5 Applications in Fluid Mechanics

We discuss the use of the DWR method for the finite element approximation of models for viscous incompressible and compressible flow including also chemical reactions. The examples presented include the computation of the drag and lift coefficient of a blunt body in two- and three-dimensional channel flows, the mean Nusselt number in a heat exchanger, line-averages of species concentrations in a flow reactor, the mean temperature in a methane flame.

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5.1 Incompressible viscous flow

'Navier-Stokes operator'

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

- 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 of 'optimal' solution $\hat{u}$ by solving the eigenvalue problem

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

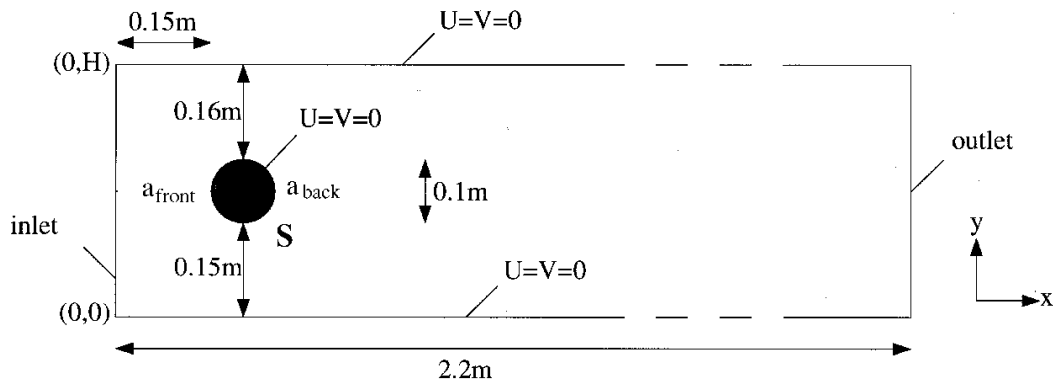**Question:** Are stationary solutions obtained by the Newton method dynamically stable?

A model configuration

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

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

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

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

Computation '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
$\tau = \frac{1}{2}\nu(\nabla v + \nabla v^T) - pI$ strain tensor

Finite Element Discretization

Solution and test spaces

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

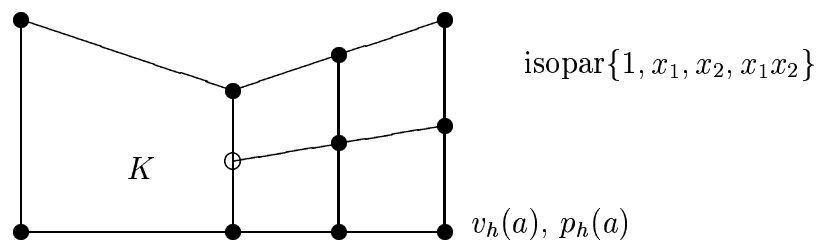Semi-linear form ('energy form'): $u = \{v, p\}, \ \varphi = \{\varphi^v, \varphi^p\}$

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

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

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

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

K

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

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-velocity coupling and advection:

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

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: $\qquad \qquad \delta_T(\nabla p_h, \nabla\varphi_h^p)_T$

- Stabilization of transport: $\qquad \qquad \delta_T(v_h\cdot\nabla v_h, v_h\cdot\nabla\varphi_h^v)_T$

- Stabilization of mass conservation: $\quad \delta_T(\nabla\cdot v_h, \nabla\cdot\varphi_h^v)_T$

- Adaptive determination of stabilization parameter:

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

Solution by quasi-Newton or pseudo-time iteration:

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

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

- 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*

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

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

Remark. Evaluation of error estimator:

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

for arbitrary ψ_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.

Primal residual:

$$\rho(u_h)(z - i_h z) := \sum_{K \in \mathbb{T}_h} \left\{ (R(u_h), \underbrace{z^v - i_h z^v}_{weight})_K + (r(u_h), \underbrace{z^v - i_h z^v}_{weight})_{\partial K} \right.$$
$$\left. + (\underbrace{z^p - i_h z^p}_{weight}, \nabla \cdot v_h)_K + \dots \right\}$$

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

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

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

Dual residual:

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

$$\left. + (\underbrace{p - i_h p}_{\text{weight}}, \nabla \cdot z_h)_K + \dots \right\}$$

cell and edge residuals

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

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

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

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

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

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		

Table. Results for drag computation on adaptively refined meshes
(error level of $< 1\%$, indicated by bold face; $N = \#$ cells).

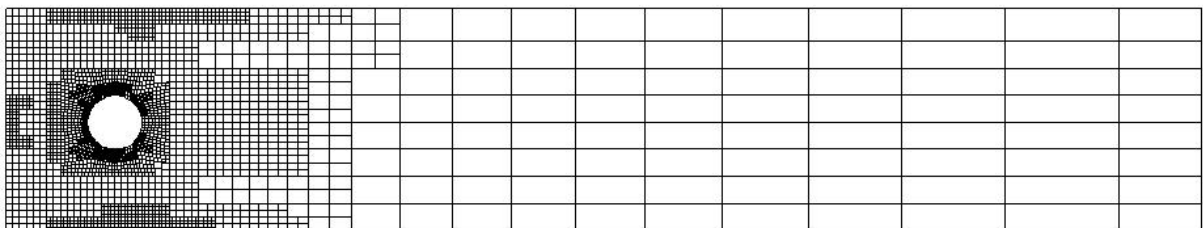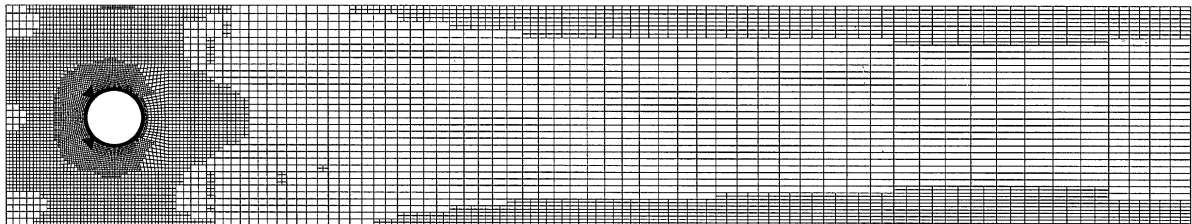**Figure.** Refined meshes by 'smoothness-based' strategies and by the DWR method.

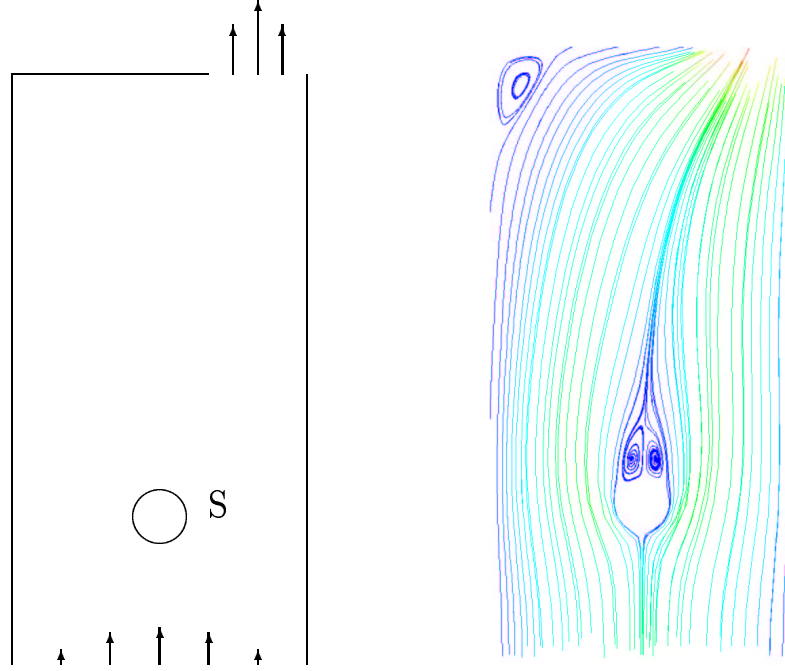**Comparison with ad-hoc adaptation (R. Becker/M. Braack 1999)**

Figure. Configuration and streamline plot (Re = 50).

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

Heuristic refinement indicators:

- *Vorticity:* $\eta_K := h_K^{-1} \|\nabla \times v_h\|_K$

- *Pressure-gradient:* $\eta_K := h_K^{-1} \|\nabla p_h\|_K$

- *"Energy-error":* $\eta_K := h_K^{-1} \|R_h\|_K + h_K^{-1/2} \|r_h\|_{\partial K} + h_K^{-1} \|\nabla \cdot v_h\|_K$

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

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

The vorticity and the pressure-gradient indicators measure the "smoothness" of $\{v_h, p_h\}$, while the "energy-error" indicator additionally contains information about local conservation of mass and momentum.
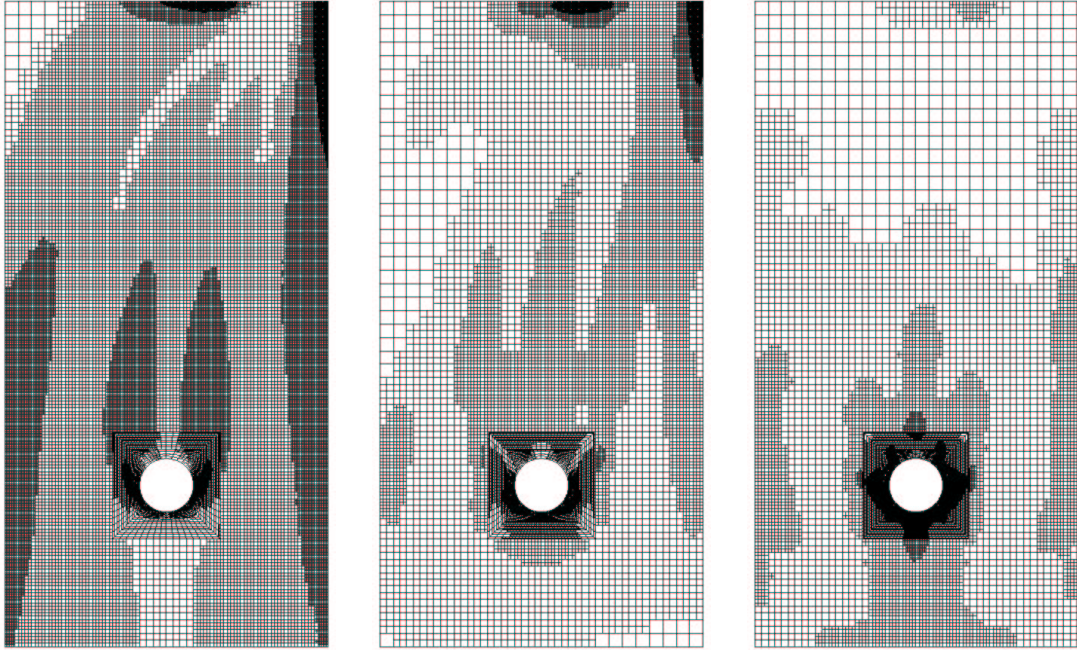
Figure. Meshes with 5 000 cells obtained by the vorticity indicator (left), the "energy" indicator (middle), and the weighted indicator (right).
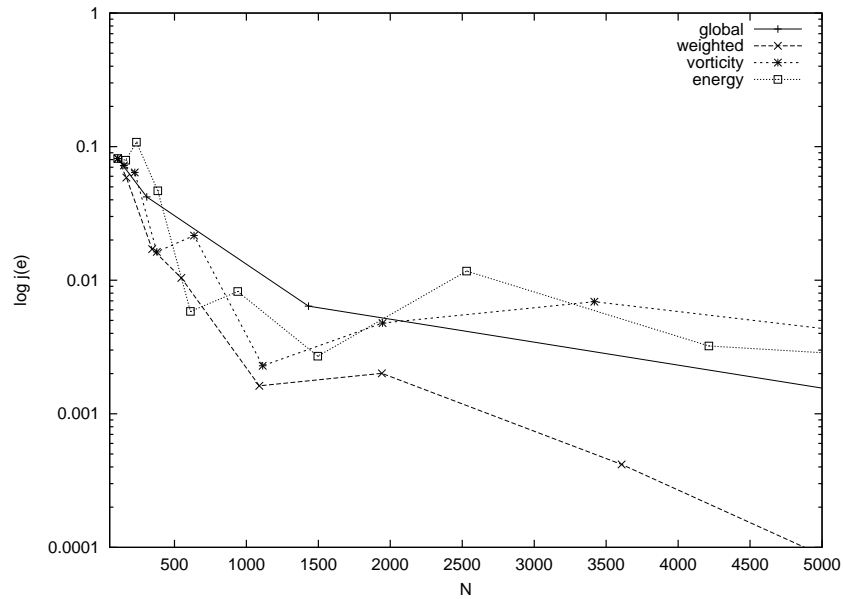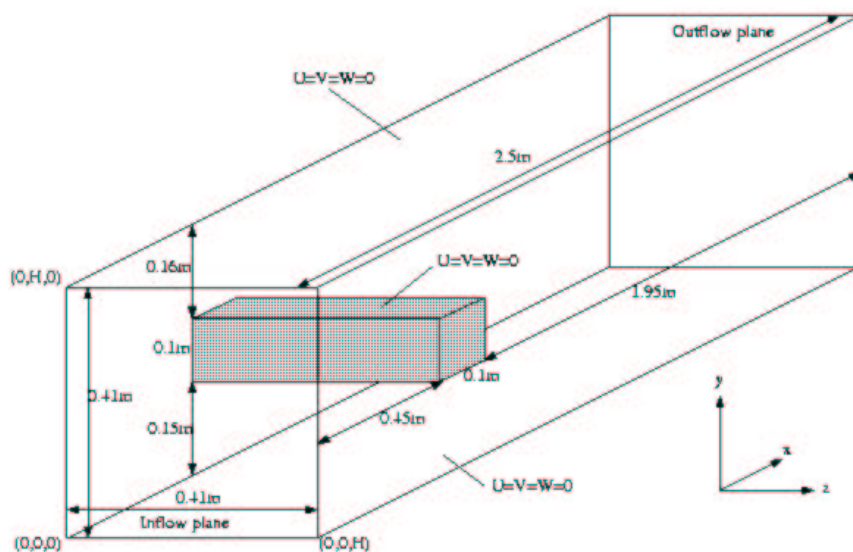

Figure. Mesh efficiency achieved by uniform refinement ("global" +), the weighted indicator ("weighted" ×), the vorticity indicator ("vorticity" ∗), and the energy indicator ("energy" □).

Computation of drag in 3-D (M. Braack, T. Richter 2002)

Computation of drag coefficient:

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

a) N_{global}	c_d	b) N_{energy}	c_d	c) $N_{weighted}$	c_d
$15,960$	8.2559	$3,696$	12.7888	$3,696$	12.7888
$117,360$	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
–	–	–	–	$162,680$	7.7788
–	–	–	–	$367,040$	7.7784
∞	7.7730	∞	7.7730	∞	7.7730

Table: Results of drag computation:
a) Q_2/Q_1-element with global uniform refinement,
b) Q_1/Q_1-element with local refinement by "energy error indicator",
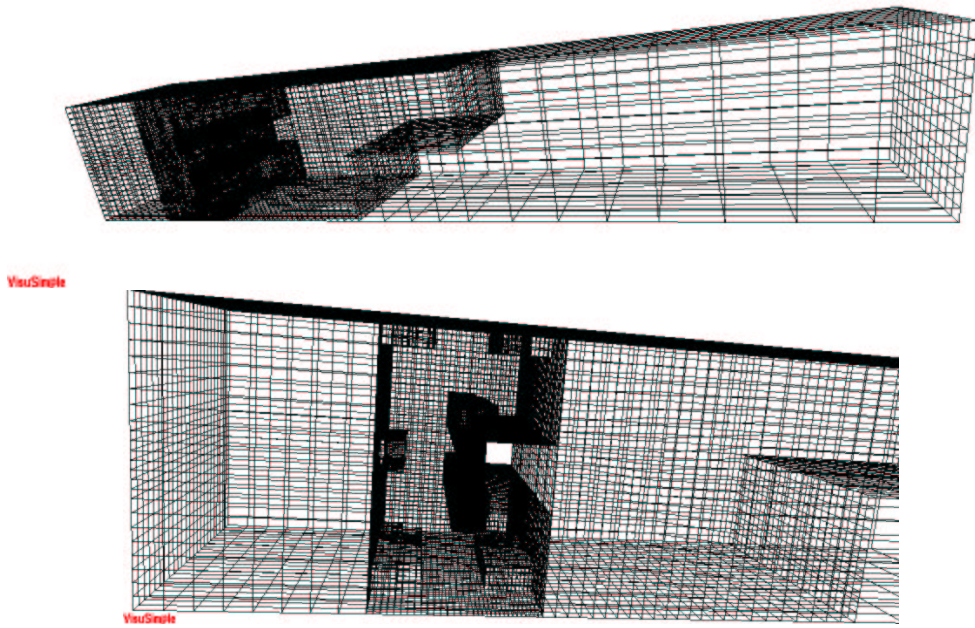c) Q_1/Q_1-element with local refinement by "weighted earor indrcator"i

Figure. Refined mesh and zoom by the "energy" error indicator.
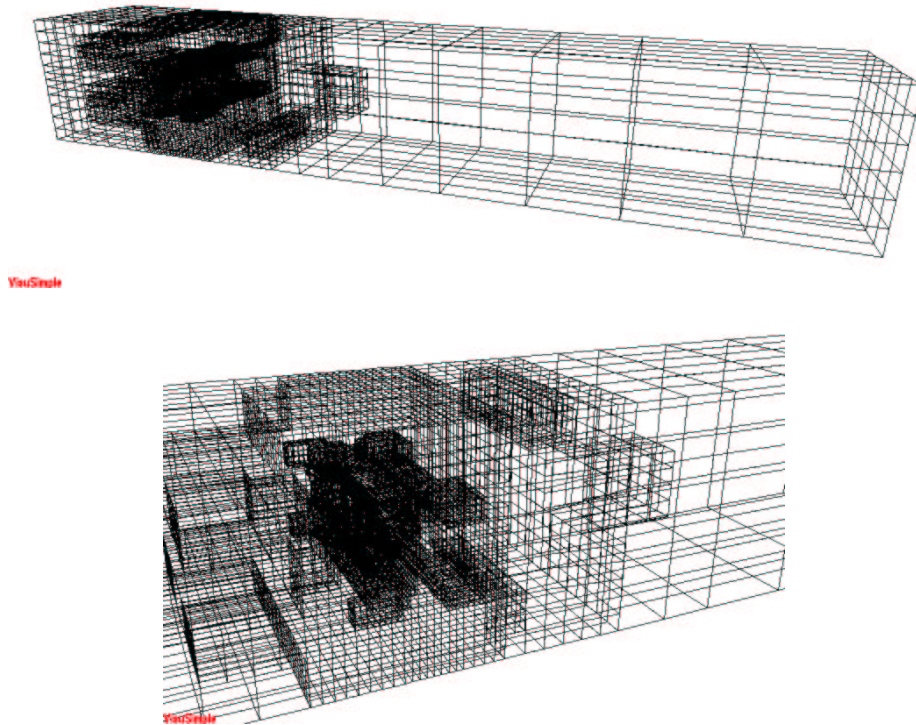

Figure. Refined mesh and zoom by the "weighted" error indicator.
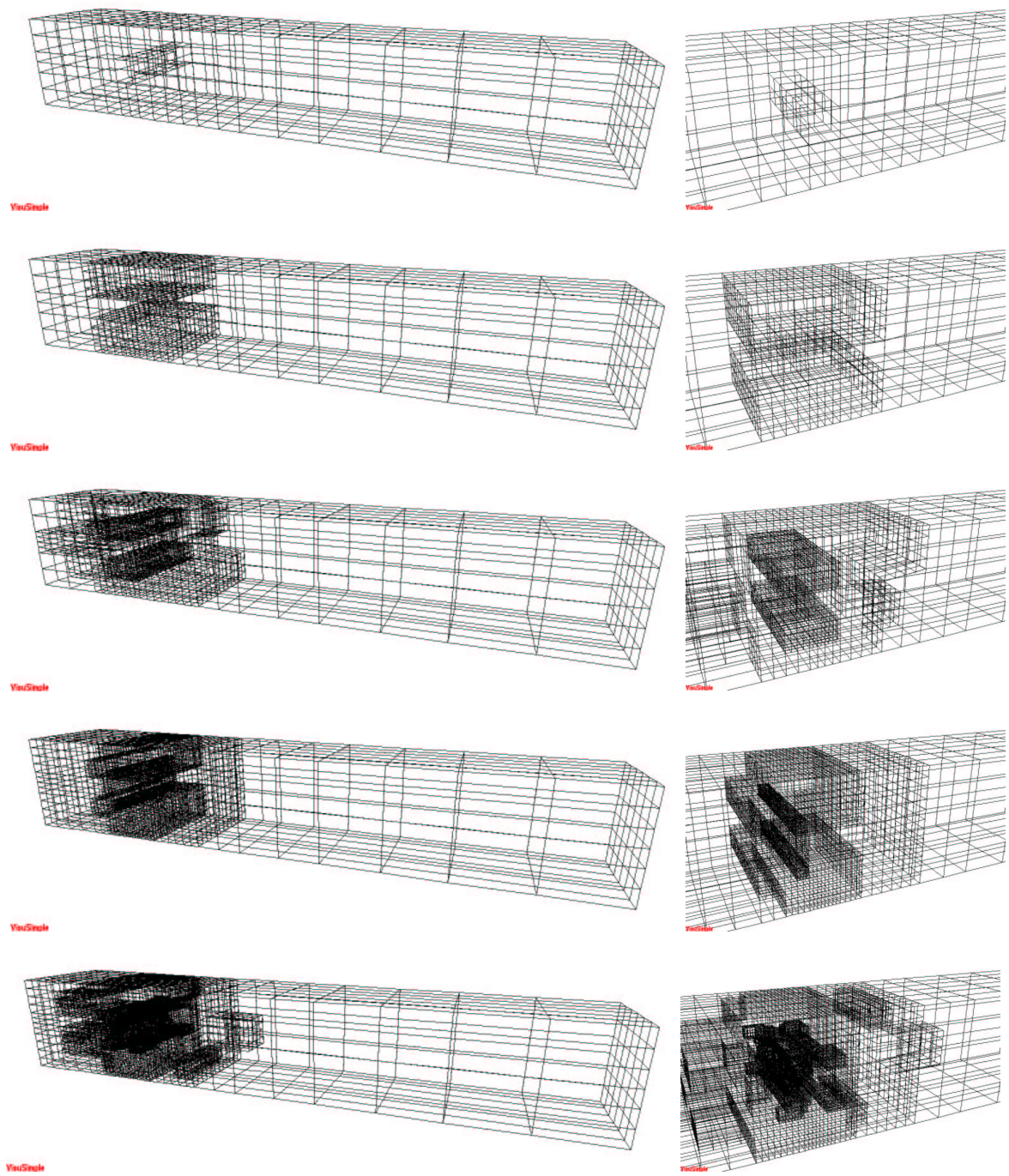
Figure. Refined mesh and zoom by the "weighted" error indicator.

5.2 Heat-driven compressible flow

The mathematical model consists of the conservation equations for the 'conservative' variables:

$$\rho \ (\text{mass}), \quad m := \rho v \ (\text{momentum}), \quad E := \rho e + \tfrac{1}{2}\rho|v|^2 \ (\text{total energy})$$

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho v) &= 0 \\
\partial_t m + \nabla \cdot (m \otimes v) &= \nabla \cdot \sigma + \rho f \\
\partial_t E + \nabla \cdot (E v) &= \rho f \cdot v + \nabla \cdot (\sigma \cdot v) + \rho h - \nabla \cdot q
\end{aligned}
$$

Conservation of torque $x \times m$ implies symmetry of stress tensor, $\sigma = \sigma^T$.
'primitive' variables: $\quad \rho$ (mass), $\quad v$ (velocity), $\quad \theta$ (temperature).

Closure equations ('equations of state'):

- Newtonian fluid ($\mu > 0$, $\lambda = -\tfrac{2}{3}\mu > 0$ viscosity parameters):

$$\sigma = -pI + \tau, \qquad \tau = \mu\{\nabla v + \nabla v^T\} + \lambda \nabla \cdot v I$$

- Law of "ideal" gas ($R > 0$ gas constant): $\quad p = p(\rho, \theta) = R\rho\theta$.

- Thermodynamic relations: $\quad e = c_v \theta, \qquad q = -\kappa(\rho, \theta)\nabla\theta$.

Velocity of sound and Mach number:

$$c(p) := \sqrt{\frac{dp}{d\rho}}, \qquad \mathrm{Ma} := \frac{|v|}{c(p)}$$

Kinematic viscosity and Reynolds number:

$$\nu := \frac{\mu}{\rho}, \qquad \mathrm{Re} := \frac{LU}{\nu}$$

The low-Mach number problem

We consider temperature driven flows for the critical case $\text{Ma} \ll 1$:

$$
\begin{aligned}
\partial_t \rho + v \cdot \nabla \rho + \rho \nabla \cdot v &= 0 \\
\rho(\partial_t v + v \cdot \nabla v) - \nabla \cdot \tau + \nabla p &= \rho f \\
\rho(\partial_t \theta + v \cdot \nabla \theta) - c_p^{-1} \nabla \cdot (\kappa \nabla \theta) &= c_p^{-1} \rho h \\
p &= R\theta\rho
\end{aligned}
$$

Scaling

$$
v \to \frac{v}{|v_{max}^0|}, \qquad \rho \to \frac{\rho}{\rho_{max}^0}, \qquad \theta \to \frac{\theta - \theta_{min}^0}{\theta_{max}^0 - \theta_{min}^0}
$$

$$
t \to \frac{|v_{max}^0|}{L} t, \qquad x \to \frac{x}{L}
$$

$$
\mu \to \frac{\mu}{|v_{max}| \rho_{max}^0}, \qquad f \to \frac{f}{|v_{max}^0|^2}
$$

yields the dimensionless form of momentum equation:

$$
\rho \partial_t v + \rho v \cdot \nabla v + \nabla \cdot \tau + \lambda^{-2} \nabla p = 0, \qquad \lambda = \sqrt{\gamma} \, \text{Ma}
$$

Warning: For $\text{Ma} \sim \lambda \ll 1$, small changes in pressure result in large changes in velocity, i.e., small errors in temperature can cause fatal errors in velocity:

$$
|v_{max}| = 1\tfrac{m}{s}, \quad \gamma = 1.4 \quad \Rightarrow \quad \lambda^{-2} \approx 8{\cdot}10^4
$$

$$
e(\nabla\theta) \approx 0.1\% \quad \Rightarrow \quad e(\nabla p) \approx 0.1\% \quad \Rightarrow \quad e(v) \approx 80\tfrac{m}{s}
$$

Consequence: The pressure should not be calculate from the gas law but through the momentum and continuity equations.

Asymptotic analysis for $Ma \to 0$ (inviscid case):

$$p = p_0 + \lambda p_1 + \lambda^2 p_2 + O(\lambda^3)$$
$$v = v_0 + \lambda v_1 + \lambda^2 v_2 + O(\lambda^3)$$

$$\lambda^{-2}(\nabla p_0 + \lambda \nabla p_1) + \rho \partial_t v_0 + \rho v_0 \cdot \nabla v_0 + \nabla p_2 = O(\lambda)$$

Assuming convergence of expansion, limit process $\lambda \to 0$ yields:

$$\nabla p_0 = \nabla p_1 = 0$$
$$\rho_0 \partial_t v_0 + \rho_0 v_0 \cdot \nabla v_0 + \nabla p_2 = 0$$

$$p_{th}(t) := p_0(t) + \lambda^{-1} p_1(t) \quad \text{``thermodynamic'' pressure}$$
$$p_{hyd}(x,t) := p_2(x,t) \qquad\qquad \text{``hydrodynamic'' pressure}$$

Low-Mach number approximation:
Neglecting of temperature creation by mechanical effects:

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

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

Determination of thermodynamic pressure p_{th} :

$$p_{th} \equiv p_{th|\Gamma_{out}} \quad (\text{``open'' flow domain})$$

$$\partial_t p_{th} = \frac{p_{th}}{|\Omega|} \int_\Omega \theta^{-1}(\partial_t \theta + v \cdot \nabla \theta)\, do \quad (\text{closed box})$$

Heat-driven flow in Boussinesq approximation:

$$|\theta - \theta_0| \ll 1, \qquad |\rho - \rho_0| \ll 1, \qquad \mu \approx \mu(\theta_0)$$

$$\nabla \cdot \tau = \mu \Delta v + \tfrac{1}{3} \nabla \cdot v$$

Expansion of forcing term about θ_0:

$$\rho g = \frac{p_{th}}{R\theta} g \quad \rightarrow \quad \beta \theta g + \alpha \nabla \Phi$$

$$\nabla{\cdot}v = 0$$
$$\partial_t v + v \cdot \nabla v - \nu \Delta v + \nabla p = \beta \theta g$$
$$c_p \rho_0 \partial_t \theta + c_p \rho_0 v \cdot \nabla \theta - \nabla \cdot (\kappa \nabla \theta) = 0$$

Incompressible Navier-Stokes equations:

Constant density: $\rho \equiv \rho_0$ (isotherm)

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

A heat-driven temperature benchmark

We consider the 'heat-driven cavity'. The flow in a square box with side length $L\!=\!1$ is driven by a temperature difference of

$$\theta_h - \theta_c = 720\,K$$

between the left ('hot') and the right ('cold') wall under the action of gravity g in the negative y-direction. The Rayleigh number is $Ra \sim 10^6$. The boundary conditions are

$$v_{|\partial\Omega} = 0, \qquad \partial_n\theta_{|\Gamma_N} = 0, \quad \theta_{|\Gamma_{hot}} = \theta_h, \quad \theta_{|\Gamma_{cold}} = \theta_c$$

Figure: Configuration of 'heat-driven cavity'

Sutherland's viscosity law:

$$\mu(\theta) \;=\; \mu^*\Big(\frac{\theta}{\theta^*}\Big)^{1/3}\frac{\theta^*+110.5\,K}{\theta+110.5\,K}, \qquad \kappa(\theta) = \mu(\theta)/\mathrm{Pr}$$

Prandtl number $\mathrm{Pr}\!=\!0.71$, $\theta^* = 273\,K$, $\mu^* = 1.68{\cdot}10^{-5}$kg/ms. The Rayleigh number is determined by

$$\mathrm{Ra} \;=\; \mathrm{Pr}\,g\,\Big(\frac{\rho_0 L}{\mu_0}\Big)^2\frac{\theta_h-\theta_c}{\theta_0}$$

Computational results (R. Becker, M. Braack 2002)

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

Average Nusselt number along the cold wall:

$$J(u) = \mathrm{Nu} : = \frac{\mathrm{Pr}}{0.3\mu_0\theta_0} \int_{\Gamma_{cold}} \kappa\partial_n\theta \, ds$$
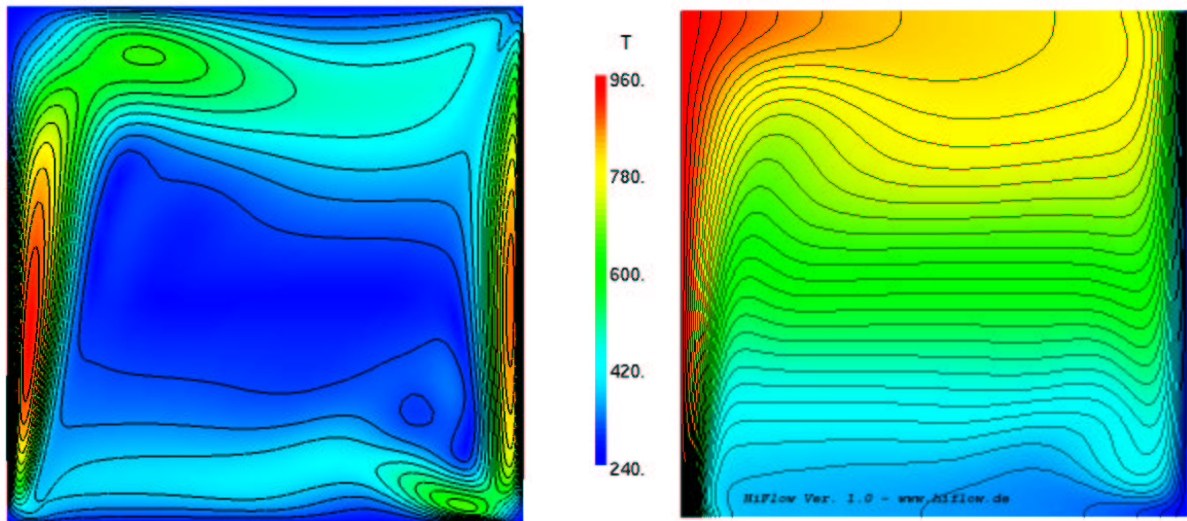
N	$\langle Nu\rangle_c$	$J(e)$		N	$\langle Nu\rangle_c$	$J(e)$
524	-9.09552	4.1e-1		523	-8.86487	1.8e-1
945	-8.67201	1.5e-2		945	-8.71941	3.3e-2
1708	-8.49286	1.9e-1		1717	-8.66898	1.8e-2
3108	-8.58359	1.0e-1		5530	-8.67477	1.2e-2
5656	-8.59982	8.7e-2		**9728**	-8.68364	3.0e-3
18204	-8.64775	3.9e-2		17319	-8.68744	8.5e-4
32676	-8.66867	1.8e-2		31466	-8.68653	6.9e-5
58678	-8.67791	8.7e-3				
79292	-8.67922	7.4e-3				

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

Figure. Optimized meshes for the 'heat-driven cavity' with $N = 523, 5530, 56077$ cells:
'energy' error indicator (left),
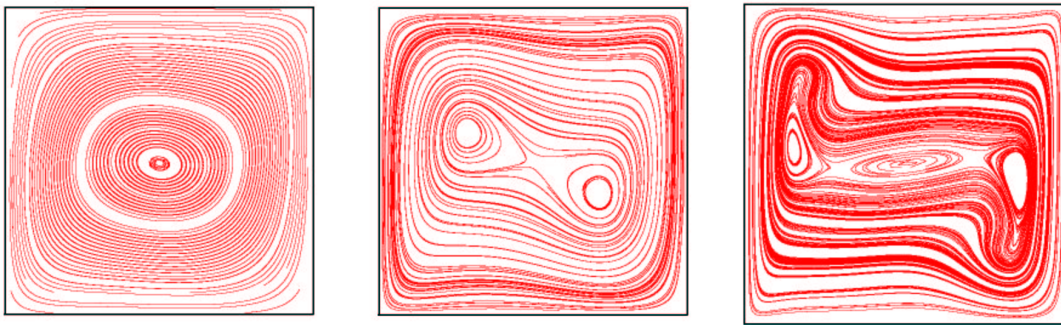'weighted' error indicator (right)

Figure: The "heat-driven cavity" flow: sequence of streamline plots for increasing
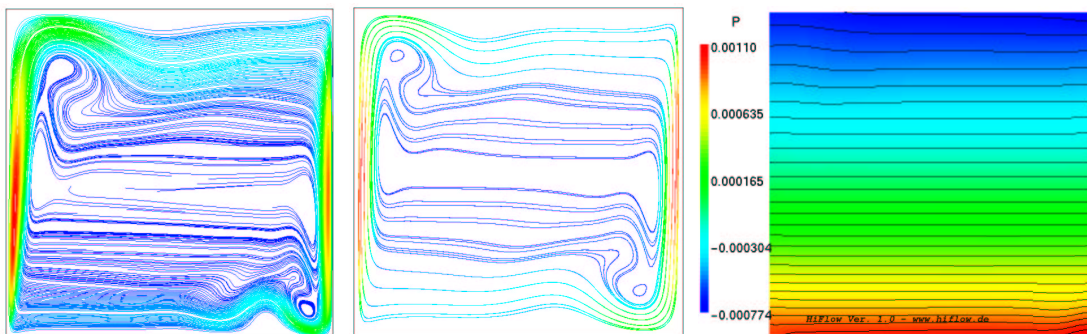Rayleigh number $\mathrm{Ra} = 10^4, 10^5, 10^6$

Figure: Stream function plots for low-Mach number approximation (left), for
Boussinesq model (middle), and pressure isolines (right)

5.3 Chemically reactive flows

Changes in energy equation and additional equations for the mass fractions of the chemical species $(w_i)_{i=1}^{N}$ (N additional PDEs):

$$\rho \partial_t \theta + \rho v \cdot \nabla \theta + c_p^{-1} \nabla \cdot (\kappa \nabla \theta) = c_p^{-1} \partial_t p_{th} + c_p^{-1} h(\theta, w)$$

$$\rho \partial_t w_i + \rho v \cdot \nabla w_i + \nabla \cdot (\rho D_i M_i^{-1} \nabla [M w_i]) = f_i(\theta, w)$$

$$p = \frac{R \rho \theta}{M}$$

Details of model:

- w_i mass fraction, M_i molar mass and c_i concentration of specie i:

$$0 \leq w_i \leq 1, \quad \sum_{i=1}^{n_s} w_i = 1, \quad M := (\sum_{i=1}^{N} M_i^{-1} w_i)^{-1}, \quad c_i = M_i^{-1} \rho w_i$$

- 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:

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

- 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:

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

"Low-Mach number" approximation of stationary reactive flow:

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

Difficulties:

i) Strongly varying spatial and time scales

- flow - turbulence - molecular transport: $10^{-2}s - 10^{-6}s$

- NO formation - methane combustion: $10^0 s - 10^{-8} s$

Fast processes lead to partial equilibrium or quasi-steady state.

ii) Strongly nonlinear source terms

- mechanical forcing: ρg "weak" nonlinearity.

- thermal forcing: $h(\theta, w)$, $f_i(\theta, w)$ "strong" nonlinearity.

Energy and species equations have to be solved "correctly".

Variational formulation (stationary case)

State space for full system of compressible Navier-Stokes equations:

$$\mathcal{V} \subset H^1(\Omega) \times H^1(\Omega)^d \times H^1(\Omega) \times H^1(\Omega)^N$$

Find $u = \{p, v, \theta, w\} \in \mathcal{V}$:

$$a(u; \varphi) = 0$$

for all test functions $\varphi = \{\varphi^p, \varphi^v, \varphi^\theta, \varphi^w\} \in \mathcal{V}$

"Energy form":

$$
\begin{aligned}
a(u; \varphi) := & \; (\rho \nabla \cdot v, \varphi^p) - (\theta^{-1} v \cdot \nabla\theta, \varphi^p) + \ldots \\
& + (\rho v \cdot \nabla v, \varphi^v) + (\mu \nabla v, \nabla \varphi^v) - (p, \nabla \varphi^v) - (\rho g, \varphi^v) \\
& + (\rho v \cdot \nabla\theta, \varphi^\theta) + (c_p^{-1} \kappa \nabla\theta, \nabla \varphi^\theta) - (h(\theta, w), \varphi^\theta) \\
& + \ldots
\end{aligned}
$$

where $\rho := p_{th}/R\theta$, and '...' indicates the additional chemistry terms. Additionally, we use appropriate boundary conditions for v, θ, w and inmitial conditions for ρ, v, θ, w.

The dual solution $z = (z^v, z^p, z^\theta, z^w)$ is determined by the system:

$$\nabla \cdot z^v = J^p$$
$$-\rho(v \cdot \nabla)z^v - \nabla \cdot \mu\nabla z^v - \rho\nabla z^p = J^v$$
$$\theta^{-1} v \cdot \nabla z^p + \theta^{-2} v \cdot \nabla\theta \cdot z^p - \rho v \cdot \nabla z^\theta - c_p^{-1}\nabla \cdot (\lambda\nabla z^\theta)$$
$$-(Df^\theta)_\theta(z^\theta, z^w)z^\theta = J^\theta$$
$$-\rho v \cdot \nabla z_i^w - \nabla \cdot (\rho D_i \nabla z_i^w) - (Df^\theta)_i(z^\theta, z^w)z_i^w = J_i^w$$

where $J = (J^p, J^v, J^\theta, J^w)$ is a suitable error functional.

Remark: In setting up the dual problem the nonlinear dependence of diffusion coefficients as well as the stabilization terms are neglected.

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])
- 39 species (C2 mechanism [Warnatz])

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
$CH_3O+O_2 = CH_2O+HO_2$	6.30e10	0	10.88
$CH_3+O_2 = CH_2O+OH$	5.20e13	0	144.66
$CH_3+O = CH_2O+H$	6.80e13	0	0
$CH_3+OH = CH_2O+H_2$	7.50e12	0	0
$HO_2+CO = CO_2+OH$	5.80e13	0	95.96
$H_2+O_2 = OH+OH$	1.70e13	0	199.91
$OH+H_2 = H_2O+H$	1.17e09	1.30	15.17
$H+O_2 = OH+O$	2.00e14	0	70.29
$O+H_2 = OH+H$	1.80e10	1.00	36.93
$H+O_2+Y = HO_2+Y$	2.30e18	-0.80	0
$H+O_2+O_2 = HO_2+O_2$	6.70e19	-1.42	0
$H+O_2+N_2 = HO_2+N_2$	6.70e19	-1.42	0
$OH+HO_2 = H_2O+O_2$	5.00e13	0	4.18
$H+HO_2 = OH+OH$	2.50e14	0	7.95
$O+HO_2 = O_2+OH$	4.80e13	0	4.18
$OH+OH = H_2O+O$	6.00e08	1.30	0
$H_2+Y = H+H+Y$	6.99e18	-1.00	436.08
$O_2+X = O+O+X$	6.91e18	-1.00	496.41
$H+OH+Z = H_2O+Z$	2.10e22	-2.00	0
$H+HO_2 = H2+O_2$	2.50e13	0	2.93

Table. C1 Mechanism of methane/air reaction with 17 species (X, Y, Z any of the participating species)

Reaction	A_r	β_r	E_{ar}
$O_2+H=OH+O$	2.00e14	0	70.3
$H_2+O=OH+H$	5.06e4	2.67	26.3
$H_2+OH=H_2O+H$	1.00e8	1.60	13.8
$OH+OH=H_2O+O$	1.50e9	1.14	0.42
$H+H+M'=H_2+M'$	1.80e18	-1.00	0
$O+O+M'=O_2+M'$	2.90e17	-1.00	0
$H+OH+M'=H_2O+M'$	2.20e22	-2.00	0
$H+O_2+M'=HO_2+M'$	2.30e18	-0.80	0
$HO_2+H=OH+OH$	1.50e14	0	4.2
$HO_2+H=H_2+O_2$	2.50e13	0	2.9
$HO_2+H=H_2O+O$	3.00e13	0	7.2
$HO_2+O=OH+O_2$	1.80e13	0	-1.7
$HO_2+OH=H2O+O_2$	6.00e13	0	0
$HO_2+HO_2=H_2O_2+O_2$	2.50e11	0	-5.2
$OH+OH+M'=H_2O_2+M'$	3.25e22	-2.00	0
$H_2O_2+H=H_2+HO_2$	1.70e12	0	15.7
$H_2O_2+H=H_2O+OH$	1.00e13	0	15.0
$H_2O_2+O=OH+HO_2$	2.803e13	0	26.8
$H_2O_2+OH=H_2O+HO_2$	5.40e12	0	4.2
$CO+OH=CO_2+H$	6.00e06	1.50	-3.1
$CO+HO_2=CO_2+OH$	1.50e14	0	98.7
$CO+O+M'=CO_2+M'$	7.10e13	0	-19.0
$CO+O_2=CO_2+O$	2.50e12	0	200.0
$CH+O=CO+H$	4.00e13	0	0
$CH+O_2=CHO+O$	3.30e13	0	0
$CH+CO_2=CHO+CO$	3.40e12	0	2.9
$CH+H_2O=3CH_2+OH$	5.70e12	0	-3.2
$CHO+M'=CO+H+M'$	7.10e14	0	70.3
$CHO+H=CO+H_2$	9.00e13	0	0
$CHO+O=CO+OH$	3.00e13	0	0
$CHO+O=CO_2+H$	3.00e13	0	0
$CHO+OH=CO+H_2O$	1.00e14	0	0
$CHO+O_2=CO+HO_2$	3.00e12	0	0
$CHO+CHO=CH_2O+CO$	3.00e13	0	0
$3CH_2+H=CH+H_2$	6.00e12	0	-7.5
$3CH_2+O\rightarrow CO+H+H$	8.40e12	0	0
$3CH_2+3CH_2=C_2H_2+H_2$	1.20e13	0	3.4
$3CH_2+3CH_2=C_2H_2+H+H$	1.10e14	0	3.4
$3CH_2+CH_3=C_2H_4+H$	4.20e13	0	0
$3CH_2+O_2=CO+OH+H$	1.30e13	0	0
$3CH_2+O_2=CO+OH+H$	1.30e13	0	6.2
$3CH_2+O_2=CO_2+H_2$	1.20e13	0	6.2
$1CH_2+M'=3CH_2+M'$	1.20e13	0	0
$1CH_2+O_2=CO+OH+H$	3.10e13	0	0
$1CH_2+H_2=CH_3+H$	7.20e13	0	0
$CH_2O+M'=CHO+H+M'$	5.00e16	0	320.0
$CH_2O+H=CHO+H_2$	2.30e10	1.05	13.7
$CH_2O+O=CHO+OH$	4.15e11	0.57	11.6
$CH_2O+OH=CHO+H_2O$	3.40e09	1.20	-1.9
$CH_2O+HO_2=CHO+H_2O_2$	3.00e12	0	54.7
$CH_2O+CH_3=CHO+CH_4$	1.00e11	0	25.5
$CH_2O+O_2=CHO+HO_2$	6.00e13	0	170.7
$CH_3+M'=3CH_2+H+M'$	1.00e16	0	379.0
$CH_3+O=CH_2O+H$	8.43e13	0	0
$CH_3+H=CH_4$	1.93e36	-7.00	38.0
$CH_3+OH\rightarrow CH_3O+H$	2.26e14	0	64.8
$CH_3O+H\rightarrow CH_3+OH$	4.75e16	-0.13	88.0
$CH_3+O_2\rightarrow CH_2O+OH$	3.30e11	0	37.4
$CH_3+HO_2=CH_3O+OH$	1.80e13	0	0
$CH_3+HO_2=CH_4+O_2$	3.60e12	0	0
$CH_3+CH_3\rightarrow C_2H_4+H_2$	1.00e16	0	134.0
$CH_3+CH_3=C_2H_6$	1.69e53	-12.0	81.24
$CH_3O+M'=CH_2O+H+M'$	5.00e13	0	105.0
$CH_3CO=CH_3+CO$	2.32e26	-5.0	75.12
$CH_3CO+H=CH_3CO+H_2$	2.00e13	0	0
$CH_2CHO+H=CH_2CO+H_2$	2.00e13	0	0
$C_2H_4+M'=C_2H_2+H_2+M'$	2.50e17	0	319.8
$C_2H_4+M'=C_2H_3+H+M'$	1.70e18	0	404.0
$C_2H_4+H=C_2H_3+H_2$	1.70e15	0	62.9
$C_2H_4+O=CH_2CHO+H$	5.20e5	2.08	0
$C_2H_4+O=CHO+CH_3$	1.21e6	2.08	0
$C_2H_4+OH=C_2H_3+H_2O$	6.50e13	0	24.9
$CH_3CHO+M'=CH_3+CHO+M'$	7.00e15	0	342.8
$CH_3CHO+H=CH_3CO+H_2$	2.10e9	1.16	10.1
$CH_3CHO+H=CH_2CHO+H_2$	2.00e9	1.16	10.1
$CH_3CHO+O=CH_3CO+OH$	5.00e12	0	7.6
$CH_3CHO+O=CH_2CHO+OH$	8.00e11	0	7.6
$CH_3CHO+O_2=CH_3CO+HO_2$	4.00e13	0	164.3
$CH_3CHO+OH=CH_3CO+H_2O$	2.30e10	0.73	-4.7
$CH_3CHO+HO_2=CH_3CO+H_2O_2$	3.00e12	0	50.0
$CH_3CHO+3CH_2=CH_3CO+CH_3$	2.50e12	0	15.9
$CH_3CHO+CH_3=CH_3CO+CH_4$	2.00e-6	5.64	10.3
$C_2H_5=C_2H_4+H$	1.02e43	-9.1	224.15
$C_2H_5+H=CH_3+CH_3$	3.00e13	0	0
$C_2H_5+O=CH_3CHO+H$	5.00e13	0	0
$C_2H_5+O=CH_2O+CH_3$	1.00e13	0	0
$C_2H_5+O_2=C_2H_4+HO_2$	1.10e10	0	-6.3
$C_2H_5+CH_3=C_2H_4+CH_4$	1.14e12	0	0
$C_2H_5+C_2H_5=C_2H_4+C_2H_6$	1.40e12	0	0
$C_2H_5O=CH_3CHO+H$	2.51e14	0	97.0
$C_2H_5O=CH_2O+CH_3$	1.00e15	0	90.4
$C_2H_5O+O_2=CH_3CHO+HO_2$	5.01e12	0	16.7
$C_2H_5O+OH=CH_3CHO+H_2O$	1.32e12	0	0
$C_2H_5O+H=CH_3CHO+H_2$	1.80e13	0	0

Reaction	A_r	β_r	E_{ar}
$CH_3O+H=CH_2O+H_2$	1.80e13	0	0
$CH_3O+O_2=CH_2O+HO_2$	4.00e10	0	8.9
$CH_2O+CH_3O\rightarrow CH_3OH+CHO$	6.00e11	0	13.8
$CH_3OH+CHO\rightarrow CH_2O+CH_3O$	6.50e9	0	57.2
$CH_3O+O=O_2+CH_3$	1.10e13	0	0
$CH_3O+O=OH+CH_2O$	1.40e12	0	0
$CH_2OH+M'=CH_2O+H+M'$	5.00e13	0	105.0
$CH_2OH+H=CH_2O+H_2$	3.00e13	0	0
$CH_2OH+O_2=CH_2O+HO_2$	1.00e13	0	30.0
$CH_3O_2+M'\rightarrow CH_3+O_2+M'$	7.24e16	0	111.1
$CH_3+O_2+M'\rightarrow CH_3O2+M'$	1.41e16	0	-4.6
$CH_3O_2+CH_2O\rightarrow CH_3O_2H+CHO$	1.30e11	0	37.7
$CH_3O_2H+CHO\rightarrow CH_3O_2+CH2O$	2.50e10	0	42.3
$CH_3O_2+CH_3=CH_3O+CH3O$	3.80e12	0	-5.0
$CH_3O+CH_3O\rightarrow CH_3O_2+CH3$	2.00e10	0	0
$CH_3O_2+HO_2\rightarrow CH_3O_2H+O_2$	4.60e10	0	-10.9
$CH_3O_2H+O_2\rightarrow CH_3O_2+HO_2$	3.00e12	0	163.3
$CH_3O_2+CH_3O_2\rightarrow CH_2O+CH_3OH+O_2$	1.80e12	0	0
$CH_2O+CH_3OH+O_2\rightarrow CH_3O_2+CH_3O_2$	0	0	0
$CH_3O_2+CH_3O_2\rightarrow CH_3O+CH_3O+O_2$	3.70e12	0	9.2
$CH_3O+CH_3O+O_2\rightarrow CH_3O_2+CH_3O_2$	0	0	0
$CH_4+H=H_2+CH_3$	1.30e4	3.0	33.6
$CH_4+O=OH+CH_3$	6.923e8	1.56	35.5
$CH_4+OH=H_2O+CH_3$	1.60e7	1.83	11.6
$CH_4+HO_2=H_2O_2+CH_3$	1.10e13	0	103.1
$CH_4+CH=C_2H_4+H$	3.00e13	0	-1.7
$CH_4+3CH_2=CH_3+CH_3$	1.30e13	0	39.9
$CH_3OH=CH_3+OH$	9.51e29	-4.3	404.1
$CH_3OH+H=CH_2OH+H_2$	4.00e13	0	25.5
$CH_3OH+O=CH_2OH+OH$	1.00e13	0	19.6
$CH_3OH+OH=CH_2OH+H_2O$	1.00e13	0	7.1
$CH_3OH+HO_2\rightarrow CH_2OH+H_2O_2$	6.20e12	0	81.1
$CH_2OH+H_2O_2\rightarrow HO_2+CH_3OH$	1.00e7	1.7	47.9
$CH_3OH+CH_3=CH_4+CH_2OH$	9.00e12	0	41.1
$CH_3O+CH_3OH\rightarrow CH_2OH+CH_3OH$	2.00e11	0	29.3
$CH_2OH+CH_3OH\rightarrow CH_3O+CH_3OH$	2.20e4	1.7	45.4
$CH_3OH+CH_2O\rightarrow CH_3O+CH_3O$	1.53e12	0	333.2
$CH_3O+CH_3O\rightarrow CH_3OH+CH_2O$	3.00e13	0	0
$CH_3O_2H=CH_3O+OH$	4.00e15	0	180.5
$OH+CH3O2H=H_2O+CH3O2$	2.60e12	0	0
$C2H+O=CO+CH$	1.00e13	0	0
$C2H+O_2=HCCO+O$	3.00e12	0	0
$HCCO+H=3CH_2+CO$	1.50e14	0	0
$HCCO+O\rightarrow CO+CO+H$	9.60e13	0	0
$HCCO+3CH2=C2H3+CO$	3.00e13	0	0
$C2H2+M'=C2H+H+M'$	3.60e16	0	446.0
$C2H2+O_2=HCCO+OH$	2.00e8	1.5	126.0
$C2H2+H=C2H+H2$	1.50e14	0	79.6
$C2H2+O=3CH_2+CO$	1.72e4	2.8	2.1
$C2H2+O=HCCO+H$	1.72e4	2.8	2.1
$C2H2+OH=H_2O+C2H$	6.00e13	0	54.2
$C2H2+C2H=C4H2+H$	3.00e13	0	0
$CH2CO+M'=3CH2+CO+M'$	1.00e16	0	248.0
$CH2CO+H=CH3+CO$	3.60e13	0	14.1
$CH2CO+O=CHO+CHO$	2.30e12	0	5.7
$CH2CO+OH=CH2O+CHO$	1.00e13	0	0
$C_2H_3=C_2H_2+H$	4.73e40	-8.8	194.50
$C_2H_3+OH=C_2H_2+H_2O$	5.00e13	0	0
$C_2H_3+H=C_2H_2+H_2$	1.20e13	0	0
$C_2H_3+O=C_2H_2+OH$	1.00e13	0	0
$C_2H_3+O=CH_3+CO$	1.00e13	0	0
$C_2H_3+O=CHO+3CH_2$	1.00e13	0	0
$C_2H_3+O_2=C_2H_2+HO_2$	5.40e12	0	0
$CH_3CHOH=CH_3CHO+H$	1.00e14	0	105.0
$CH_3CHOH+H=CH_3CHO+H_2$	3.00e13	0	0
$CH_3CHOH+OH=CH_3CHO+H_2O$	1.51e13	0	0
$CH_3CHOH+O=CH_3CHO+OH$	1.20e14	0	0
$CH_3CHOH+O_2=CH_3CHO+HO_2$	1.20e13	0	0
$CH_2CH_2OH=C_2H_4+OH$	1.00e14	0	140.0
$CH_2CH_2OH+H=CH_3CHO+H_2$	5.00e13	0	0
$C_2H_6+H=C_2H_5+H_2$	1.40e9	1.5	31.1
$C_2H_6+O=C_2H_5+OH$	1.00e9	1.5	24.4
$C_2H_6+OH=C_2H_5+H_2O$	7.20e6	2.0	3.6
$C_2H_6+HO_2=C_2H_5+H_2O_2$	1.70e13	0	85.9
$C_2H_6+O_2=C_2H_5+HO_2$	6.00e13	0	217.0
$C_2H_6+3CH_2=C_2H_5+CH_3$	2.20e13	0	36.3
$C_2H_6+CH_3=C_2H_5+CH_4$	1.500e-07	6.0	25.4
$C_2H_5OH=CH_3+CH_2OH$	2.51e16	0	353.0
$C_2H_5OH+OH=CH_3CHOH+H_2O$	5.25e6	2.0	1.9
$C_2H_5OH+OH=C_2H_5O+H_2O$	1.15e6	2.0	3.8
$C_2H_5OH+OH=CH_2CH_2OH+H_2O$	8.13e6	2.0	2.5
$C_2H_5OH+O=CH_3CHOH+OH$	7.94e12	0	13.6
$C_2H_5OH+O=C_2H_5O+OH$	4.79e13	0	28.7
$C_2H_5OH+O=CH_2CH_2OH+OH$	1.00e14	0	31.3
$C_2H_5OH+H=CH_3CHOH+H_2$	4.40e12	0	19.1
$C_2H_5OH+H=C_2H_5O+H_2$	5.90e11	0	14.4
$C_2H_5OH+HO_2=CH_3CHOH+H_2O_2$	6.30e12	0	81.1
$C_2H_5OH+CH_3=CH_3CHOH+CH_4$	2.04e11	0	36.4
$C_2H_5OH+CH_3=CH_2CH_2OH+CH_4$	2.04e11	0	36.4
$C_2H_5OH+CH_3=C_2H_5O+CH_4$	7.49e10	0	39.3
$C_2H_5OH+CH_3O=CH_3CHOH+CH_3OH$	2.00e11	0	29.3
$C_2H_5OH+CH_2O=C_2H_5O+CH_3O$	1.53e12	0	333.2
$C_2H5OH+C_2H5O=C_2H5OH+CH_3CHOH$	2.00e11	0	29.3

Table. C2 mechanism of methane combustion with (Collision efficiencies: $M=1$, $M'(O_2, H_2, H_2O, CO, CO_2, CH_4, N_2) = (0.4, 1, 6.5, 0.75, 1.5, 3, 0.4))$

Some computational details:

a) Methodology:

- quasi-Newton instead of pseudo time-stepping

- multigrid for linear systems

- local mesh refinement

- model adaptation

b) Work (M. Braack 1997-):

- Memory requirements: 10KB per mesh cell (52MB for 5500 cells)

- Cost of mesh adaptation: 10% of total CPU time

- CPU time with pseudo-time stepping for 17 species:
  > 5 days (SGI R10000)

- CPU time with Newton iteration for 17 species:
  < 5 hs (Pentium II)

- CPU-time on tensor-product grid with 10^6 nodes:
  ~ 1 week (17 species)

- CPU-time on adapted grid with 10^4 nodes:
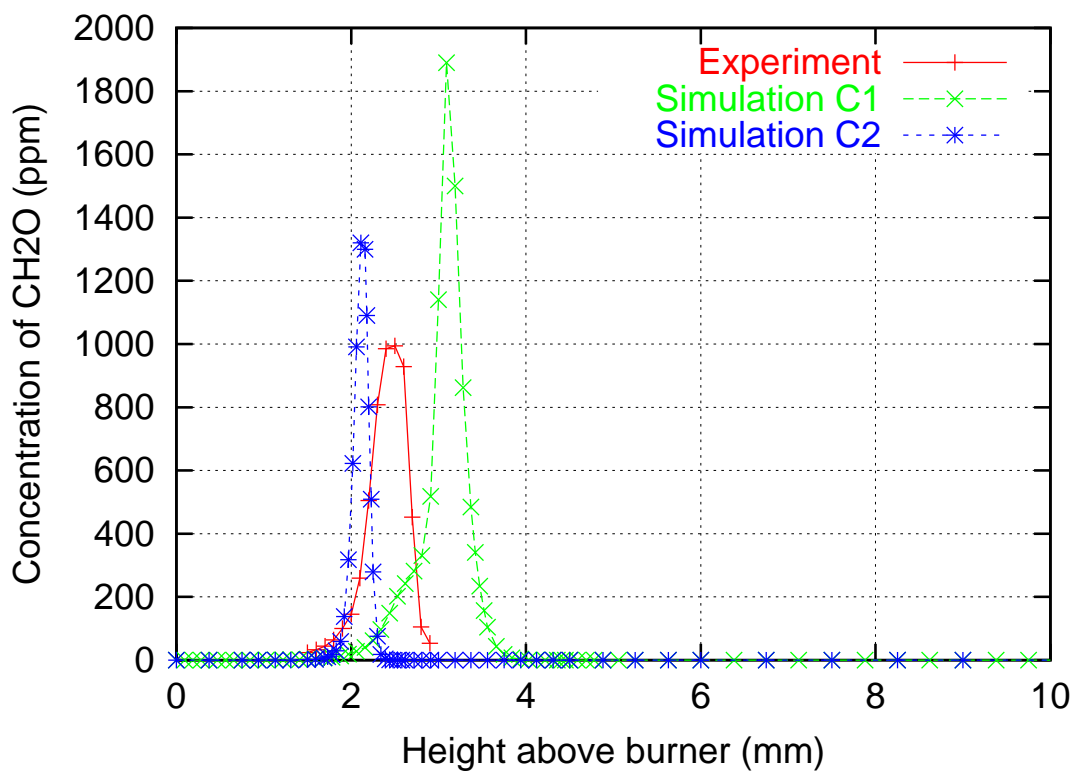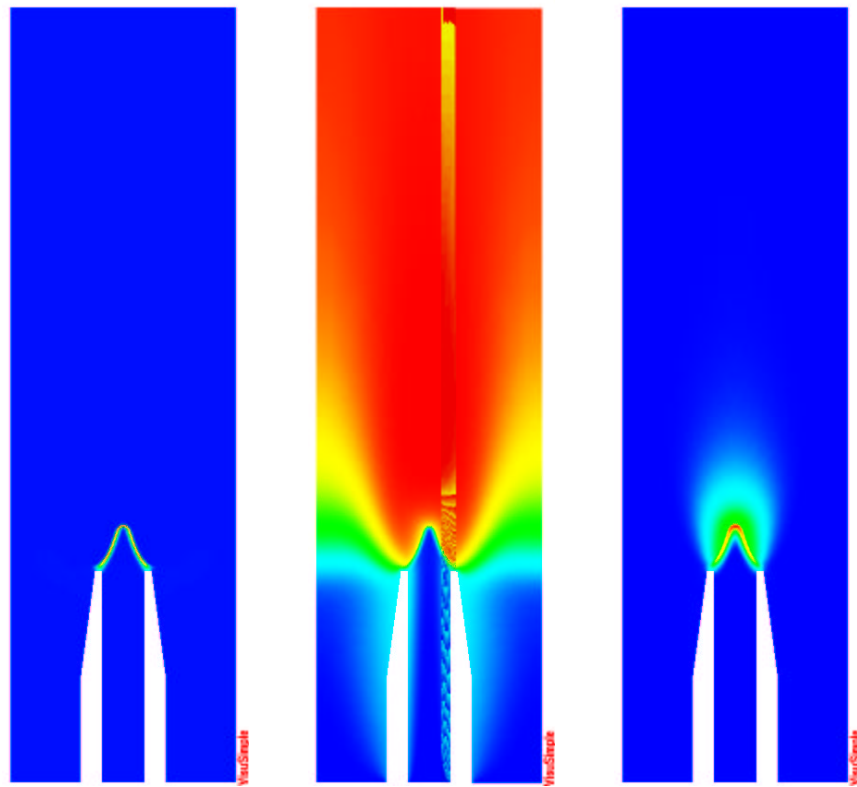 $\sim$ **4 hours** (17 species), 23 hours (39 species)
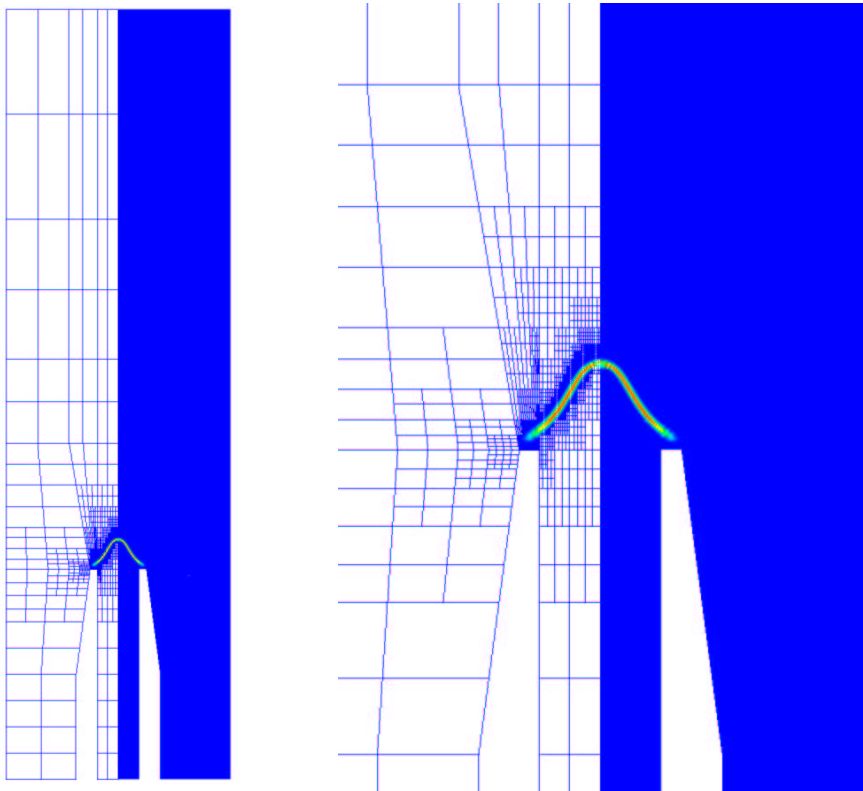
Figure. Comparison simulation - measurements
(PCI Heidelberg, J. Wolfrum)

Figure. Locally adapted mesh