6 Model Adaptivity

The concept of residual-based adaptivity used in the DWR method can be extended to the hierarchical approximation or enrichment of mathematical models. At first, the underlying idea will be illustrated for simple model cases, and then a more advanced application to chemically reactive flow will be presented. This is closely related to parameter estimation which will be treated in the last lecture.

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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):

$$\mathcal{F}_i^M = -\rho w_i \sum_{j\in\mathcal{S}} D_{ij}\Big(\nabla x_j + \chi_l \nabla(\log T)\Big)$$

Configuration of test problem:

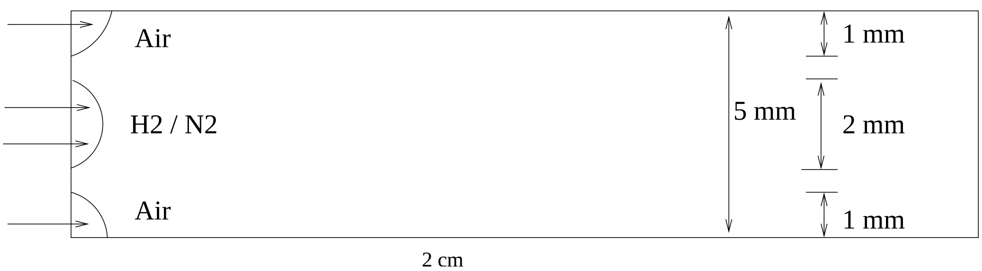

Figure. Inflow: outer inlet N_2, O_2, inner inlet H_2, N_2

Remark. The choice of the diffusion model affects also the transport model in the temperature equation which is neglected here for simplicity.

The diffusion model has substantial impact on flame front:

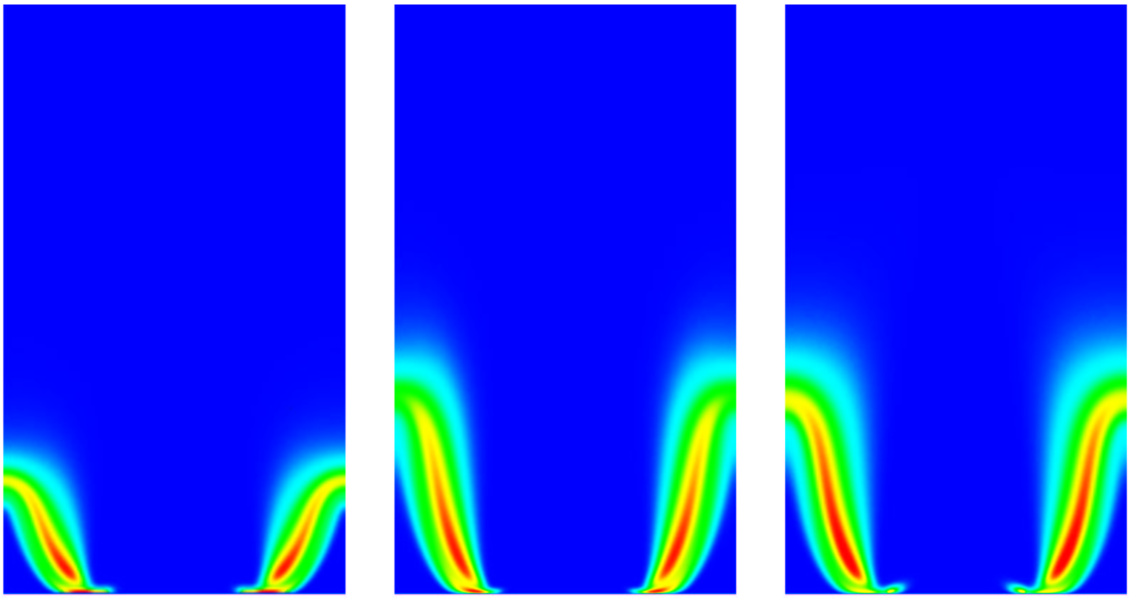

Figure. Initial solution with $\mathcal{F}_k^F$, optimized D_k w.r.t. 'experimental' data, and reference solution with $\mathcal{F}_k^M$ (M. Braack 2003).

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 caused by numerical integration)

$$a(u)(\psi_h) - a(u_h^m)(\psi_h) = -d(u)(\psi_h), \quad \psi \in V$$

Dual problems

$$\begin{aligned} a'(u)(\varphi,z) + d'(u)(\varphi,z) &= J'(u)(\varphi) \quad \varphi \in V \\ a'(u_h^m)(\varphi_h,z) &= J'(u)(\varphi) \quad \varphi \in V \end{aligned}$$

Redurced primal and dual residuals:

$$\begin{aligned} \rho(u_h^m)(\cdot) &:= -a(u_h^m)(\cdot) \\ \rho^* &:= J'(u_h^m)(\cdot) - a'(u_h^m)(\cdot, z_h^m) \end{aligned}$$

Proposition (Braack/Ern 2003). *For the combined disretization and modeling error, there holds the error identity*

$$\begin{aligned} J(u) - J(u_h) = &\frac{1}{2}\big\{\rho(u_h^m)(z - i_h z) + \rho^*(u_h^m, z_h^m)(u - i_h u)\big\} \\ &- \frac{1}{2}\big\{d(u_h^m)(e_z) + d'(u_h^m)(e_u, z_h^m)\big\} - d(u_h^m)(z_h^m) + \frac{1}{2}R \end{aligned}$$

where the remainder R is cubic in the errors e^u, e^z.

Proof. The proof uses a modification of the argument already 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:

$$J(u) - J(u_h) \approx \eta_h + \eta_m$$

$$\begin{aligned} \eta_h &:= \frac{1}{2}\big\{\rho(u_h^m)(i_{2h}^{(2)} z_h^m - z_h^m) + \rho^*(u_h^m, z_h^m)(i_{2h}^{(2)} u_h^m - u_h^m)\big\} \\ \eta_m &:= -d(u_h^m)(z_h^m) \end{aligned}$$

Localization of modeling error indicator:

$$-d(u_h^m)(z_h^m) = \sum_{K \in \mathbb{T}_h} \Big(\sum_{i=1}^{N} (\mathcal{F}_i^M(u_h^m) - \mathcal{F}^F(u_h^m), \nabla z_{i,h}^m)_K \Big)$$

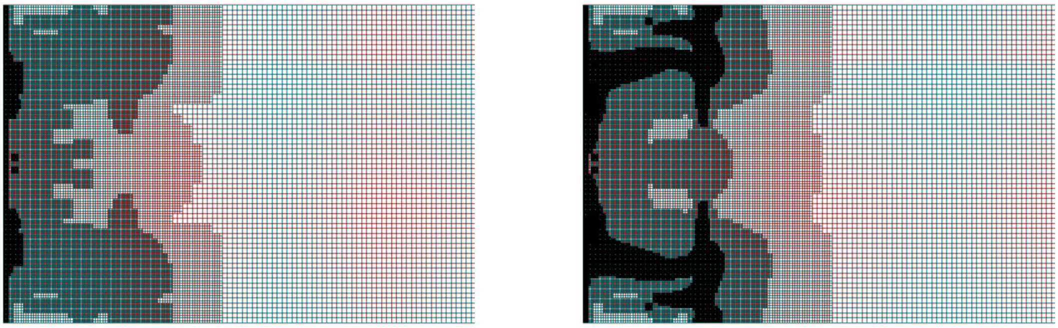

Figure. Adapted meshes with 25 040 and 47 360 cells.

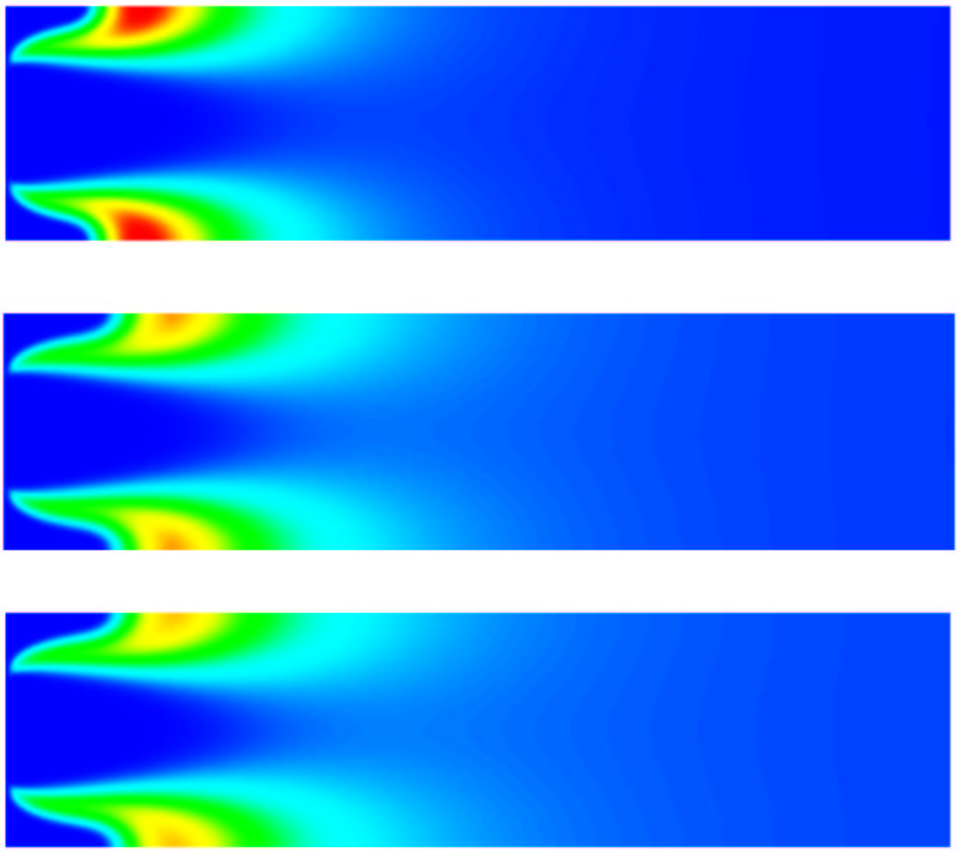

Figure. Flame front obtained using Fick's law (left), 15% multicomponent diffusion, 100% multicomponent diffusion (gain in CPU time 50%)