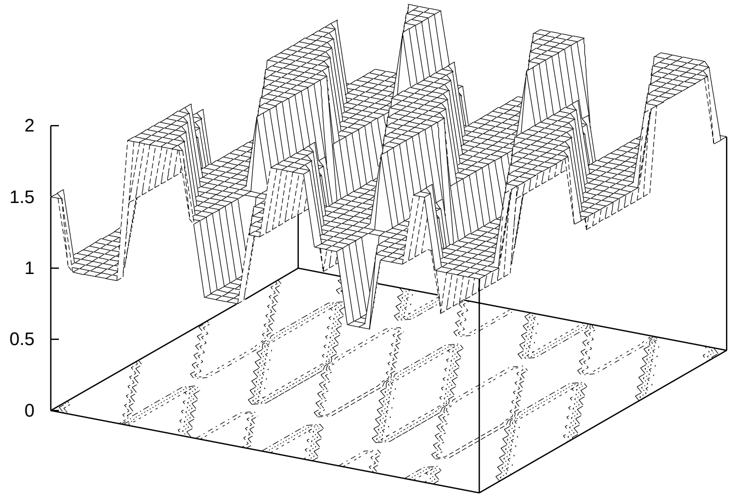
and the edge residuals

$$r(w_h)_{|\Gamma \times I_m} := \begin{cases} -\frac{1}{2} n\cdot[a\nabla w_h], & \text{if } \Gamma \subset \partial K \setminus \partial\Omega, \\ 0, & \text{if } \Gamma \subset \partial\Omega. \end{cases}$$

Numerical test (W. Bangerth 1999)

We consider the propagation of an outward travelling wave on $\Omega = (-1, 1)^2$ with a strongly heterogeneous coefficient.





Layout of the domain (left) and the coefficient $a(x)$ (right)

Boundary and initial conditions are chosen as follows:

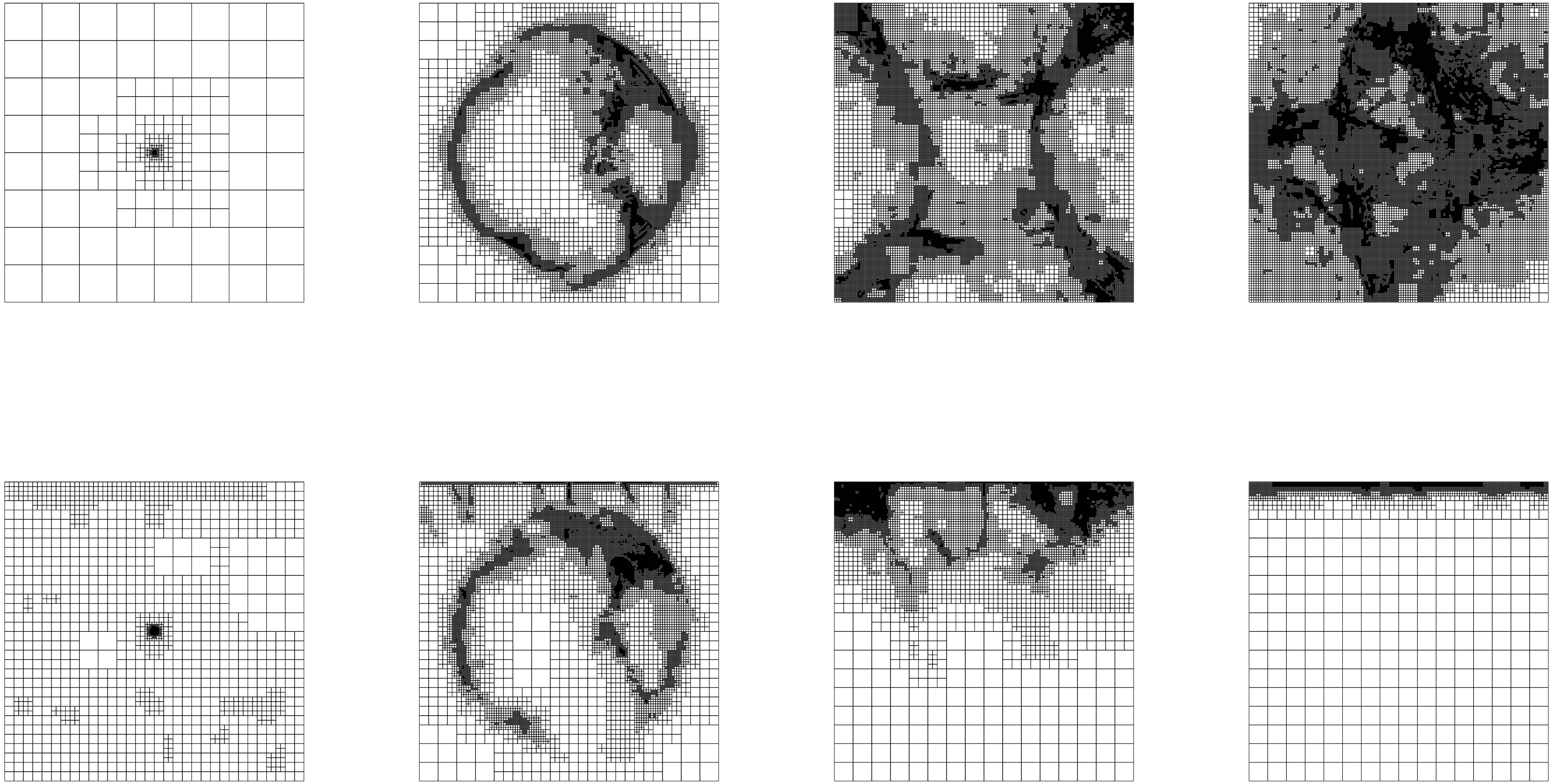
$$n \cdot \{a\nabla w\} = 0 \quad \text{on } \; y = 1, \qquad w = 0 \quad \text{on } \; \partial\Omega \backslash \{y = 1\},$$

$$w_0 = 0, \quad v_0 = \theta(s - r)\mathsf{exp}\left(-|x|^2/s^2\right)\left(1 - |x|^2/s^2\right),$$

with $s = 0.02$ and $\theta(\cdot)$ the jump function. If this example is taken as a model of propagation of seismic waves in a faulted region of rock, then the seismograms at the surface, the top line Γ of the domain, are to be recorded. A corresponding functional output is

$$J(w) = \int_0^T \int_\Gamma w(x,t)\; \omega(\xi,t)\, \mathrm{d}\xi\, \mathrm{dt},$$

with a weight $\omega(\xi,t) = \sin(3\pi\xi)\sin(5\pi t/T)$, and end-time $T = 2$.



Grids produced by the energy-error indicator (upper row)

and by the weighted estimator (lower row), at times $t = 0,\ \frac{2}{3},\ \frac{4}{3},\ 2$

7.22

8. Applications in structural mechanics

The Lamé-Navier equations of linear elasticity theory:

$$-\nabla \cdot \sigma = f, \quad \sigma = A\epsilon(u), \quad \epsilon(u) = \tfrac{1}{2}(\nabla u + \nabla u^T) \quad \text{in } \Omega$$

$$u = 0 \quad \text{on } \Gamma_D\,, \qquad n \cdot \sigma = g \quad \text{on } \Gamma_N$$

Describes the (small) deformation of an elastic body in a bounded (polyhedral) domain $\Omega \subset \mathbb{R}^d$ ($d{=}2$ or 3), which is fixed along a part Γ_D $(\mathrm{meas}(\Gamma_D) \neq 0)$ of its boundary $\partial\Omega$, loaded by a body force with density f and a surface traction g along $\Gamma_N = \partial\Omega \setminus \Gamma_D$.

Linear–elastic isotropic material law (Hooke's law),

$$\sigma = A\epsilon(u) = 2\mu\epsilon^D(u) + \kappa\nabla \cdot uI$$

with constants $\mu > 0$ and $\kappa > 0$, and ϵ^D the deviatoric part of ϵ.

Primal variational formulation:

$$a(u,\psi) := (A\epsilon(u),\epsilon(\psi)) = (f,\psi) + (g,\psi)_{\Gamma_N} \quad \forall\,\psi\in V$$

where $V = \{v \in H^1(\Omega)^d,\ v=0 \text{ on } \Gamma_D\}$.

Finite element discretization with linear/bilinear elements in subspaces $V_h\subset V$ on meshes matching the decomposition $\partial\Omega = \Gamma_u \cup \Gamma_\sigma$.

$$a(u_h,\psi_h) = (f,\psi_h) + (g,\psi_h)_{\Gamma_\sigma} \quad \forall\,\psi_h \in V_h$$

Galerkin orthogonality relation for error $e = u - u_h$:

$$a(e,\psi_h) = 0, \quad \psi_h \in V_h$$

A posteriori error analysis

For error functional $J(\cdot)$ solve dual problem:

$$a(\varphi, z) = J(\varphi) \quad \forall\, \varphi \in V$$

Taking $\varphi = e$ and using Galerkin orthogonality,

$$J(e) = a(e, z) = a(e, z - \psi_h), \quad \psi_h \in V_h$$

Splitting the global integration over Ω into the contributions of the mesh cells $T \in \mathbb{T}_h$ and integrating cell-wise by parts yields

$$J(e) = \sum_{K \in \mathbb{T}_h} \left\{ (-\nabla \cdot A\epsilon(e), z - \psi_h)_K + (n \cdot A\epsilon(e), z - \psi_h)_{\partial K} \right\}$$

Observing $-\nabla\cdot A\epsilon(u)=f$ and the continuity of $n\cdot A\epsilon(u)$ across interelement edges,

$$J(e)=\sum_{K\in\mathbb{T}_h}\Big\{(R(u_h),z-\psi_h)_K+(r(u_h),z-\psi_h)_{\partial K}\Big\}$$

with cell residuals $R(u_h)_{|K}:=f+\nabla\cdot A\epsilon(u_h)$ and the edge residuals:

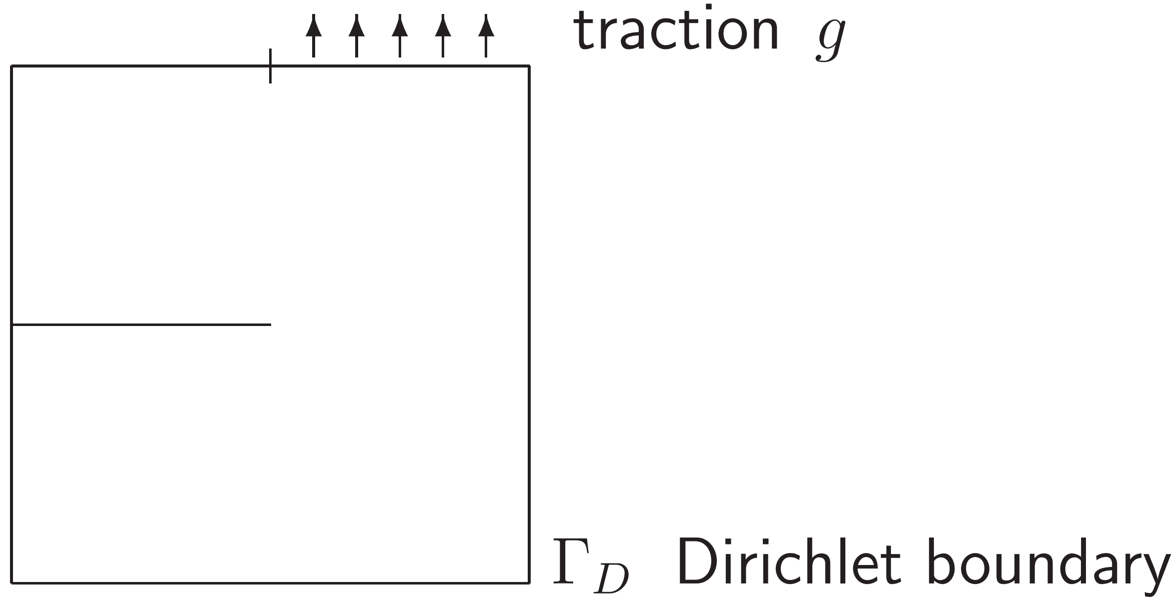
$$r(u_h)_{|\Gamma}:=\begin{cases}-\frac{1}{2}n\cdot[A\epsilon(u_h)], & \text{if } \Gamma\subset\partial K\setminus\partial\Omega\\ 0, & \text{if } \Gamma\subset\Gamma_D\\ g-n\cdot A\epsilon(u_h), & \text{if } \Gamma\subset\Gamma_N\end{cases}$$

Energy-norm error estimate (derived analogously as in the case of the Poisson model problem):

$$\|e\|_E\le\eta_E(u_h):=c_Sc_I\Big(\sum_{K\in\mathbb{T}_h}\rho_K^2\Big)^{1/2}.$$

Numerical example (F.-T. Suttmeier 1997)

A square elastic disc with a crack is subjected to a constant boundary traction acting along half of the upper boundary. Along the right-hand and lower parts of the boundary the disc is clamped and along the remaining part of the boundary (including the crack) it is left free.



The solution has a singularity with a stress singularity (expressed in terms of polar coordinates (r, θ)): $\sigma \approx r^{-1/2}$

The material parameters are chosen as commonly used for aluminium, i.e., $2\mu \sim \lambda \sim 0.16 N/m^2$. The surface traction is of size $g \equiv 0.1 N/m^2$.

Goal functional: Normalstress along Γ_D

$$J(u) = \int_{\Gamma_u} n \cdot A\epsilon(u) \cdot n \, ds$$

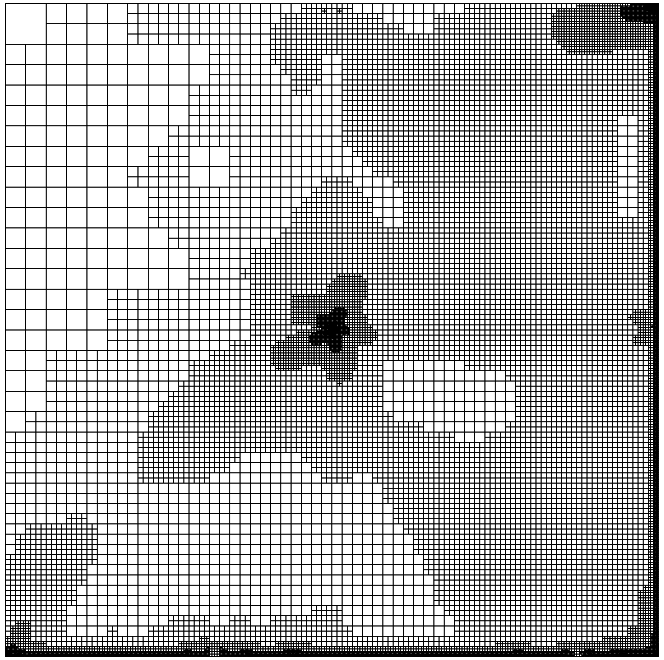
Regularization with $\epsilon = TOL$. The reference solution is σ_{ref}.

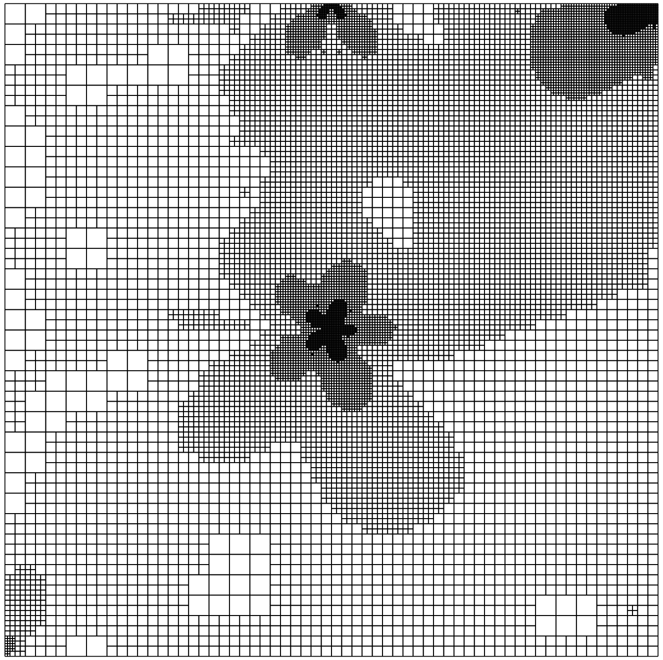
$$E^{\mathrm{rel}} := \left| \frac{J_\epsilon(\sigma_h - \sigma_{\mathrm{ref}})}{J_\epsilon(\sigma_{\mathrm{ref}})} \right|, \quad I_{\mathrm{eff}} := \left| \frac{\eta_\omega(u_h, \sigma_h)}{J_\epsilon(\sigma_h - \sigma_{\mathrm{ref}})} \right|$$

L	N	$J(u_h)$	E^{rel}	I_{eff}
1	256	0.017080	0.0283	1.80
2	484	0.019542	0.0180	1.96
3	1060	0.021138	0.0113	1.95
4	2113	0.022157	0.0070	1.96
5	4435	0.022795	0.0044	1.92
6	8830	0.023198	0.0027	1.86
7	15886	0.023428	0.0017	1.79
8	29947	0.023593	0.0010	1.79

L	N	$J(u_h)$	E^{rel}
1	256	0.017080	0.0283
2	544	0.018174	0.0237
3	1180	0.019363	0.0188
4	2659	0.020528	0.0139
5	6193	0.021538	0.0096
6	13423	0.022319	0.0064
7	31336	0.022811	0.0043
8	65332	0.023153	0.0029

Results for $\eta_\omega(u_h)$ (left) and $\eta_E(u_h)$ (right)





Results for $\eta_\omega(u_h)$ (left) and $\eta_E(u_h)$ (right)

A model problem in elasto-plasticity theory (a non-differentiable nonlinearity)

Fundamental problem in the static deformation theory of linear–elastic perfect–plastic material (*Hencky* model):

$$-\nabla\cdot\sigma = f, \quad \epsilon(u) = A{:}\sigma + \lambda, \quad \epsilon(u) = \tfrac{1}{2}(\nabla u + \nabla u^T) \quad \text{in } \Omega$$

$$\lambda : (\tau-\sigma) \le 0 \quad \forall\,\tau \quad \text{with} \quad F(\tau) \le 0$$

$$u = 0 \;\text{ on } \Gamma_D, \quad \sigma\cdot n = g \;\text{ on } \Gamma_N$$

λ plastic growth.

This system describes the deformation of an elasto-plastic body occupying a bounded domain $\Omega\subset\mathbb{R}^d$ ($d{=}2$ or 3) which is fixed along a part Γ_D $(\mathrm{meas}(\Gamma_D)\neq 0)$ of its boundary $\partial\Omega$, under the action of a body force with density f and a surface traction g along $\Gamma_N = \partial\Omega\backslash\Gamma_D$.

Linear–elastic isotropic material law (Hooke's law):

$$\sigma = 2\mu\epsilon^D(u) + \kappa\nabla\cdot uI$$

with constants $\mu > 0$ and $\kappa > 0$, while the plastic behavior follows the von Mises flow rule, with some $\sigma_0 > 0$:

$$F(\sigma) = |\sigma^D| - \sigma_0 \leq 0$$

Primal variational formulation:

$$A(u)(\psi) := (C(\epsilon(u)), \epsilon(\psi)) = (f, \psi) + (g, \psi)_{\Gamma_N} =: F(\psi), \quad \forall\psi \in V$$

where $C(\epsilon(u)) = \Pi(2\mu\epsilon^D(u)) + \kappa\nabla\cdot uI$,

$$\Pi(2\mu\epsilon^D(u)) = \begin{cases} 2\mu\epsilon^D(u) & , \text{ if } \quad |2\mu\epsilon^D(u)| \leq \sigma_0, \\ \dfrac{\sigma_0}{|\epsilon^D(u)|}\epsilon^D(u) & , \text{ if } \quad |2\mu\epsilon^D(u)| > \sigma_0 \end{cases}$$

This nonlinearity is only Lipschitz continuous.

Finite element approximation (Q_1-elements):

$$A(u_h)(\psi_h) = F(\psi_h) \qquad \forall \psi_h \in V_h,$$

Associated stress σ_h :

$$\sigma_h = \Pi(2\mu\epsilon^D(u_h)) + \kappa\nabla \cdot u_h I.$$

Given a (linear) error functional $J(\cdot)$, we have the a posteriori error representation, with second-order remainder,

$$J(e) = \rho(u_h)(z - \psi_h) + R^{(2)}, \quad \psi_h \in V_h$$

where

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

Linear dual problem:

$$(C'(u)\epsilon(\psi), \epsilon(z)) = J(\psi) \quad \forall \psi \in V$$

$$C'(\tau)\epsilon := \begin{cases} C\epsilon, & \text{if} \quad |2\mu\tau^D| \le \sigma_0, \\ \dfrac{\sigma_0}{|\tau^D|}\Big\{I - \dfrac{(\tau^D)^T\tau^D}{|\tau^D|^2}\Big\}\epsilon^D + \kappa\,\mathrm{tr}(\epsilon)I, & \text{if} \quad |2\mu\tau^D| > \sigma_0 \end{cases}$$

The remainder term is $R^{(2)} = \mathcal{O}(e^2)$ in regions where the form $A(\cdot)(\cdot)$ is C^2, i.e. outside the elastic-plastic transition zone $\{|2\mu\tau^D| = \sigma_0\}$. The residual term in the error identity has the form

$$\rho(u_h)(z-\psi_h) = \sum_{K\in\mathbb{T}_h} \Big\{(R(u_h), z-\psi_h)_K + (r(u_h), z-\psi_h)_{\partial K}\Big\}$$

with the cell and edge residuals $R(u_h)_{|K} = f - \nabla\cdot C(\epsilon(u_h))$,

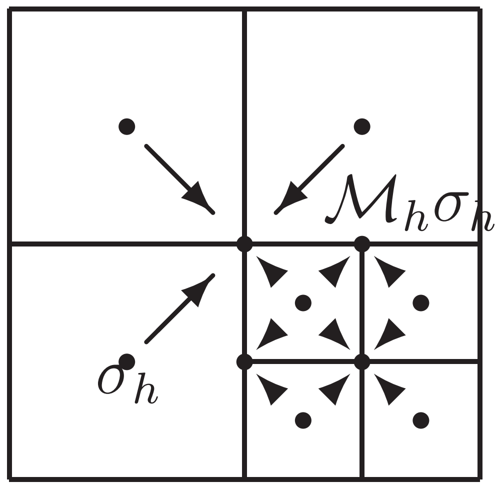
$$r(u_h)_{|\Gamma} = \begin{cases} -\frac{1}{2}n\cdot[C(\epsilon(u_h))], & \text{if } \Gamma \subset \partial K \setminus \partial\Omega \\ 0, & \text{if } \Gamma \subset \Gamma_D \\ g - n\cdot C(\epsilon(u_h)), & \text{if } \Gamma \subset \Gamma_N \end{cases}$$

Alternative heuristic error indicators for comparison:

(1) *ZZ-error indicator (à la Zienkiewicz/Zhu):*
An approximation $\sigma \approx M_h\sigma_h$ to σ by local averaging,

$$\|e_\sigma\| \approx \eta_{ZZ}(u_h) = \Big(\sum_{K\in\mathbb{T}_h} \|M_h\sigma_h - \sigma_h\|_K^2 \Big)^{1/2}$$

The nodal value at a point of the triangulation determining $\mathcal{M}_h\sigma_h$ is obtained by averaging the cell-wise constant values of σ_h of those cells having this point in common.



(2) *An energy-error indicator (à la Johnson/Hansbo):*

This heuristic energy-error estimator is based on decomposing the domain Ω into *discrete* plastic and elastic zones, $\Omega = \Omega_h^p \cup \Omega_h^e$. Accordingly the error estimator has the form

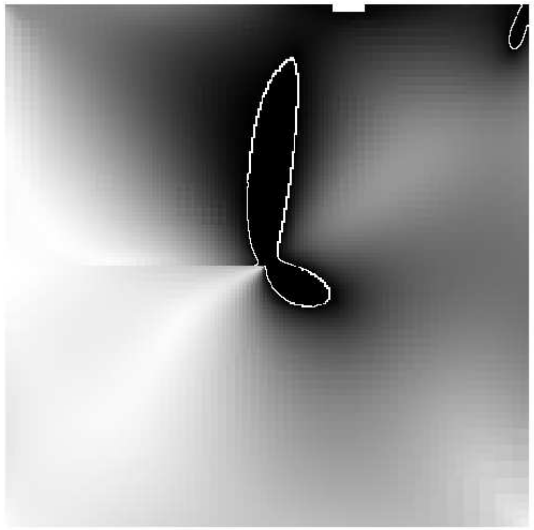
$$\|e_\sigma\| \approx \eta_E(u_h) = c_i \Big(\sum_{K \in \mathbb{T}_h} \eta_K^2 \Big)^{1/2}$$

with the local error indicators defined by

$$\eta_K^2 := \begin{cases} h_K^2 \{\rho_K + \rho_{\partial K}\}^2, & \text{if } K \subset \Omega_h^e \\ \{\rho_K + \rho_{\partial K}\} \|M_h \sigma_h - \sigma_h\|_K, & \text{if } K \subset \Omega_h^p \end{cases}$$

Numerical tests (F.-T. Suttmeier 1998)

a) Square plate with a slit:



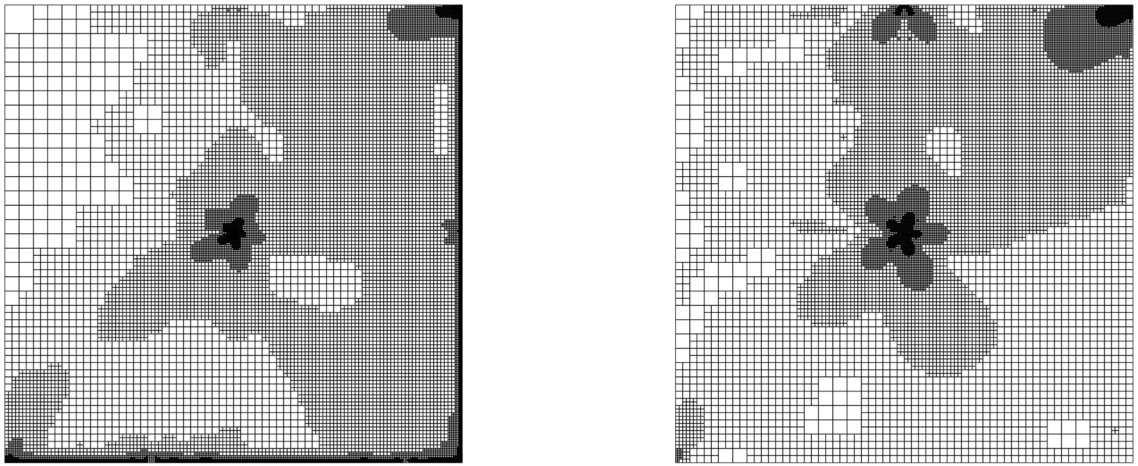
Plot of $|\sigma^D|$ (plastic regions black) computed on a mesh with $N \approx 64\,000$ cells

Goal functional: Mean normal stress along Γ_D

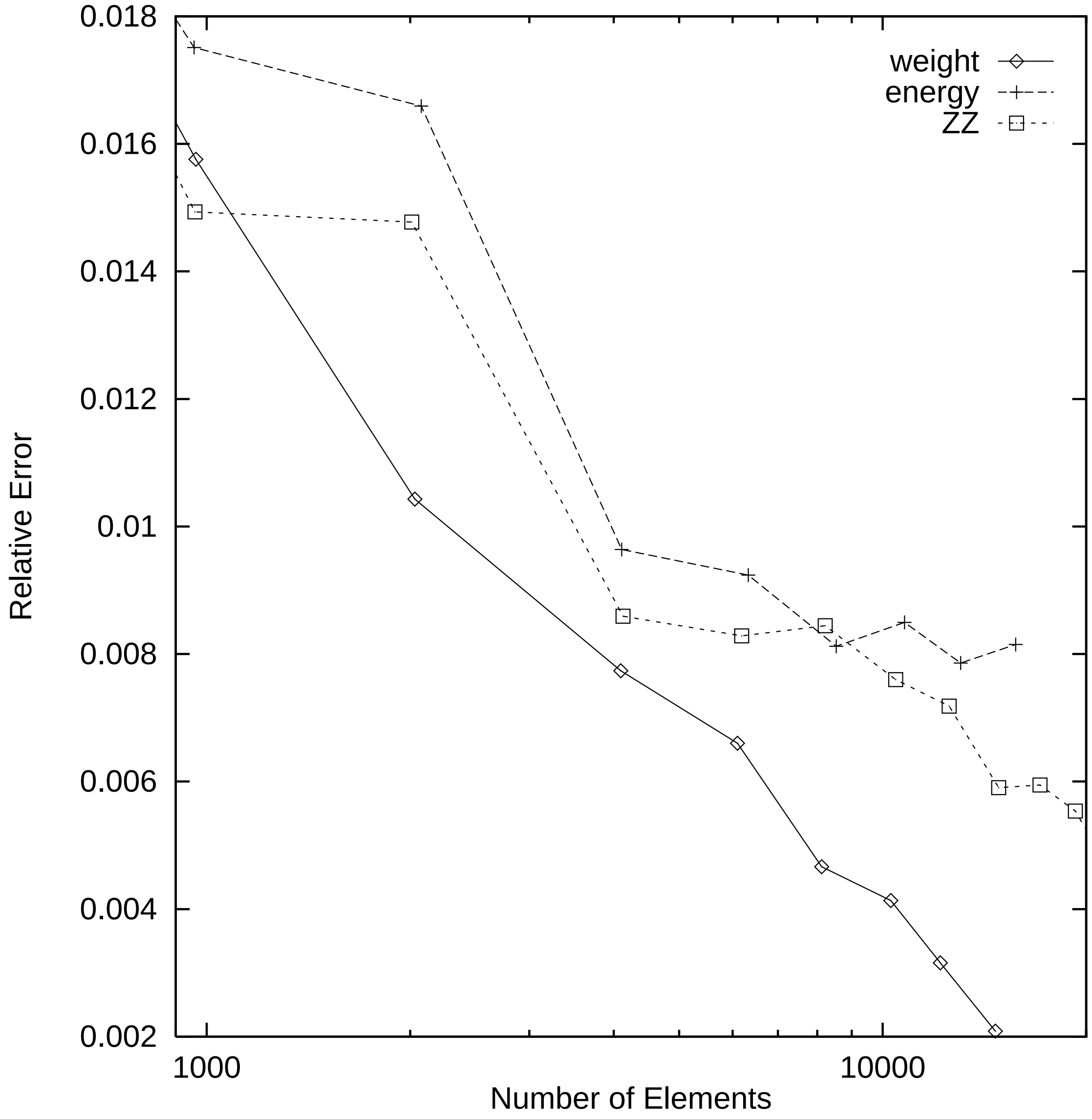
$$J(\sigma) = \int_{\Gamma_D} n \cdot \sigma \cdot n \, ds$$

L	N	$J_\epsilon(\sigma_h)$	E^{rel}	I_{eff}
1	256	0.017080	0.0283	1.80
3	1060	0.021138	0.0113	1.95
5	4435	0.022795	0.0044	1.92
7	15886	0.023428	0.0017	1.79
9	52288	0.023697	0.0006	1.86

Results obtained by the *weighted* error estimator $\eta_\omega(u_h)$

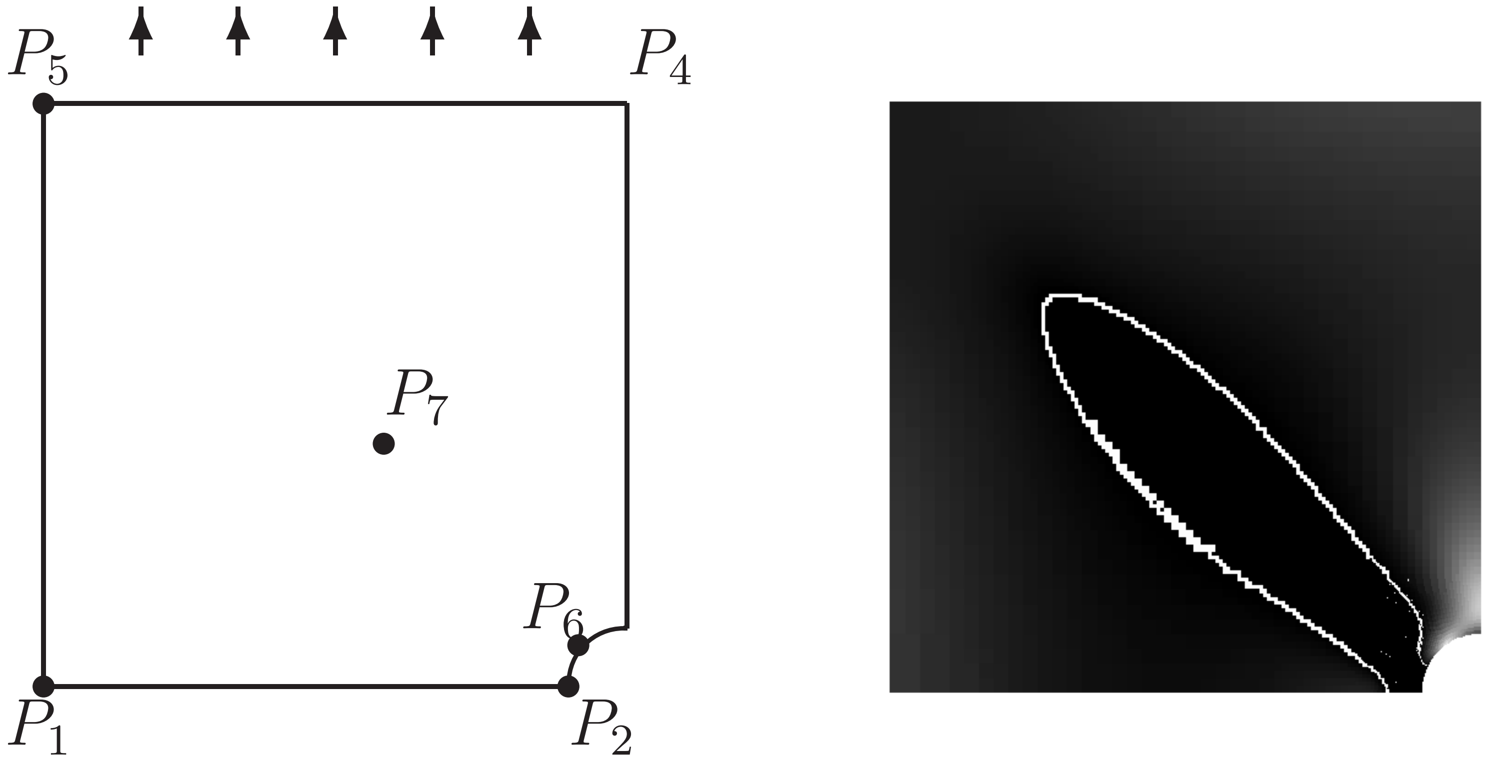


Finest meshes obtained by $\eta_\omega(u_h)$ (left) and $\eta_E(\sigma_h)$ (right)



Relative error for $J(\sigma)$ on grids based on the different error indicators

b) Benchmark square plate with a hole:



Geometry of the benchmark problem and plot of $|\sigma^D|$ (plastic region black, transition zone white) computed on a mesh with $N \approx 10\,000$ cells

Geometrically two-dimensional model (restriction to a quarter-domain) with plane-strain approximation, i.e., $\epsilon_{i3} = 0$, and perfectly plastic material behavior. The material parameters are chosen as those of aluminium, $\kappa = 164,206\, N/mm^2$, $\mu = 80,193.80\, N/mm^2$, $\sigma_0 = \sqrt{2/3}\,450$. The boundary traction is given in the form $g(t) = tg_0$, $g_0 = 100$, $t \in [0,6]$. For the stationary Hencky model, the calculations are performed with one load step from $t=0$ to $t=4.5$.

The quantities to be computed are:

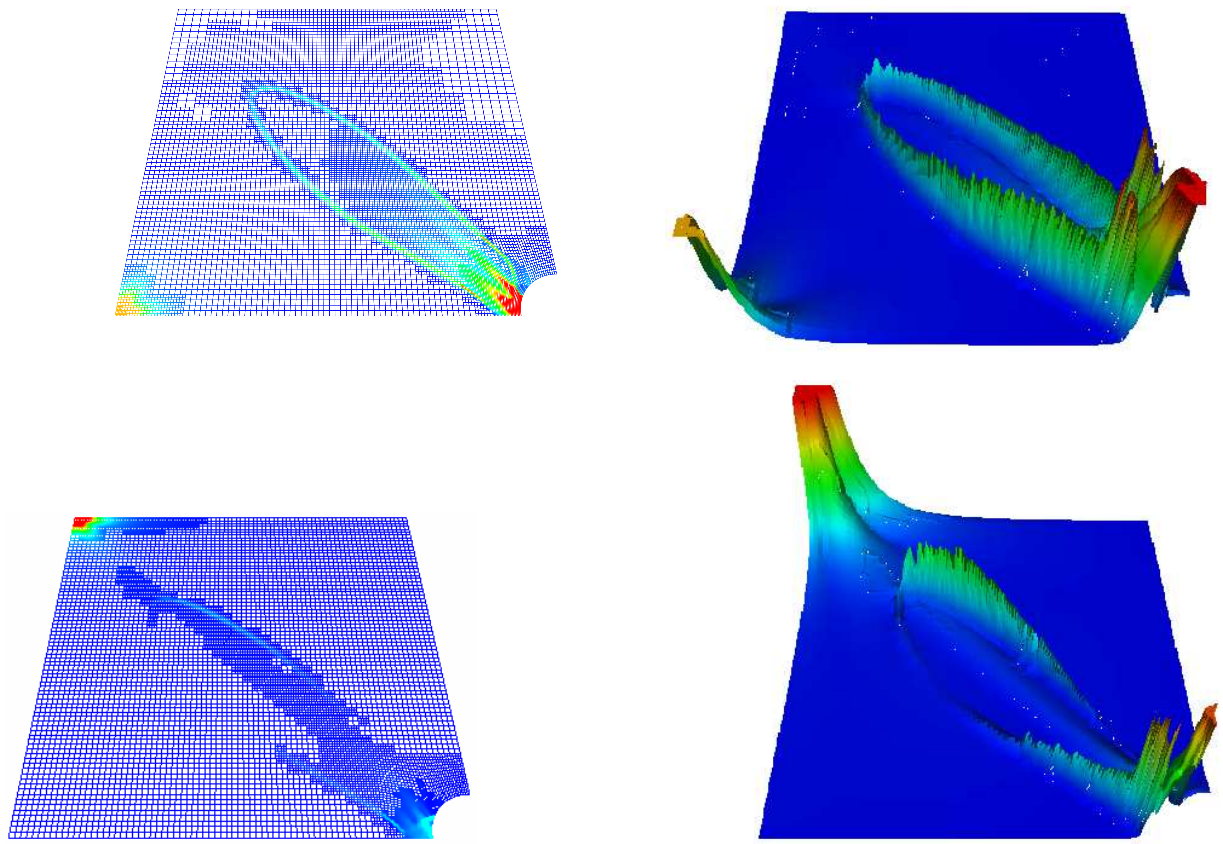
- Displacements u_1 and u_2 at various points and stress $\sigma_{22}(P_2)$.

The solutions on very fine (adapted) meshes with about $200,000$ cells are taken as reference solutions u_{ref} for determining the relative errors E^{rel} and the effectivity indices I_{eff} of the error estimator.

N	$u_1(P_5)$	E^{rel}	I_{eff}
1000	6.5991e-02	7.7403e-02	0.64
2000	6.3462e-02	3.6121e-02	0.83
6000	6.1687e-02	7.1352e-03	1.35
10000	6.1479e-02	3.7331e-03	1.69
14000	6.1408e-02	2.5833e-03	1.75
18000	6.1370e-02	1.9605e-03	1.80
∞	6.1251e-02		

Results for $u_1(P_5)$ based on the error estimator $\eta_\omega(u_h)$

The weighted error estimator turns out to be efficient even on coarse meshes. This indicates that the strategy of evaluating the weights ω_T computationally works also for the present irregular nonlinear problem.



Optimized meshes for computing $u_1(P_1)$ (top) and $u_1(P_5)$ (bottom) together with corresponding weight distributions ω_T

8.22

9. Applications in fluid mechanics

(I) Incompressible viscous flow: Navier-Stokes equations

$$u := \{v, p\} : \qquad \mathcal{A}(u) := \left\{ \begin{array}{c} -\nu\Delta v + v\cdot\nabla v + \nabla p - f \\ \nabla\cdot v \end{array} \right\} = 0$$

- Compute $J(u)$ from the solution of

$$\mathcal{A}(u) = 0$$

- Minimize $J(u)$ under the constraint

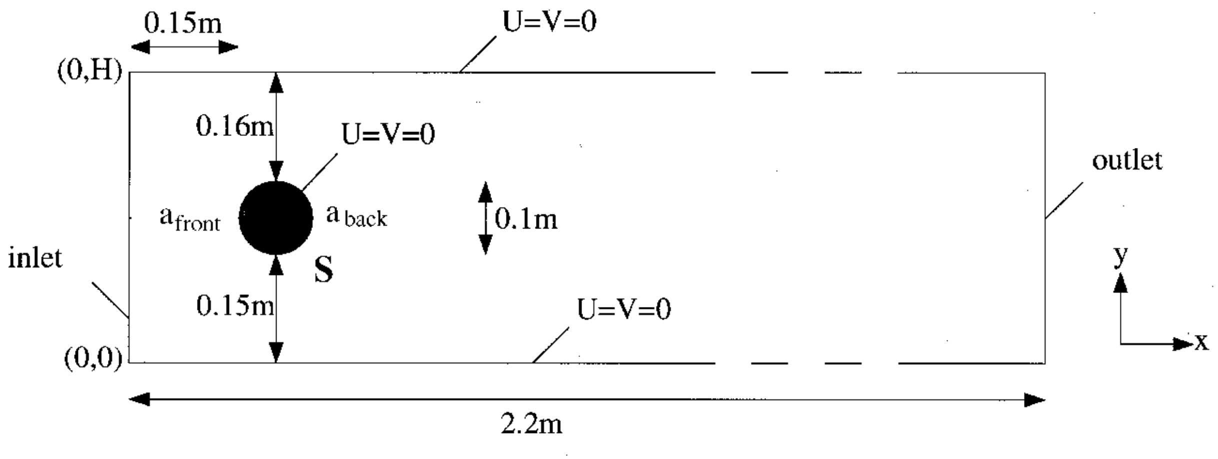
$$\mathcal{A}(u) + Bq = 0$$

- Determine the stability (i.e. physical relevance) of "optimal" state $\hat{u}$ by solving the eigenvalue problem

$$\mathcal{A}'(\hat{u})u = \lambda\mathcal{M}u$$

v velocity, p pressure, ν viscosity ($\rho \equiv 1$), $f = 0$,

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



Reynolds number
$\mathrm{Re} = \frac{\bar{\mathrm{U}}^2\mathrm{D}}{\nu} = 20$
(stationary flow)

Computation of "drag coefficient":

$$J(u) := \frac{2}{\bar{U}^2 D} \int_S n^T(\tau - pI)e_1 \,\mathrm{ds}$$

S surface of cylinder, D diameter, $\bar{U}$ reference velocity
$\tau = \nu(\nabla v + \nabla v^T) - pI$ strain tensor (evaluated in volume form)

Finite Element Discretization

Solution and test spaces

$$L := L^2(\Omega), \quad H := \{v \in H^1(\Omega)^2 : v_{|\Gamma_{\rm in}\cup\Gamma_{\rm rigid}} = 0\}, \quad V := H\times L$$

Semi-linear form ("energy form"): $\quad u = \{v,p\},\ \varphi = \{\varphi^v, \varphi^p\}$

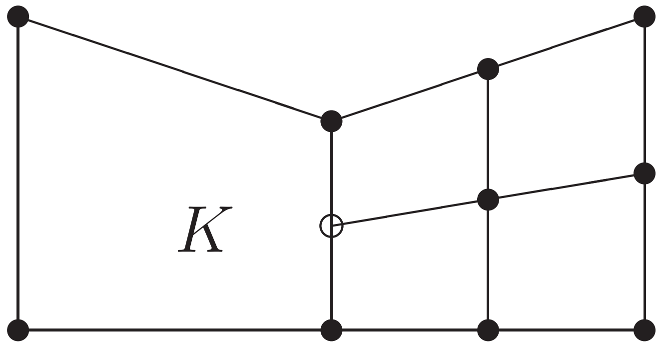
$$a(u)(\varphi) := \underbrace{(\nabla v, \nabla\varphi^v) + (v\cdot\nabla v - f, \varphi^v) - (p, \nabla\cdot\varphi^v)}_{\text{momentum}} + \underbrace{(\varphi^p, \nabla\cdot v)}_{\text{continuity}}$$

Variational Navier-Stokes problem $\ u \in u^{\rm in} + V$:

$$a(u)(\varphi) = 0 \qquad \forall\varphi\in V$$

Discretization by quadrilateral Q_1/Q_1-Stokes element:

$$L_h \subset L, \quad H_h \subset H, \quad V_h := H_h \times L_h$$



isopar$\{1, x_1, x_2, x_1x_2\}$

$v_h(a),\ p_h(a)$

Problem of "inf-sup" stability (stability of pressure):

$$\inf_{q_h \in L_h} \sup_{v_h \in H_h} \frac{(q_h, \nabla \cdot v_h)}{\|q_h\| \, \|\nabla v_h\|} =: \beta_h \ \geq \ \beta \ > \ 0\,!$$

Simultaneous "least-squares" stabilization of pressure and transport:

$$\mathcal{S}(u)\varphi := \left\{ \begin{array}{c} v\cdot\nabla\varphi^v + \nabla\varphi^p \\ \nabla\cdot\varphi^v \end{array} \right\}, \qquad (\varphi,\psi)_\delta := \sum_{T\in\mathbb{T}_h} \delta_T\,(\varphi,\psi)_T$$

Stabilized discrete problems $u_h \in u_h^{in} + V_h$:

$$a_\delta(u_h)(\varphi_h) := a(u_h)(\varphi_h) + (\mathcal{A}(u_h), \mathcal{S}(u_h)\varphi_h)_\delta = 0 \qquad \forall \varphi_h \in V_h$$

Fully consistent stabilization $\quad a_\delta(u)(\varphi_h) = 0$

- Stabilization of pressure: $\delta_T(\nabla p_h, \nabla\varphi_h^p)_T$
- Stabilization of transport: $\delta_T(v_h\cdot\nabla v_h, v_h\cdot\nabla\varphi_h^v)_T$
- Stabilization of mass conservation: $\delta_T(\nabla\cdot v_h, \nabla\cdot\varphi_h^v)_T$
- Adaptive determination of stabilization parameter:

$$\delta_T = \alpha\big(\nu h_T^{-2}, \beta\,|v_h|_{T;\infty} h_T^{-1}\big)^{-1}$$

Solution by quasi-Newton or pseudo-time iteration:

- correction equation: $\quad \forall \varphi_h \in V_h$,

$$\Big(\underbrace{k_t^{-1}(\delta u_h^t, \varphi_h)}_{\text{time part}} \Big) + \underbrace{\tilde{a}'_\delta(u_h^t)(\delta u_h^t, \varphi_h)}_{\text{Newton part}} = \underbrace{-a_\delta(u_h^t)(\varphi_h)}_{\text{residual}}$$

- update: $\quad u_h^{t+1} = u_h^t + \kappa_t \delta u_h^t \quad$ (κ_t damping parameter)

A posteriori error estimation

Proposition. *We have the* $a\ posteriori$ *error representation*

$$J(u) - J(u_h) \; = \; \tfrac{1}{2}\underbrace{\rho(u_h)(z - i_h z)}_{\textit{primal residual}} + \tfrac{1}{2}\underbrace{\rho^*(u_h, z_h)(u - i_h u)}_{\textit{dual residual}} + R_h^{(3)}$$

for interpolations $i_h z,\, i_h u \in V_h$ *. The remainder* $R_h^{(3)}$ *is cubic in the errors* $e := u - u_h$ *and* $e^* := z - z_h$ *.*

Remark. Evaluation of error estimator:

$$\eta_\omega(u_h, z_h) := \tfrac{1}{2}\rho(u_h)(\tilde{z}_h - z_h) + \tfrac{1}{2}\rho^*(u_h, z_h)(\tilde{u}_h - u_h),$$

for arbitrary $\psi_h,\, \varphi_h \in V_h$ by using approximations $\tilde{u}_h \approx u$ and $\tilde{z}_h \approx z$ to the exact primal and dual solutions.

Approximation of weights by patch-wise higher-order interpolation:

$$z - i_h z \;\approx\; i_{2h}^{(2)} z_h - z_h, \qquad u - i_h u \;\approx\; i_{2h}^{(2)} u_h - u_h$$

Primal residual:

$$\rho(u_h)(z-i_h z) := \sum_{K\in\mathbb{T}_h} \Big\{ (R(u_h), \underbrace{z^v - i_h z^v}_{\text{weight}})_K + (r(u_h), \underbrace{z^v - i_h z^v}_{\text{weight}})_{\partial K}$$

$$+ (\underbrace{z^p - i_h z^p}_{\text{weight}}, \nabla\cdot v_h)_K + \dots \Big\}$$

cell and edge residuals ($[\dots]$ jump across an interior edge Γ)

$$R(u_h)_{|K} := f - \nu\Delta v_h + v_h\cdot\nabla v_h + \nabla p_h,$$

$$r(u_h)_{|\Gamma} := \left\{ \begin{array}{ll} -\frac{1}{2}[\nu\partial_n v_h - n p_h], & \text{if } \Gamma \not\subset \partial\Omega \\ \quad 0, & \text{if } \Gamma \subset \Gamma_{\text{rigid}} \cup \Gamma_{\text{in}} \\ -\nu\partial_n v_h + n p_h, & \text{if } \Gamma \subset \Gamma_{\text{out}} \end{array} \right\}$$

Dual residual:

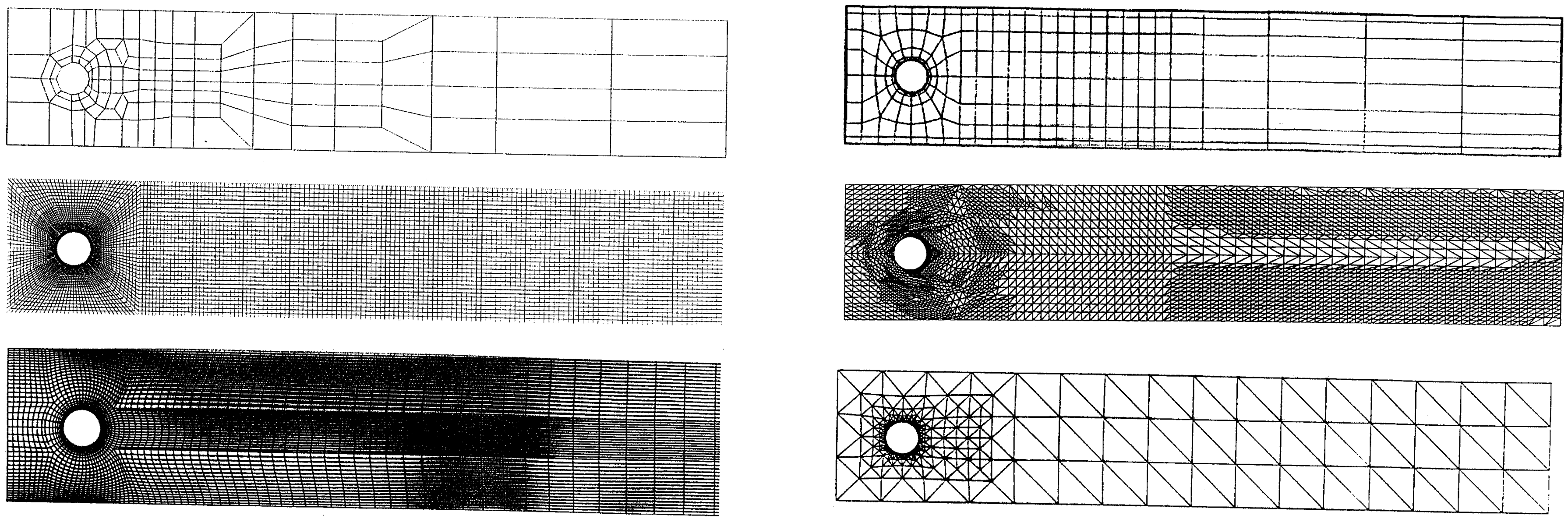
$$\rho^*(u_h, z_h)(u - i_h u) := \sum_{K \in \mathbb{T}_h} \Big\{ (R^*(z_h), \underbrace{v - i_h v}_{\text{weight}})_K + (r^*(z_h), \underbrace{v - i_h v}_{\text{weight}})_{\partial K}$$
$$+ (\underbrace{p - i_h p}_{\text{weight}}, \nabla \cdot z_h)_K + \dots \Big\}$$

cell and edge residuals

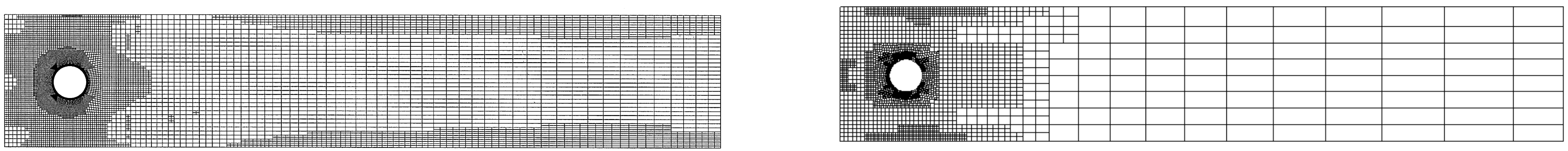
$$R^*(z_h)_{|K} := j - \nu \Delta z_h^v - v_h \cdot \nabla z_h^v + \nabla v_h^T z_h^v - \nabla \cdot v_h z_h^v + \nabla z_h^p$$

$$r^*(z_h)_{|\Gamma} := \left\{ \begin{array}{ll} -\frac{1}{2}[\nu \partial_n z_h^v + n \cdot v_h z_h^v - z_h^p n], & \text{if } \; \Gamma \not\subset \partial\Omega \\ \quad 0, & \text{if } \; \Gamma \subset \Gamma_{\text{rigid}} \cup \Gamma_{\text{in}} \\ -\nu \partial_n z_h^v - n \cdot v_h z_h^v + z_h^p n, & \text{if } \; \Gamma \subset \Gamma_{\text{out}} \end{array} \right\}$$

(Ia) Computation of drag in 2-D (R. Becker 1997)



Examples of “hand-made’meshes for the drag computation



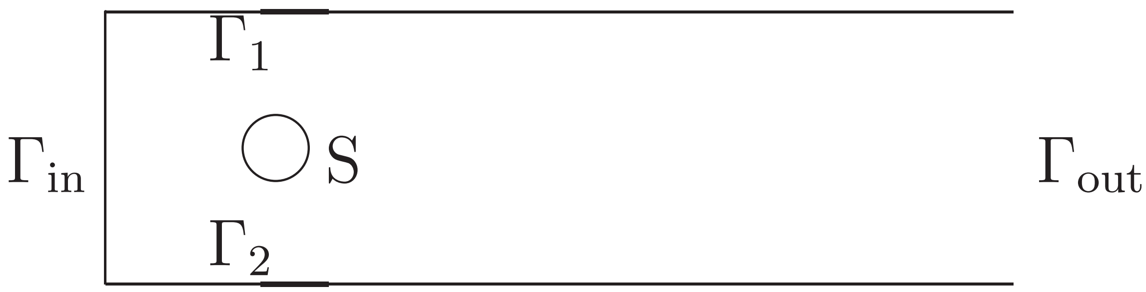
Refined meshes by “smoothness-based” strategies and by the DWR method

Computation of drag				
L	N	c_{drag}	η_{drag}	I_{eff}
4	984	5.66058	$1.1e{-}1$	0.76
5	**2244**	5.59431	$3.1e{-}2$	0.47
6	4368	5.58980	$1.8e{-}2$	0.58
6	7680	5.58507	$8.0e{-}3$	0.69
7	9444	5.58309	$6.3e{-}3$	0.55
8	22548	5.58151	$2.5e{-}3$	0.77
9	41952	5.58051	$1.2e{-}3$	0.76
	∞	5.57953		

Results for drag computation on adaptively refined meshes

(error level of $< 1\%$, indicated by bold face; $N = \#$ cells)

(Ib) Minimization of drag by pressure control (R. Becker 1999)



$u \in u^{\text{in}} + V$ state variable

q "boundary control" (piecewise constant at $\Gamma_Q := \Gamma_1 \cup \Gamma_2$)

$$J(u,q) := J_{\text{drag}} \;\to\; \min, \qquad \mathcal{A}(u) + \mathcal{B}q = 0$$

Variational formulation:

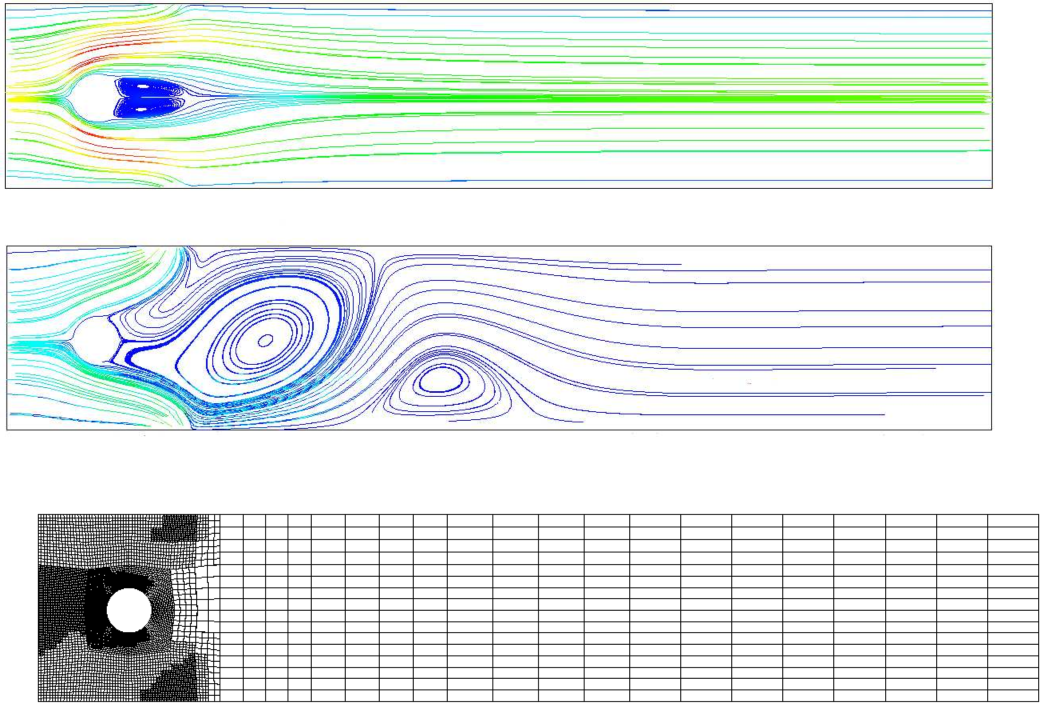
$$a_\delta(u)(\varphi) + b(q,\varphi) = 0 \qquad \forall \varphi \in V$$

"control form" $\quad b(q,\varphi) := -(q, n \cdot \varphi^v)_{\Gamma_Q}$

Computational results

Uniform refinement		Adaptive refinement	
N	$J_{\rm drag}$	N	$J_{\rm drag}$
10 512	3.31321	1 572	3.28625
41 504	3.21096	4 264	3.16723
164 928	3.11800	11 146	3.11972

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



Velocity of the uncontrolled flow (top), controlled flow (middle), and corresponding adapted mesh (bottom)

Problem: Stability of "optimal" stationary flow (computed by Newton method)?

(Ic) Stability of flows (V. Heuveline 2001)

Stability of base solution $\hat{u} = \{\hat{v}, \hat{q}\}$ by linear theory ("spectral argument"):

Non-sym. eigenvalue problem for $u := \{v, p\} \in V$ and $\lambda \in \mathbb{C}$:

$$\mathcal{A}'(\hat{u})u := -\nu\Delta v + \hat{v}\cdot\nabla v + v\cdot\nabla\hat{v} + \nabla p = \lambda v, \qquad \nabla\cdot v = 0$$

$$\mathrm{Re}\,\lambda \geq 0 \quad \Rightarrow \quad \hat{u} \;\text{ stable (?)}$$

Variational formulation:

$$\begin{aligned} a'(\hat{u})(\psi,\varphi) &:= \nu(\nabla\psi^v, \nabla\varphi^v) + (\hat{v}\cdot\nabla\psi^v, \varphi^v) + (\psi^v\cdot\nabla\hat{v}, \varphi^v) \\ &\qquad - (\psi^p, \nabla\cdot\varphi^v) + (\varphi^p, \nabla\cdot\psi^v), \\ m(\psi,\varphi) &:= (\psi^v, \varphi^v). \end{aligned}$$

Primal and dual eigenvalue problems: $u,\ u^* \in V$:

$$a'(\hat{u})(u,\varphi) = \lambda\, m(u,\varphi) \qquad \forall \varphi \in V$$
$$a'(\hat{u})(\varphi,u^*) = \lambda\, m(\varphi,u^*) \quad \forall \varphi \in V$$

Normalization: $m(u,u) = m(u,u^*) = 1\,.$

Degenerate case:

If $m(u,u^*) = 0\,$, the boundary value problem

$$a'(\hat{u})(\tilde{u},\varphi) - \lambda\, m(\tilde{u},\varphi) = m(u,\varphi) \quad \forall \varphi \in V$$

has a solution $\tilde{u} \in V$ ('generalized eigenfunction')
$\Rightarrow \quad \mathrm{defect}(\lambda) > 0$

Discretization

Stabilized sesquilinear form

$$\tilde{a}'_\delta(\hat{v}_h)(u_h, \varphi_h) := a'(\hat{u})(u_h, \varphi) + (\mathcal{A}'(\hat{u})u - \lambda_h v, \mathcal{S}(\hat{u})\varphi)_\delta$$

Discrete primal and dual eigenvalue problems $u_h,\ u_h^* \in V_h,\ \lambda_h \in \mathbb{C}$:

$$\tilde{a}'_\delta(\hat{u}_h)(u_h, \varphi_h) = \lambda_h\, m(u_h, \varphi_h) \quad \forall \varphi_h \in V_h$$
$$\tilde{a}'_\delta(\hat{u}_h)(\varphi_h, u_h^*) = \lambda_h\, m(\varphi_h, u_h^*) \quad \forall \varphi_h \in V_h$$

Stabilization $\quad m(u_h, u_h) = m(u_h, u_h^*) = 1$

Blow-up criterion:

$$m(u_h^*, u_h^*) \to \infty \quad (h \to 0) \quad \Rightarrow \quad \mathrm{defect}(\lambda) > 0$$

A posteriori error estimation

Embedding into the general framework of variational equations:

$$\mathcal{V} := V \times V \times \mathbb{C}, \quad \mathcal{V}_h := V_h \times V_h \times \mathbb{C}$$

$$U := \{\hat{u}, u, \lambda\}, \quad U_h := \{\hat{u}_h, u_h, \lambda_h\}, \quad \Phi = \{\hat{\varphi}, \varphi, \mu\} \in \mathcal{V}$$

$$A(U)(\Phi) := \underbrace{-a_\delta(\hat{u})(\hat{\varphi})}_{\text{base solution}} + \underbrace{\lambda\, m(u,\varphi) - \tilde{a}'_\delta(\hat{u})(u,\varphi)}_{\text{eigenvalue equation}}$$
$$+ \underbrace{\overline{\mu}\{m(u,u) - 1\}}_{\text{normalization}}$$

Compact variational formulation:

$$A(U)(\Phi) = 0 \quad \forall \Phi \in \mathcal{V}$$
$$A(U_h)(\Phi_h) = 0 \quad \forall \Phi_h \in \mathcal{V}_h$$

Error control functional:

$$J(\Phi) := \mu\, m(\varphi,\varphi) \quad \Rightarrow \quad J(U) = \lambda m(u,u) = \lambda.$$

Dual solutions $Z = \{\hat z, z, \pi\} \in \mathcal{V}$, $Z_h = \{\hat z_h, z_h, \pi_h\} \in \mathcal{V}_h$:

$$A'(U)(\Phi, Z) = J'(U)(\Phi) \qquad \forall \Phi \in \mathcal{V}$$
$$A'(U_h)(\Phi_h, Z_h) = J'(U_h)(\Phi_h) \quad \forall \Phi_h \in \mathcal{V}_h$$

Observation: $\hat z = \hat u^*, \quad z = u^*, \quad \pi = \lambda$

$$a'(\hat u)(\psi, \hat u^*) = -\, a''(\hat u)(\psi, u, u^*) \quad \forall \psi \in V$$

Residuals:

$$\rho(\hat u_h)(\cdot) := -a_\delta(\hat u_h)(\cdot)$$
$$\rho^*(\hat u_h^*)(\cdot) := -a_\delta''(\hat u)(\cdot, u_h, u_h^*) - \tilde a_\delta'(\hat u_h)(\cdot, \hat u_h^*)$$
$$\rho(u_h, \lambda_h)(\cdot) := \lambda_h\, m(u_h, \cdot) - \tilde a_\delta'(\hat u_h)(u_h, \cdot)$$
$$\rho^*(u_h^*, \lambda_h)(\cdot) := \lambda_h\, m(\cdot, u_h^*) - \tilde a_\delta'(\hat u_h)(\cdot, u_h^*)$$

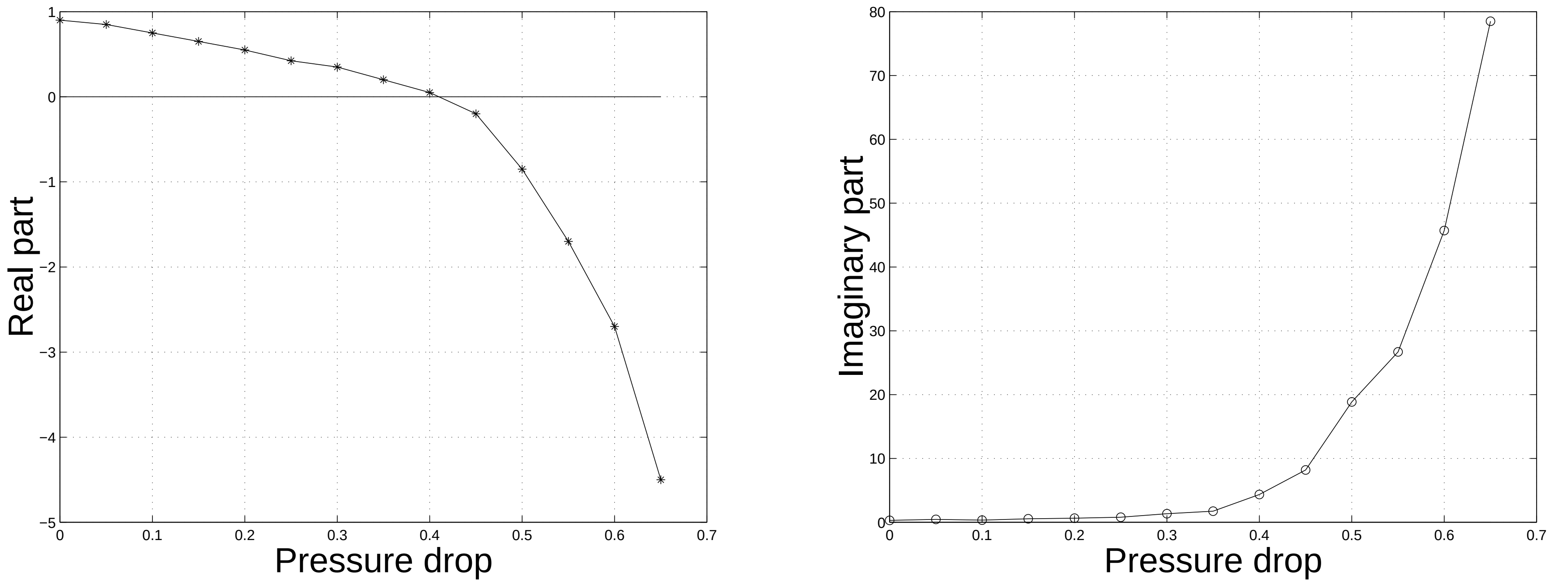
Proposition. *We have the error representation*

$$\lambda - \lambda_h = \underbrace{\tfrac{1}{2}\,\rho(\hat{u}_h)(\hat{u}^* - \hat{\psi}_h) + \tfrac{1}{2}\rho^*(\hat{u}_h^*)(\hat{u} - \hat{\varphi}_h)}_{\textit{base solution residuals}}\ \}$$

$$+\ \underbrace{\tfrac{1}{2}\,\rho(u_h, \lambda_h)(u^* - \psi_h) + \tfrac{1}{2}\rho^*(u_h^*, \lambda_h)(u - \varphi_h)}_{\textit{eigenvalue residuals}} + R_h^{(3)},$$

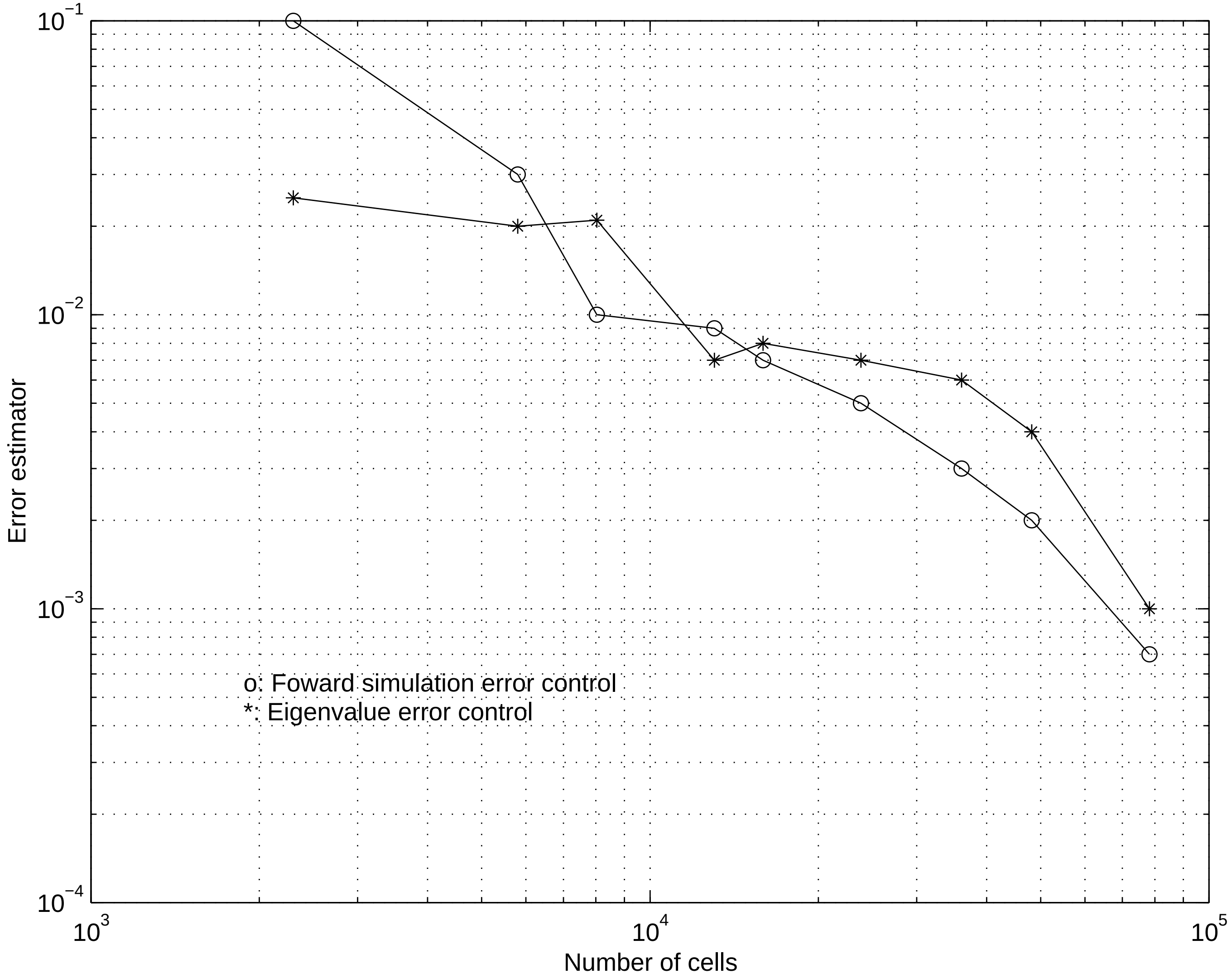
for arbitrary $\hat{\psi}_h,\, \psi_h,\, \hat{\varphi}_h,\, \varphi_h \in V_h$*. The remainder* $R_h^{(3)}$ *is cubic in the errors* $\hat{e}^v := \hat{v} - \hat{v}_h$ *,* $\hat{e}^{v*} := \hat{v}^* - \hat{v}_h^*$ *and* $e^\lambda := \lambda - \lambda_h$ *,* $e^v := v - v_h$ *,* $e^{v*} := v^* - v_h^*$ *.*

Computational results



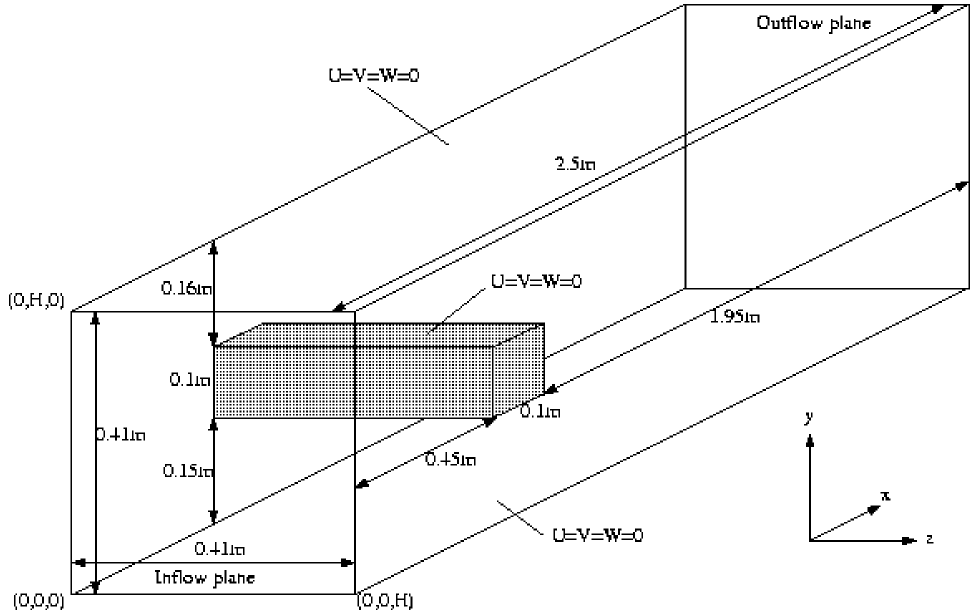
Real part and imaginary part of critical eigenvalue as function of imposed pressure

($q_{\text{opt}} \approx 0.5 \;\; \Rightarrow$ **solution unstable**)



Dominance of error indicator contributions, “base solution-part” and “eigenvalue part”

(II) The potential of goal-oriented adaptivity: drag computation in 3-D cylinder flow (M. Braack and Th. Richter 2002)



Drag coefficient:

$$J(u) \;:=\; c_d \;=\; \kappa \int_S n^T \sigma(v,p) e_2 \, ds$$

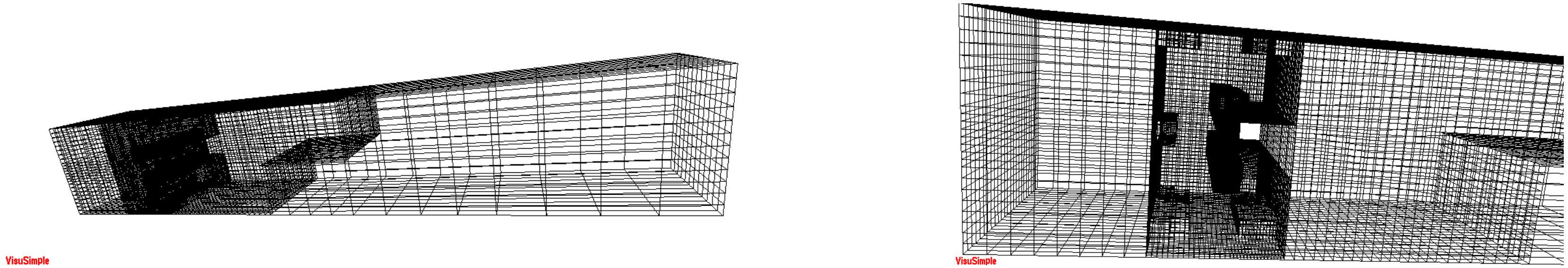
a) Q_2/Q_1-element with global uniform refinement,

b) Q_1/Q_1-element with local refinement by “smoothness indicator”,

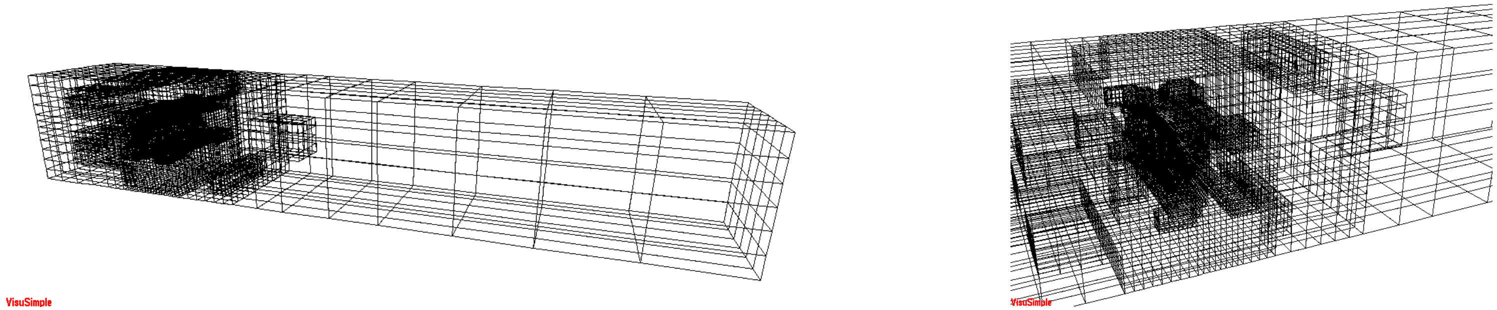
c) Q_1/Q_1-element with local refinement by DWR method.

a) N_{global}	c_d	b) N_{energy}	c_d	c) N_{weighted}	c_d
117 360	7.9766	21 512	8.7117	8 456	9.8262
899 040	7.8644	80 864	7.9505	15 768	8.1147
7 035 840	7.8193	182 352	7.9142	30 224	8.1848
55 666 560	7.7959	473 000	7.8635	**84 832**	7.8282
–	–	**1 052 000**	7.7971	162 680	7.7788
–	–	–	–	367 040	7.7784
–	–	–	–	700 904	7.7769
∞	7.7730	∞	7.7730	∞	7.7730

Results of drag computation (1% error)

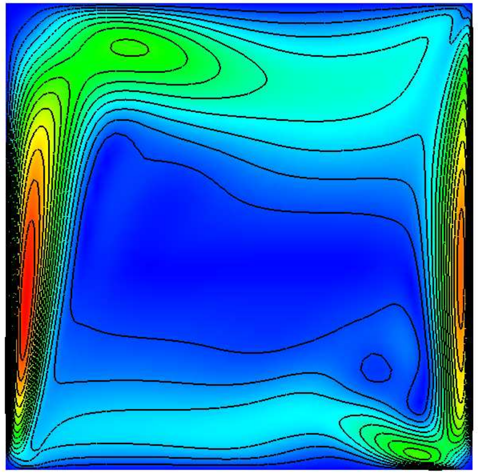


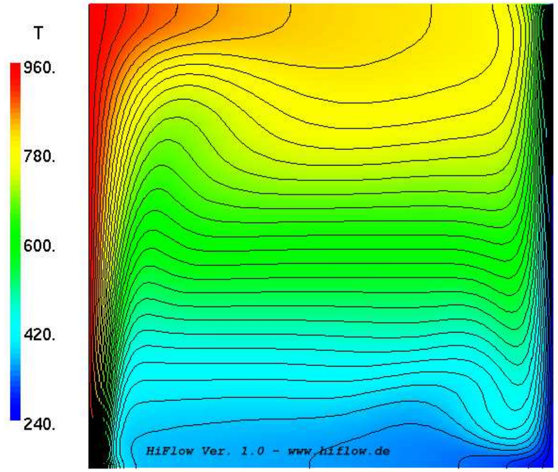
Refined mesh and zoom by the “energy” error indicator



Refined mesh and zoom by the “weighted” error indicator

(III) Multifield problem: heat-driven compressible flow (R. Becker and M. Braack 2002)





"Heat-driven cavity" ($\theta_h - \theta_c = 720\,K$): velocity norm and temperature isolines

"Low-Mach number" approximation for "primitive" variables ρ (mass), v (velocity), θ (temperature):

$$p = p_{th} + p_{\rm hyd}, \quad \rho \approx \frac{p_{\rm th}}{R\theta}, \quad \sigma : \nabla v \approx 0, \quad \partial_t p_{\rm hyd} + v \cdot \nabla p_{\rm hyd} \approx 0$$

"Compressible" Navier-Stokes equations in low-Mach number approximation:

$$\begin{aligned} \nabla \cdot v - \theta^{-1} \partial_t \theta - \theta^{-1} v \cdot \nabla \theta &= -p_{th}^{-1} \partial_t p_{th} \\ \rho \partial_t v + \rho v \cdot \nabla v + \nabla \cdot \tau + \nabla p_{hyd} &= \rho g \\ \rho c_p \partial_t \theta + \rho c_p v \cdot \nabla \theta - \nabla \cdot (\kappa \nabla \theta) &= \partial_t p_{th} + \rho h \end{aligned}$$

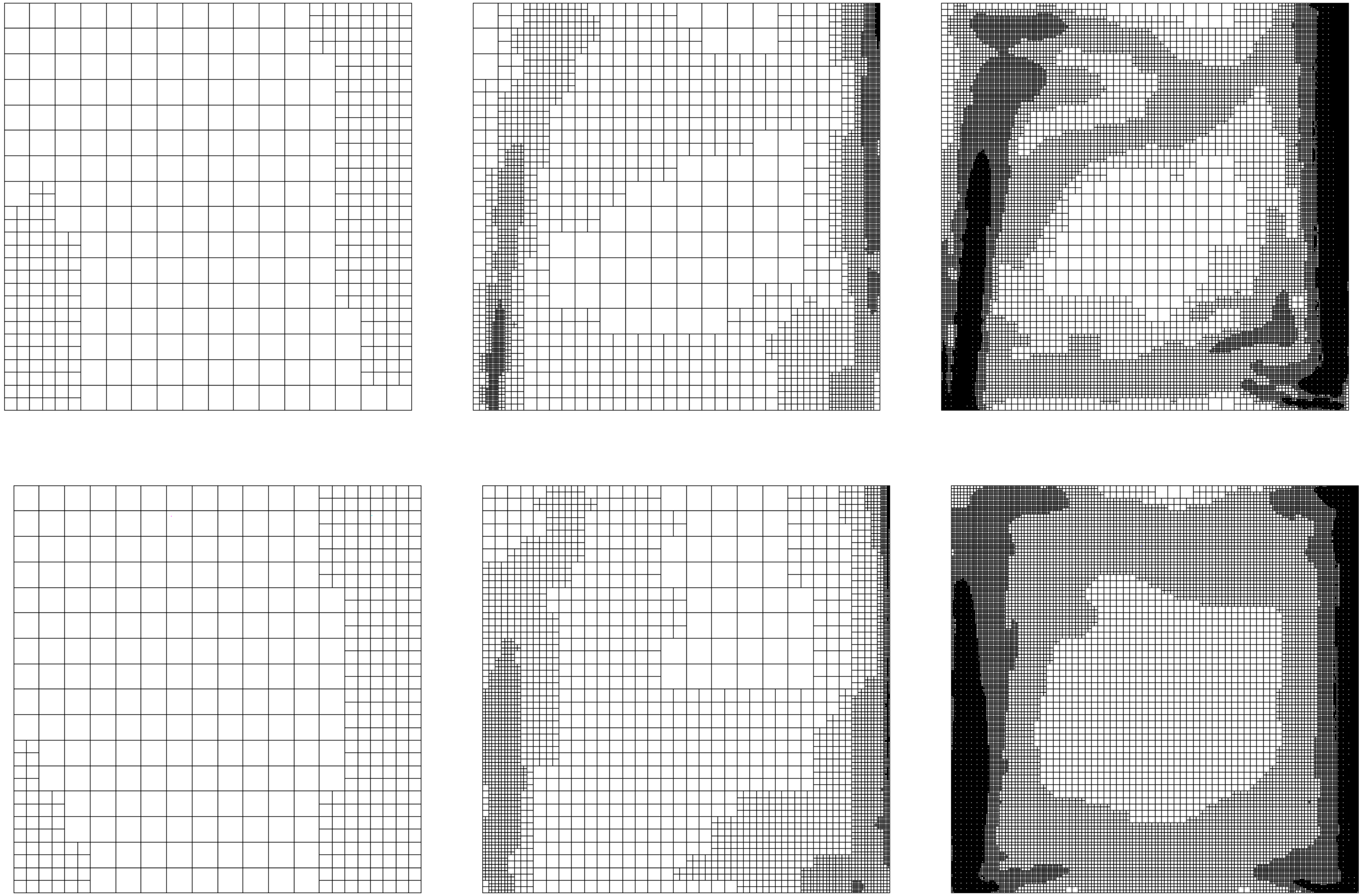
Target quantity: average Nusselt number along the cold wall

$$J(u) = \mathrm{Nu} := \frac{\mathsf{Pr}}{0.3 \mu_0 \theta_0} \int_{\Gamma_{cold}} \kappa \partial_n \theta \, ds$$

N	$\langle Nu \rangle_c$	$J(e)$
524	-9.09552	4.1e-1
945	-8.67201	1.5e-2
1 708	-8.49286	1.9e-1
3 108	-8.58359	1.0e-1
5 656	-8.59982	8.7e-2
18 204	-8.64775	3.9e-2
32 676	-8.66867	1.8e-2
58 678	-8.67791	8.7e-3
79 292	-8.67922	7.4e-3

N	$\langle Nu \rangle_c$	$J(e)$
523	-8.86487	1.8e-1
945	-8.71941	3.3e-2
1 717	-8.66898	1.8e-2
5 530	-8.67477	1.2e-2
9 728	-8.68364	3.0e-3
17 319	-8.68744	8.5e-4
31 466	-8.68653	6.9e-5

Computation of the Nusselt number in the "heat-driven cavity" by the "energy error indicator" (left), "weighted indicator" (right)



Sequence of refined meshes for the "heat-driven cavity" with $N = 523, 5530, 56077$ cells: "energy" error indicator (upper row), "weighted" error indicator (lower row)

(IV) Complex interaction: Chemically reactive flows (M. Braack 2001)

"Low-Mach number" approximation of stationary reactive flow (Changes in energy equation and additional equations for the mass fractions of the chemical species $(w_i)_{i=1}^N$:

$$
\begin{aligned}
\rho\nabla\cdot v - \theta^{-1} v\cdot\nabla\theta + M^{-1} v\cdot\nabla M &= 0 \\
\rho v\cdot\nabla v + \nabla\cdot(\mu\nabla v) + \nabla p &= \rho g \\
\rho v\cdot\nabla\theta + c_p^{-1}\nabla\cdot(\kappa\nabla\theta) &= c_p^{-1} h(\theta, w) \\
\rho v\cdot\nabla w_i + \nabla\cdot(\rho D_i M_i^{-1}\nabla[M w_i]) &= f_i(\theta, w), \quad i = 1, \dots, N \\
\rho &= \frac{p_{\mathrm{th}}}{R\theta}
\end{aligned}
$$

Details of model:

- w_i mass fraction, M_i molar mass and c_i concentration of specie i: $\quad 0 \le w_i \le 1\,,$

$$\sum_{i=1}^{n_s} w_i = 1, \quad M := \Big(\sum_{i=1}^{N} M_i^{-1} w_i\Big)^{-1}, \quad c_i = M_i^{-1} \rho w_i$$

- Elementary chemical reaction:

$$\sum_{i=1}^{n_s} a_{ir} \chi_i \xrightarrow{k_r} \sum_{i=1}^{n_s} \tilde{a}_{ir} \chi_i$$

- Production rate $\dot{\omega}_i$ for species i:

$$\dot{\omega}_i(T, w) = \sum_{r=1}^{n_r} \Big\{ (\tilde{a}_{ir} - a_{ir}) k_r(T) \prod_{j=1}^{n_s} c_j^{a_{jr}}(w) \Big\}$$

- Chemical source term for specie i :

$$f_i(T,w) = M_i\,\dot{\omega}_i(T,w), \qquad \sum_{i=1}^{n_s} f_i = 0$$

- Arrhenius-law for temperature-dependence:

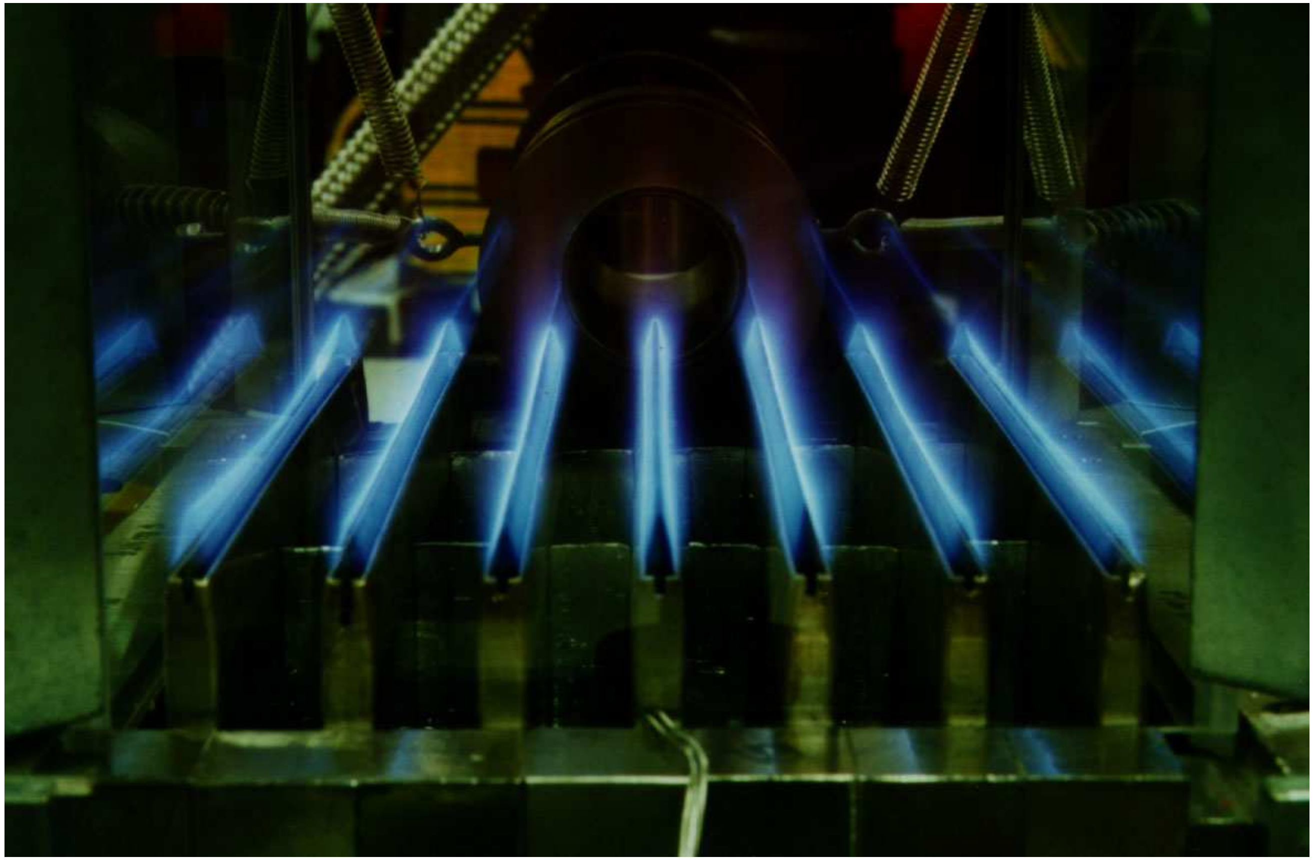
$$k_r(T) = A_r T^{\beta_r} \exp\left\{\frac{-E_{ar}}{RT}\right\}$$

- Further quantities to be modelled:

$$\mu(\theta,w), \quad \kappa(\theta,w), \quad c_p(\theta,w), \quad D_i(\theta,w), \quad h(\theta,w)$$

Application: flame diagnostics of a 2-D lamella burner

Laminar combustion of methane in a gas burner; control the production of the critical pollutants NO_x .



The inflow is CH_4, O_2, and N_2, with a flow velocity of $0.2\,m/s$, and a thermodynamical pressure of $P_{th} = 1\,bar$. The flow velocity increases up to $1.0\,m/s$ and the combustion is kept laminar.

The error control functional is a weighted line-mean value of CH_2O,

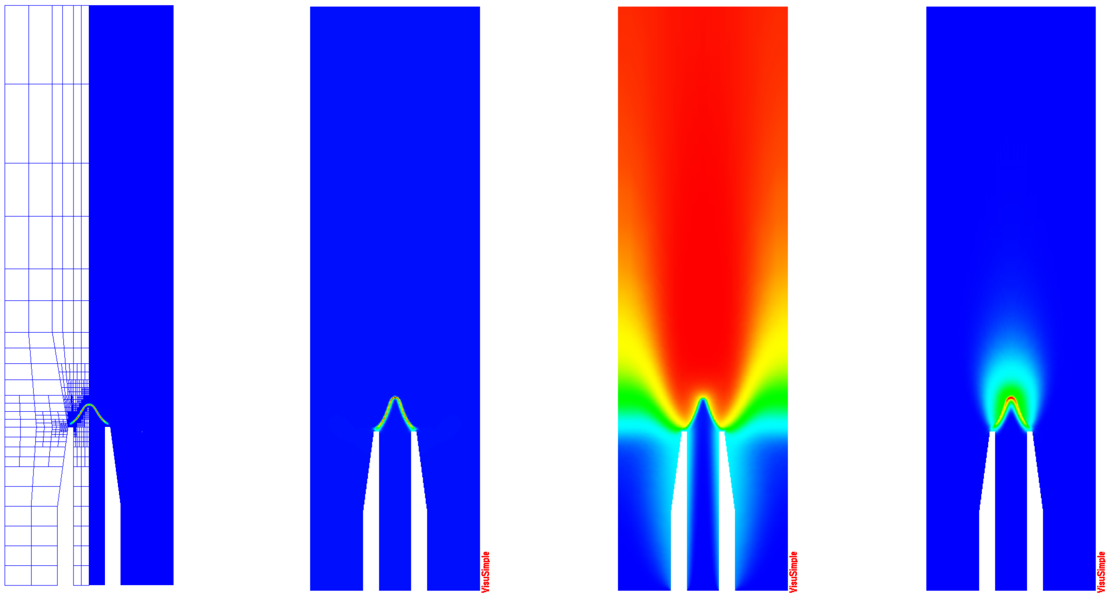
$$J(u) := \int_\Gamma w_{CH_2O}(s)\sigma(s)\,ds$$

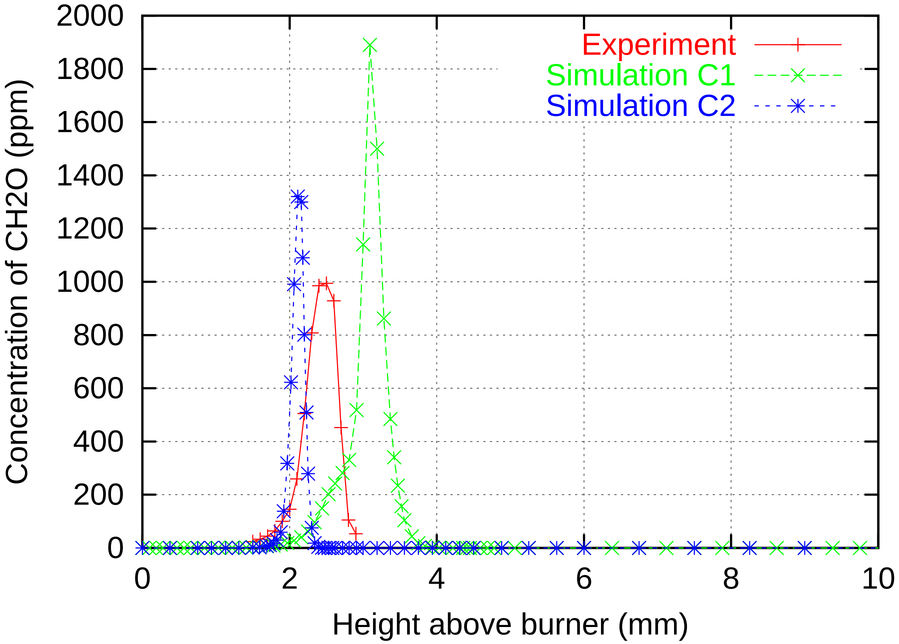
Chemistry model:

- 17 species (C1 mechanism [Smooke]) $-$ **22 PDE**
- 39 species (C2 mechanism [Warnatz]) $-$ **44 PDE**

Reaction	A_i	β_i	$E_{a,i}$
$CH_4+X = CH_3+H+X$	$6.30e14$	0	435.14
$CH_4+O_2 = CH_3+HO_2$	$7.90e13$	0	234.30
$CH_4+H = CH_3+H_2$	$2.20e04$	3.00	36.61
$CH_4+O = CH_3+OH$	$1.60e06$	2.36	30.96
$CH_4+OH = CH_3+4H_2O$	$1.60e06$	2.10	10.29
$CH_2O+OH = HCO+H_2O$	$7.53e12$	0	0.70
$CH_2O+H = HCO+H_2$	$3.31e14$	0	43.93
$CH_2O+X = HCO+H+X$	$3.31e16$	0	338.90
$CH_2O+O = HCO+OH$	$1.81e13$	0	12.90
$HCO+OH = CO+H_2O$	$5.00e12$	0	0
$HCO+X = CO+H+X$	$7.14e14$	0	70.29
$HCO+H = CO+H_2$	$4.00e13$	0	0
$HCO+O = OH+CO$	$1.00e13$	0	0
$HCO+O_2 = CO+HO_2$	$3.00e12$	0	0
$CO+O+X = CO_2+X$	$7.10e13$	0	-19.00
$CO+OH = CO_2+H$	$1.51e07$	1.30	-3.17
$CO+O_2 = CO_2+O$	$1.60e13$	0	171.54
$CH_3+O_2 = CH_3O+O$	$7.00e12$	0	107.33
$CH_3O+X = CH_2O+H+X$	$2.40e13$	0	120.55
$CH_3O+H = CH_2O+H_2$	$2.00e13$	0	0
$CH_3O+OH = CH_2O+H_2O$	$1.00e13$	0	0
$CH_3O+O = CH_2O+OH$	$1.00e13$	0	0

Part of C1 mechanism of methane/air reaction with 17 species (X, Y, Z any of the participating species)





Zoom into C_2H_3-concentration (not contained in the smaller mechanism) and refined mesh (left), CH_2O-concentration (middle), OH-concentration (right)

Comparison simulation - measurements (PCI Heidelberg, J. Wolfrum)

Computational cost:

- "Small" mechanism with **17 species in 2D**:
  number of cells $65\,880$, number of unknowns $1\,415\,842$
  CPU time **14 hours** on a single PC

- "Large" mechanism with **39 species in 3D**:
  number of cells $291\,102$, number of unknowns $14\,299\,478$
  CPU time **24 hours** on a 32-PC-system

- not treatable on uniform meshes

Need for complexity reduction

- by "goal-oriented" mesh adaptation

- by model reduction

9.38

9.40

10. Miscellaneous and open problems

Topics to be discussed:

1. *Use of error representations for postprocessing*
2. *Anisotropic mesh adaptation*
3. h/p adaptivity
4. Model adaptivity
5. *Towards theoretical justification*
6. Current developments and open problems

10.1 Use of error representations for postprocessing

Poisson equation in 2D written in variational form

$$a(u,\varphi) = (f,\varphi) \quad \forall \varphi \in V$$

$$a(u_h,\varphi_h) = (f,\varphi_h) \quad \forall \varphi_h \in V_h$$

The target functional is $J(\cdot)$ and $z \in V$ the corresponding dual solution with $z_h \in V_h$ its Ritz projection. There holds

$$J(u) = a(u,z) = (f,z)$$

$$J(u) = J(u_h) + a(e,z) = J(u_h) + \rho(u_h)(z - z_h)$$

$$\rho(u_h)(z - z_h) = (f, z - z_h) - a(u_h, z - z_h)$$

With the patchwise biquadratic interpolation $\tilde{z}_h := I_{2h}^{(2)} z_h$ of z_h on the mesh $\mathbb{T}_h$:

$$J(e) \approx \rho(u_h)(\tilde{z}_h - z_h) = \rho(u_h)(\tilde{z}_h)$$

Rewriting this relation as

$$J(u) \approx \tilde{\mathbf{J}}_{\mathbf{1}}(\mathbf{u_h}) := \mathbf{J}(\mathbf{u_h}) + (\mathbf{f}, \tilde{\mathbf{z}}_{\mathbf{h}}) - \mathbf{a}(\mathbf{u_h}\tilde{\mathbf{z}}_{\mathbf{h}})$$

we obtain a new (better?) approximation to $J(u)$. Indeed,

$$J(u) - \tilde{J}_1(u_h) = J(e) - \rho(u_h)(\tilde{z}_h) = a(e, z) - a(u_h, \tilde{z}_h) = a(e, z - \tilde{z}_h)$$

which implies

$$|J(u) - \tilde{J}_1(u_h)| \leq \|\nabla e\| \, \|\nabla(z - \tilde{z}_h)\|$$

Since it is not clear whether $\tilde{z}_h$ is a reasonably better approximation to z than z_h, this estimate is of only questionabls value. Further, the two energy-norm errors correspond both to the "primal" mesh $\mathbb{T}_h$ and can therefore not be minimized independently.

Proposition. *Let $\mathbb{T}_h$ and $\mathbb{T}_h^*$ be two independent meshes and V_h and V_h^* corresponding finite element spaces in which the Ritz projections u_h and z_h^* of u and z are computed. Further, denote by $\tilde{z}_h^*$ the patchwise biquadratic interpolation of z_h^* on the dual mesh $\mathbb{T}_h^*$. Then, for the post-processed approximation*

$$\tilde{\mathbf{J}}_{\mathbf{2}}(\mathbf{u_h}) := \mathbf{J}(\mathbf{u_h}) + (\mathbf{f}, \tilde{\mathbf{z}}_{\mathbf{h}}^*) - \mathbf{a}(\mathbf{u_h}, \tilde{\mathbf{z}}_{\mathbf{h}}^*),$$

there holds the estimate

$$|\mathbf{J}(\mathbf{u}) - \tilde{\mathbf{J}}_{\mathbf{2}}(\mathbf{u_h})| \leq \|\nabla \mathbf{e}\| \, \|\nabla(\mathbf{z} - \tilde{\mathbf{z}}_{\mathbf{h}}^*)\|.$$

Here, the two energy-norm terms can be minimized independently by optimizing the primal and dual meshes $\mathbb{T}_h$ and $\mathbb{T}_h^*$.

Proof. We have

$$\begin{aligned} J(u) - \tilde{J}_2(u_h) &= J(u) - J(u_h) - \rho(u_h)(\tilde{z}_h^*) \\ &= (f, z) - a(u_h, z) - (f, \tilde{z}_h^*) + a(u_h, \tilde{z}_h^*) \\ &= (f, z - \tilde{z}_h^*) - a(u_h, z - \tilde{z}_h^*) \\ &= a(e, z - \tilde{z}_h^*) \end{aligned}$$

This implies the assertion. Q.E.D.

One may hope to obtain an even better approximation by

$$\mathbf{\tilde{J}_3(u_h) := \tilde{J}_2(\tilde{u}_h) = J(\tilde{u}_h) + (f, \tilde{z}_h^*) - a(\tilde{u}_h, \tilde{z}_h^*)},$$

where $\tilde{u}_h$ is the patchwise biquadratic interpolation of u_h .

Numerical test (Th. Richter 2002)

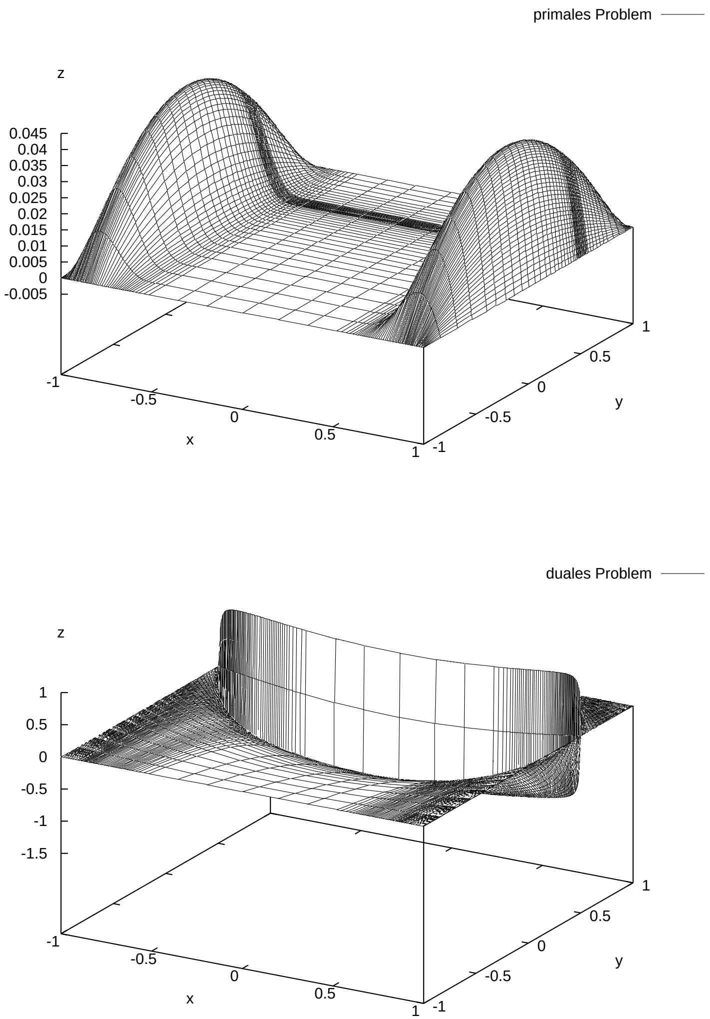
Model Poisson problem with $\Omega = (-1,1)^2$,

$$u(x) = (1-x_1^2)(1-x_2^2)\exp(1-x_2^{-4})$$

and the error functional

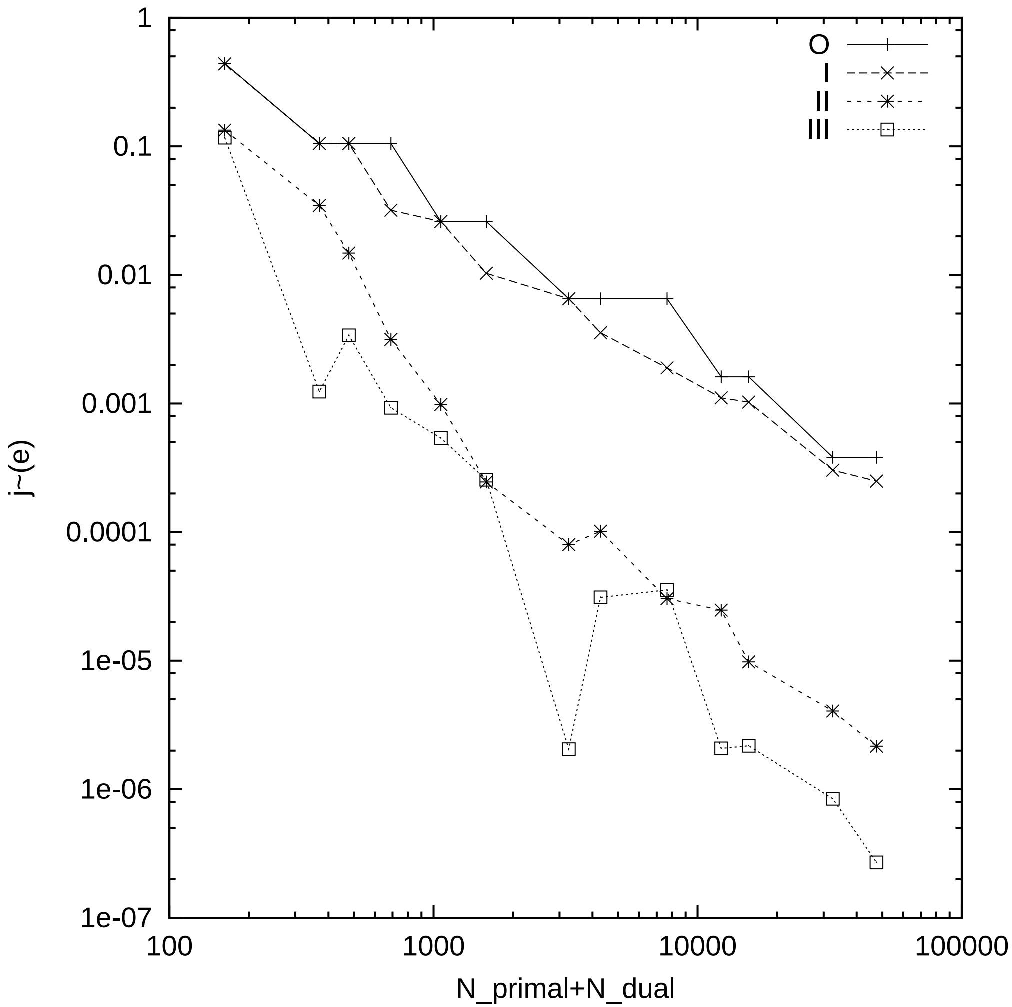
$$J(u) = \int_{-1}^{1} u(x_1,0)\,dx$$

In this example primal and dual solution have irregularities at different locations such that is is to expected that maximal efficiency is achieved using different meshes for u_h and z_h.



Primal (left) and dual (right)

solution of the model problem



Mesh efficiencies of postprocessing

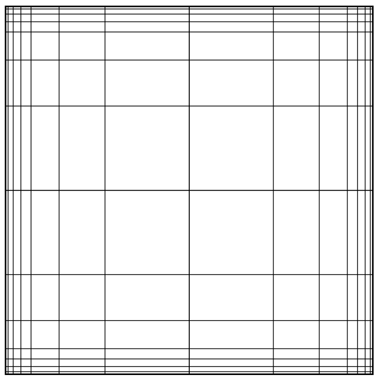
The results show the mesh efficiencies of $J(u_h)$ and the three post-processed approximations $\tilde{J}_1(u_h)$, $\tilde{J}_2(u_h)$ and $\tilde{J}_3(u_h)$. The mesh refinements are driven by energy-norm error indicators as derived before separately on the primal and dual meshes $\mathbb{T}_h$ and $\mathbb{T}_h^*$, respectively. We see that $\tilde{J}_1(u_h)$ does not bring significant adventages over the original approximation $J(u_h)$. The two other approximations $\tilde{J}_2(u_h)$ and $\tilde{J}_3(u_h)$ which use different meshes for u and z are clearly superior and show a mesh complexity like $TOL \approx N^{-2}$ ($N = N_{\text{primal}} + N_{\text{dual}}$).

10.2 Towards anisotropic mesh adaptation

Sometimes *isotropic* mesh refinement as discussed so far is not efficient for properly resolving certain features of the solution. For example, in singular perturbed problems of the form

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

with small coefficient ϵ, boundary layers may occur in which the solution has large derivative in normal direction to the boundary derivative while it varies only slowly in tangential direction.



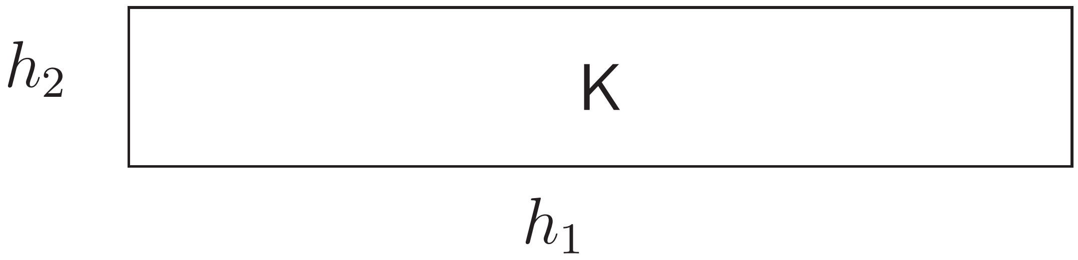
We consider adaptive cell stretching alone and, for simplicity, concentrate on the construction of "optimal" cartesian tensor-product meshes. Starting form an error representation of the form

$$J(e) = \sum_{K\in\mathbb{T}_h} \left\{ (f+\Delta u_h, z-I_h z)_K - \tfrac{1}{2}([\partial_n u_h], z-I_h z)_{\partial K\setminus\partial\Omega} \right\}$$

we have to adress the following questions:

- How to detect anisotropic behavior of the true solutiopn u?
- How to detect anisotropic behavior of the dual solution z?
- How to obtain an indicator for "optimal" cell stretching?
- *How to obtain an indicator for "optimal" cell orientation?*

Suppose that the domain's boundary and the mesh are oriented along the coordinate axes. Then any cell $K \in \mathbb{T}_h$ is characterized by its widths h_i in the x_i-directions.



On an edge Γ the edge-residual terms contain information about second derivatives of the primal and dual solutions u and z, e.g., on a vertical edge:

- jump terms: $\quad [\partial_1 u_h]_\Gamma \approx h_1 \partial_1^2 u_{|\Gamma}$
- weights: $\quad (z - I_h z)_{|\Gamma} \approx h_2^2 \partial_2^2 z_{|\Gamma}$

Assuming the second-order derivatives of u as constant, we obtain

$$
\begin{aligned}
|([\partial_n u_h], z - I_h z)_{\partial K}| &\approx h_1^3 h_2 |\partial_2^2 u|\,|\partial_1^2 z| + h_1 h_2^3 |\partial_1^2 u|\,|\partial_2^2 z| \\
&= |K|\big\{h_1^2 |\partial_2^2 u|\,|\partial_1^2 z| + |K|^2 h_1^{-2} |\partial_1^2 u|\,|\partial_2^2 z|\big\}
\end{aligned}
$$

Minimizing this with respect to h_1, for fixed $|K|$, yields the necessary condition

$$
2h_1 |\partial_2^2 u|\,|\partial_1^2 z| - 2|K|^2 h_1^{-3} |\partial_1^2 u|\,|\partial_2^2 z| = 0 \quad \Rightarrow \quad h_1^4 = |K|^2 \frac{|\partial_1^2 u|\,|\partial_2^2 z|}{|\partial_2^2 u|\,|\partial_1^2 z|}
$$

and, consequently,

$$
(I) \qquad \frac{h_1^2}{h_2^2} \approx \frac{|\partial_1^2 u|\,|\partial_2^2 z|}{|\partial_2^2 u|\,|\partial_1^2 z|}
$$

Remark. This result is counter-intuitive as it does not indicate the optimal cell stretching in accordance with interpolation theory:

Consider the case that u is linear in x_1-direction, i.e., $\partial_1^2 u \equiv 0$, and that z is isotropic. Then, the formula would suggest to refine the cell in x_1 direction which is evidently the wrong decision. It seems that considering only the edge terms in the error estimate, as commonly suggested for low-order elements, is not appropriate.

In view of this observation, we now follow a more heuristic approach and base the anisotropic cell adaptation on an estimate for the interpolation error. We recall the anisotropic interpolation error

$$\|\nabla(u - I_h u)\|_K \le c\left(h_1^2\|\partial_1\nabla u\|_K^2 + h_2^2\|\partial_2\nabla u\|_K^2\right)^{1/2}$$

Hence, assuming the second derivatives as constant on K, we have

$$\|\nabla(u - I_h u)\|_K \le c|K|^{1/2}\left(h_1^2|\partial_1\nabla u|^2 + |K|^2 h_1^{-2}|\partial_2\nabla u|^2\right)^{1/2}$$

Minimizing this with respect to h_1, for fixed $|K|$, results in

$$2h_1|\partial_1\nabla u|^2 - 2|K|^2 h_1^{-3}|\partial_2\nabla u|^2 = 0 \quad \Rightarrow \quad h_1^2 = |K|\frac{|\partial_2\nabla u|}{|\partial_1\nabla u|}$$

and, consequently,

$$\frac{h_1}{h_2} \approx \frac{|\partial_2\nabla u|}{|\partial_1\nabla u|}$$

In view of this result, we now consider the heuristic error indicator

$$\eta_K := \|\nabla(u - I_h u)\|_K \|\nabla(z - I_h z)\|_K$$

which is minimized for

$$(II) \qquad \frac{h_1^2}{h_2^2} \approx \frac{|\partial_2\nabla u|\,|\partial_2\nabla z|}{|\partial_1\nabla u|\,|\partial_1\nabla z|}$$

This relation simultaneously reflects possible anisotropies in the primal and also the dual solution.

Numerical tests (Th. Richter 2001)

Test problem

$$-\Delta u = f \quad \text{in } \Omega = (-1,1)^2, \qquad u_{|\partial\Omega} = 0$$

Test case 1. Solution

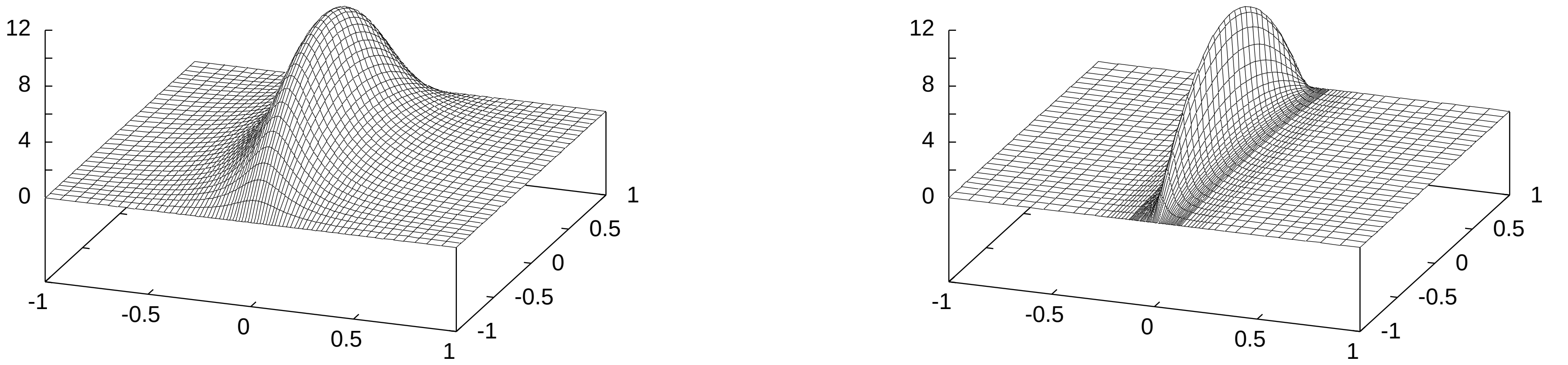
$$u(x) = (1-x_1^2)^2(1-x_2)^2(kx_1^2+0.1)^{-1}$$

where the parameter $k = 1, 4, 16, 64, \ldots,$ determines the strength of the anisotropy. The right hand side is determined as $f := -\Delta u$.

Target quantity:

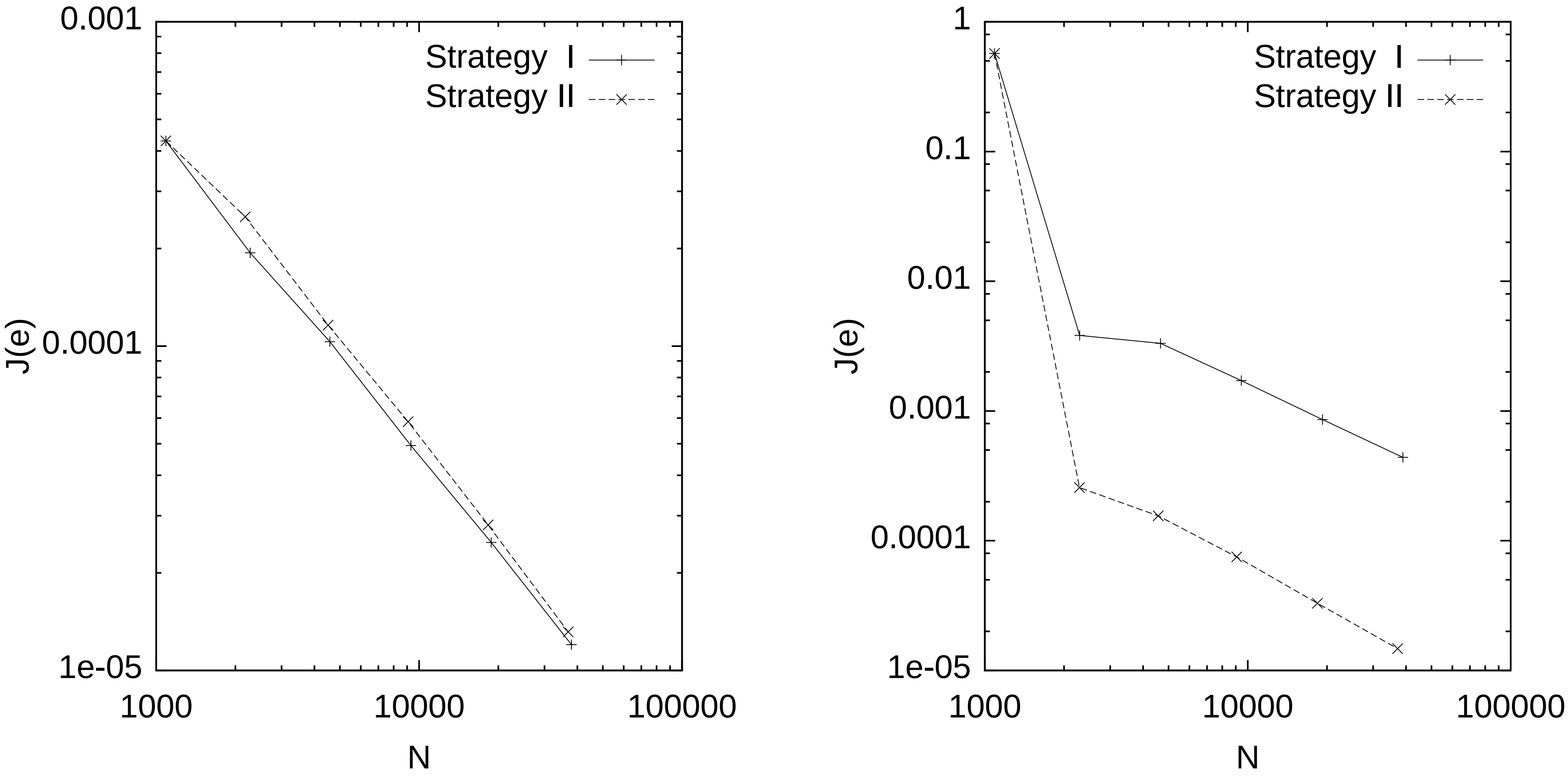
$$J(u) := |\Omega|^{-1} \int_\Omega u \, dx$$

The anisotropy is only in the primal solution while the dual solution satisfies $-\Delta z = 1$ and is isotropic.



Anisotropic solutions for $k = 4$ (left) and $k = 64$ (right)

The computation starts from a coarse uniform tensor-product mesh which is then successively adapted on the basis of the relations (I) and (II)

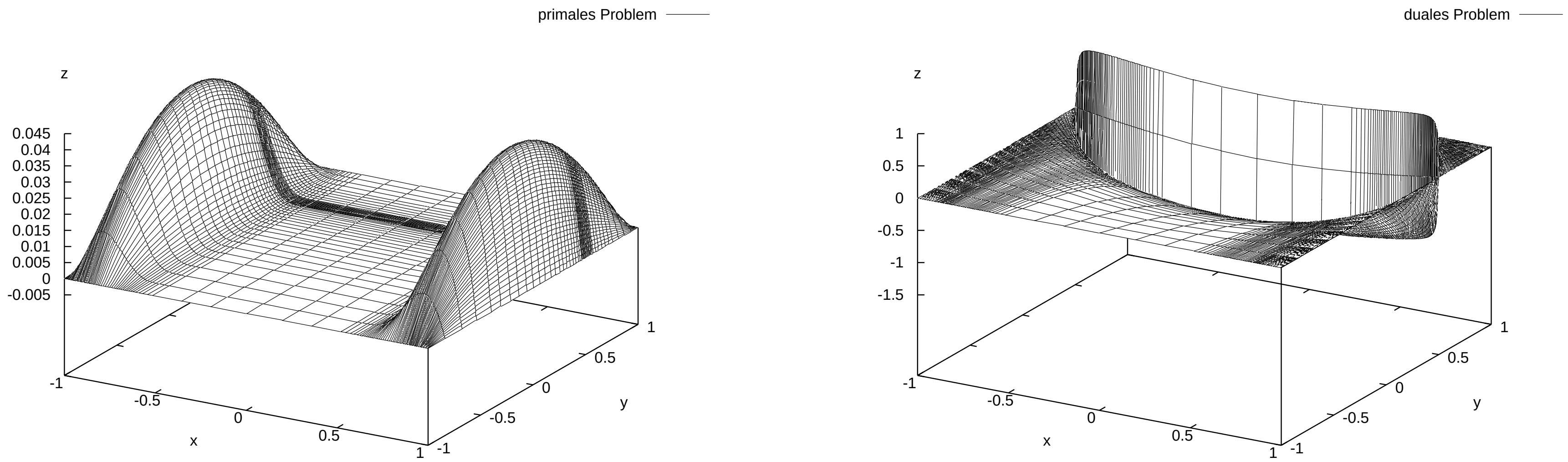


Mesh efficiencies of anisotropic refinement by Strategy I and Strategy II,

for $k = 1$ (left) and $k = 64$ (right)

Test 2. Solution and functional

$$u(x) := (-x_1^2)(1-x_2^2)\exp(-x_1^{-4}), \qquad J(u) := \int_{-1}^{1} \partial_2 u(x_1, 0.5)\, dx_1$$



Primal and dual solution of Test 2

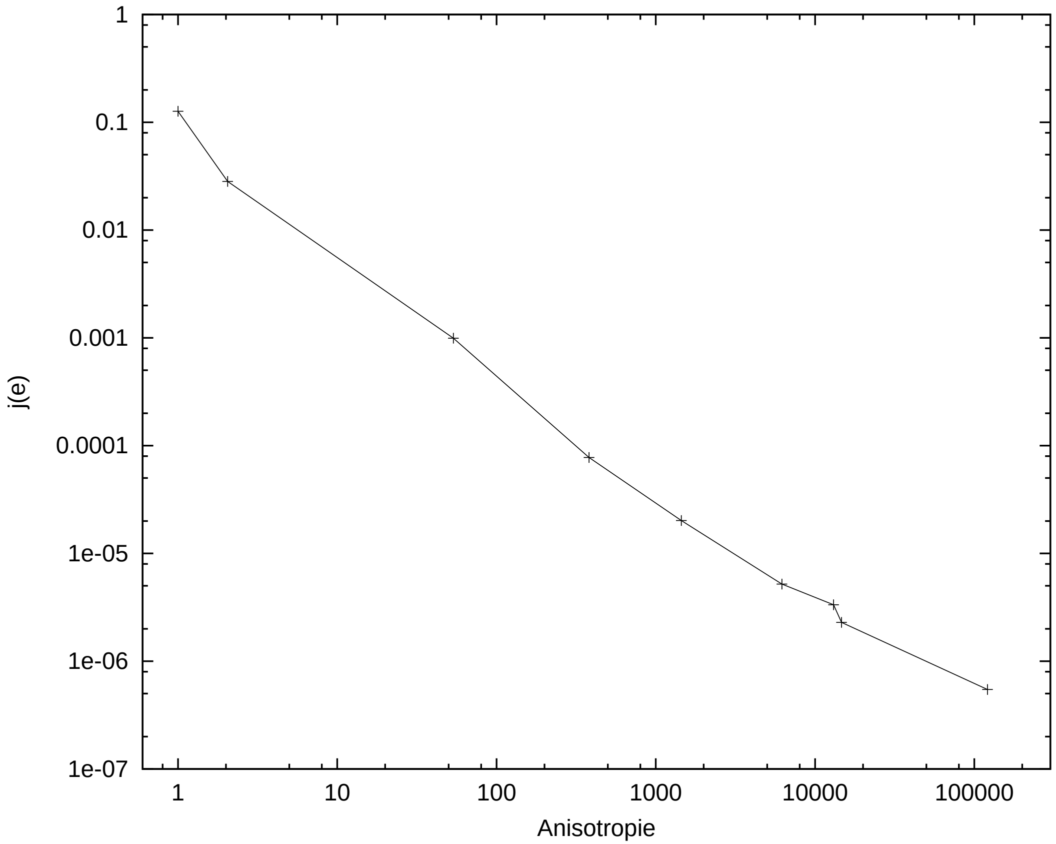
N	$J(e)$	I_{eff}	$A_{\max}$
81	$4.5 \cdot 10^{-1}$	1.82	1
289	$7.4 \cdot 10^{-2}$	2.34	22
1035	$2.5 \cdot 10^{-3}$	2.11	25
3735	$1.2 \cdot 10^{-3}$	1.73	163
13137	$2.3 \cdot 10^{-4}$	2.18	782
46269	$1.2 \cdot 10^{-5}$	13.72	20 433

Computation of $J(u)$ following strategy (I)

($A_{\max}$ maximum aspect ratio of cells)

Test 3. Solution and functional

$$u(x) := (1-x_1^2)(1-x_2^2)(1-x_1), \qquad J(u) := \int_{\partial\Omega} \partial_n u \, ds$$



Mesh efficiency $TOL \sim 1/N$ in Test 3

10.3 h/p adaptivity

In the following, we will briefly discuss the extension of the DWR approach to a posteriori error control to higher-order finite elements. Let $V_h^{(p)} \subset V$, be finite element spaces of oder $p+1$. We recall the error representation,

$$J(e) = \sum_{K \in \mathbb{T}_h} \left\{ (R(u_h), z - I_h^{(p)} z)_K + (r(u_h), z - I_h^{(p)} z)_{\partial K} \right\}$$

with the cell and edge residuals $R(u_h)$ and $r(u_h)$ as defined above and some local interpolation $I_h^{(p)} z \in V_h^{(p)}$. The evaluation of this identity for use as an error estimator may be done in a similar way as in the low-order case $p = 1$ employing a patchwise $(p+1)$-degree interpolation $I_{2h}^{(p+2)} z_h$ of the Ritz projection $z_h \in V_h^{(p)}$.

On the basis of the a posteriori error estimator $\eta(u_h)$ and the resulting local error indicators η_K, "optimal" distributions of h_K and p_K are constructed by a series of adaptation cycles such that at the final stage the equilibration property is achieved:

$$\eta_K \approx \frac{TOL}{N_h}, \qquad N_h = \#\{K \in \mathbb{T}_{\text{opt}}\}$$

Let a tolerance TOL be given. In solving a stationary problem the adaptation process usually starts from a coarse mesh $\mathbb{T}_h^{(0)}, k = 1, 2, \dots,$ with mesh-size distribution $h^{(0)}$ and polynomial degree $p^{(0)} \equiv 1$. Then, a sequence of meshes $T_h^{(k)}, k = 1, 2, \dots,$ with corresponding distributions $h_K^{(k)}$ and $p_K^{(k)}$ is constructed by the following process:

1. On the mesh $\mathbb{T}_h^{(k)}$ compute $u_h^{(k)}$, $z_h^{(k)}$, and evaluate $\eta_\omega(u_h^{(k)})$ and the cell-error indicators η_K. If $\eta(u_h^{(k)}) < TOL$, then STOP.

2. Order cells according to the size of η_K. On each cell $K \in \mathbb{T}_h^{(k)}$ test whether

$$\eta_K < \frac{1}{2}\frac{TOL}{N_h}? \qquad N_h = \#\{K \in \mathbb{T}_h^{(k)}\}$$

   If YES, procede to next cell. If NO, consider the three cases:

   - Cell K and the polynomial degree p_K had been left unchanged in the preceding cycle. Then, leave K again unchanged but increase p_K to $p_K + 1$.

   - Cell K had been left unchanged in the preceding cycle, but p_K had been increased. Check whether

$$\eta_K < h_K \eta_K^{\text{old}}.$$

If YES, then again increase p_K to $p_K + 1$. If NO, then refine K into 2^d cells.

- Cell K had been obtained by refinement of a mother cell $K_m \in \mathbb{T}_h^{(k-1)}$ (without changing p_K). Check whether

$$\eta_K \leq 2^{-p_K - 1} \eta_{K_m}^{\text{old}} \,?$$

If YES, increase p_K to $p_K + 1$ and keep h_K. If NO, keep p_K and refine K into 2^d cells.

3. The local changes of h_K and p_K may cause additional hanging nodes and discontinuity of functions. To keep conformity neighboring cells need to be refined and polynomial degrees raised.

We try to raise p_K whenever possible. The philosophy underlying this rule is that usually for enhancing accuracy on a cell K it is more economical to raise p_K rather than to reduce h_K.

Numerical test (V. Heuveline 2003)

The computational domain is $\Omega = (-1,1) \times (-1,3)$ with and without a vertical slit with tip at $(0,0)$. The error $J(e)$ is estimated by the error estimator $\eta_\omega := \eta_\omega(u_h)$ which is evaluated by the procedure described above. The quality of the error estimate is expressed in terms of the "effectivity index"

$$I_{\text{eff}} := \left| \frac{\eta_\omega(u_h)}{J(e)} \right|.$$

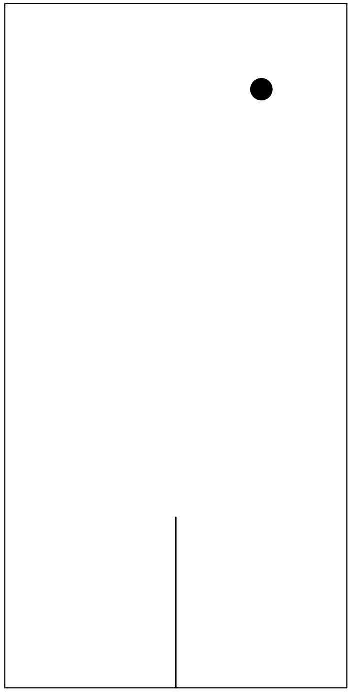
We monitor the number of degrees of freedom $N := \dim V_h^p$, the actual error $J_\omega = J_\omega(e)$ obtained by the DWR method, and the error $J_{\mathrm{E}}(e)$ obtained by a standard energy-type error estimator:

$$\eta_{\mathrm{E}}(u_h) := \Big(\sum_{K \in \mathbb{T}_h} h_K^2 p_K^{-2} \|f + \Delta u_h\|_K^2 + \tfrac{1}{2} h_K p_K^{-1} \|[\partial_n u_h]\|_{\partial K}^2 \Big)^{1/2}$$

The semi-singular case: On $\Omega_0 = (-1,1) \times (-1,3)$, we compute the derivative point value $J(u) := \partial_1 u(x_0)$, $x_0 = (0.5, 2.5)$. The solution is $u(x) = \sin(\pi(x_1+1)/2)\sin(3\pi(x_2+1)/4)$.

N	$J_\omega(e)$	$N/\ln(J_\omega)^2$	$\eta_w(u_h)$	I_{eff}	$J_{\mathrm{E}}(e)$	J_{E}/J_ω
125	$3.50e-01$	113	$7.40e+00$	21.1	$4.33e-01$	1
233	$2.59e-02$	17	$3.42e-01$	13.2	$7.93e-02$	3
297	$4.19e-03$	10	$3.10e-02$	7.4	$3.59e-02$	8
412	$3.21e-04$	6	$6.75e-04$	2.1	$9.98e-03$	3
581	$3.09e-05$	5	$4.02e-05$	1.3	$5.34e-03$	173
812	$4.32e-06$	5	$5.19e-06$	1.2	$1.34e-03$	310
1113	$4.21e-07$	5	$5.06e-07$	1.1	$3.29e-04$	781

Computation of $\partial_1 u(x_0)$ for smooth solution



3	4	5	6	6	7	7	6
3	4	5	6	7	7	7	7
3	4	5	6	7	7	7	7
3	4	5	6	6	7	7	6
3	3	4	5	6	6	6	6
3	3	3	4	5	5	5	5
3	3	3	3	4	4	4	4
3	3	3	3	3	3	3	3
3	3	3	3	3	3	3	3
2	2	3	3	3	3	3	3
2	2	2	2	2	2	2	2
1	1	2	2	2	2	2	2
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1

6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6
6	7	7	7	7	7	7	6
6	7	7	7	7	7	7	6
6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6
6	7	7	7	7	7	7	6
6	7	7	7	7	7	7	6
6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6
6	7	7	7	7	7	7	6
6	7	7	7	7	7	7	6
6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6

Configuration (left), optimized distribution of p by η_ω (middle), and by η_{E} (right)

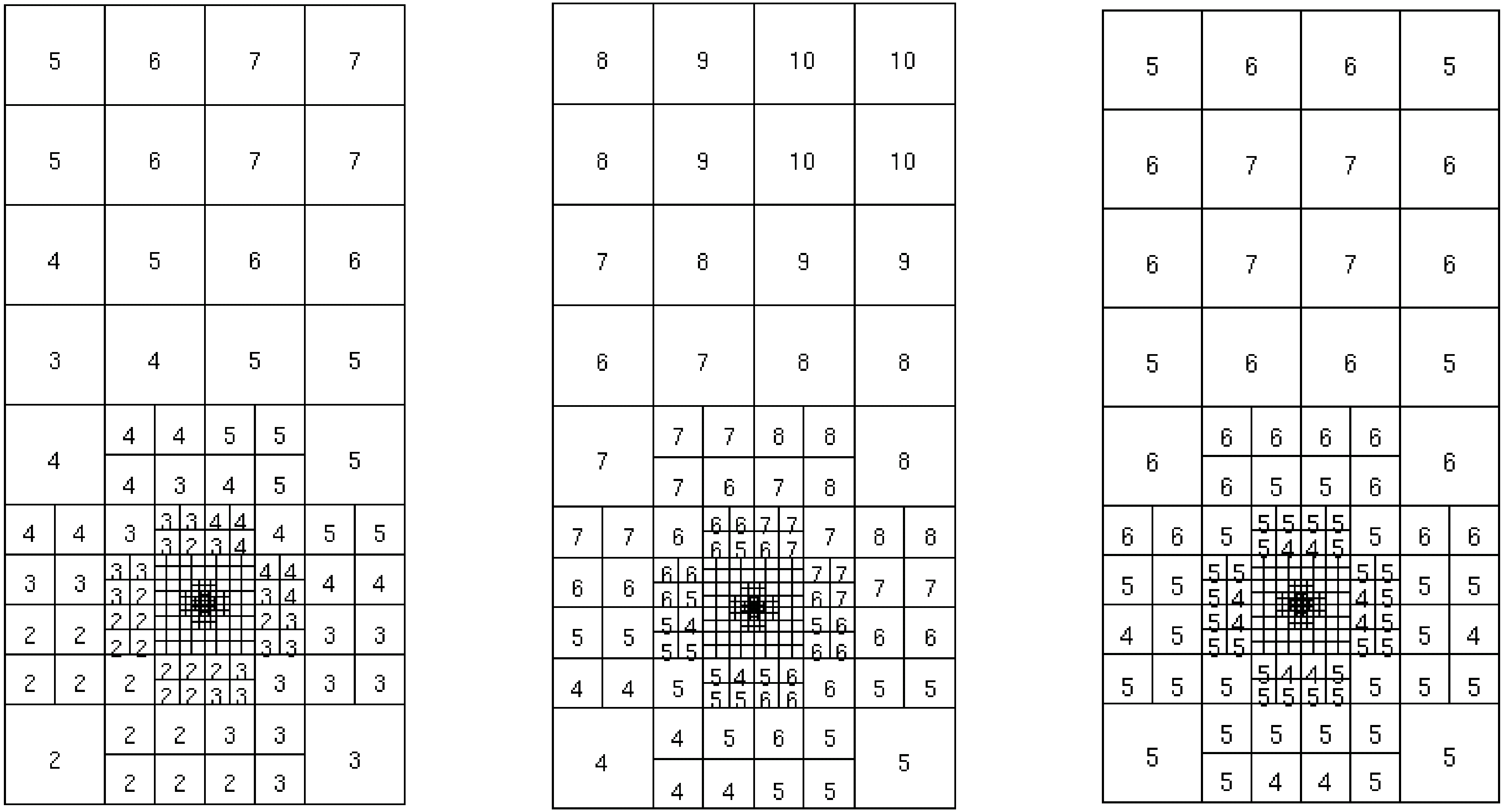
As expected the automatic adaptation process keeps the initial mesh unrefined and only raises p. We see that for computing point values, hp adaptivity based on the weighted error estimator η_ω is more efficient than that using the energy error estimator η_{E}.

The fully singular case: On the slit domain

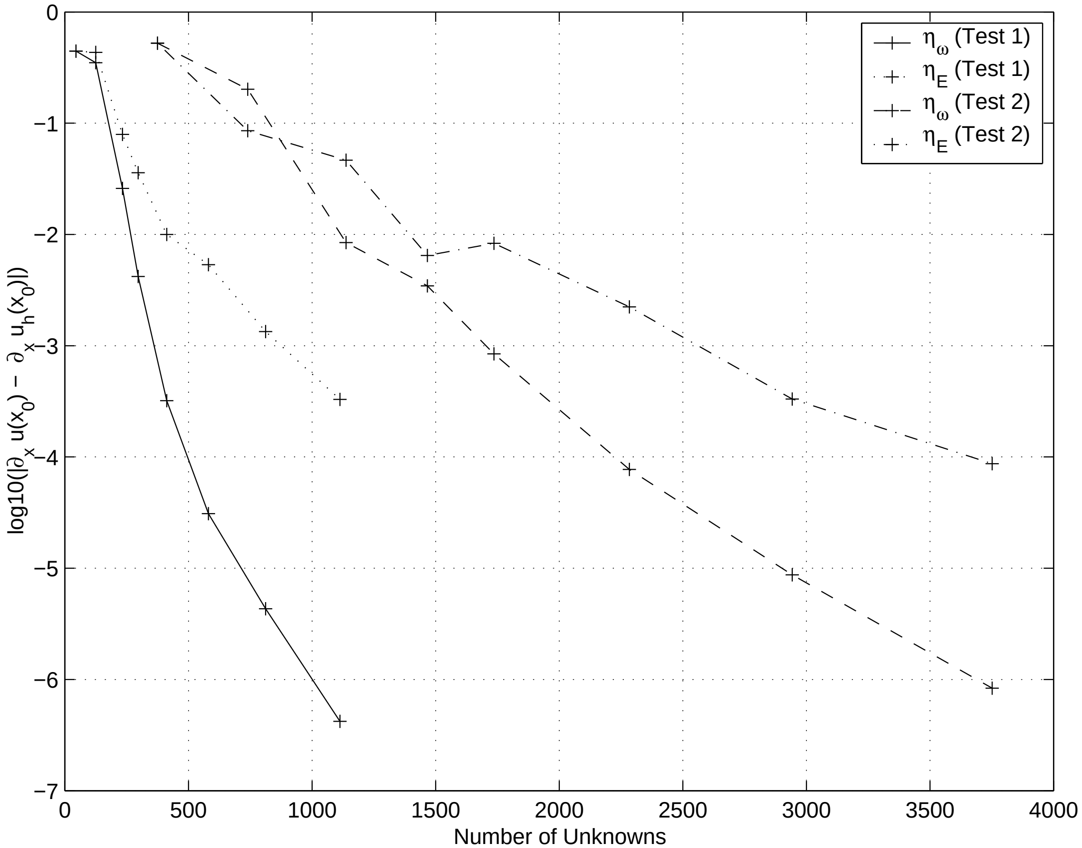
$$\Omega_1 = (-1,1) \times (-1,3) \setminus \{x \in \mathbb{R},\ x_1 = 0, -1 < x_2 < 0\},$$

we compute the derivative point value $J(u) := \partial_1 u(x_0)$. The exact solution is $u(x) = r^{1/2} \sin(\theta/2)(x_1 - 1)(x_1 + 1)(x_2 - 3)(x_2 + 1)$.

N	$J_\omega(e)$	$N/\ln(J_\omega)^2$	$\eta_w(u_h)$	I_{eff}	$J_{\mathrm{E}}(e)$	J_{E}/J_ω
1467	$3.45e-03$	45	$4.31e-02$	12.5	$6.48e-03$	2
1736	$8.43e-04$	34	$6.65e-03$	7.9	$8.32e-03$	10
2284	$7.73e-05$	25	$2.47e-04$	3.2	$2.23e-03$	29
2943	$8.72e-06$	22	$2.00e-05$	2.3	$3.32e-04$	38
3752	$8.34e-07$	19	$1.50e-06$	1.8	$8.71e-05$	104
5372	$3.34e-08$	18	$3.60e-08$	1.1	$9.32e-06$	282
6156	$4.43e-10$	15	$4.87e-10$	1.1	$1.37e-07$	309



Optimized h and p by η_ω for $TOL \approx 10^{-6}$ (left) and $TOL \approx 10^{-9}$ (middle), and by η_{E} (right)



Efficiency of hp adaptation using the weighted and the energy-error estimators

The weighted error estimator η_ω is asymptotically sharp and more efficient for computing the point value $\partial_1 u(x_0)$ than the energy-error estimator η_{E}.

10.4 Model adaptivity

The concept of residual-based adaptivity in the DWR method can be extended to the hierarchical approximation of mathematical models.

Example: Adaptation of the diffusion model in flame simulation

Balance equations for mass fractions of the chemical species w_i :

$$\rho\partial_t w_i + \rho v\cdot\nabla w_i + \nabla\cdot\mathcal{F}_i^F \;=\; f_i(\theta, w)$$

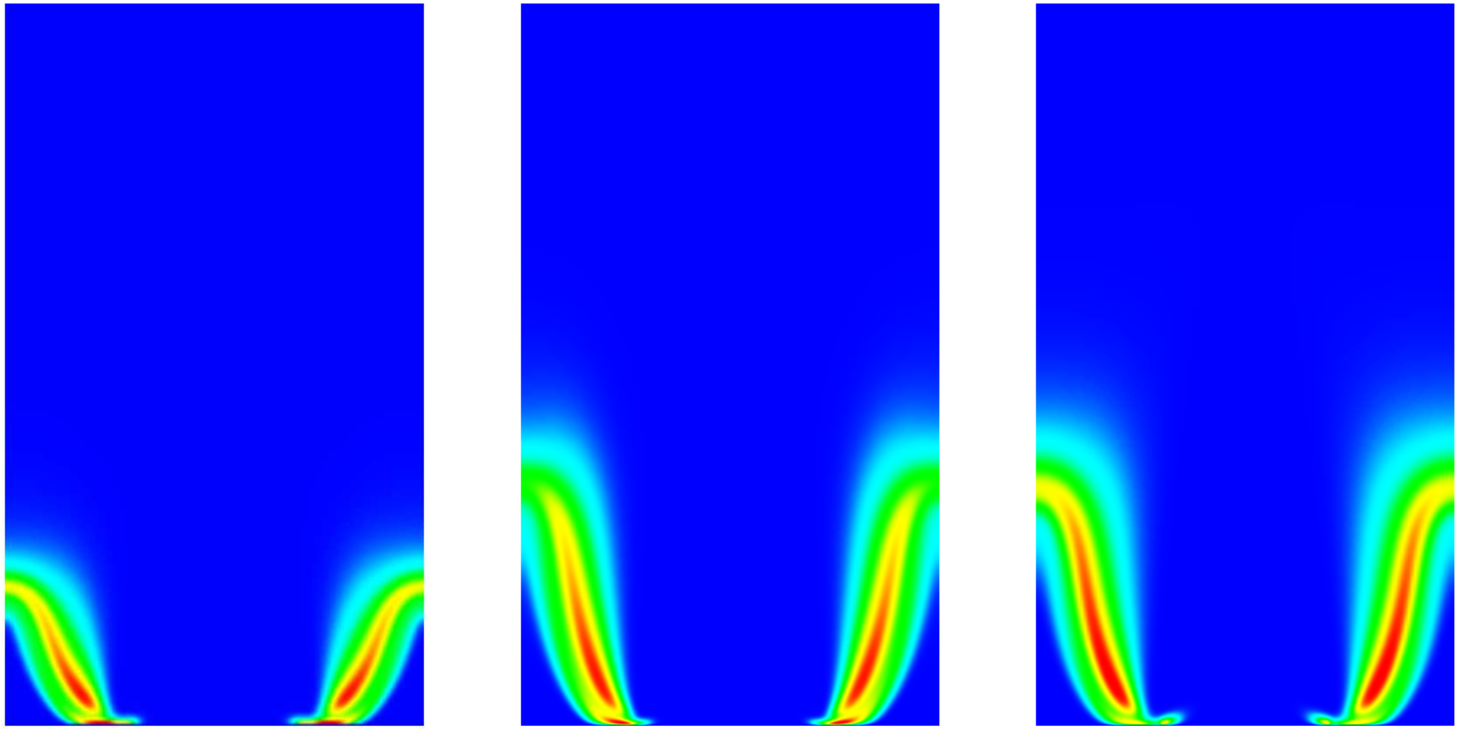
Fick's law:

$$\mathcal{F}_i^F = -\rho D_i \frac{w_i}{x_i}\nabla x_i, \quad i = 1, \dots, N$$

Reference solution obtained by taking a more accurate diffusion model (multicomponent diffusion):

$$\mathcal{F}_i^M = -\rho w_i \sum_{j\in\mathcal{S}} D_{ij}\Big(\nabla x_j + \chi_l \nabla(\log T)\Big)$$

The diffusion model has substantial impact on flame front (M. Braack and A. Ern 2002):



Initial solution with $\mathcal{F}_k^F$, optimized D_k w.r.t. "experimental" data, and reference solution with $\mathcal{F}_k^M$

Start with simple diffusion model on coarse mesh and simultaneously refine mesh and model locally on the basis of an a posteriori error estimate.

Full model

$$a(u)(\psi) + d(u)(\psi) = 0 \quad \forall \psi \in V$$

where $d(\cdot)(\cdot)$ represents the difference between the multicomponent and the Fick's diffusion model. The approximate discrete problem reads

$$a(u_h^m)(\psi_h) = 0 \quad \forall \psi_h \in V_h$$

For the error $e_h^m := u - u_h^m$, we have a perturbed Galerkin orthogonality (such as would be caused by numerical integration)

$$a(u)(\psi_h) - a(u_h^m)(\psi_h) = -d(u)(\psi_h), \quad \psi \in V$$

Dual problems

$$a'(u)(\varphi, z) + d'(u)(\varphi, z) = J'(u)(\varphi) \quad \varphi \in V$$

$$a'(u_h^m)(\varphi_h, z) = J'(u)(\varphi) \quad \varphi \in V$$

Reduced primal and dual residuals:

$$\rho(u_h^m)(\cdot) := -a(u_h^m)(\cdot)$$

$$\rho^* := J'(u_h^m)(\cdot) - a'(u_h^m)(\cdot, z_h^m)$$

Proposition. *For the combined disretization and modeling error, there holds the error identity*

$$J(u) - J(u_h) = \tfrac{1}{2}\big\{\rho(u_h^m)(z - i_h z) + \rho^*(u_h^m, z_h^m)(u - i_h u)\big\}$$
$$- \tfrac{1}{2}\big\{d(u_h^m)(e_z) + d'(u_h^m)(e_u, z_h^m)\big\} - d(u_h^m)(z_h^m) + \tfrac{1}{2} R_h^{(3)}$$

where the remainder $R_h^{(3)}$ *is cubic in the errors* e^u, e^z *.*

Proof. The proof uses a modification of the argument employed for deriving the error representation for the Galerkin approximation of general nonlinear variational equations. The difference is caused by the non-Galerkin character of the model perturbation.

Practical error estimator:

$$J(u) - J(u_h) \approx \eta_h + \eta_m$$

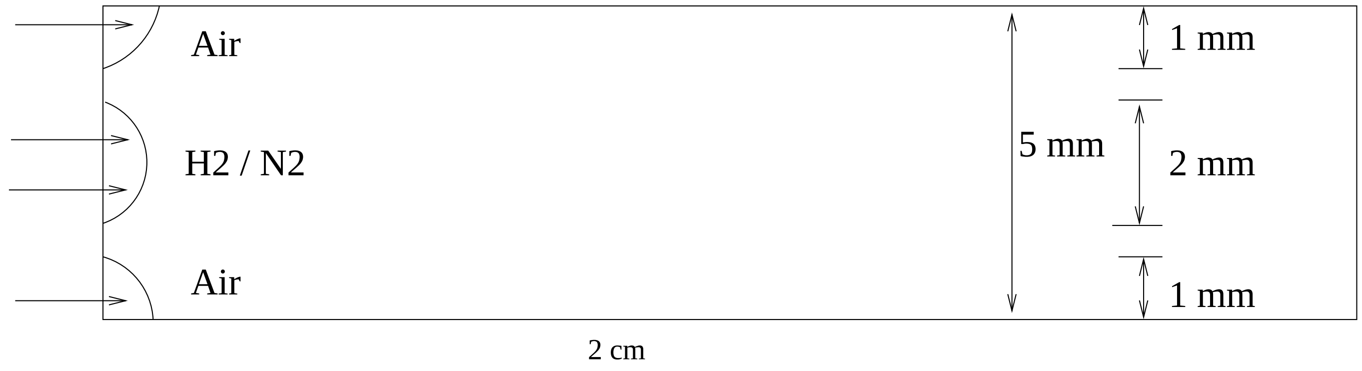
$$\begin{aligned}
\eta_h &:= \frac{1}{2}\{\rho(u_h^m)(i_{2h}^{(2)} z_h^m - z_h^m) + \rho^*(u_h^m, z_h^m)(i_{2h}^{(2)} u_h^m - u_h^m)\} \\
\eta_m &:= -d(u_h^m)(z_h^m)
\end{aligned}$$

Localization of modeling error indicator:

$$-d(u_h^m)(z_h^m) = \sum_{K \in \mathbb{T}_h} \Big(\sum_{i=1}^{N} (\mathcal{F}_i^M(u_h^m) - \mathcal{F}^F(u_h^m), \nabla z_{i,h}^m)_K \Big)$$

Configuration of test problem: Laminar ozon flame:

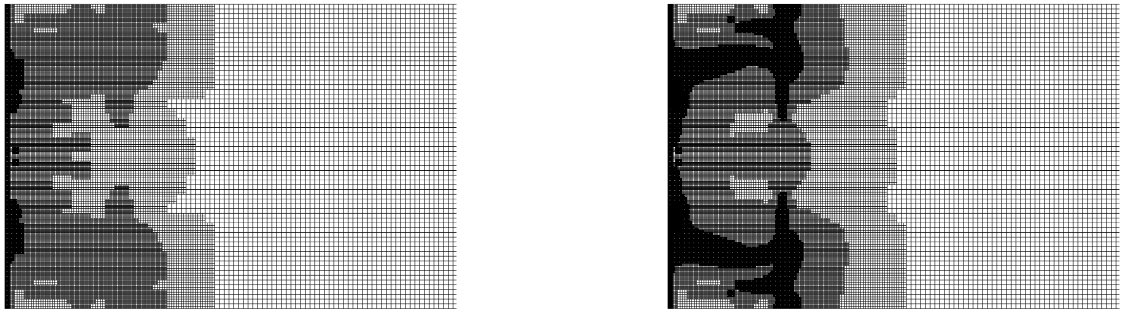
$$\begin{aligned} O_3 + M &\leftrightarrow O_2 + O + M \\ O + O + M &\leftrightarrow O_2 + M \\ O + O_3 &\leftrightarrow O_2 + O_2 \end{aligned}$$



Inflow: outer inlet N_2, O_2, inner inlet H_2, N_2

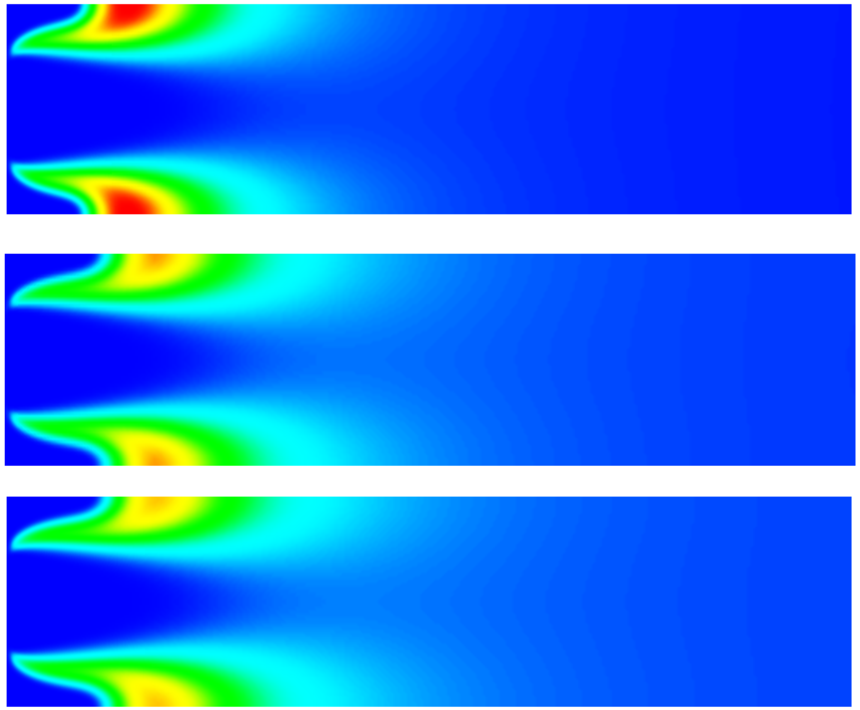
Error control functional: mass fraction of O-atoms along the middle axis:

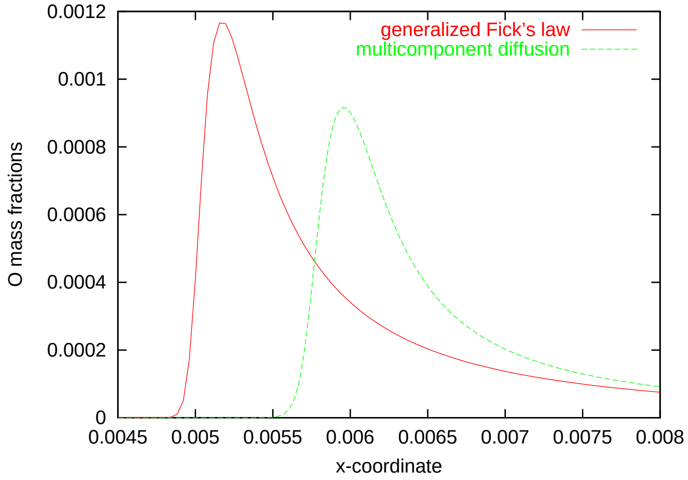
$$J(u) = \int_\Gamma y_O \, dx$$

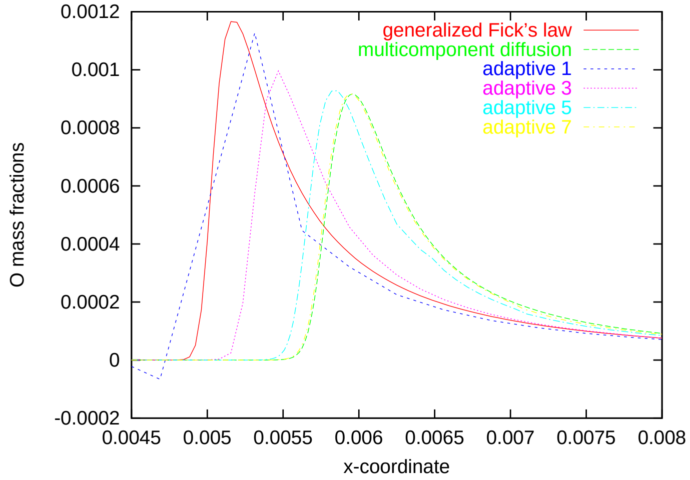


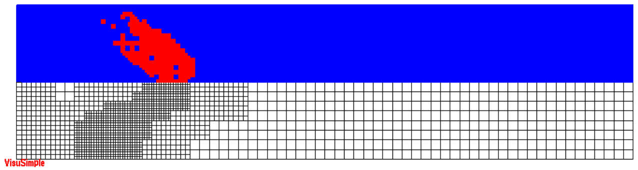
Adapted meshes with $25\,040$ and $47\,360$ cells.

Flame front obtained using Fick's law (left), 15% multicomponent diffusion, 100% multicomponent diffusion (gain in CPU time 50%)



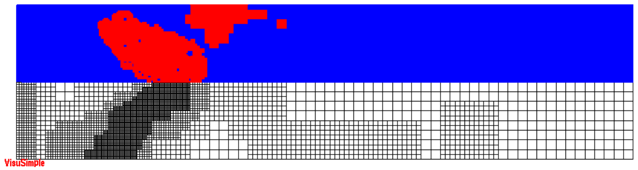






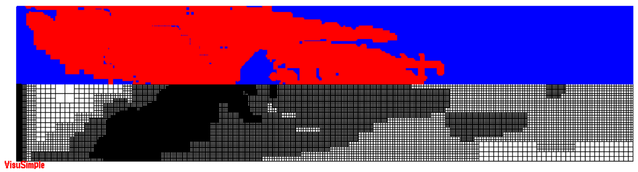
2117 nodes,

32% multi-comp' diffusion



4879 nodes,

60% multi-comp' diffusion



34477 nodes,

72% multi-comp' diffusion

Total gain: $\approx 50\%$ CPU time

4.5 Towards theoretical justification

To illustrate the problem, let us consider the special case of the evaluation of the derivative of a smooth solution $u \in C^2(\bar{\Omega})$ at some point $P \in \Omega \subset \mathbb{R}^2$. For this, we use the regularized output functional

$$J_\epsilon(u) := \frac{1}{|B_\epsilon(P)|} \int_{B_\epsilon(P)} \partial_1 u(P)\, dx = \partial_1 u(P) + \mathcal{O}(\epsilon^2)$$

with $\epsilon := TOL$.

The corresponding dual solution behaves like a regularized "derivative Green function" of the Laplacian:

$$|\nabla^k z(x)| \approx r(x)^{-k-1} := (|x-a|^2 + \epsilon^2)^{-(k+1)/2}, \quad k = 0, 1, 2.$$

Then, for bilinear elements, the a posteriori error estimate takes the form

$$|J_\epsilon(e)| \approx \eta := \sum_{K\in\mathbb{T}_h} \rho_K \frac{h_K^3}{d_K^3}, \qquad d_K := \max_{x\in K} |x-P|.$$

Assumption (may be checked a posteriori in the course of the mesh adaptation process; recall that u is assumed to be smooth):

$$\boldsymbol{\rho_K \approx h_K}$$

Then,

$$\eta \approx \sum_{K\in\mathbb{T}_h} \frac{h_K^4}{r_K^3}.$$

The optimal mesh for prescribed accuracy TOL is characterized by the equilibration property

$$\eta_K = \frac{h_K^4}{r_K^3} \approx \frac{TOL}{N} \quad \Rightarrow \quad |J_\epsilon(e)| \approx \sum_{K\in\mathbb{T}_h} \frac{\mathrm{TOL}}{N} \approx \mathrm{TOL}.$$

From this, we obtain

$$h_K^2 \approx r_K^{3/2}\Big(\frac{TOL}{N}\Big)^{1/2},$$

and consequently,

$$N = \sum_{K\in\mathbb{T}_h} h_K^2 h_K^{-2} = \Big(\frac{N}{TOL}\Big)^{1/2} \sum_{K\in\mathbb{T}_h} h_K^2 r_K^{-3/2} \approx \Big(\frac{N}{TOL}\Big)^{1/2}.$$

This implies that $\mathbf{N \approx TOL^{-1}}$, which is better than the $N \approx TOL^{-2}$ achieved on uniformly refined meshes.

This predicted behavior is confirmed by numerical tests:

TOL	N	L	$\|J_\epsilon(e)\|$	η
4^{-3}	940	9	$4.10{\cdot}10^{-1}$	$1.42{\cdot}10^{-2}$
4^{-4}	4912	12	$4.14{\cdot}10^{-3}$	$3.50{\cdot}10^{-3}$
4^{-5}	20980	15	$2.27{\cdot}10^{-4}$	$9.25{\cdot}10^{-4}$
4^{-6}	86740	17	$5.82{\cdot}10^{-5}$	$2.38{\cdot}10^{-4}$

Remarks: We emphasize that in this example strong mesh refinement occurs, although the solution is smooth. In fact, this phenomenon should rather be interpreted as “mesh coarsening” away from the point of evaluation.

Remark: The assumption $\boldsymbol{\rho_K \approx h_K}$ is decisive for the optimality of a refined mesh. To see this, suppose that only

$$\rho_K \approx h_K^{1-\epsilon}$$

holds, for some small $\epsilon > 0$. Then, the above calculation would result in

$$h_K^2 \approx r_K^{6/(4-\epsilon)} \Big(\frac{TOL}{N}\Big)^{2/(4-\epsilon)},$$

and consequently,

$$N = \sum_{K\in\mathbb{T}_h} h_K^2 h_K^{-2} = \Big(\frac{N}{TOL}\Big)^{2/(4-\epsilon)} \sum_{K\in\mathbb{T}_h} h_K^2 r_K^{-6/(4-\epsilon)} \approx \Big(\frac{N}{TOL}\Big)^{2/(4-\epsilon)}.$$

This would give us the asymptotic complexity $\mathbf{N \approx TOL^{-1-\epsilon/2}}$, which growths faster than TOL^{-1}.

Remark: The traditional energy-norm error estimator η_E is known to be *reliable* as well as *efficient*, i.e., it is asymptotically sharp in the sense that

$$c_1\|\nabla e\| \le \eta_E \le c_2\big\{\|\nabla e\| + \|f-\bar f_h\|\big\},$$

where $\bar f_h$ is the piecewise constant interpolation of f. A similar result is not possible in general for estimators η_ω of locally defined error quantities. Already the transition from the *error representation* to the *error estimate* in terms of (non-negative) cell-wise error indicators is critical, since by this localization the asymptotic sharpness of the global error representation may get lost. To illustrate this, consider the case $J(u) = u(0)$ and assume that the exact and the approximate solution are anti-symmetric with respect to the x_1-axis. Then, $e(0) = 0$, but $\sum_{K\in\mathbb{T}_h} \eta_K \neq 0$.

Convergence of residuals

For analyzing this question in the case of d-linear finite elements, it suffices to consider the edge-residual part $\|[\partial_n u_h]\|_{\partial K}$, since on Cartesian meshes the cell-residual term automatically satisfies

$$\|f + \Delta u_h\|_K = \|f\|_K \le c(f) h_K,$$

for bounded f . Now, notice that

$$h_K^{-1/2} \|r(u_h)\|_{\partial K} = h_K^{-1/2} \|[\partial_n u_h]\|_{\partial K} =: h_K \left| \mathbf{D_h^2 u_{h|K}} \right|$$

can be viewed as a mean value of a second-order difference quotient of u_h on the cell-patch $\tilde{K}$ containing K and its neighbors. Hence, we have to seek for an estimate of the form

$$\sup_{\mathbf{h>0}} \|\mathbf{D_h^2 u_h}\|_\infty \le \mathbf{c(u)}$$

Proof on quasi-uniform meshes ($h_{\max}/h_{\min} \le c$) by known L^∞ error estimates and inverse property:

$$
\begin{aligned}
|D_h^2 u_{h|K}| &\le h_K^{-1}\|D_h^2 u_h\|_K \\
&\le h_K^{-1}\|D_h^2(u_h - I_h u)\|_K + h_K^{-1}\|D_h^2 I_h u\|_K \\
&\le \mathbf{c h_K^{-2}\|\nabla e\|_K} + c h_K^{-2}\|\nabla(u - I_h u)\|_K + h_K^{-1}\|D_h^2 I_h u\|_K \\
&\le \mathbf{c h_K^{-1}\|\nabla e\|_{\infty;K}} + c\|\nabla^2 u\|_{\infty;\tilde K} \\
&\le c\|\nabla^2 u\|_\infty
\end{aligned}
$$

where again $\tilde K$ denotes a cell-patch neighborhood of K .

The local error estimate

$$\|\nabla \mathbf{e}\|_{\infty;\mathbf{K}} \le \mathbf{h_K c(u)}$$

does not hold on meshes with $h_{\max}/h_{\min} \to \infty$.

By standard localization techniques one can prove is the weaker version (all estimates modulo possibly logarithms $\log(1/h)$)

$$\|\nabla e\|_{\infty;K} \le c(u)\{\max_{K'\in\hat{S}(K)} h_{K'} + h^2\}$$

where $h := h_{max}$, and $\hat{S}(K)$ is some $\mathcal{O}(1)$-neighborhood of K.

This estimate may be sharpened by assuming certain additional mesh properties:

$$\|\nabla e\|_{\infty;K} \le c(u)\{\max_{K'\in\hat{S}(K)} h_{K'} + h^2\}$$

Numerical experiments: No evidence is observed for the deterioration of the bound

$$h_K^{-3/2}\|[\partial_n u_h]\|_{\partial K} \le c(u)$$

on irregular meshes (e.g., refinement towards points or lines).

Approximation of weights

We analyze the effect of approximating the dual solution z in the weights ω_K, on the accuracy of the error estimate.

i) Approximation by a higher-order method.

Let the dual solution z be approximated by its Ritz projection $z_h^{(2)}$ into the space $V_h^{(2)}$ of biquadratic finite elements:

$$(\nabla\varphi_h, \nabla z_h^{(2)}) = J(\varphi_h) \quad \varphi_h \in V_h^{(2)}.$$

Resulting approximate error representation:

$$\tilde{\eta}(\mathbf{u_h}) := \sum_{\mathbf{K}\in\mathbb{T}_\mathbf{h}} \{(\mathbf{R_h}, \mathbf{z_h^{(2)}} - \mathbf{I_h z_h^{(2)}})_\mathbf{K} + (\mathbf{r_h}, \mathbf{z_h^{(2)}} - \mathbf{I_h z_h^{(2)}})_{\partial\mathbf{K}}\}$$

Error for $\tilde{e}^* := z - z_h^{(2)}$:

$$\eta(\mathbf{u_h}) - \tilde{\eta}(\mathbf{u_h}) = \rho(\mathbf{u_h})(\tilde{\mathbf{e}}^* - \mathbf{I_h}\tilde{\mathbf{e}}^*)$$

a) First error estimate with $\tilde{e}^* := z - z_h^{(2)}$ and $\tilde{e} := u - u_h^{(2)}$:

$$
\begin{aligned}
|\eta(u_h) - \tilde{\eta}(u_h)| &= |\rho(u_h)(\tilde{e}^* - I_h\tilde{e}^*)| = |\rho(u_h)(\tilde{e}^*)| \\
&= |(\nabla e, \nabla\tilde{e}^*)| = |(\nabla\tilde{e}, \nabla\tilde{e}^*)| \\
&\le \|\nabla\tilde{e}\|\|\nabla\tilde{e}^*\| \\
&\le c\Big(\sum_{K\in\mathbb{T}_h} h_K^4\|\nabla^3 u\|_K^2\Big)^{1/2}\Big(\sum_{K\in\mathbb{T}_h} h_K^4\|\nabla^3 z\|_K^2\Big)^{1/2}
\end{aligned}
$$

This estimate allows the primal as well as the dual solution to be irregular. Otherwise, we estimate further

$$|\eta(\mathbf{u_h}) - \tilde{\eta}(\mathbf{u_h})| \le \mathbf{ch^4}\|\nabla^3\mathbf{u}\|\|\nabla^3\mathbf{z}\|$$

b) Second error estimate for the special case u smooth and $J_\epsilon(u) \approx u(P)$ (L^∞/L^1 duality):

$$
\begin{aligned}
|\eta(u_h) - \tilde{\eta}(u_h)| = |(\nabla\tilde{e}, \nabla\tilde{e}^*)| &= |(\nabla(u - I_h^{(2)}u), \nabla\tilde{e}^*))| \\
&\le c \max_K \{h_K^2 \|\nabla^3 u\|_{L^\infty(K)}\} \|\nabla\tilde{e}^*\|_{L^1} \\
&\le ch|\log(h_{min})| \max_K \{h_K^2 \|\nabla^3 u\|_{L^\infty(K)}\}
\end{aligned}
$$

The L^1-error estimate for the regularized Green function

$$
\|\nabla\tilde{e}^*\|_{L^1} \le c\,|\log(h_{min})|
$$

can be shown by the usual weighted-norm technique also on locally refined meshes.

These estimates are useful provided that $\mathbf{h^3 \ll TOL}$ on the current mesh (e.g., point-value evaluation: $TOL \approx h^2$).

Numerical test

The effectivity of the strategies for estimating the weights $\omega_K(z)$

1. approximation by higher-order global Ritz projection: $z \approx z_h^{(2)}$
2. approximation by high-order local interpolation: $z \approx I_{2h}^{(2)} z_h$

are is tested for the 2-D Poisson model problem with the solution $u(x) = (1 - x_1^2)(1 - x_2^2)\sin(4x_1)\sin(4x_2)$ for the two output functionals

$$J_1(u) := |S|^{-1} \int_S u\,dx, \quad S := [-\tfrac{1}{2}, 0] \times [0, \tfrac{1}{2}], \qquad J_2(u) := u(\tfrac{1}{2}, \tfrac{1}{2}).$$

Effectivity index

$$I_{\text{eff}} := \frac{\eta(u_h)}{|J(e)|}$$

Effectivity of weighted error indicators for the mean error $J_1(e)$ (left) and the point-error $J_2(e)$ (right)

N	$J_1(e)$	$I_{\mathrm{eff}}^{(1)}$	$I_{\mathrm{eff}}^{(2)}$
81	$7.6\cdot10^{-2}$	1.01	1.05
151	$2.7\cdot10^{-2}$	1.00	1.07
653	$3.6\cdot10^{-3}$	0.99	0.99
1435	$1.4\cdot10^{-3}$	1.00	1.00
2937	$6.5\cdot10^{-4}$	1.00	0.98
6249	$3.2\cdot10^{-4}$	1.00	1.00
12995	$1.2\cdot10^{-4}$	1.00	0.99
26603	$7.2\cdot10^{-5}$	1.00	1.00
56073	$2.7\cdot10^{-6}$	1.00	0.99

N	$J_2(e)$	$I_{\mathrm{eff}}^{(1)}$	$I_{\mathrm{eff}}^{(2)}$
81	$4.2\cdot10^{-1}$	0.17	0.18
151	$1.4\cdot10^{-1}$	0.26	0.20
635	$1.0\cdot10^{-2}$	0.30	0.28
1443	$2.9\cdot10^{-3}$	0.39	0.40
2875	$9.4\cdot10^{-4}$	0.52	0.51
6229	$2.8\cdot10^{-4}$	0.61	0.60
12521	$1.0\cdot10^{-4}$	0.74	0.72
26903	$3.9\cdot10^{-5}$	0.82	0.80
55287	$1.6\cdot10^{-5}$	0.89	0.88

ii) Approximation by higher-order interpolation.

Next, we consider the approximate error estimator

$$\tilde{\eta}(\mathbf{u_h}) := \sum_{\mathbf{K}\in\mathbb{T}_\mathbf{h}} \left\{ (\mathbf{R_h}, \mathbf{I^{(2)}_{2h}z_h} - \mathbf{z_h})_\mathbf{K} + (\mathbf{r_h}, \mathbf{I^{(2)}_{2h}z_h} - \mathbf{z_h})_{\partial\mathbf{K}} \right\}$$

where $I^{(2)}_{2h}z_h$ is the patch-wise *biquadratic* interpolation of the *bilinear* Ritz projection z_h .

Remark: Why should $I^{(2)}_{2h}z_h$ be a better approximation to z than z_h? In fact, the construction of $I^{(2)}_{2h}z_h$ is based on nodal point information of z_h , and the point error $(z-z_h)(a)$ behaves generally not better then $\mathcal{O}(h^2)$, even on uniform meshes. Hence, it seems unlikely that

$$\|z - I^{(2)}_{2h}z_h\|_K \ll \|z - z_h\|_K .$$

More reasonable concept reflecting "global" super-approximation:

$$|\rho(u_h)(z-I_{2h}^{(2)}z_h)| \ll |\rho(u_h)(z-z_h)|,$$

We rewrite the error identity $J(e)=\rho(u_h)(z-z_h)$ in the form

$$J(e)=\rho(u_h)(z-I_{2h}^{(2)}z)+\rho(u_h)(I_{2h}^{(2)}z-I_{2h}^{(2)}z_h)+\boldsymbol{\rho(u_h)(I_{2h}^{(2)}z_h-z_h)}$$

where the last term is our error estimator. There holds

$$\Big(\|z-I_{2h}^{(2)}z\|_K^2+\tfrac{1}{2}h_K\|z-I_{2h}^{(2)}z\|_{\partial K}^2\Big)^{1/2}\le ch_K^3\|\nabla^3 z\|_{S(K)}$$

and, therefore, if $\boldsymbol{\rho_K \le c(u)h_K}$,

$$\begin{aligned}|\rho(u_h)(z-I_{2h}^{(2)}z)| &\le c\sum_{K\in\mathbb{T}_h}\rho_K h_K^3\|\nabla^3 z\|_{S(K)}\\ &\le c\Big(\sum_{K\in\mathbb{T}_h}\rho_K^2 h_K^6\Big)^{1/2}\|\nabla^3 z\| \le \mathbf{ch^3\|\nabla^3 z\|}\end{aligned}$$

The second term is the "hard" one which requires more work, as it relates to properties of the non-local Ritz projection and the local interpolation. Its estimation strongly relies on uniformity properties of the mesh $\mathbb{T}_h$. The idea is that the scaled error $h^{-2}e$ is a "smooth" function, such that it can be approximated in V_h. To make this concept clear, suppose that the mesh $\mathbb{T}_h$ is $uniform$ with mesh-width h. Then, it is known that in the nodal points, the error $z - z_h$ allows an asymptotic expansion in powers of h of the form

$$I_h z - z_h = I_h(z - z_h) = h^2 I_h w + h^3 \tau_h,$$

with some h-independent function $w \in H_0^1(\Omega)$ and a remainder satisfying $\|\tau_h\| \le c\|\nabla^3 z\|$. Hence, noting that $I_{2h}^{(2)} z = I_{2h}^{(2)} I_h z$,

$$\rho(u_h)(I_{2h}^{(2)} z - I_{2h}^{(2)} z_h) = h^2 \rho(u_h)(I_{2h}^{(2)} w) + h^3 \rho(u_h)(\tau_h)$$

Then, using Galerkin orthogonality,

$$\rho(u_h)(I_{2h}^{(2)}z - I_{2h}^{(2)}z_h) = h^2\rho(u_h)(I_{2h}^{(2)}w - I_h w) + h^3\rho(u_h)(\tau_h).$$

Assuming that the interpolation operators I_h and $I_{2h}^{(2)}$ behave like the H^1-stable Clément operator, we have

$$\|I_{2h}^{(2)}w - I_h w\|_K + \tfrac{1}{2}h_K^{1/2}\|I_{2h}^{(2)}w - I_h w\|_{\partial K} \leq ch_K\|\nabla w\|_{S_K}$$

This implies, assuming again $\boldsymbol{\rho_{\mathbf{K}} \leq \mathbf{ch_K}}$,

$$|\rho(u_h)(I_{2h}^{(2)}z - I_{2h}^{(2)}z_h)| \leq c(u,z)h^3$$

Collecting the foregoing estimates, we obtain

$$\mathbf{J(e) = \tilde{\eta}(u_h, z_h) + \mathcal{O}(h^3)}$$

for smooth dual solution z.

A really meaningful analysis has to deal with the following three complications:

- The estimates are to be proven on locally refined meshes with only limited uniformity properties.
- The estimates are to be localized in order to allow for singularities in the dual solution.
- Cases of non-smooth solutions u, either due to data irregularities or due to reentrant corners (the more severe case) should be considered.

10.6 Current developments and open problems

- *3-D applications:* The full power of the DWR method is expected to be seen in applications to 3D problems. Those are currently developed in the context of the nonstationary Navier-Stokes equations.

- *Multi-physics and multi-scale problems:* The DWR method allows the systematic treatment of rather complex systems involving various physical mechanisms and spatial or temporal scales. A typical example is seen in chemically reacting flow where the chemical reaction usually induces much faster time scales and smaller spatial scales compared to those of the flow.

- *Adaptivity in optimal control:* Most numerical simulation eventually is optimization. Goal-oriented model reduction by adaptive discretization has the potential of facilitating large-scale optimization problems in structural and fluid mechanics, such as for example, minimization of drag or control of flow-induced structural vibrations, as well as in the estimation of distributed parameters in PDE.

- *Model adaptivity:* The concept of *a posteriori* error control for single quantities of interest via duality may also be applicable to other situations when a full model, such as a differential equation, is reduced by projection to a subproblem, such as a finite element model. Model reduction within scales of hierarchical sub-models is a recent development in structural as well as fluid mechanics.

- *Open areas for applications:* There are several very promising and almost untouched areas for the application of the DWR method such as, e.g., electro-magnetics, semi-conductor theory, porous media flow, and fluid-structure interactio (currently under development).
- *"Non-standard" finite element methods:* The DWR method can also be used in the context of "non-standard" finite element methods such as *non-conforming* and *mixed* methods as well as the "least-squares" stabilized cG-FEM for transport-dominated problems.

Open problems (partially solved)

- *How to organize anisotropic mesh refinement?* The rigorous extension of the DWR concept for generating solution-adapted *anisotropic* meshes, either by simple cell stretching or by more sophisticated mesh reorientation, is still to be fully developed. In the context of "global" error estimation with respect to energy norm and L^2 norm a posteriori error estimates on anisotropic meshes have been derived.

- *How to effectively control the error caused by "variational crimes"?* These are deviations from the pure Galerkin method such as numerical integration, boundary approximation, cutting off unbounded domains, transport stabilization, etc.

- *How to apply the DWR method to non-variational problems?* Residual-based methods for *a posteriori* error estimation like the DWR method rely on the variational formulation and the Galerkin orthogonality property of the finite element scheme. This allows us to locally extract additional powers of the mesh size, leading to sensitivity factors of the form $h_K^2\|\nabla^2 z\|_K$. Other "non-variational" discretizations such as the finite volume method usually have a different error behavior, governed by sensitivity factors like $h_K\|\nabla z\|_K$. This may be seen by reinterpreting these discretizations as perturbed finite element schemes obtained by evaluating local integrals by special low-order quadrature rules.

- *How to solve the technical problems discussed in the course for providing theoretical support for the DWR method?*

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