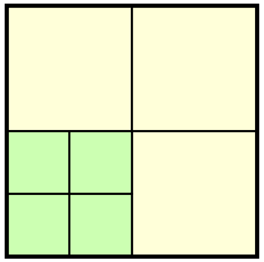
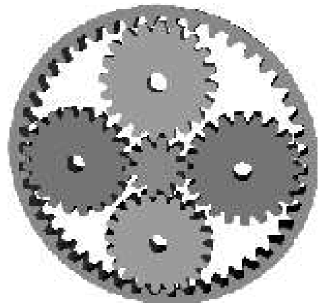
LECTURE 2

Goal-Oriented Adaptivity



Rolf Rannacher

Institute of Applied Mathematics
Interdiscipl. Center for Scientific Computing
University of Heidelberg



12th School "Mathematical Theory in Fluid Mechanics",
Kacov, May 27 - June 3, 2011

2.0 Content

References

- R. Becker and R. Rannacher: *An optimal control approach to error estimation and mesh adaptation in finite element methods*, Acta Numerica 2000 (A. Iserles, ed.), pp. 1-102, Cambr. Univ. Press, 2001.
- **W. Bangerth and R. Rannacher: *Adaptive Finite Element Methods for Differential Equations*, Lectures in Mathematics, Birkhäuser, 2003.**
- D. Meidner, R. Rannacher, and J. Vihharev: *Goal-oriented error control of the iterative solution of finite element equations*, J. Numer. Math. 17(2), 143 (2009).
- R. Rannacher: *Adaptive Finite Element Discretization of Flow Problems for Goal-Oriented Model Reduction*, in CFD Review, World Scientific Publishing, 2010 (for examples and references).
- M. Besier and R. Rannacher: *Goal-oriented space-time adaptivity in the finite element Galerkin method for the computation of nonstationary incompressible flow*, Preprint (see my homepage), submitted to Int. J. Numer. Meth. Fluids, 2011.

2.1 Goal-oriented adaptivity

i) Simulation: Compute a quantity $J(u)$ on a mesh $\mathbb{T}_h$ from a discrete model

$$\mathcal{A}_h(u_h) = 0 \quad \approx \quad \mathcal{A}(u) = 0$$

---

ii) Error estimation: Optimize mesh $\mathbb{T}_h$ and model $\mathcal{A}_h$ on the basis of an a posteriori error representation

$$J(u) - J(u_h) \;\approx\; \eta(u_h) := \sum_{K \in \mathbb{T}_h} \underbrace{\rho_K(u_h)\omega_K}_{\eta_K}$$

cell residuals $\rho_K(u_h)$ and **weights (sensitivity)** ω_K

---

iii) Mesh and model adaptation:

$$\eta_K \gg \delta \;\Rightarrow\; \text{refine}, \quad \dots, \quad \eta_K \ll \delta \;\Rightarrow\; \text{coarsen}$$

Mesh adaptation for a set of physical quantities $u = (u^i)_{i=1}^n$ is based on "smoothness" or "residual" information like

$$\eta_K := \sum_{i=1}^n \omega_K^i \|D_h^2 u_h^i\|_K \quad \text{or} \quad \eta_K = \sum_{i=1}^n \omega_K^i \|R_i(u_h)\|_K$$

The complex error interaction has to be detected by computation (**solution of an adjoint problem**):

- error propagation in space (**pollution effect**)
- interaction of physical error sources (**sensitivities**)

$\Rightarrow$ Feed-back process for economical computation

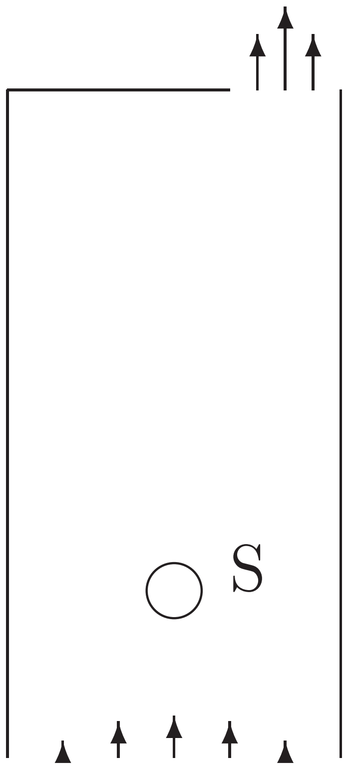
$\Rightarrow$ **D**ual **W**eighted **R**esidual (DWR) Method

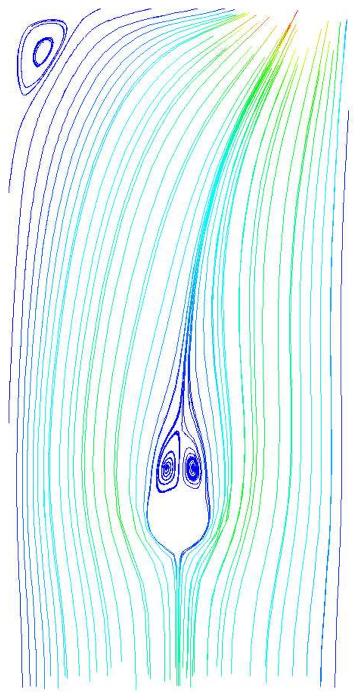
Ex. 1: Drag computation in 2-d viscous flow

Stationary Navier-Stokes system for velocity/pressure:

$$-\nu\Delta v + v\cdot\nabla v + \nabla p = f, \quad \nabla\cdot v = 0$$

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





$\text{Re} = 50$

$$c_{\text{drag}} := c\int_S n\cdot\sigma\cdot d\,\text{ds}$$

$$\sigma := \nu(\nabla v + \nabla v^T) - pI$$

$$d := (0,1)^T \text{ flow direction}$$

Discretization by standard (2nd-order) **FE method**.

Mesh refinement indicators for each mesh cells K :

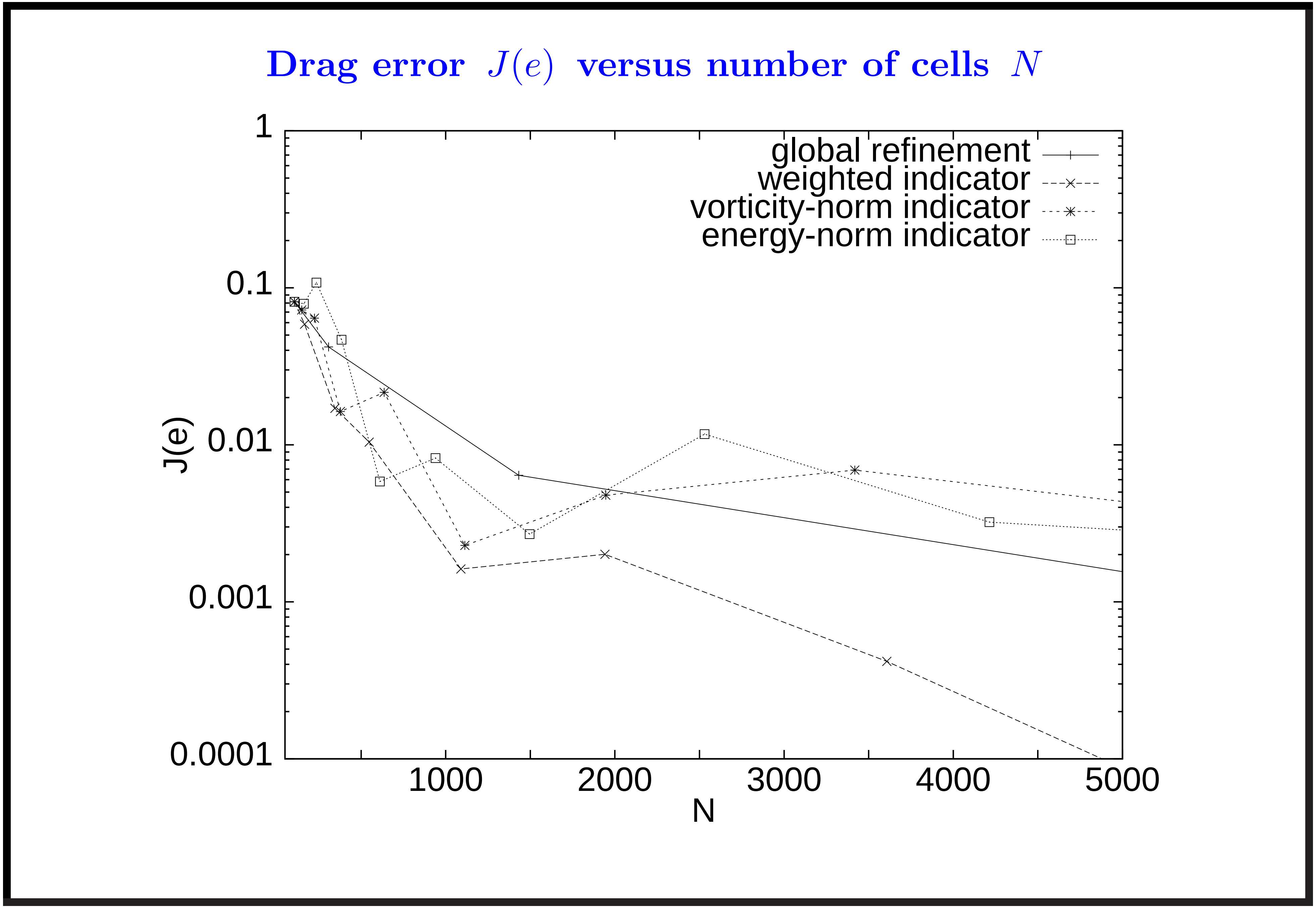
- *Vorticity*: $\eta_K := h_K \|\nabla \times v_h\|_K$
- *Pressure gradient*: $\eta_K := h_K \|\nabla p_h\|_K$
- *Velocity gradient*: $\eta_K := h_K \|\nabla_h^2 v_h\|_K$
- *Residual indicator*: $\eta_K = \rho_K(v_h, p_h)$

$$\rho_K(v_h, p_h) := h_K \|R_h\|_K + h_K^{1/2} \|r_h\|_{\partial K} + h_K \|\nabla \cdot v_h\|_K$$

$$R_{h|K} := f + \nu \Delta v_h - v_h \cdot \nabla v_h - \nabla p_h,$$

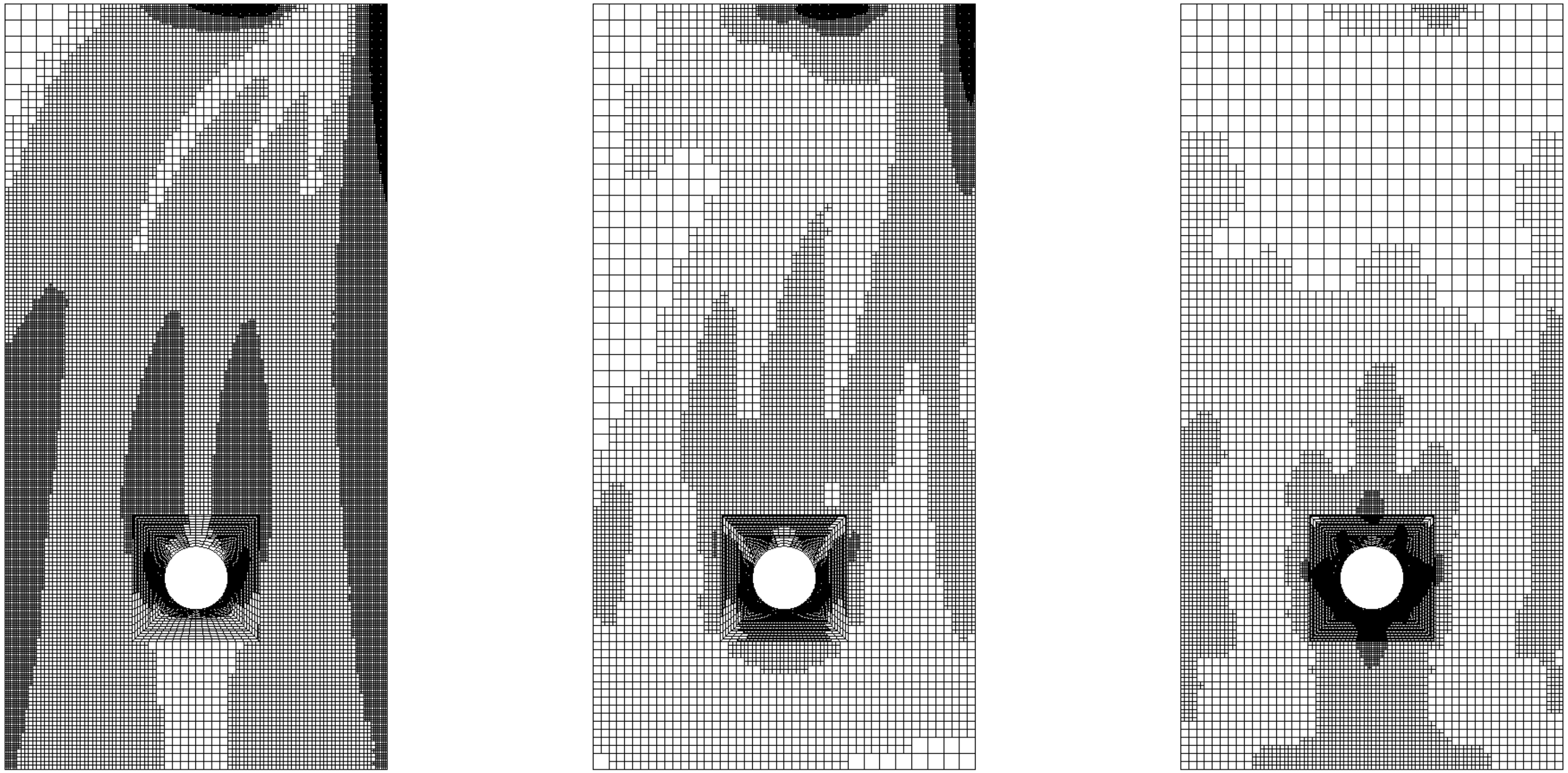
$$r_{h|\Gamma} := \tfrac{1}{2}[\nu \partial_n v_h - n p_h], \quad \text{if } \Gamma \not\subset \partial\Omega$$

- **“Weighted” indicator**: $\eta_K := \rho_K(v_h, p_h)\, \omega_{\mathbf{K}}$

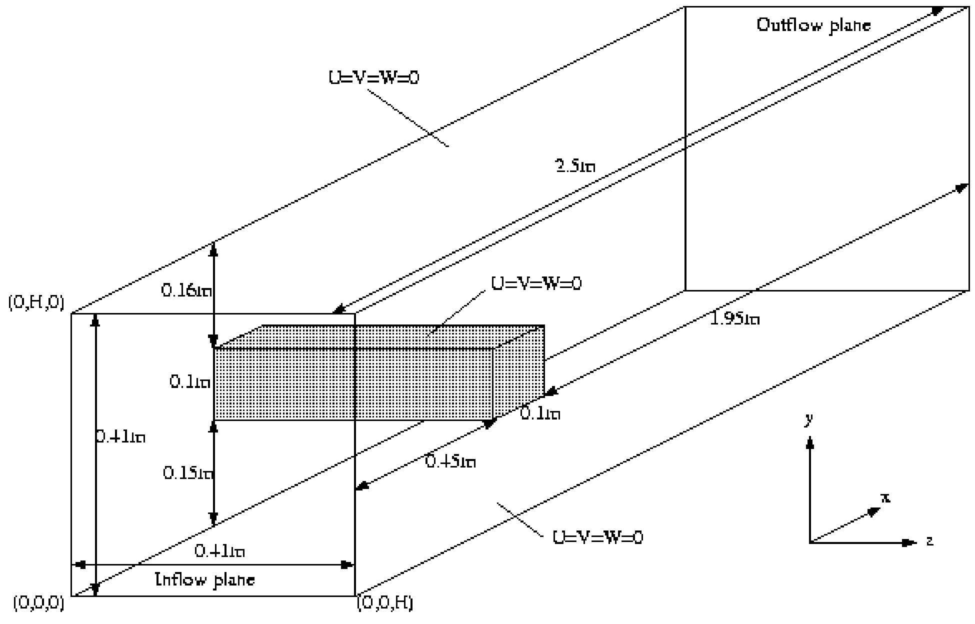

Drag error $J(e)$ versus number of cells N
1
0.1
0.01
0.001
0.0001
J(e)
1000
2000
3000
4000
5000
N
global refinement
weighted indicator
vorticity-norm indicator
energy-norm indicator

Adapted meshes with 5,000 cells

vorticity indicator   residual indicator   weighted indicator



Ex. 2: Drag computation in 3-d viscous flow



a) Q_2/Q_1-element - uniform refinement,

b) Q_1/Q_1-element - local refinement by "smoothness" indicator,

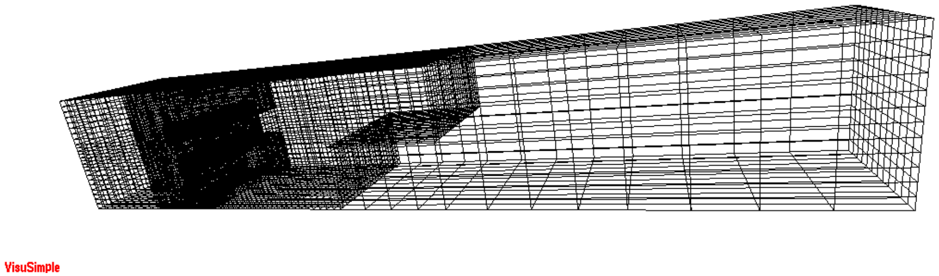
c) Q_1/Q_1-element - local refinement by "weighted" indicator

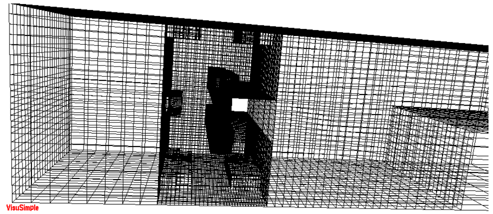
Error level of $\approx 1\%$ indicated by red

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

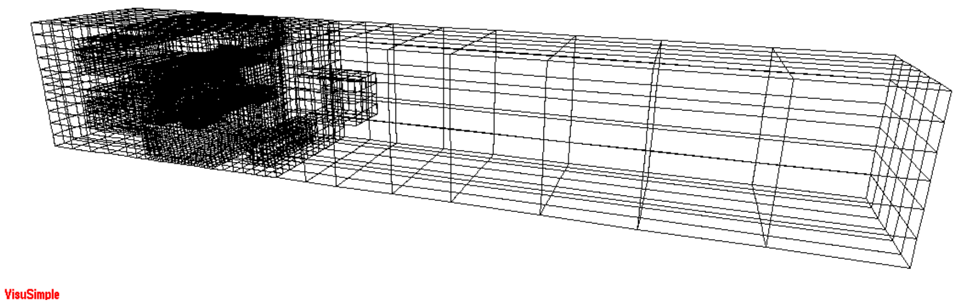
Adapted mesh and zoom

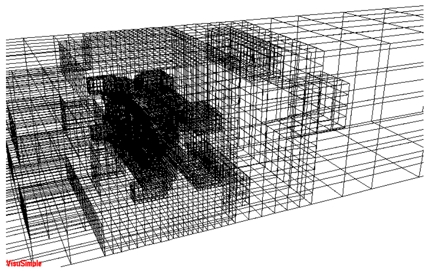
b) Mesh refinement by "smoothness" indicator:





c) Mesh refinement by weighted indicator:





Ex. 3: Inviscid 2-d Euler equations

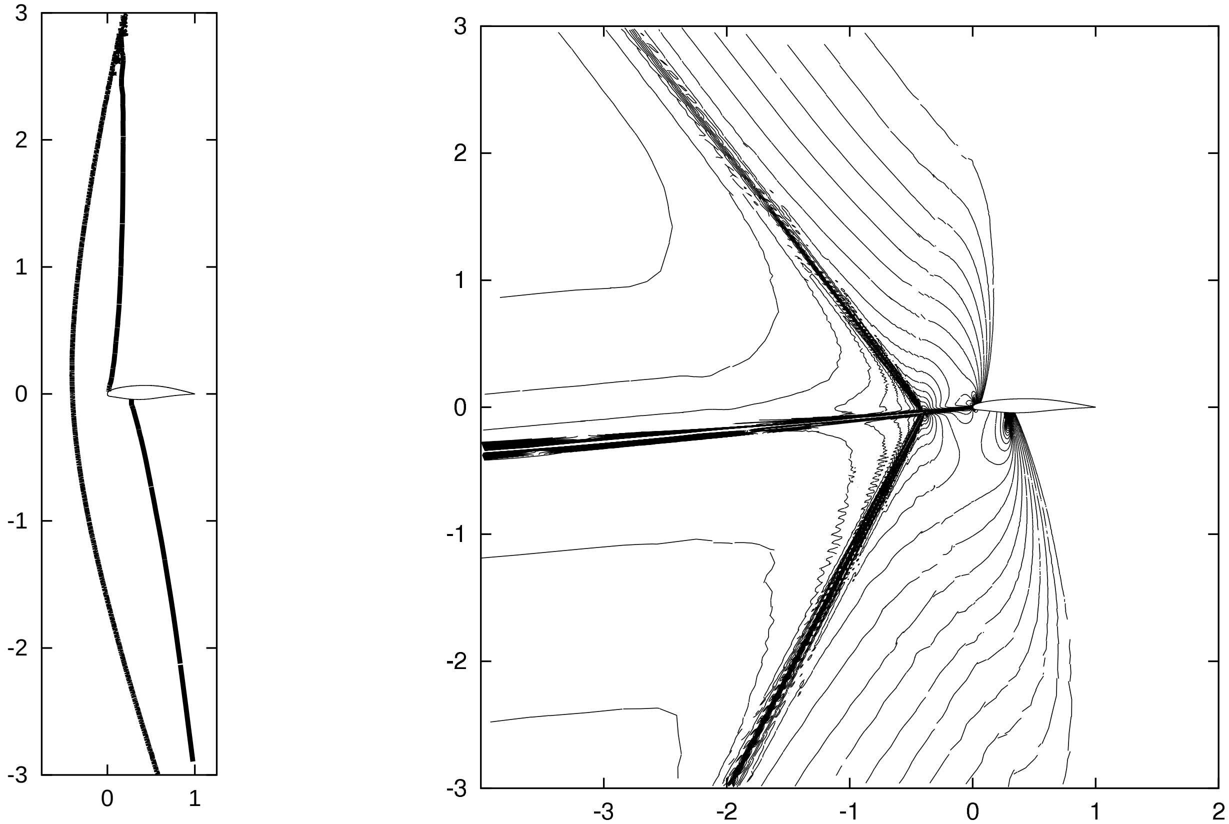
$$\partial_t \rho + \nabla \cdot (\rho v) = 0,$$
$$\partial_t (\rho v) + \nabla \cdot (\rho v \otimes v) + \nabla p = \rho g,$$
$$c_p \partial_t (\rho e) + c_p \nabla \cdot (\rho e v + p v) = h.$$

Supersonic flow around a BAC3-11 airfoil (AGARD Report 1994) inflow $\mathrm{Ma} = 1.2$, angle of attack $\alpha = 5°$

The solution develops two shocks. The quantity of interest is the **pressure point value**

$$J(\rho, v, e) := p(a) = (\gamma - 1)(e(a) - \tfrac{1}{2}\rho v(a)^2),$$

at the (subsonic) leading edge of the airfoil.



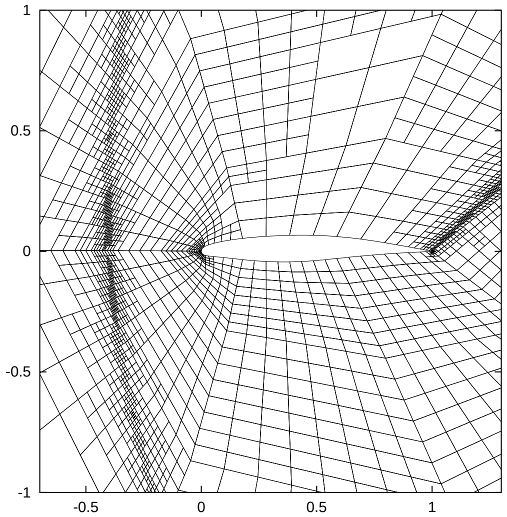
left: Ma = 1 isolines of primal solution

right: isolines of z_ρ component of dual solution

Heuristic error indicators (1% accuracy):

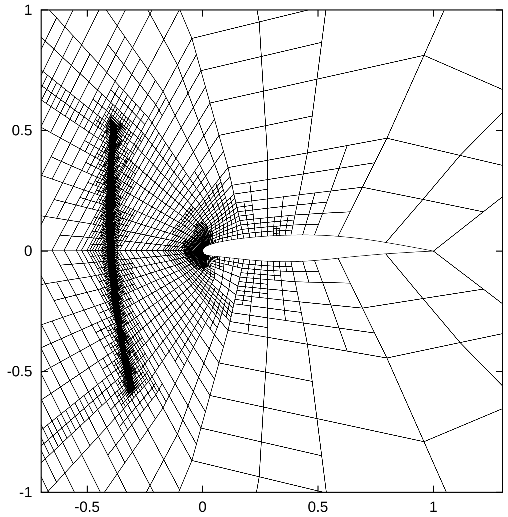
$$\eta_K^{\text{res}} := h_K \|R_h\|_K + h_K^{1/2} \|r_h\|_{\partial K}$$

$$\tilde{\eta}_K^{\text{res}} := \begin{cases} \eta_K^{\text{res}}, & \text{if } K \cap C \neq \emptyset, \quad C = 90^\circ\!-\!\text{cone} \\ 0, & \text{otherwise.} \end{cases}$$



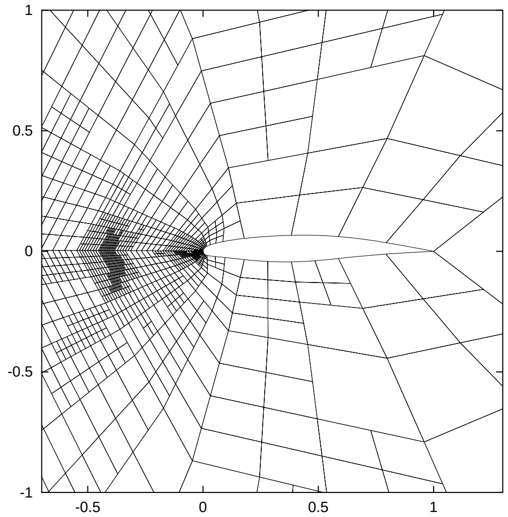
$N = 13,719$

residual



$N = 9,516$

modified indicator



$N = 1,803$

weighted

2.2 The theoretical framework

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

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

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

Proposition 1 *There holds the error representation*

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

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

Proof. By elementary calculus, trapezoidal rule and Galerkin orthogonality ($e = x - x_h$):

$$L(x) - L(x_h) = \int_0^1 L'(x_h + se)(e)\,\mathrm{ds}$$

$$= \underbrace{\tfrac{1}{2}\Big\{L'(x)(e) + L'(x_h)(e)\Big\}}_{\textbf{trapezoidal rule}}$$

$$+ \underbrace{\tfrac{1}{2}\int_0^1 L'''(x_h + se)(e,e,e)\,\sigma(s)\,\mathrm{ds}}_{\textbf{remainder}}$$

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

Application in flow simulation

Variational equation in function space V :

$$a(u)(\psi) = 0 \quad \forall \psi \in V, \qquad \text{target quantity} \;\; J(u).$$

Galerkin approximation in $V_h \subset V$:

$$a(u_h)(\psi_h) = 0 \quad \forall \psi_h \in V_h, \qquad \text{error} \;\; J(u) - J(u_h).$$

Lagrangian functional with “dual” variable z :

$$\mathcal{L}(u,z) := J(u) - a(u)(z)$$

$$\mathcal{L}'(u,z) = 0\,!$$

Determine stationary point $\{u, z\} \in V \times V$:

$$\left\{ \begin{array}{ll} J'(u)(\varphi) - a'(u)(\varphi, z) & \\ -a(u)(\psi) & \forall \{\varphi, \psi\} \end{array} \right\} = 0$$

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

$$\left\{ \begin{array}{ll} J'(u_h)(\varphi_h) - a'(u_h)(\varphi_h, z_h)\rangle & \\ -a(u_h)(\psi_h) & \forall \{\varphi_h, \psi_h\} \end{array} \right\} = 0$$

"primal" and **"dual"** residuals

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

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

Embedding in abstract theory: $X := V \times V,\ X_h := \dots$

$$x := \{u, z\} \in X, \qquad x_h := \{u_h, z_h\} \in X_h$$

$$\mathbf{L(x) := \mathcal{L}(u, z) = J(u) - a(u)(z)}$$

$$L(x) - L(x_h) = \mathbf{J(u)} - \underbrace{a(u)(z)}_{=0} - \mathbf{J(u_h)} - \underbrace{a(u_h)(z_h)}_{=0}$$

Proposition 2 *There holds the error representation*

$$J(u) - J(u_h) \;=\; \tfrac{1}{2}\underbrace{\rho(u_h)(z - \psi_h)}_{\textbf{primal}} + \tfrac{1}{2}\underbrace{\rho^*(z_h)(u - \varphi_h)}_{\textbf{dual}} + \mathcal{R}_h$$

for arbitrary $\varphi_h, \psi_h \in V_h$ *, with a remainder* $\mathcal{R}_h$ *cubic in the errors* $u - u_h$ *and* $z - z_h$.

2.3 Practical aspects

2.3.1 The main steps in the DWR method

- Solution of discrete **linear** dual problem:

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

  (work load of one additional Newton step).

- **Linearization** by neglecting remainder terms
- **Approximation of weights** by patch-wise higher-order interpolation:

$$(z - z_h)_{|K} \approx (\tilde{I}_{2h}^{(2)} z_h - z_h)_{|K}$$

- Mesh adaptation on the basis of cell-wise **error indicators** η_K by one of the common strategies: "error balancing", "fixed fraction", "fixed error reduction", or "look-ahead mesh optimization.

2.3.2 Balancing of discretization and iteration error

Problem: The "exact" discrete solution $\mathbf{u_h}$ is not available, but rather an approximation $\tilde{\mathbf{u}}_\mathbf{h}$ obtained by some iterative methods. This approximation spoils "Galerkin orthonality", which is used in the derivation of the a posteriori error identity.

Goal: Design a strategy for controlling the (discrete) iteration based on a posteriori information: **"balancing iteration error against discretization error"**.

Basic identity (linear case):

(i) **with** Galerkin orthogonality:

$$\mathbf{J}(\mathbf{e}) = \eta := \rho(\mathbf{u_h})(\mathbf{z} - \psi_\mathbf{h})$$

(ii) **without** Galerkin orthogonality:

$$\mathbf{J}(\tilde{\mathbf{e}}) \approx \tilde{\eta} := \rho(\tilde{\mathbf{u}}_\mathbf{h})(\mathbf{z} - \psi_\mathbf{h}) + ?$$

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 representation*

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

If an MG method has been used with canonical components, the following refined representation holds:

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

Here, $\hat{z}_j \in V_j$ *can be chosen arbitrarily and* $R_j(\tilde{v}_j)$ *is the iteration residual on mesh level* j *.*

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

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

Proof. In general there holds

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

If the multigrid method has been used, the second term corresponding to the iteration error can be rewritten in the form

$$\rho(\tilde{u}_L)(\hat{z}_L) = \sum_{j=1}^{L} \big\{ (f, \hat{z}_j - \hat{z}_{j-1}) - a(\tilde{u}_L, \hat{z}_j - \hat{z}_{j-1}) \big\} + \big\{ (f,\hat{z}_0) - a(\tilde{u}_L,\hat{z}_0) \big\}$$

Since $V_j \subset V_L$ for $j \le L$, we observe by the definitions of Q_j, P_j, and A_j that for $\varphi_j \in V_j$ there holds

$$(f,\varphi_j) - a(\tilde{u}_L,\varphi_j) = (P_j f, \varphi_j) - (A_j Q_j \tilde{u}_L, \varphi_j)$$

Further, by the identity $A_j Q_j = P_j A_L$ for $j \leq L$, we have

$$(P_j f, \varphi_j) - (A_j Q_j \tilde{u}_L, \varphi_j) = (P_j(f - A_L \tilde{u}_L), \varphi_j) = (R_j(\tilde{u}_L), \varphi_j).$$

Using the particular structure of the multigrid method the holds

$$\begin{aligned}
R_j(\tilde{u}_L) &= P_j(f_L - A_L \tilde{u}_L) \\
&= P_j f_L - P_j A_L S_L^{\nu}(\tilde{u}_L^{(0)}) - P_j A_L p_{L-1}^{L} \tilde{v}_{L-1} \\
&= P_j(d_L - A_{L-1} \tilde{v}_{L-1}) \\
&= P_j d_L - P_j A_{L-1} S_{L-1}^{\nu}(\tilde{v}_{L-1}^{(0)}) - P_j A_{L-1} p_{L-2}^{L-1} \tilde{v}_{L-2} \\
&\vdots \\
&= P_j(d_{j+2} - A_j \tilde{v}_{j+1}) \\
&= P_j d_{j+2} - P_j A_{j+1} S_{j+1}^{\nu}(\tilde{v}_{j+1}^{(0)}) - P_j A_{j+1} p_j^{j+1} \tilde{v}_j \\
&= P_j(d_{j+1} - A_j \tilde{v}_j) = R_j(\tilde{v}_j).
\end{aligned}$$

Using this for $\varphi_j = \hat{z}_j - \hat{z}_{j-1}$ and $\varphi_0 = \hat{z}_0$ completes the proof.

Remarks.

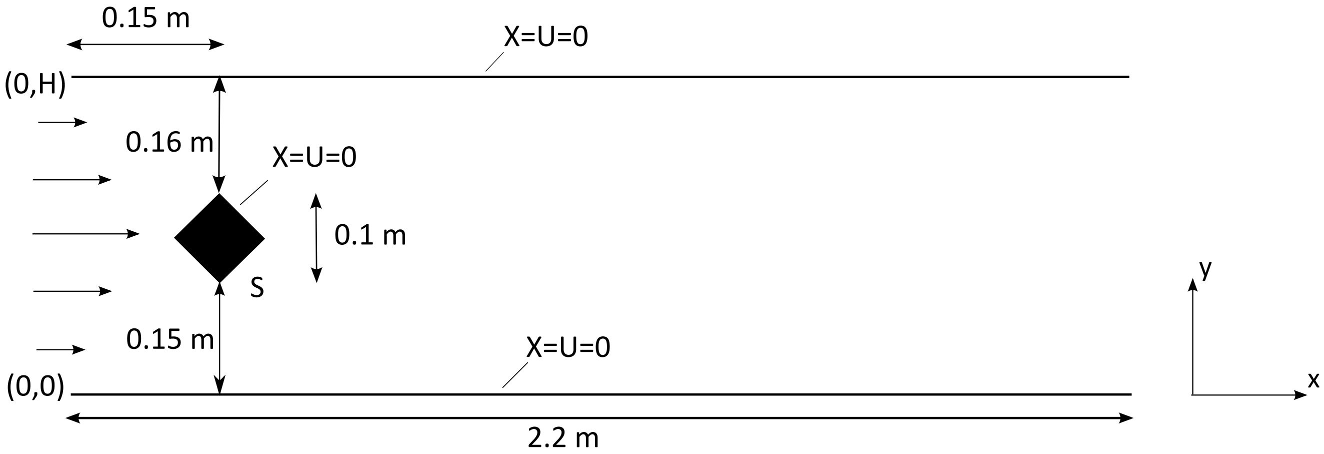
- The proof of the proposition for "energy-norm" and L^2-norm error control is due to Becker/Johnson/Ra. (1995).
- The first error representation can be used for approximative solutions $\tilde{u}_L$ obtained by any solution process,

$$J(\tilde{e}_L) = \rho(\tilde{u}_L)(z - \hat{z}_L) + \rho(\tilde{\mathbf{u}}_\mathbf{L})(\hat{\mathbf{z}}_\mathbf{L}),$$

  where $\rho(\tilde{\mathbf{u}}_\mathbf{L})(\hat{\mathbf{z}}_\mathbf{L})$ measures Galerkin orthogonality.
- 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,

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

Ex. Stokes equations: channel flow



Stokes equations of fluid mechanics describing the behavior of a creeping incompressible fluid, $\partial\Omega = \Gamma_{\text{rigid}} \cup \Gamma_{\text{in}} \cup \Gamma_{\text{out}}$,

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

$$v = 0 \quad \text{on} \;\; \Gamma_{\text{rigid}}, \quad v = v^{\text{in}} \quad \text{on} \;\; \Gamma_{\text{in}}, \quad \nu\partial_n v - pn = 0 \quad \text{on} \;\; \Gamma_{\text{out}},$$

Quantity of interest drag coefficient

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

Discretization by stabilized Q_1/Q_1 Stokes element and solution by an (geometric) MG method with canonical mesh transfer operations and a $4+4$ "block ILU" smoothing.

MG iteration towards round-off error level)

N	#It	$J(e)$	$\eta_h + \eta_{\text{it}}$	η_h	η_{it}	$I_{\text{eff}}^{\text{tot}}$
1 754	9	3.12e-05	2.81e-05	2.81e-05	1.05e-16	0.90
4 898	9	1.83e-05	1.21e-05	1.21e-05	2.20e-15	0.66
11 156	9	1.05e-05	7.01e-06	7.01e-06	9.49e-15	0.67
22 526	10	5.34e-06	3.77e-06	3.77e-06	8.36e-17	0.71
44 874	10	2.75e-06	2.12e-06	2.12e-06	3.39e-16	0.77
82 162	10	1.26e-06	1.09e-06	1.09e-06	4.29e-17	0.86
159 268	11	5.76e-07	6.11e-07	6.11e-07	1.26e-17	1.06
306 308	12	1.85e-07	2.98e-07	2.98e-07	8.74e-19	1.60

MG iteration with adaptive stopping criterion

N	#It	$J(e)$	$\eta_h + \eta_{\text{it}}$	η_h	η_{it}	$I_{\text{eff}}^{\text{tot}}$
1 754	2	3.12e-05	2.82e-05	2.81e-05	6.81e-08	0.90
4 898	2	1.83e-05	1.21e-05	1.21e-05	1.60e-08	0.66
11 156	2	1.05e-05	7.05e-06	7.01e-06	3.42e-08	0.67
22 526	2	5.34e-06	3.82e-06	3.77e-06	5.48e-08	0.72
44 874	2	2.75e-06	2.16e-06	2.12e-06	4.04e-08	0.78
82 162	2	1.27e-06	1.11e-06	1.09e-06	2.63e-08	0.88
159 268	2	5.76e-07	6.41e-07	6.10e-07	3.07e-08	1.11
306 308	2	1.86e-07	3.10e-07	2.97e-07	1.31e-08	1.67

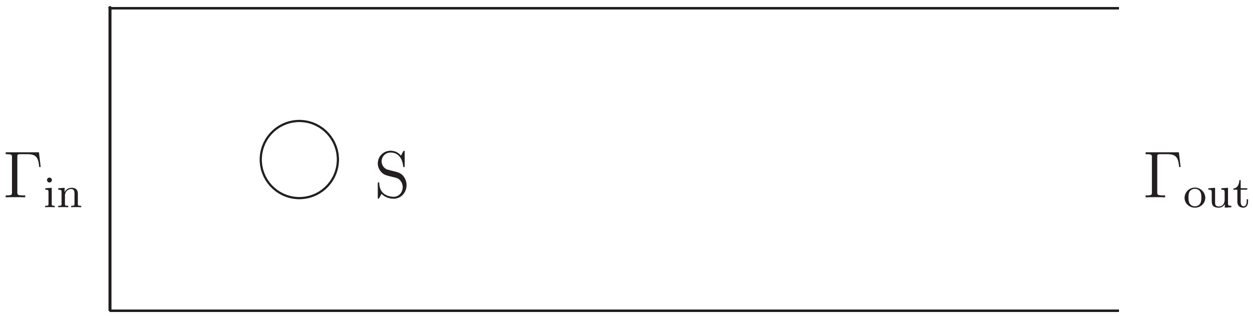
2.4 Applications

2.4.1 Drag computation

a) Simulation:

Stationary Navier-Stokes equations for v, p

Discretization by standard (2nd-order) **FE method**.



$$\mathrm{Re} = \frac{\bar{\mathrm{U}}^2 \mathrm{D}}{\nu} = 20$$

(stationary flow).

$$J(v,p) = c_{\text{drag}} := \frac{2}{\bar{U}^2 D} \int_S n^T (2\nu\tau(v) - pI) e_1 \, \mathrm{ds},$$

Primal and dual residuals:

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

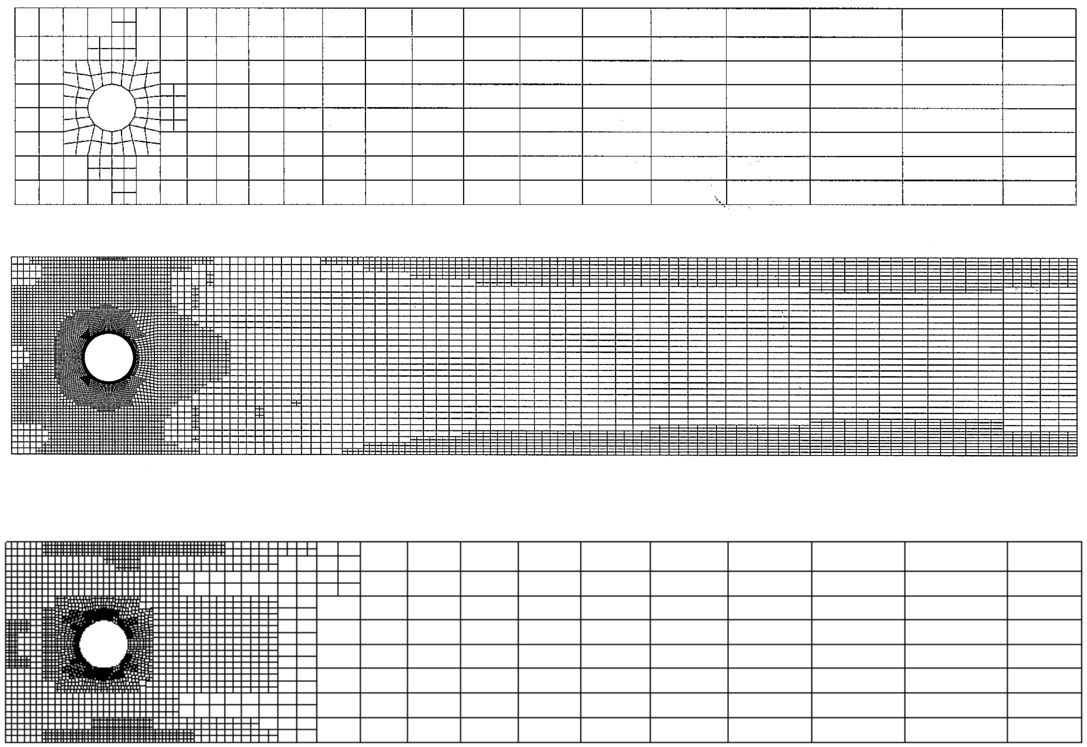
$$+ (r(u_h), \underbrace{z^v - z_h^v}_{\textbf{weight}})_{\partial K} + (\underbrace{z^p - z_h^p}_{\textbf{weight}}, \nabla\cdot v_h)_K \Big\}$$

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

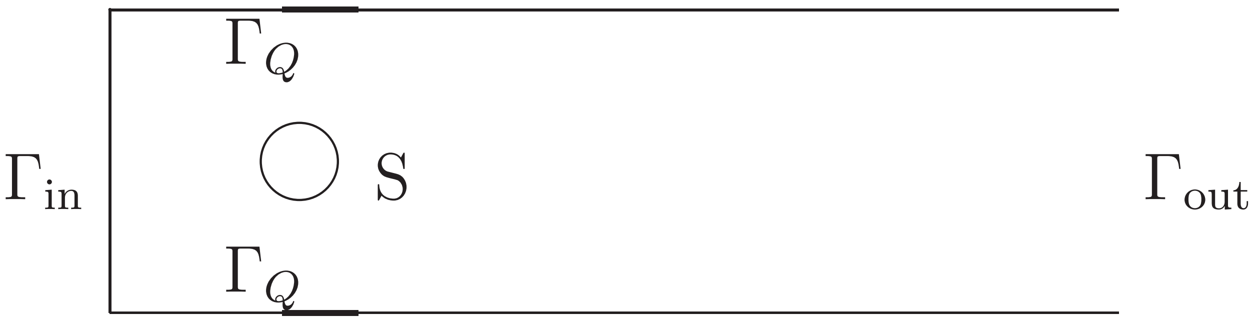
$$r(u_h)_{|\partial K} := -\tfrac{1}{2}\nu n\cdot[\nabla v_h - p_h I], \quad \Gamma \not\subset \partial\Omega$$

$$\rho^*(z_h)(u-u_h) := \dots$$

Refined meshes obtained by “smoothness-based” strategies and by the DWR method starting from a coarse mesh



b) Optimization (drag minimization by Neumann boundary control)

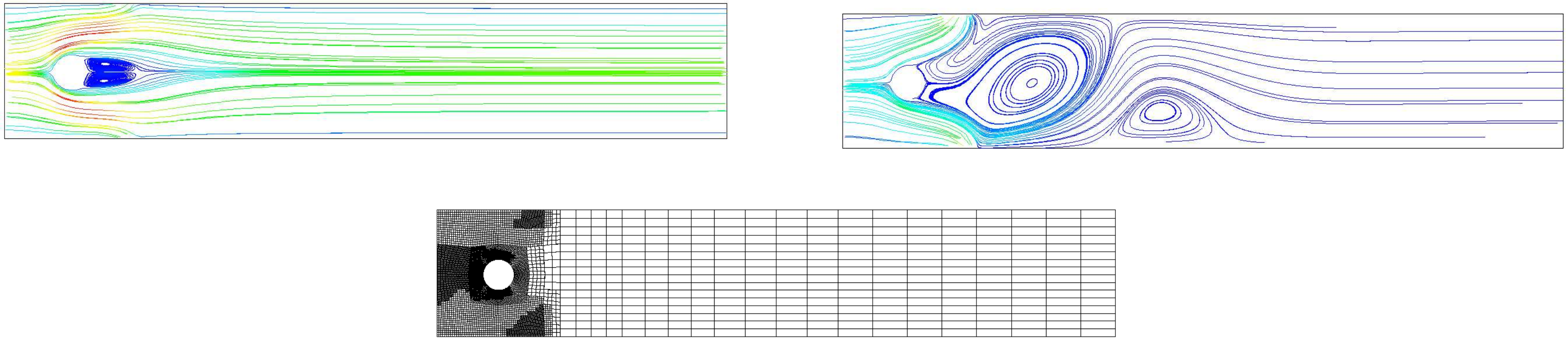


$$\mathrm{Re} = \frac{\bar{\mathrm{U}}^2 \mathrm{D}}{\nu} = 40$$

(stationary flow).

Variational formulation:

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



Velocity of the uncontrolled flow, controlled flow, adapted mesh

Uniform refinement		**Adaptive** refinement	
N	J_{drag}	N	J_{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 versus adaptive refinement

Question. Stability of "optimal" flow?

c) Flow stability analysis

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

linear stability theory:

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

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

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

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

Embedding into framework of variational equations:

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

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

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

Compact variational formulation:

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

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

Proposition 3 *There holds the error representation*

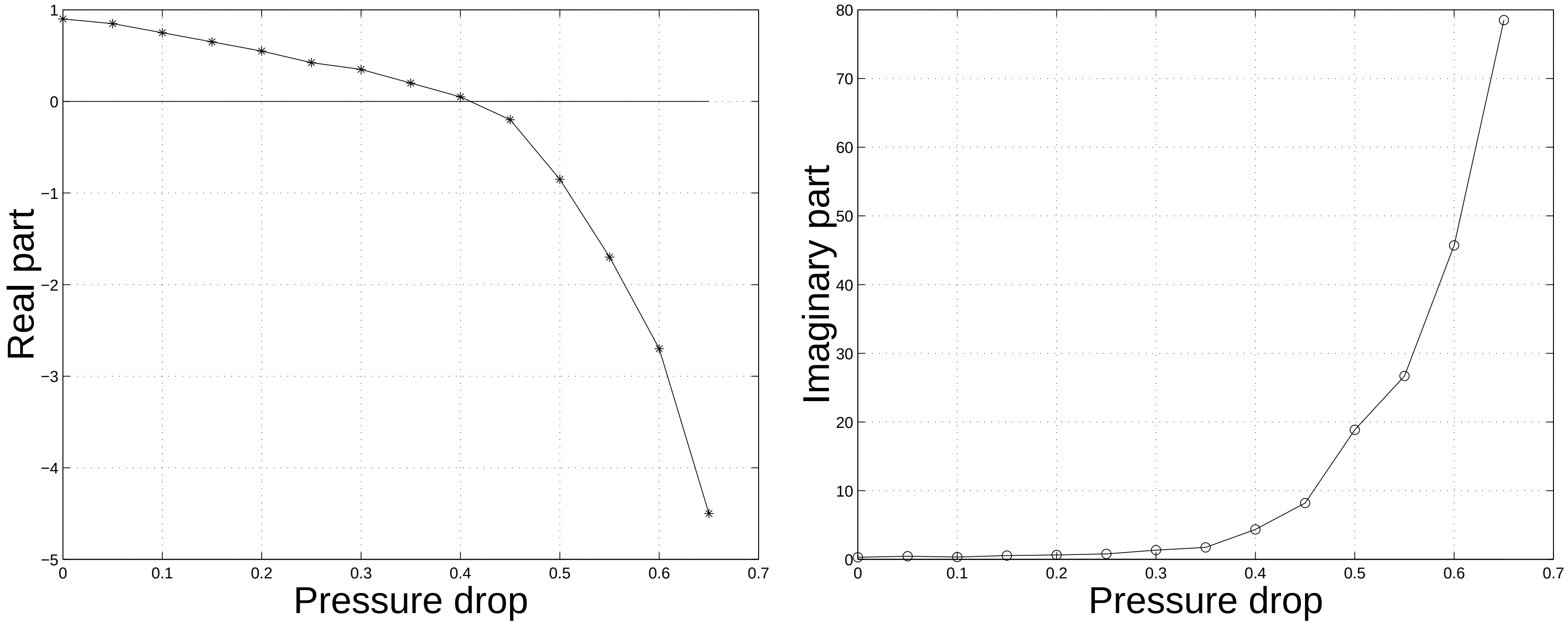
$$\lambda - \lambda_h = \underbrace{\tfrac{1}{2}\rho(\hat{u}_h)(\hat{u}^* - \hat{\psi}_h) + \tfrac{1}{2}\rho^*(\hat{u}_h^*)(\hat{u} - \hat{\varphi}_h)}_{\textbf{base solution residuals}}$$

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

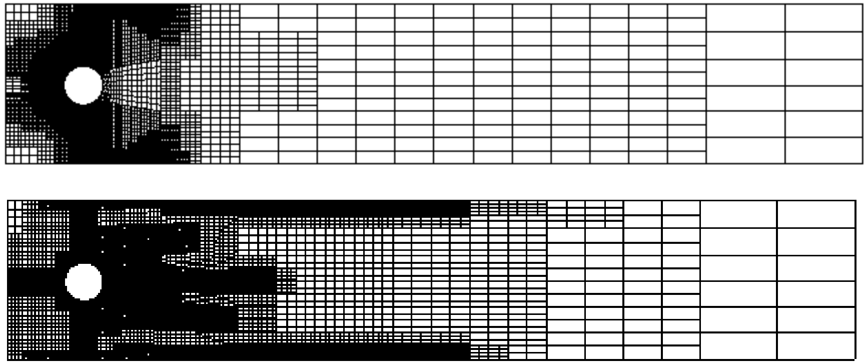
$$+ \mathcal{R}_h,$$

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

Stability of drag minimal flow



Real and imaginary parts of the critical eigenvalue as function of the control pressure (optimal pressure $q_{\text{opt}} \sim 0.5 \quad \Rightarrow \quad$ **instability**)



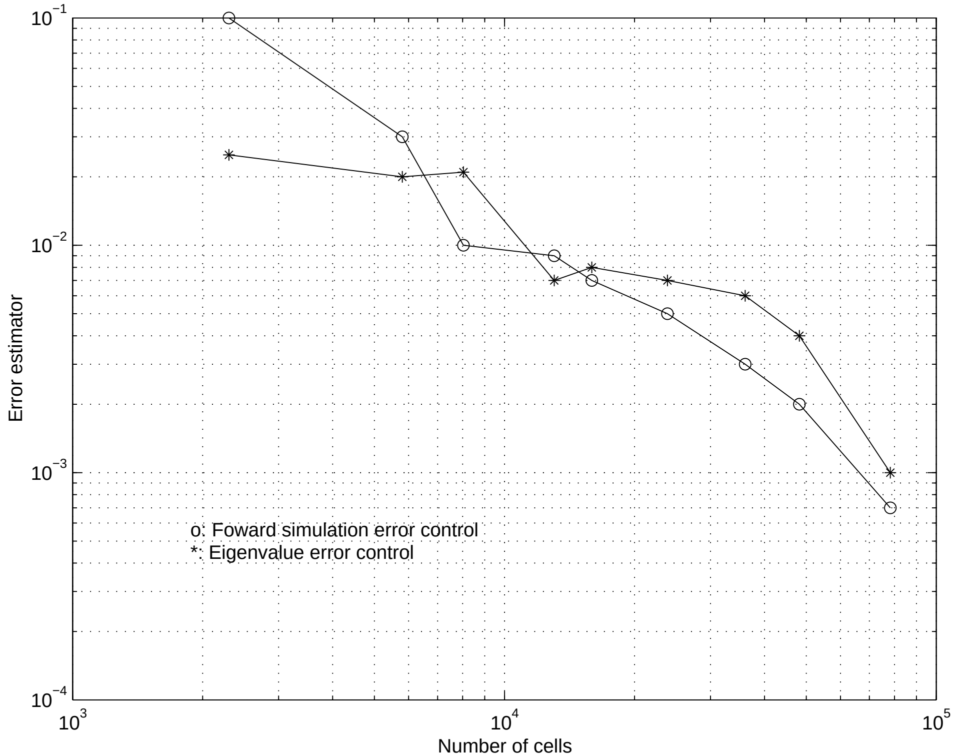
Meshes obtained by the error estimators for the drag minimization (top) and the eigenvalue computation (bottom)

Error estimator and

balancing criterion:

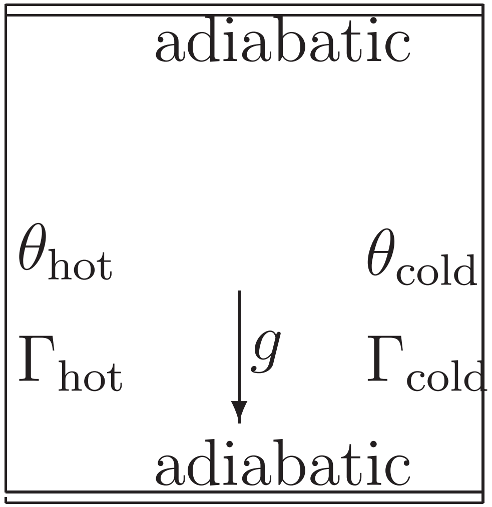
$$|\lambda - \lambda_h| \approx \sum_{K \in \mathbb{T}_h} \{\hat{\eta}_K + \eta_K^\lambda\}$$

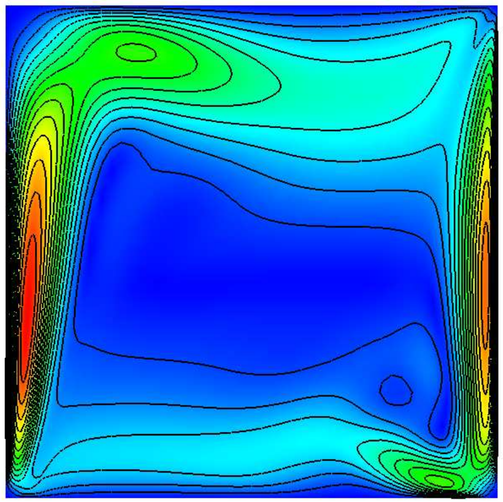
$$\sum_{K \in \mathbb{T}_h} \hat{\eta}_K \leq \sum_{K \in \mathbb{T}_h} \eta_K^\lambda \quad !$$



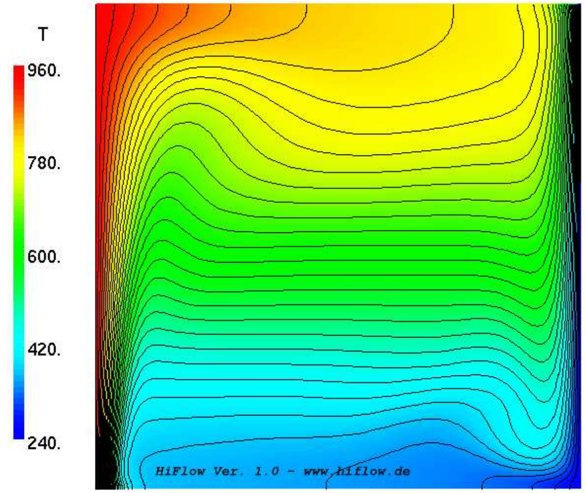
2.4.2 A 2d heat-driven cavity benchmark

Square cavity driven by temperatur difference $\theta_h - \theta_c = 720\,K$ and gravity g; Rayleigh number $Ra \sim 10^6$.





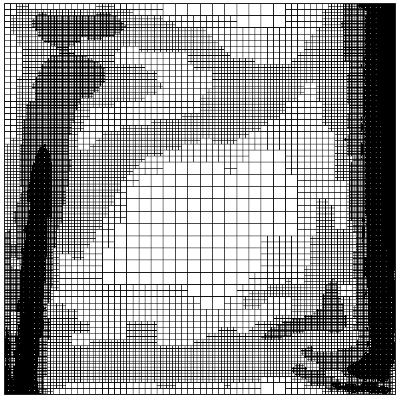
Velocity norm isolines



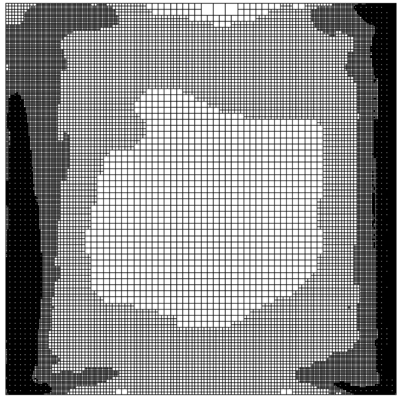
temperature isolines

Nusselt number (mean heat flux) along the cold wall

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

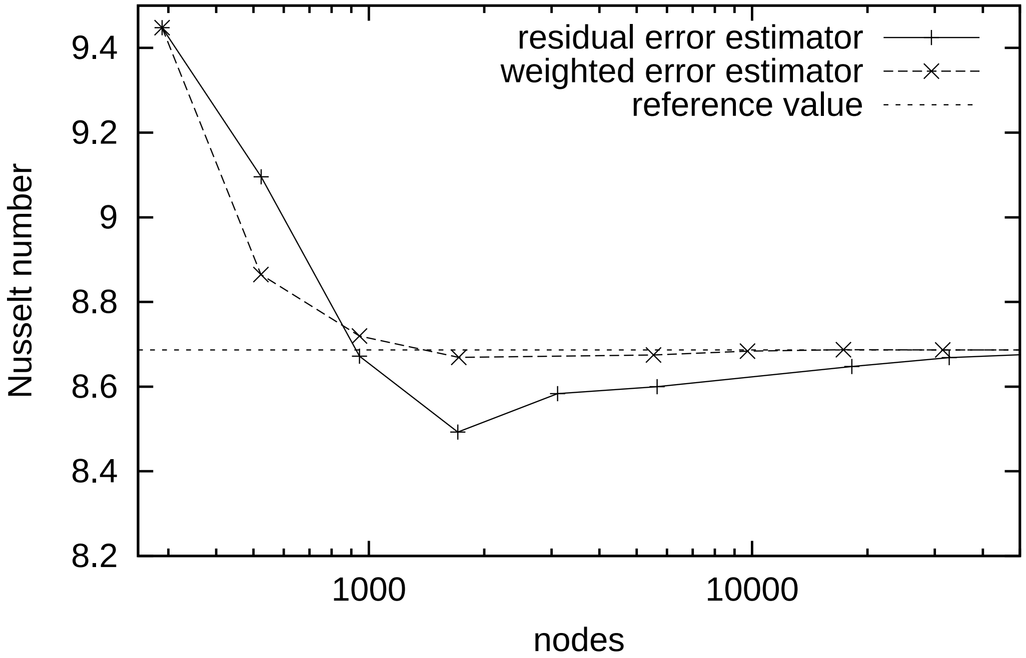


residual



weighted

Adapted meshes with about $58,000$ cells for a 1% error



Efficiency

2.4.3 Viscous flow with chemistry

Example: diffusion model in reactive flow

1) **Compressible** Navier-Stokes equations

2) Species mass conservation, **diffusion fluxes** F_i :

$$\rho \frac{\partial y_i}{\partial t} + \rho v \cdot \nabla y_i + \nabla \cdot F_i = f_i$$

Sophisticated (diffusion) models have disadvantage:

- large computational costs
- introduction of nonlinearities
- additional couplings between variables

3) **Diffusion models:**

- Fick's law: $\mathcal{F}_i = -D\nabla y_i$

- Generalized Fick's law:

$$F_i = -\rho D_i \left(\nabla y_i + \frac{y_i}{\overline{m}} \nabla \overline{m} \right)$$

- **Multicomponent** diffusion:

$$F_i = -\rho y_i \left\{ \sum_{j \in \mathcal{S}} D_{ij} d_j + \theta \nabla (\log T) \right\}$$

$$d_j = \nabla x_j + (x_j - y_j) \nabla (\log p)$$

$$D_{ij} = \text{solutions of } N \text{ linear problems of dimension } N$$

$\Rightarrow$ **enormous computational work**.

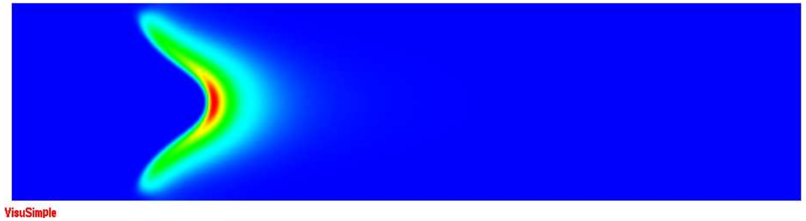
Example: Ozon recombination (laminar ozon flame)

$$O_3 + M \leftrightarrow O_2 + O + M, \quad O + O + M \leftrightarrow O_2 + M, \quad O + O_3 \leftrightarrow O_2 + O_2$$

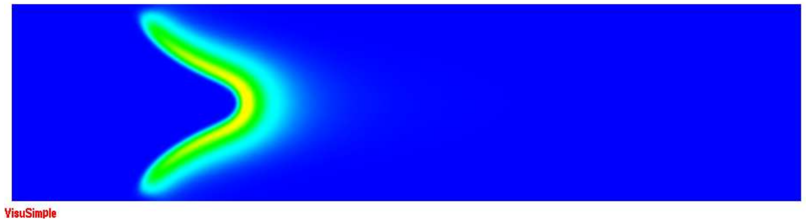
Error functional: Total mass fraction of O-atoms

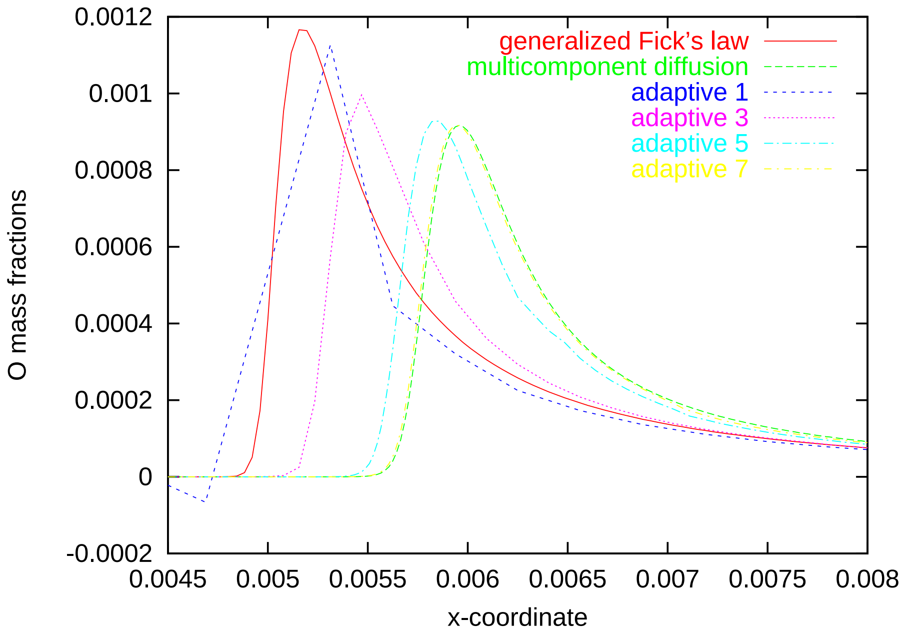
$$J(u) = \int_\Omega y_O \, dx$$

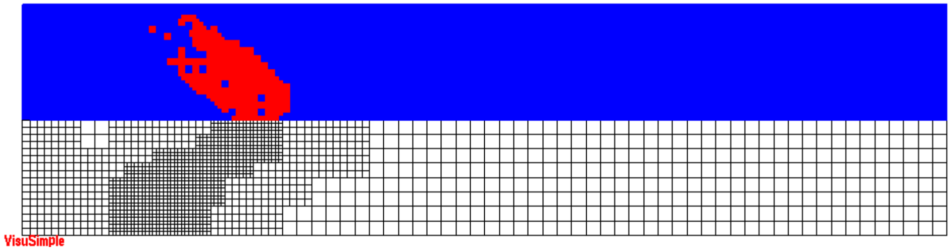
Fick's law



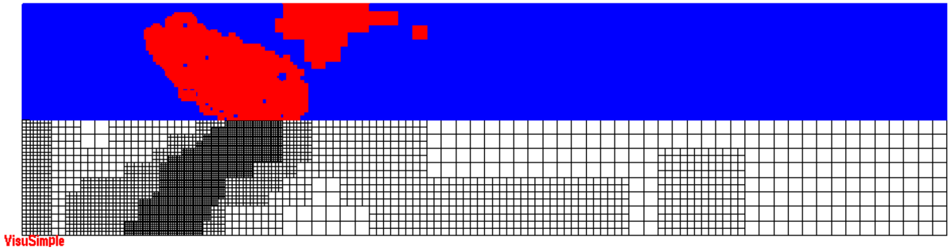
Multicomponent diffusion



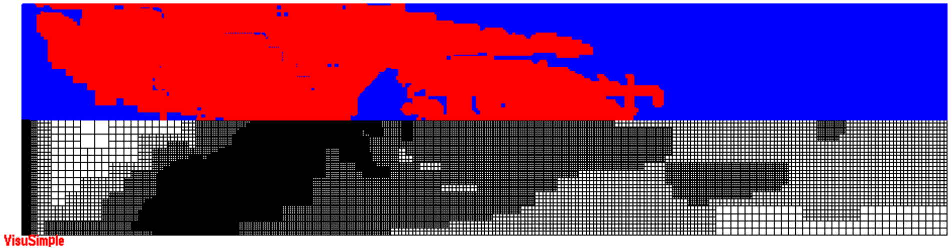




2117 nodes,
32% multi diffusion



4879 nodes,
60% multi diffusion

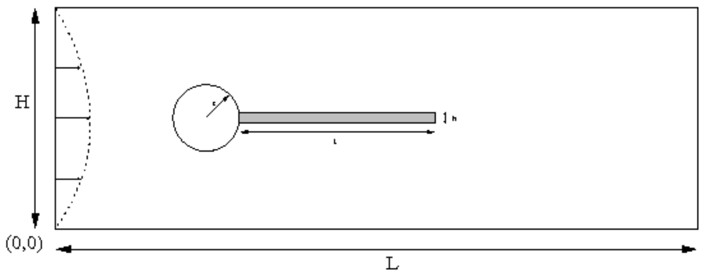


34477 nodes,
72% multi diffusion

Total gain: $\approx 50\%$ CPU time

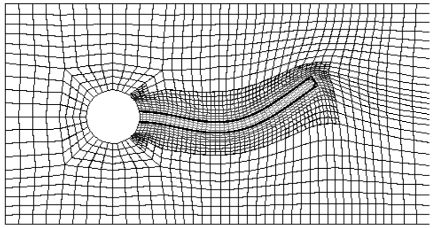
2.4.4 Fluid-structure interaction

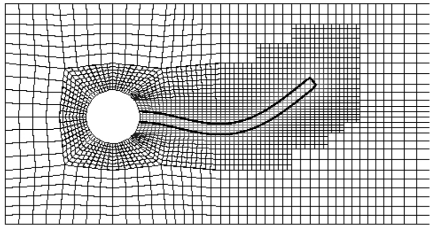
FSI benchmark "Vibrating Thin Plate"



Computation by FEM based on fully coupled (monolitic) formulations:

- arbitrary **Lagrian-Eulerian** (ALE) formulation (left)
- fully **Eulerian** formulation (right)





Outline of models and methods used

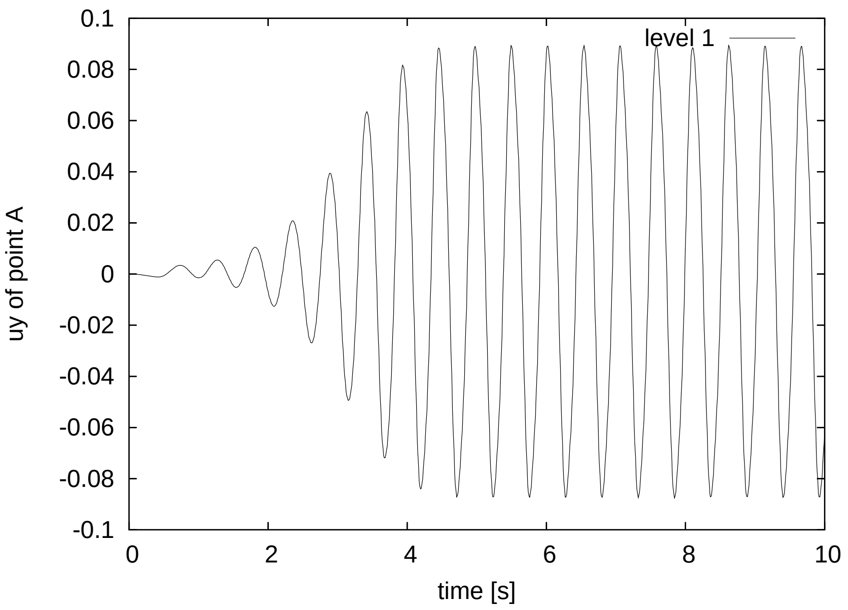
- **Material models:**
  - **Fluid:** incompressible Newtonian
  - **Structure:** compressible St. Venant-Kirchhoff
  - Fully coupled **monolitic** formulation
- **Numerics:**
  - Galerkin FE method for fluid and structure
  - Newton/functional iteration (for interface Γ_i)
  - GMRES/multigrid for linear subproblems
- Error estimation and mesh adaption by **DWR method**

Vertical displacement of end point A:

ALE:

$\max = 0.0882m,$

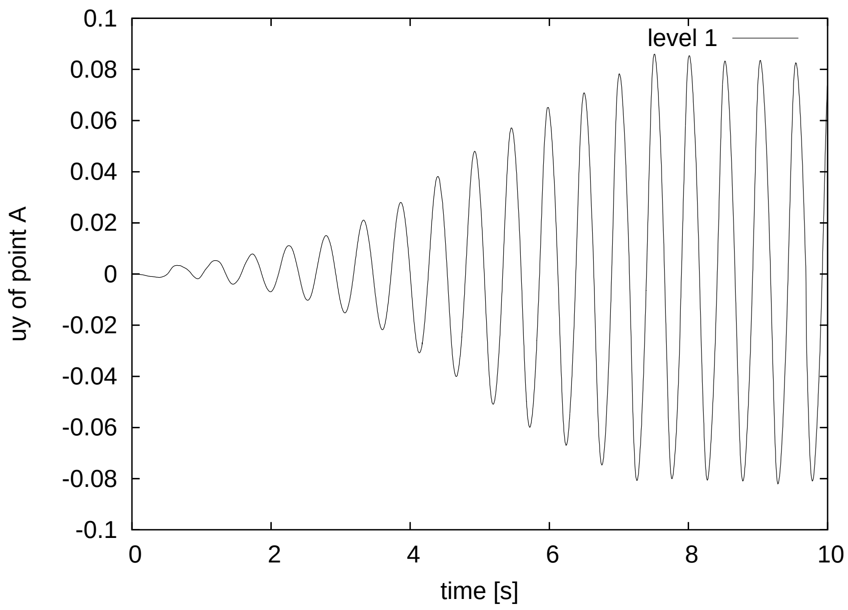
$\nu = 1.95\, s^{-1}$



Eulerian:

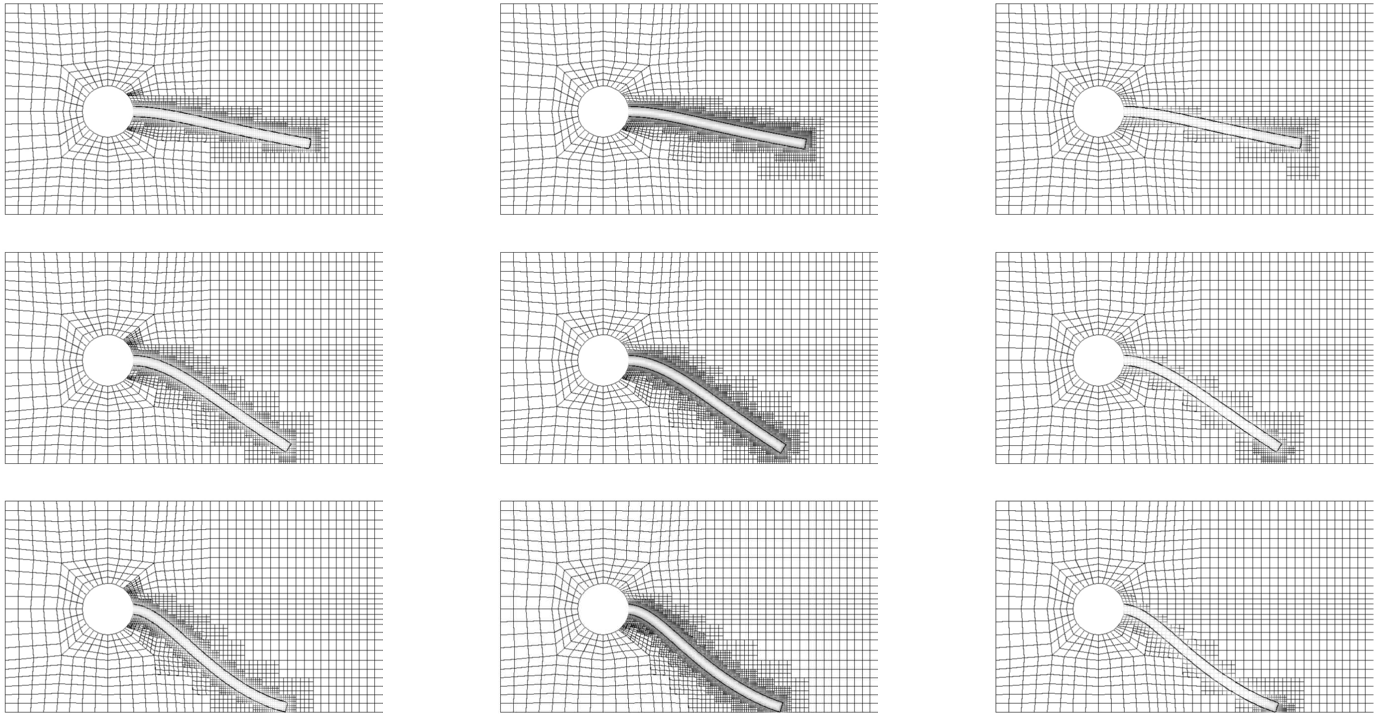
$\max = 0.0822m\,,$

$\nu = 1.92\, s^{-1}$

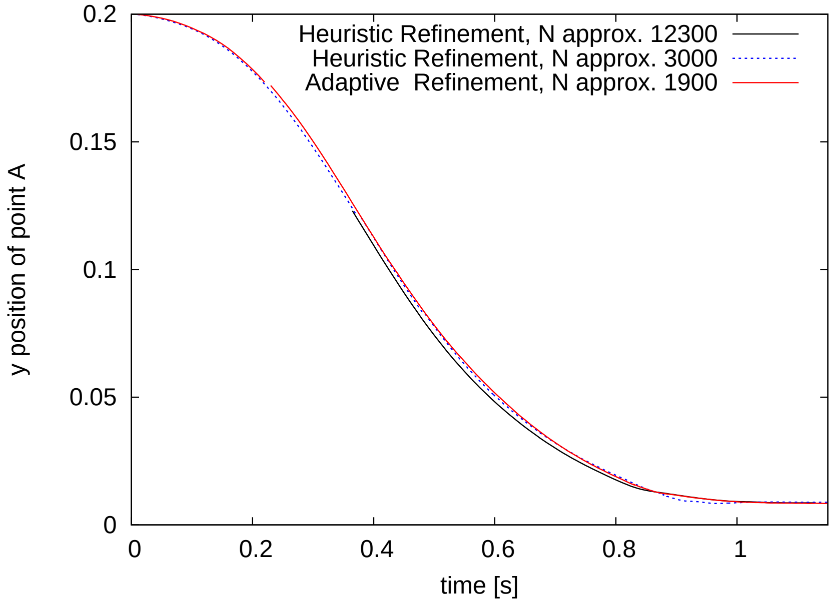


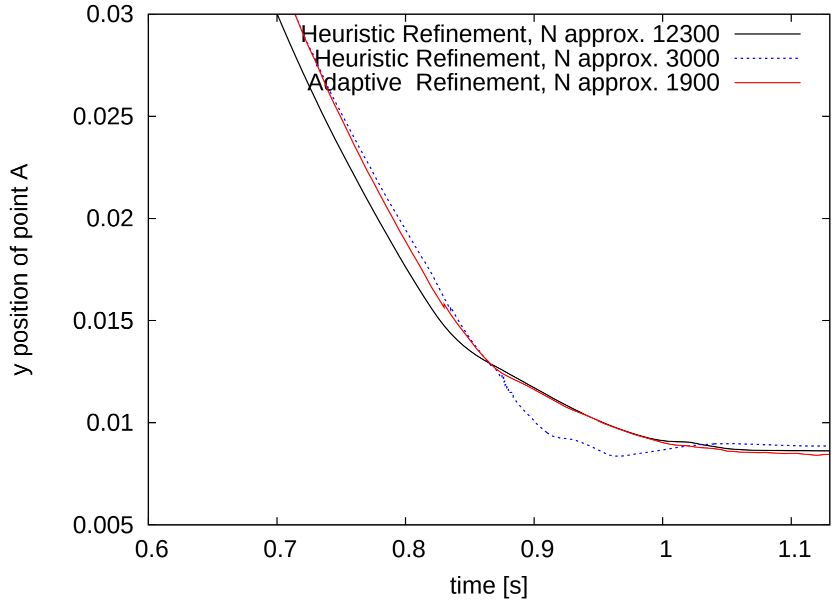
Large deformation (touching the wall)

Eulerian approach: zonal versus local refinement



$N \sim 3,000$ $\quad N \sim 12,000$ $\quad N \sim 1,900$





Position $x_A(t)$ of end point A

CPU time: **zonal 30 h**, **local 4 h**

Subject of ongoing work (Th. Richter)