The DWR method for numerical simulations related to nuclear waste disposals

Roland Becker
Laboratoire de Mathématiques Appliquées
Université de Pau et de Pays de l'Adour

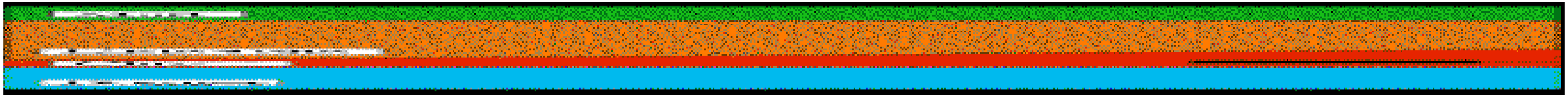
joint work with
Malte Braack (Universität Kiel), Dominik Meidner (Universität Heidelberg), Boris Vexler (RICAM Linz)

1. The couplex 1 - benchmark
2. The DWR-method
3. Time-dependent problems
4. Inverse problems
5. Convergence of adaptive methods

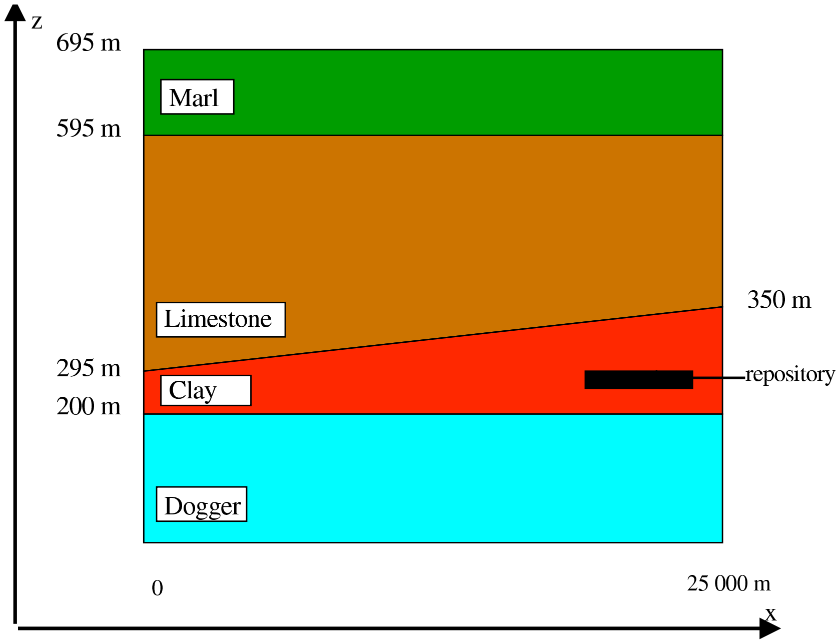
1. The couplex 1 - benchmark

- benchmark definition
- our tool: Gascoigne
- some thoughts about adaptivity

benchmark definition: couplex 1



(il manque encore un facteur 3)



$$R_i\omega(\frac{\partial C_i}{\partial t} + \lambda_i C_i) - \nabla \cdot (\mathbf{D}_i \nabla C_i) + \mathbf{u} \cdot \nabla C_i = f_i$$

$$\mathbf{u} = -K\nabla H \quad \nabla \cdot (K\nabla H) = 0$$

+ boundary conditions...

- linear problem
- tremenduous scales
- long-time integration
- rection-diffusion-advection with changing regimes

weak formulation

Find (C,H) in $(C_0,H_0)+V\times W$ such that:

$$a(C,\phi)+b(C,H,\phi)=l(\phi) \qquad \forall\phi\in V$$

$$d(H,\psi)=0 \qquad \forall\psi\in W$$

$$a(C,\phi):=\langle(C_t+\lambda C),\phi\rangle+\langle K\nabla C,\nabla\phi\rangle$$

$$b(C,H,\phi):=-\langle K\nabla H\cdot\nabla C,\nabla\phi\rangle$$

$$d(H,\psi):=\langle K\nabla H,\nabla\psi\rangle$$

$$u=(C,H),\quad v=(\phi,\psi),\quad X=V\times W$$

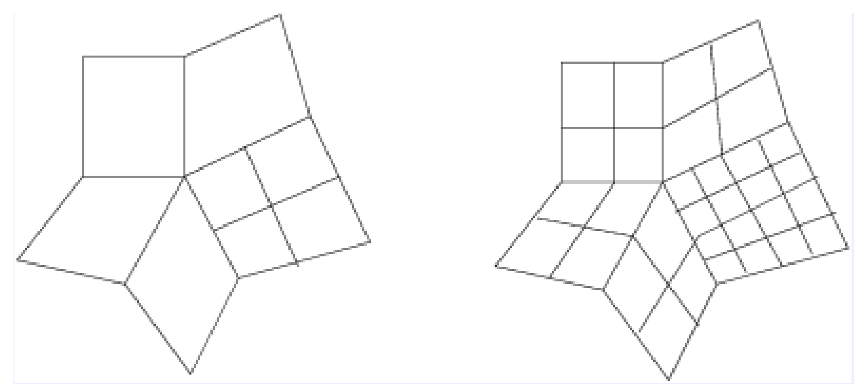
$$u\in u_0+X_0:\quad A(u,v)=F(v) \qquad \forall v\in X$$

3D Gascoigne

http://www.numerik.uni-kiel.de/~mabr/gascoigne/index.html

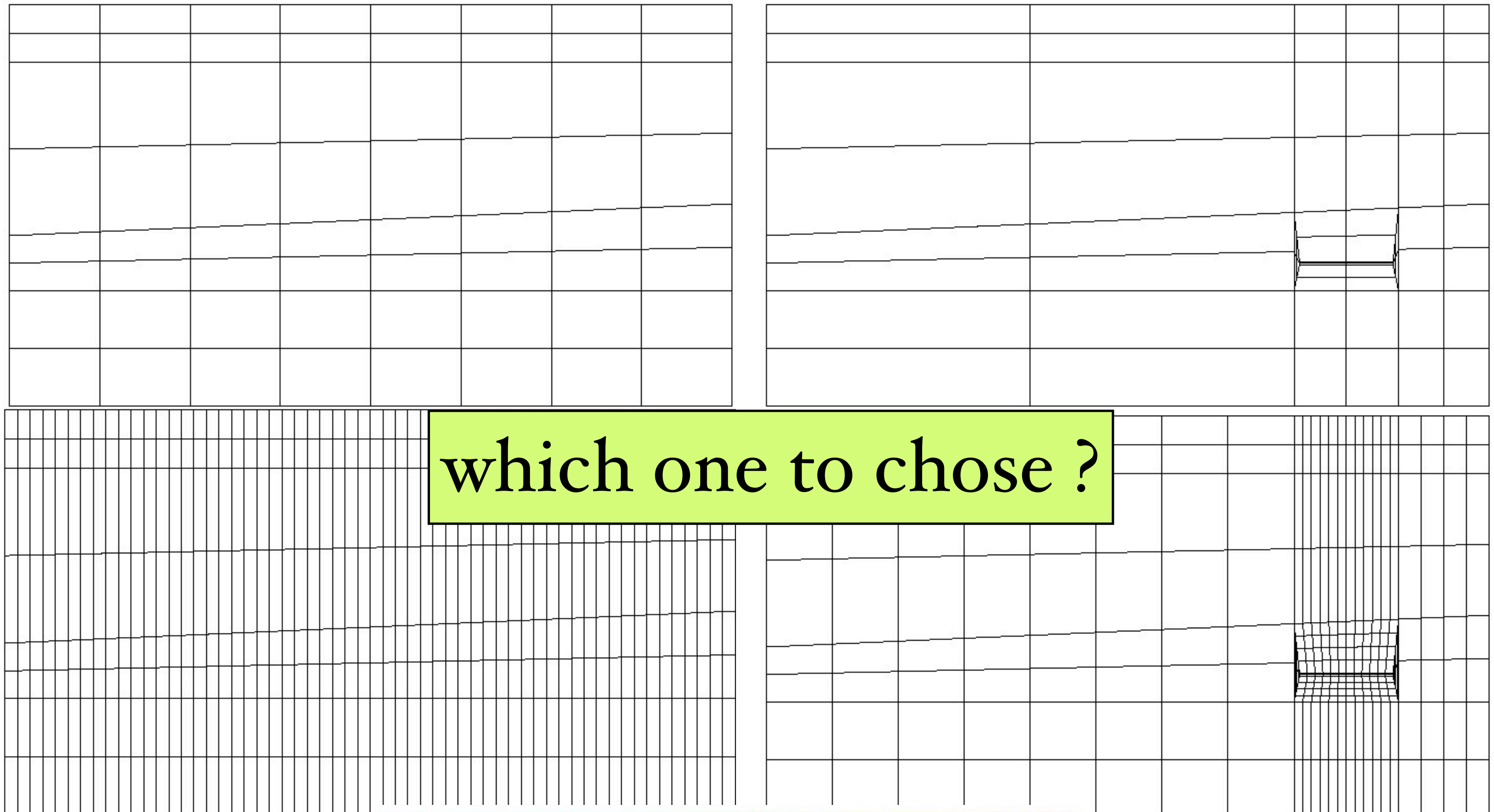
- adaptive mesh refinement
- quad (hex) - meshes with hanging nodes
- Newton, multigrid
- flexibility / modelling
- discretization: Q1, Q2 with stabilization

- local refinement with hanging nodes
- multigrid
- LPS - local projection stabilization
  - similar to the schemes of Guermond, Codina, Burman,...

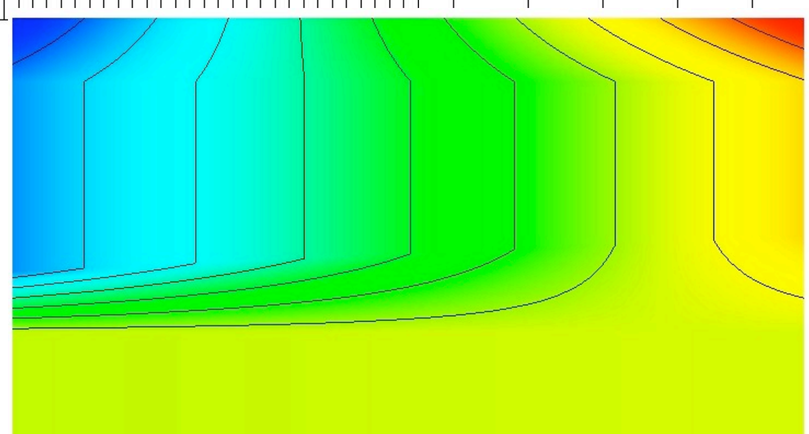


[1] R. Becker and M. Braack. A finite element pressure gradient stabilization for the Stokes equations based on local pro jections. Calcolo, 38(4):173–199, 2001.

starting mesh



which one to chose ?



hydrodynamic load H

adaptive strategy I

What quantity(ies) to compute ?

1.6 Output requirements

The following output quantities are expected from the simulations(both tables and graphical representations):

- Contour levels of C_i at times 200, 10110, 50110, 10^6, 10^7 years (the following level values should be used: $10^{-12}, 10^{-10}, 10^{-8}, 10^{-6}, 10^{-4}$);
- Pressure field (10 values uniformly distributed between 180 and 340;
- Darcy velocity field, along the 3 vertical lines given by $x = 50$, $x = 12500$, $x = 20000$, using 100 points along each line;
- Places where the Darcy velocity is zero;
- Cumulative total flux through the top and the bottom clay layer boundaries, as a function of time;
- Cumulative total fluxes through the left boundaries of the dogger and limestone layers;
- The discretization grid of the domains and the time stepping used in the simulations should also be given.

J(t)

$$
\begin{aligned}
J(t) &= \int_{\Gamma} K \frac{\partial C(t)}{\partial n} ds \\
&= \int_{\partial\Omega} z K \frac{\partial C(t)}{\partial n} ds \quad (z|_{\partial\Omega\setminus\Gamma} = 0) \\
&= \int_{\Omega} K \nabla C \cdot \nabla z \, dx.
\end{aligned}
$$

relates the functional to the operator !

...

stationary problem

- suppose we are interested in mean total flux
- equations are linear, stationary coefficients
  - time-derivative drop out

$$\overline{J} := \frac{1}{T}\int_0^T J(t)\,dt = J(\overline{C})$$
$$\overline{C} := \frac{1}{T}\int_0^T C(t)\,dt$$

Find $(\overline{C},\overline{H})$ in $(\overline{C}_0,\overline{H}_0)+\overline{V}\times\overline{W}$ such that:

→
$$\overline{a}(\overline{C},\phi)+b(\overline{C},\overline{H},\phi)=l(\phi) \qquad \forall\phi\in\overline{V}$$
$$d(\overline{H},\psi)=0 \qquad \forall\psi\in\overline{W}$$

stationary problem

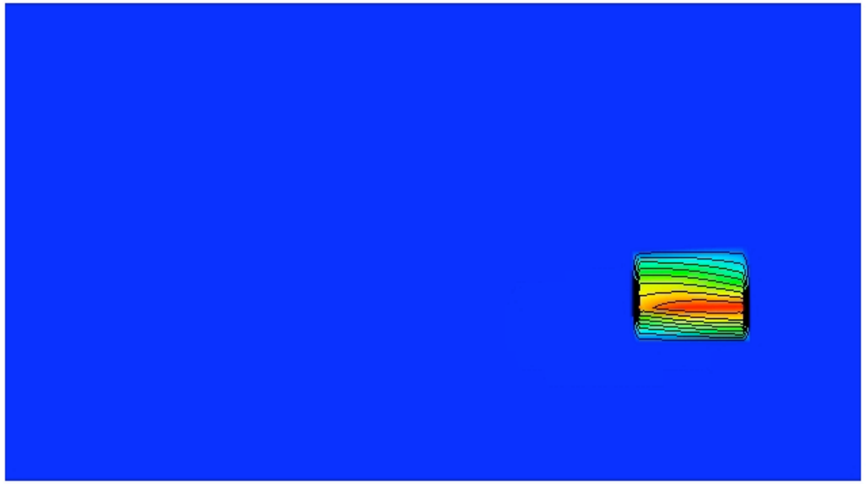
- simplify notation: drop overline

$$J(u) = A'(u)(u,z) \approx F(z) - A(u)(z)$$

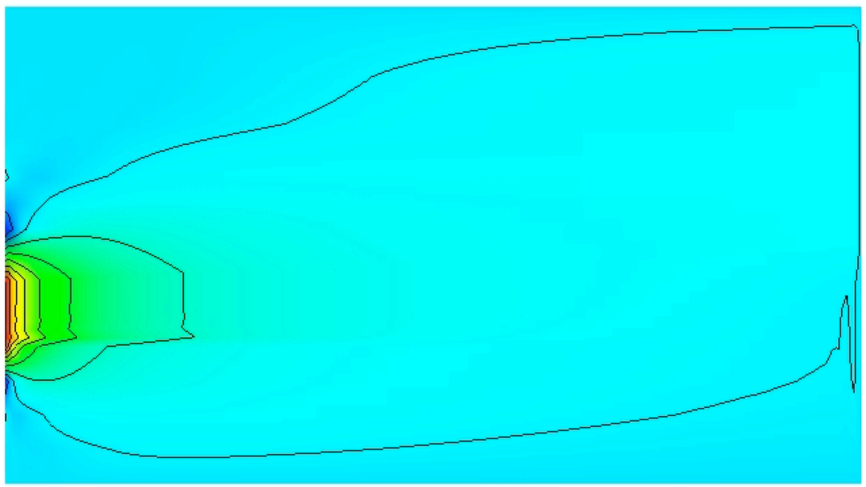
$$z \in z_0 + X$$
$$A'(u)(v,z) = 0 \quad \forall v \in X.$$

$$z = (D,G)$$
$$a(\phi,D) + b_C(\phi,H,D) = 0,$$
$$b_H(C,\psi,D) + d(\psi,G) = 0.$$

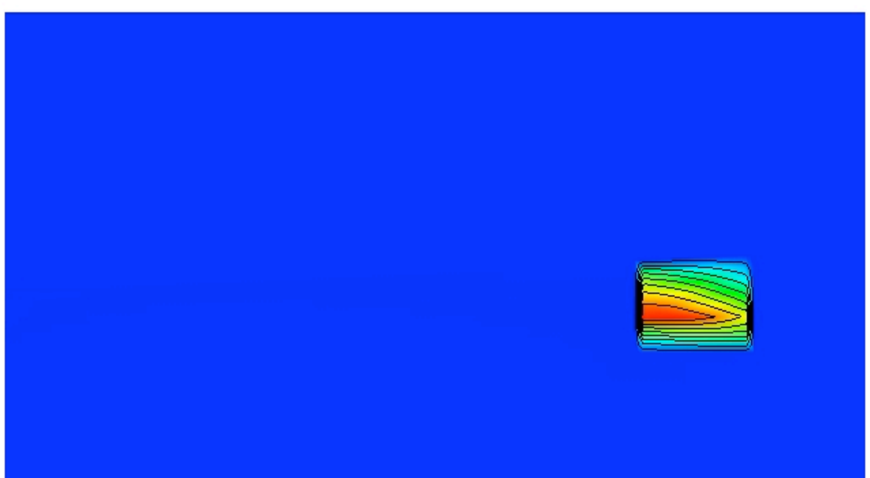
influence sur G



time-averaged solution

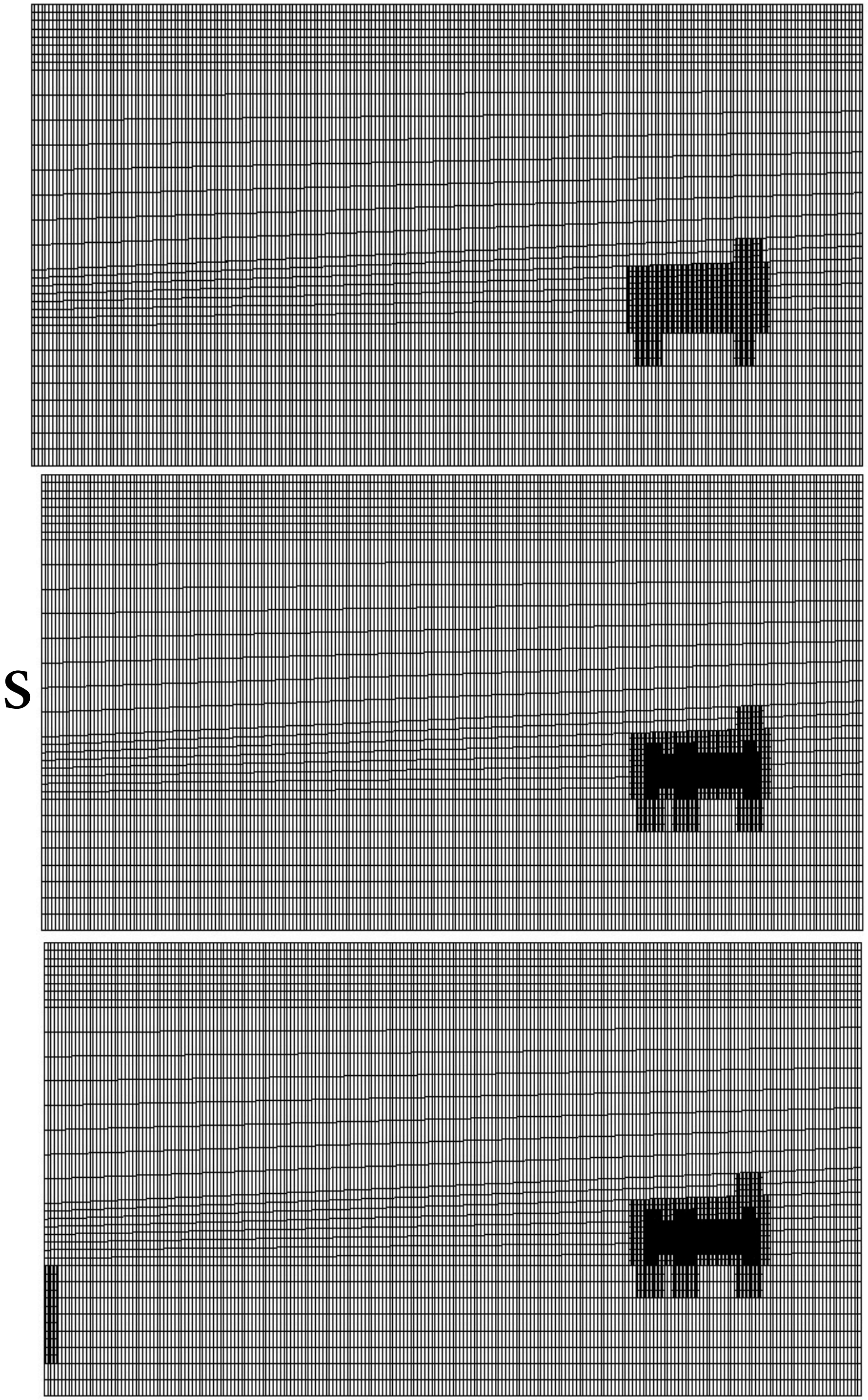


dual concentration



dual pressure

sequence of meshes
time-averaged pb



back to the full problem

- static adapted meshes
  - compute dynamic problem on the meshes as above…
  - what can be said ? how to improve ?
- dynamic meshes
  - needs space-time (finite element) discretization
  - H needs to be recomputed
  - adjoint problem is backward in time !!

2. The DWR-method

- Task: estimate the (discretization) error with respect to a given quantity
- Task: automatically construct efficient meshes to compute this quantity

idea (1): the quantity is a functional on the solution space

$$u \in V: \quad A(u,v) = F(v) \quad \forall v \in V$$

$$u_h \in V_h: \quad A(u_h,v) = F(v) \quad \forall v \in V_h$$

suppose linear...

estimate $G(u) - G(u_h) \quad (G \in V^*)$

idea (2): represent the functional by duality (c.f. Aubin-Nitsche, Lagrange,...)

$$z \in V: \quad A(v,z) = G(v) \quad \forall v \in V$$

$$\longrightarrow \quad G(u) - G(u_h) = A(u - u_h, z) = A(u - u_h, z - z_h)$$

error estimation

- many standard techniques can be used
  - residual estimators
  - hierarchical estimators
  - recovery
- our proposal: use hierarchy
  - I patchwise higher order interpolation (B/R,...)
  - II compute the finer solution(s)

$$G(u) - G(u_h) \approx G(u_{h/2}) - G(u_h) = A(u_{h/2} - u_h, z_{h/2} - z_h)$$

mesh adaptation

- needs to capture influence of local residuals on quantity of interest
- error density

$$G(u) - G(u_h) = \int_\Omega \eta(x)\, dx$$

example

model problem:

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

$$J(u) = \frac{\partial u}{\partial x}(x_0)$$

dual problem:

$$-\Delta z = J_\varepsilon \quad \text{in } \Omega,$$
$$z = 0 \quad \text{on } \partial\Omega.$$

$$J(u) - J(u_h) =$$

$$(\nabla(u - u_h), \nabla z) =$$

$$(\nabla(u - u_h), \nabla z - v_h) =$$

$$\ldots$$

$$\sum_K (\Delta u_h + f, z - v_h)_K +$$

$$\sum_K \frac{1}{2}([\partial_n u_h], z - v_h)_{\partial K} \leq$$

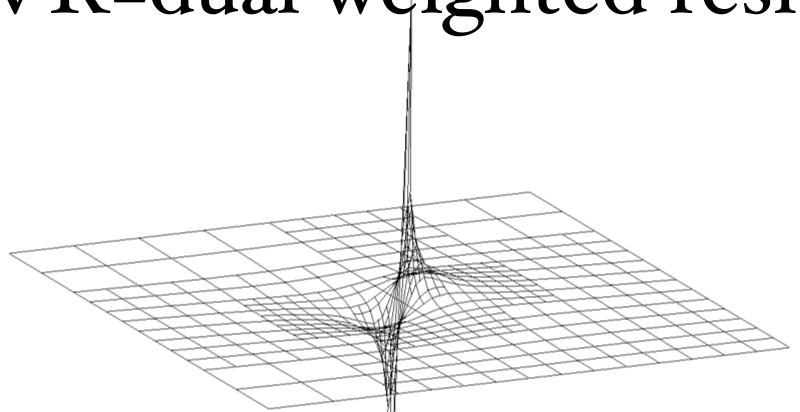
behaves like r^{-3}

$$\sum_{K \in \mathcal{T}_h} \rho_K \omega_K$$

$$\omega_K = \|z - v_h\|_K$$

$$\rho_K = \max(\|f + \Delta u_h\|_K, h_K^{-1/2}\|[\partial_n u_h]\|_{\partial K})$$

DWR=dual weighted residual



z

$\eta_{1,point}^{regular}$					
TOL	N	L	$\lvert\partial_1 e(0)\rvert$	η	I_{eff}
1	40	4	2.57e-0	1.09e-2	-
4^{-1}	64	4	1.47e-0	5.16e-2	-
4^{-2}	148	6	7.51e-1	5.92e-2	-
4^{-3}	940	9	4.10e-1	1.42e-2	3.33
4^{-4}	4912	12	4.14e-3	3.50e-3	1.25
4^{-5}	20980	15	2.27e-4	9.25e-4	0.24
4^{-6}	86740	17	5.82e-5	2.38e-4	0.24

behaves like second-order !!

for comparison: energy estimator

η_{energy}					
TOL	N	L	$\lvert\partial_1 e(0)\rvert$	η	I_{eff}
1	736	6	3.91e-1	8.80e-1	0.43
4^{-1}	11020	8	9.91e-2	2.28e-1	0.43
4^{-2}	166360	10	2.48e-2	5.88e-2	0.42

a general approach

$$J(u) - J(u_h) = \frac{1}{2}\mathcal{L}'(u_h, z_h)(u - \phi_h, z - \psi_h) + R,$$

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

$$\begin{cases} \rho(u_h)(\psi) := f(\psi) - a(u_h)(\psi) \\ \rho^*(z_h)(\phi) := J'(u_h)(\phi) - a'(u_h)(\phi, z_h) \end{cases}$$

$$J(u) - J(u_h) = \frac{1}{2}\underbrace{\rho(u_h)(z - \psi_h)}_{\text{primal}} + \frac{1}{2}\underbrace{\rho^*(z_h)(u - \phi_h)}_{\text{dual}} + R.$$

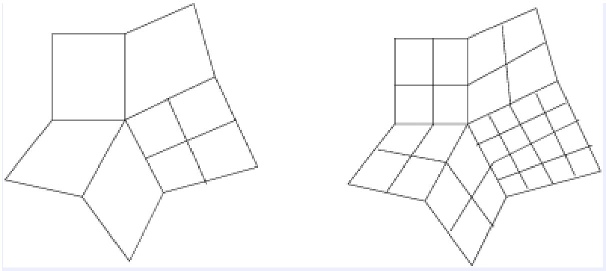
[1] R. Becker and R. Rannacher. Weighted a posteriori error control in FE methods. In e. a. H. G. Bock, editor, ENUMATH'97. World Sci. Publ., Singapore, 1995.
[2] R. Becker and R. Rannacher. A feed-back approach to error control in finite element methods: Basic analysis and examples. East-West J. Numer. Math., 4:237–264, 1996.
[3] **R. Becker and R. Rannacher. An optimal control approach to a-posteriori error estimation. In A. Iserles, editor, Acta Numerica 2001, pages 1–102. Cambridege University Press, 2001.**

pour Couplex

$$J(u) - J(u_h) = \frac{1}{2}\rho(u_h)(z - \psi_h) + \frac{1}{2}\rho^*(u_h, z_h)(u - \phi_h)$$

- no linearization error
- approximation of weights

algorithm



- standard adaptive algorithm: SOLVE-ESTIMATE-MARK-REFINE
- patched meshes → $V_h \approx Q_h^1 \qquad W_h \approx Q_{2h}^2$
  $I_h : V_h \to W_h$ natural
- approximation of weights
  - ActaNumerica → $z - \psi_h \approx I_h z_h - z_h$
  - gendarmes → do the mesh refinement on $2h$
    $z - \psi_{2h} \approx z_h - i_{2h} z_h$

3. Time-dependent problems

with D. Meidner, M. Schmich, B. Vexler

- need all the data in space and time
  - even for evaluation of estimator
  - known problem in optimal control

- windowing/checkpointing for storage reduction
- generalization of DWR to time-dependent problems

storage reduction

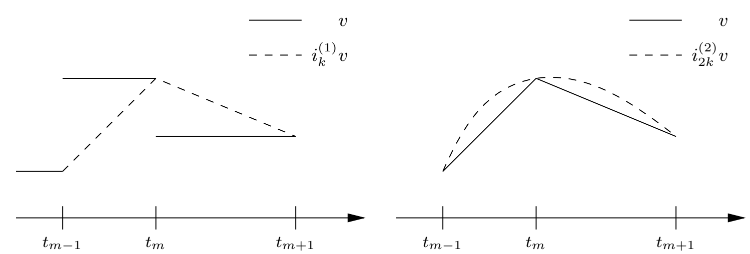
- divide and conquer: replace storage by computation
- can be done optimally up to logs
- see Griewank/Walther for AD
- for optimization of parabolic equations

[1] R. Becker, D. Meidner, and B. Vexler. Efficient numerical solution of parabolic optimization problems by finite element methods. Technical report, UPPA, 2005.

DWR for parabolic problems

[1] **M. Schmich and B. Vexler.** Adaptivity with dynamic meshes for space-time finite element discretizations of parabolic equations. Technical report, RICAM, 2006.

- variational framework:
  - space-time finite elements
  - requires special care !
- use ‘patched time-steps’



(a) Piecewise linear interpolation (b) Piecewise quadratic interpolation

Fig. 4.1: Interpolation operators

- we need to distinguish between space and time

an example: reaction-diffusion

$$\partial_t \theta - \Delta\theta = \omega(\theta, Y) \qquad \text{in } \Omega \times I,$$
$$\partial_t Y - \frac{1}{\mathrm{Le}}\Delta Y = -\omega(\theta, Y) \qquad \text{in } \Omega \times I,$$

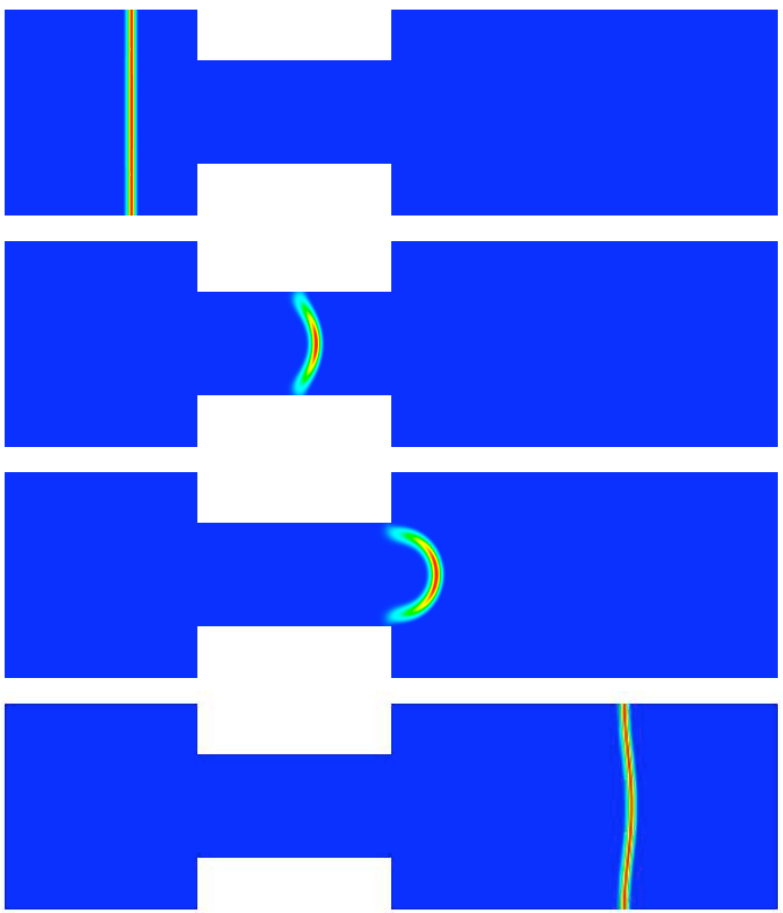


Fig. 5.4: Example 1: Reaction rate ω at $t = 1.0, 20.0, 40.0, 60.0$

compute:

$$J(u) = \frac{1}{60|\Omega|}\int_0^{60}\int_\Omega \omega(\theta, Y)\,dx\,dt$$

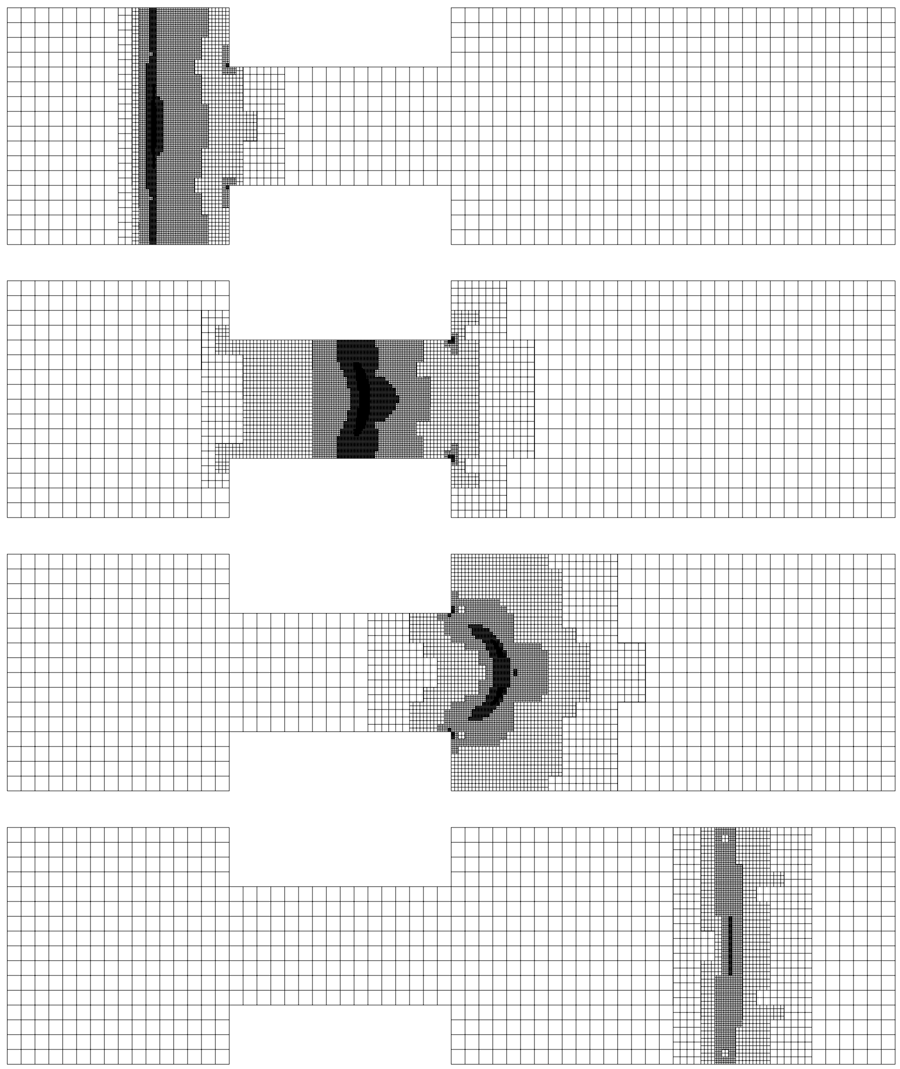
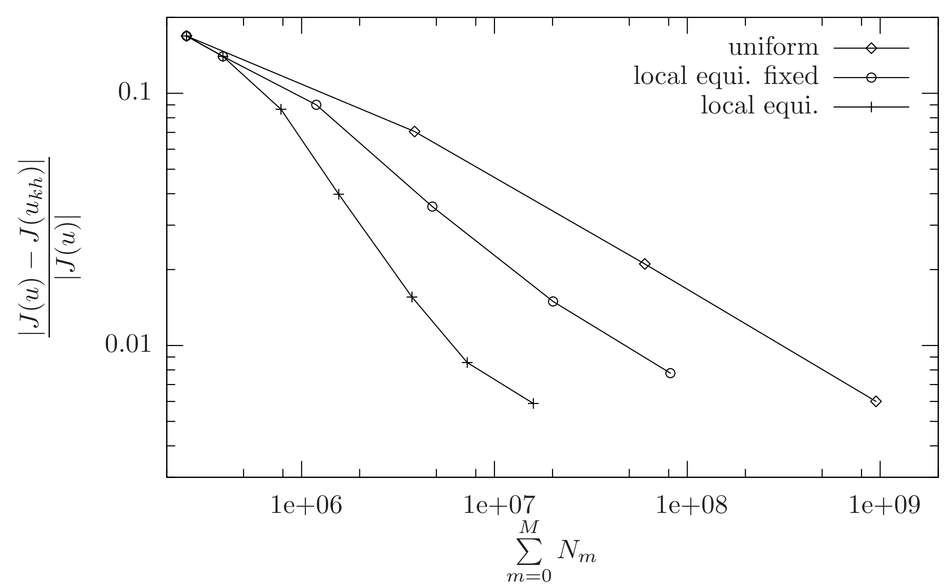


Fig. 5.5: Example 1: Corresponding meshes at $t = 1.0$, 20.0, 40.0, 60.0



4. Inverse problems

- an example problem
- a systematic approach
- numerical sensitivities

an example problem

Find $q \in \mathbb{R}$

$$\frac{1}{2}\Big|\int_\Omega \omega u \, dx - \bar{C}\Big|^2 \longrightarrow \inf, \qquad \omega > 0$$

$$\begin{aligned} -\Delta u &= qf \qquad \text{in } \Omega = (0,1)^2, \\ u &= 0 \qquad \text{on } \partial\Omega, \qquad f > 0 \end{aligned}$$

objective: compute q !

solution operator: $S : Q \to V \qquad q \mapsto u$

$$u = S(q) = q u_1,$$

with

$$\begin{aligned} -\Delta u_1 &= f && \text{in } \Omega \\ u_1 &= 0 && \text{on } \partial\Omega. \end{aligned}$$

optimal solution:

$$q = \bar{C}\mu, \qquad \mu := \frac{1}{\int_\Omega \omega u_1 \, dx}.$$

discrete solution:

$$q_h = \bar{C}\mu_h, \qquad \mu_h := \frac{1}{\int_\Omega \omega u_{1h} \, dx},$$

Ritz projection: $u_{1h} \in V_h$

adjoint problem:

$$\begin{aligned} -\Delta y &= -\mu\omega && \text{in } \Omega \\ y &= 0 && \text{on } \partial\Omega. \end{aligned}$$

$$\begin{aligned} q - q_h &= \overline{C}\mu - \mu \int_\Omega \omega u_1 \, dx \, q_h \\ &= \int_\Omega \omega u_h \, dx \, q_h + q_h(\nabla u_1, \nabla y) \\ &= -(\nabla u_h, \nabla y) + (q_h f, y) \end{aligned}$$

$\longrightarrow$ $$q - q_h = \rho(y), \qquad \rho(\phi) := (q_h f, \phi) - (\nabla u_h, \nabla \phi)$$

Proposition 1 *For the discretization of the simple example (12,13), we have the a posteriori error estimate:*

$$|q - q_h| \;\leq\; \eta := \sum_{K \in \mathcal{T}_h} \rho_K \omega_K, \tag{20}$$

with the cell residual and cell weights defined by:

$$\rho_K \;=\; \|q_h f + \Delta u_h\|_K + \tfrac{1}{2} h_K^{-1/2} \|[\partial_n u_h]\|_{\partial K}, \tag{21}$$

$$\omega_K \;=\; \|y - i_h y\|_K + h_K^{1/2} \|y - i_h y\|_{\partial K}, \tag{22}$$

where the second term in (21) involves the jump of the normal derivative over the interiori faces of the mesh and is understood to be zero on boundary faces. The weights are local interpolation errors involving an arbitrary interpolation operator $i_h : V \to V_h$.

a systematic approach

$$\begin{aligned} \text{Minimize} \quad & \tfrac{1}{2}\|C(u) - C_0\|^2 \\ \text{under the constraint} \quad & a(u, q)(\phi) = f(\phi) \qquad \forall \phi \in V. \end{aligned}$$

- Functional estimate $J - J_h$ useless
- Few paramaters: $Q = \mathbb{R}^l, l \approx 10$
- Gauß–Newton

objective: compute E(q) !

(E is a functional on control space)

Unconstrained least squares formulation

Minimize $\frac{1}{2}\|c(q) - C_0\|^2, \quad c(q) := C(u(q)), \quad J := c'(q_k)$

$$(J^T J)(q_{k+1} - q_k) = -J^T(c(q_k) - C_0)$$

$$E(q) - E(q_h) = \frac{1}{2}\{\rho(\delta z) + \rho^*(\delta u)\} + R_{GN} + R_{NL}$$

$$a'_u(u,q)(\phi,z) = - < J(J^tJ)^{-1}\nabla E(q), C'(u)(\phi) >$$

$$\begin{aligned} \rho(\phi) &:= (f,\phi) - a(u_h,q_h)(\phi) \\ \rho^*(\phi) &:= < J_h(J_h^tJ_h)^{-1}\nabla E(q_h), C'(u_h)(\phi) > + a'_u(u_h,q_h)(\phi, z_h \end{aligned}$$

Remarks

- R_{NL} is cubic
- $R_{GN} \leq C\,\|e\|\,\|C(u)\|$

[1] R. Becker and B. Vexler. A posteriori error estimation for finite element discretizations of parameter identification problems. *Numer. Math.*, 96(3):435–459, 2004.

How does this fit into the framework ?

$$Au = Bq, \quad \|Cu - C_0\| \to \inf$$

Then

$$c(q) = Jq - C_0, \quad J = CA^{-1}B, \quad (J^*J)q = J^*C_0$$

$$\mathcal{M}(u, z, q, \lambda) := b(q, z) - a(u, z) + < Cu - C_0, \lambda > + E(q),$$

$$\lambda \in R(J)$$

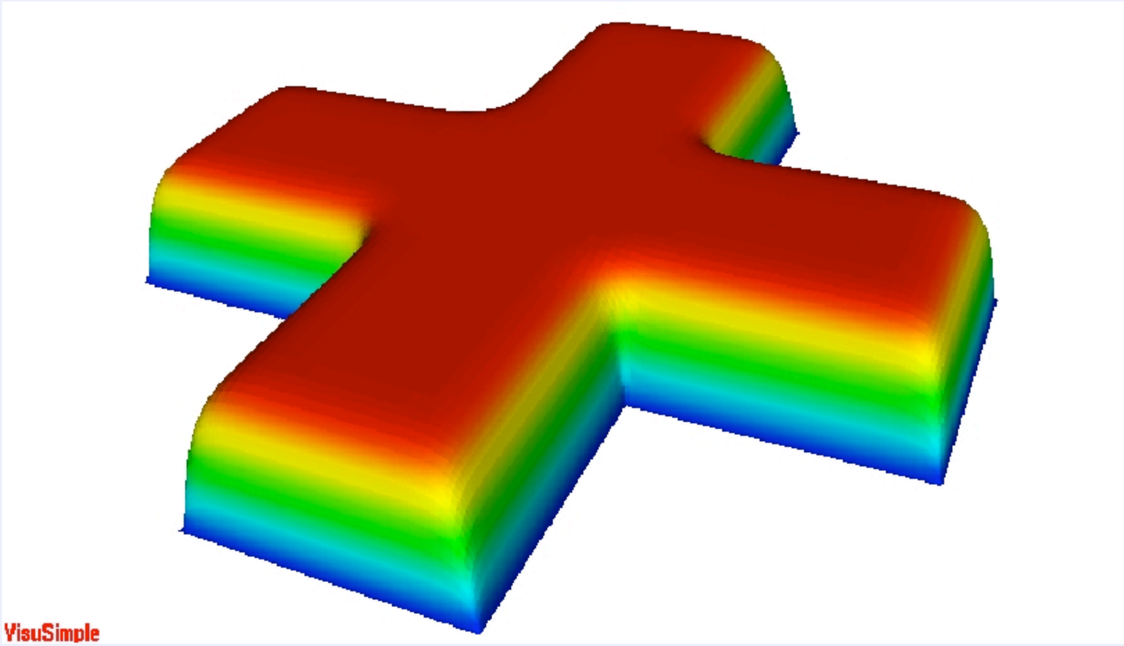
We find:

- $Au = Bq$
- $Jq = P_{R(J)}C_0$
- $A^*z = C^*J\mu, \quad \lambda = J\mu, \quad (J^*J)\mu = E$

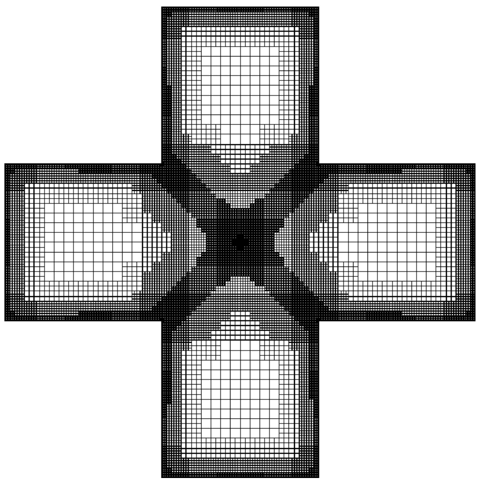
Example

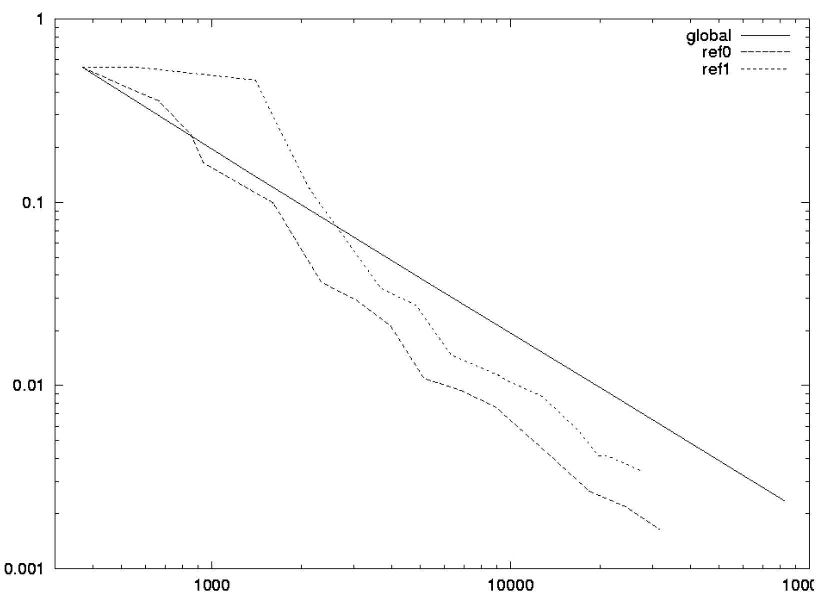
$$\begin{aligned} -q_0 \Delta u + q_1 u &= 2 \qquad \text{in } \Omega, \\ u &= 0 \qquad \text{on } \partial\Omega. \end{aligned}$$

$$C_1(u) = u(0.5, 0.5) - \overline{u}_1, \qquad C_2(u) = \int_\Omega u - \overline{u}_2$$

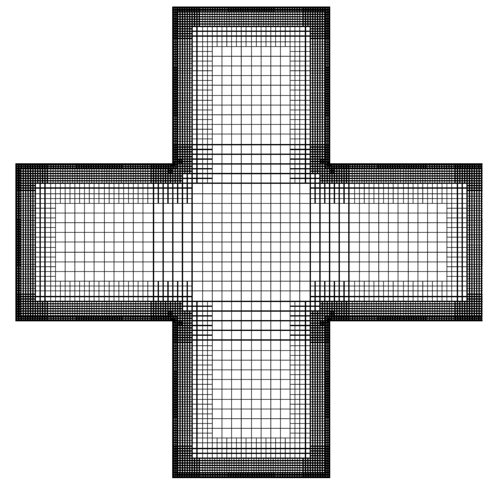


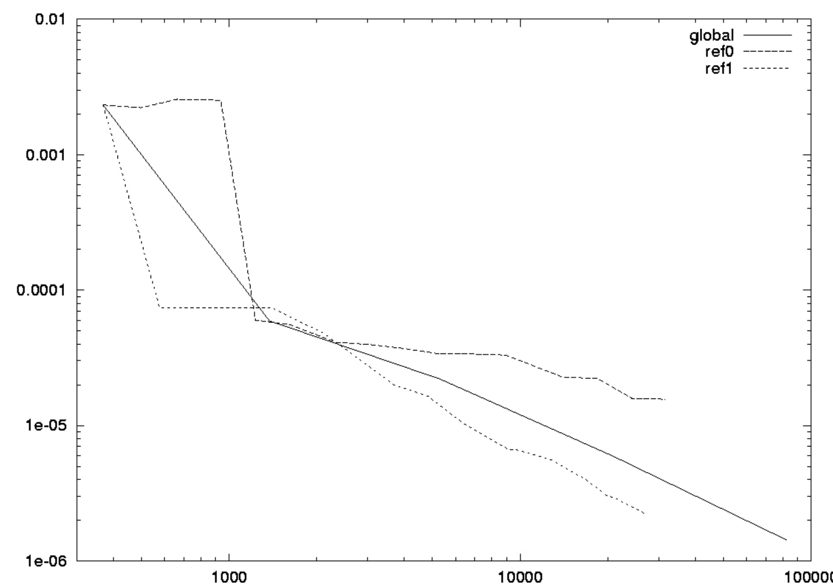
C_1




global
ref0
ref1
1
0.1
0.01
0.001
1000
10000
1000

C_2




global
ref0
ref1
0.01
0.001
0.0001
1e-05
1e-06
1000
10000
100000

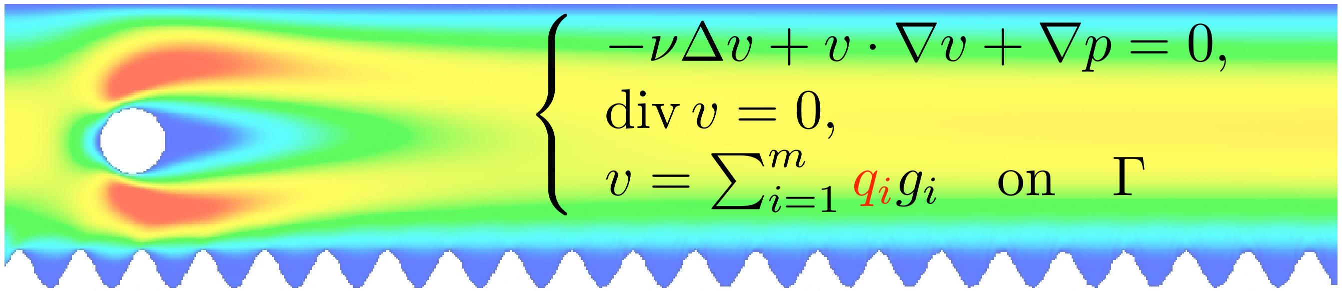
numerical sensitivities

- there is a more general approach:
  - functionals depending on control and state
  - inequality constraints
  - numerical sensitivities

[1] R. Becker and B. Vexler. Mesh refinement and numerical sensitivity analysis for parameter calibration of partial differential equations. *J. Comp. Phs.*, 206(1):95–110, 2005.

[2] R. Griesse and B. Vexler. Numerical sensitivity analysis for the quantity of interest in pde-constrained optimization. *SIAM Journal on Scientific Computing*, 2007.

an example

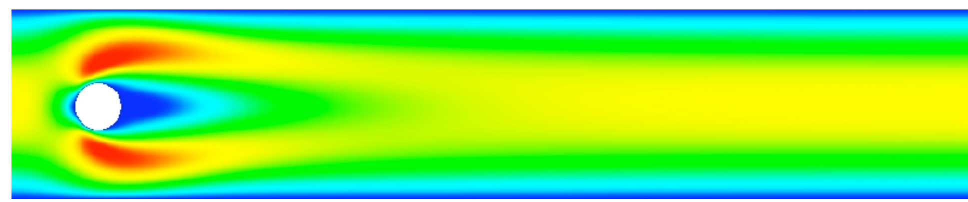


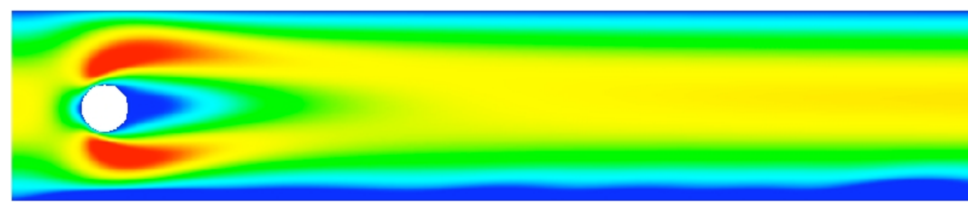
$$\begin{cases} -\nu \Delta v + v \cdot \nabla v + \nabla p = 0, \\ \operatorname{div} v = 0, \\ v = \sum_{i=1}^{m} q_i g_i \quad \text{on} \quad \Gamma \end{cases}$$

$$J(u, c) = \frac{1}{2} \sum_{i=1}^{n} |C_i(u) - \bar{C}_i|^2$$

C_i = measurements of p, v

- (How to solve this ?)
- What are the most important **modes** ?
- What are most important **mesuraments** ?





consider modes/mesures as "parameters"...
compute (relaticve) condition numbers

5. Convergence of adaptive methods

- few results known for Poisson's equation
- <u>much less</u> known for NON-Poisson
- nothing known for DWR

▸ we need more theory !

what is the problem ?

- do adaptive FEM-discretizations converge at all ?
- at what speed ? (what means ‘speed’ ?)
- are these questions useful for development of algorithms ?

what we have

- Dörfler/Verfürth: P1, bulk chasing: *convergence*
- Cohen/Dahmen/de Vore: bulk chasing for <u>wavelets</u>: *quasi-optimal convergence*
- Morin/Nochetto /Siebert: P1, newest vertex, data oscillation: *convergence*
- Binev/Dahmen/de Vore--Stevenson: bulk chasing for P1, newest vertex: *quasi-optimal convergence*

what we do not have

- non-nested refinement
- non-conforming, mixed FEM
- hp- methods
- DWR-method
- non bulk chasing algorithm

A new algorithm: the Gendarme Algorithm

- as bad as the others, but more complex (nearly)
- <u>two</u> estimators
- <u>two</u> meshes
- nested spaces
- quasi-optimal convergence

The Gendarme Algorithm

$$\begin{array}{ccccccccc} \ldots & \subset & V_{k-1} & \subset & V_k & \subset & V_{k+1} & \subset & \ldots \\ \ldots & & & & \cap & & & & \ldots \\ \ldots & \subset & \overline{V_{k-1}} & \subset & \overline{V_k} & \subset & \overline{V_{k+1}} & \subset & \ldots \end{array}$$

- do a global refinement
- if $\quad |||\overline{u_{k+1}} - u_k|||^2 \leq \alpha\, \eta^{(2)}(V_k)$ refine "osc"
- else use simple estimator to refine

$$C_1\eta^{(1)}(\widetilde{V},\widehat{V}) \le |||\widehat{u}-\widetilde{u}|||^2 \le C_2\eta^{(1)}(\widetilde{V},\widehat{V}).$$

$$|||u-\widetilde{u}|||^2 \le \eta^{(2)}(\widetilde{V}).$$

we need:

$$\eta^{(2)}(\widetilde{V}) \le C_\eta |||u-\widetilde{u}|||^2 + osc(\widetilde{\mathcal{T}}),$$

$$osc(\widetilde{\mathcal{T}}) := \sum_{K\in\widetilde{\mathcal{T}}} h_K^2 \|f-P_{\widetilde{V}}f\|_K^2.$$

$$\mathcal{A}^s := \{u \in H_0^1(\Omega) : \sup_{N\in\mathbb{N}} N^s \inf_{V\in\mathcal{V}_N} |||u-v|||^2 < +\infty\}.$$

Theorem 6. *Let for $s>0$ $u\in\mathcal{A}^s$. There exists a constant C such for $\varepsilon>0$ the following holds. If the gendarme algorithm terminates with error $|||u-u_V|||^2 \le \varepsilon$ then the dimensions N of V is bounded by:*

$$N \le C\varepsilon^{-1/s}. \tag{28}$$