# 8 Application in Parameter Estimation

We discuss the use of the DWR method in the finite element discretization of parameter estimation and eigenvalue problems. This will be illustrated by several examples ranging from the determination of diffusion coefficients to problems in hydrodynamic stability. The lecture will close with an outlook to further developments and open problems.

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**Formulation of the Problem**

Model problem

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

Determine the coefficient $q$ by comparison with given data

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

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

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

determined by:

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

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

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

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

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

**Remedy.**

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

**General setup of (discrete) parameter estimtion**

- Least Squares Method:

  Minimize $J(u) := \frac{1}{2}\|C(u) - \bar{C}\|_Z^2$ for $u \in V$, $q \in Q = \mathbb{R}^{n_p}$, such that

  $$a(u,q)(\varphi) = f(\varphi) \quad \forall \varphi \in V$$

- Discretization by Finite Elements:

  Minimize $J(u_h) = \frac{1}{2}\|C(u_h) - \bar{C}\|_Z^2$ for $u_h \in V_h$, $q_h \in Q$, such that

  $$a(u_h, q_h)(\varphi_h) = f(\varphi_h) \quad \forall \varphi_h \in V_h$$

- Unconstrained Formulation:

  Minimize $j(q) := \frac{1}{2}\|c(q) - \bar{C}\|_Z^2$, with $c(q) := C(S(q))$ for $q \in Q$

Derivatives: $\quad G_{ij} := \frac{\partial}{\partial q_j} c_i(q) = C_i'(u)(w_j),$

Tangent Equations:

$$a_u'(u,q)(w_j,\varphi) = -a_{q_j}'(u,q)(1,\varphi) \quad \forall \varphi \in V$$

**Optimization algorithm**

- Necessary Optimality Condition:

$$j'(q) = 0 \quad \Leftrightarrow \quad G^*(c(q) - \bar{C}) = 0$$

- Iteration:

$$q_{k+1} = q_k + \delta q, \quad H_k\, \delta q = G_k^*(\bar{C} - c(q_k)), \quad G_k = c'(q_k)$$

- Choice of the Matrix $H_k$:
  - Full Newton Algorithm

$$H_k := G_k^* G_k + \langle c(q_k) - \bar{C}, c''(q_k)\rangle_Z$$

  - Gauß-Newton Algorithm $H_k := G_k^* G_k,$
  - Update Methods

$$H_k := G_k^* G_k + M_k, \quad \text{with updates for } \; M_k$$

- Globalization Strategies:
  - Line Search
  - Trust Region Techniques

A posteriori error estimate for target quantity $E(u)$

$$E(q) - E(q_h) = \eta + P + R$$

- Estimator:
$$\eta = \frac{1}{2}\rho(x_h)(y - i_h y) + \frac{1}{2}\rho^*(x_h)(u - i_h u)$$

- Adjoint problem:
$$a'_u(u,q)(\varphi, y) = -\langle G(G^*G)^{-1}\nabla E(q), C'(u)(\varphi)\rangle_Z \quad \forall \varphi \in V$$

- Residuals:
$$\begin{aligned} \rho(\psi) &:= (f,\psi) - a(u_h, q_h)(\psi) \\ \rho^*(\varphi) &:= \langle G_h(G_h^* G_h)^{-1}\nabla E(q_h), C'(u_h)(\varphi)\rangle - a'_u(u_h, q_h)(\varphi, y_h) \end{aligned}$$

- Remainder terms:
  - R is a cubic remainder term due to linearization
  - $|P| \le \widetilde{C}\,\|e\|\,\|C(u) - \bar{C}\|$

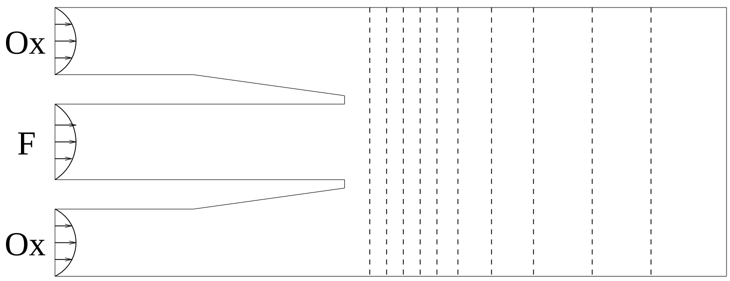
**Example 1: Fitting of reaction parameters (B. Vexler 2003)**

Reaction-diffusion problem

$$\beta \cdot \nabla u - \mu \Delta u + f(u) = 0 \quad \text{in} \;\; \Omega$$
$$u = \hat{u} \quad \text{on} \;\; \Gamma_{in}, \qquad \partial_n u = 0 \quad \text{on} \;\; \partial\Omega \setminus \Gamma_{in}$$

Arrhenius-type reaction law

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




Measurements:
vertical line-integrals of concentration

**Figure.** Configuration

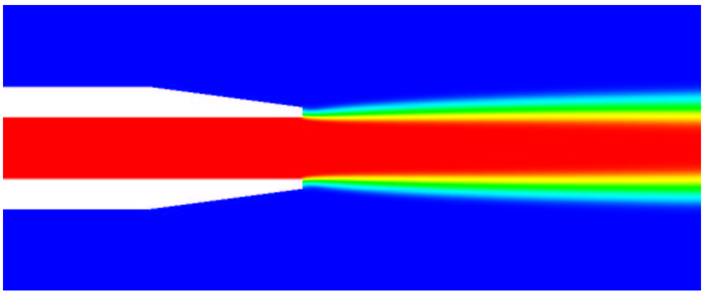


**Figure.** Initial solution ($A = 54.6$, $E = 0.15$)

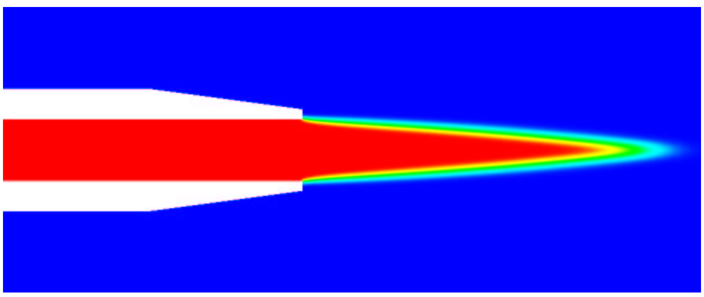


**Figure.** Estimated solution ($A = 992.3$, $E = 0.07$)

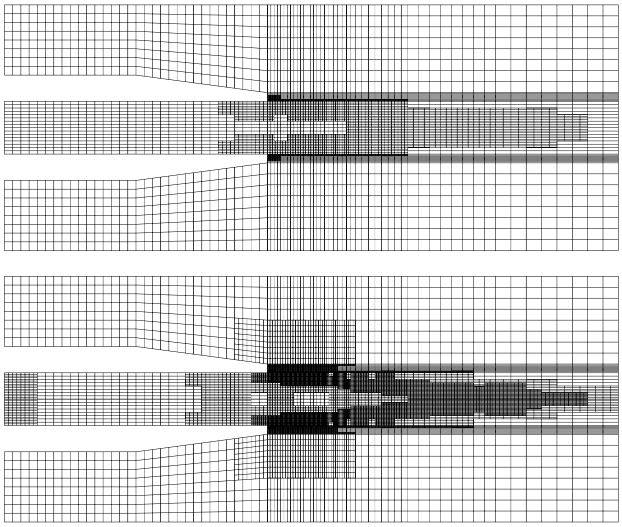


**Figure.** Locally refined meshes

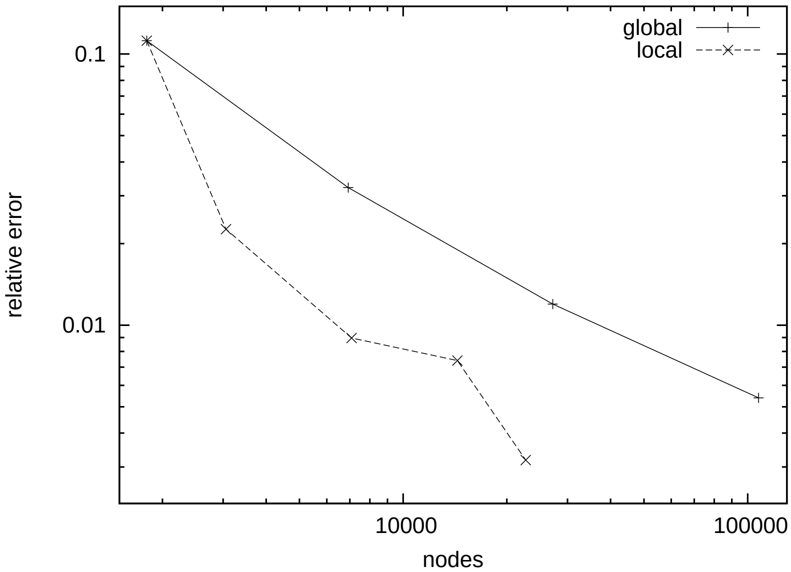
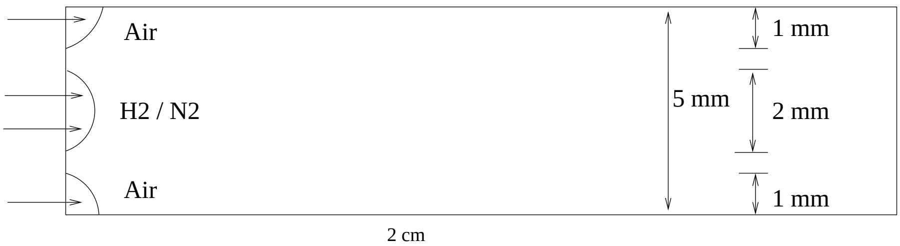



**Figure.** Quality of generated meshes

## Example 2: Fitting of diffusion parameters

Reactive flow problem

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




Measurements: point-values of concentrations

**Figure.** Configuration

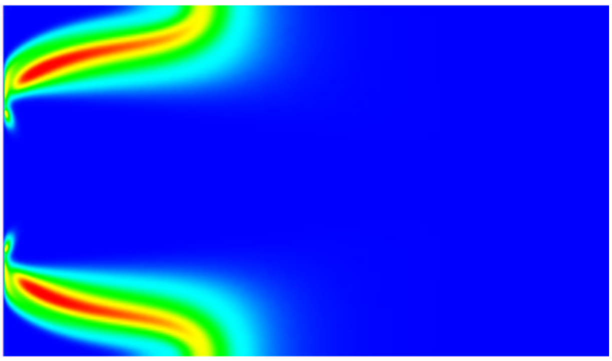


**Figure.** Multicomponent diffusion (reference solution)

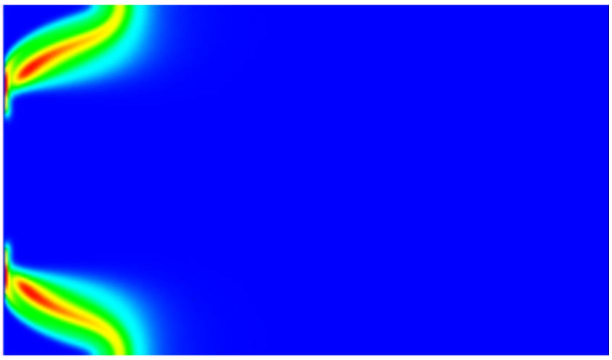


**Figure.** Fick's law (initial parameters)

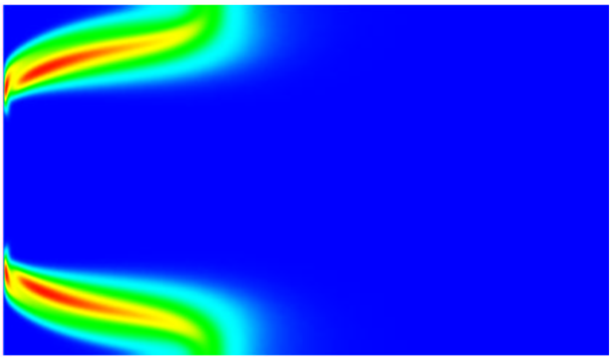


**Figure.** Fitted Fick's law (estimated parameters)

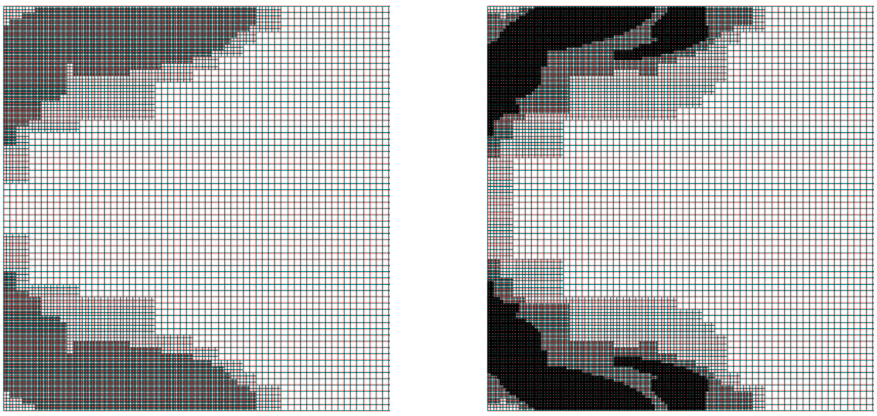


**Figure.** Locally refined meshes (zooms)

**Example 3: Fitting of outflow boundary condition**

Navier-Stokes equations (bypass simulation)

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

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

$$v = 0 \text{ on } \Gamma_0$$

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

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

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

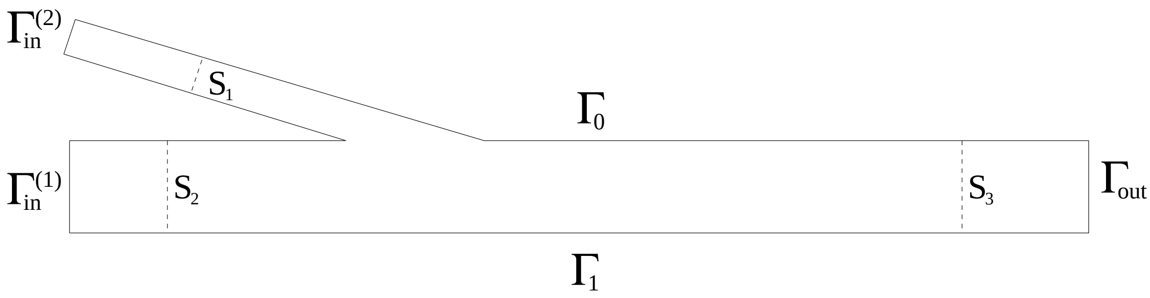



**Figure.** Configuration

Measurements: point-values of pressure

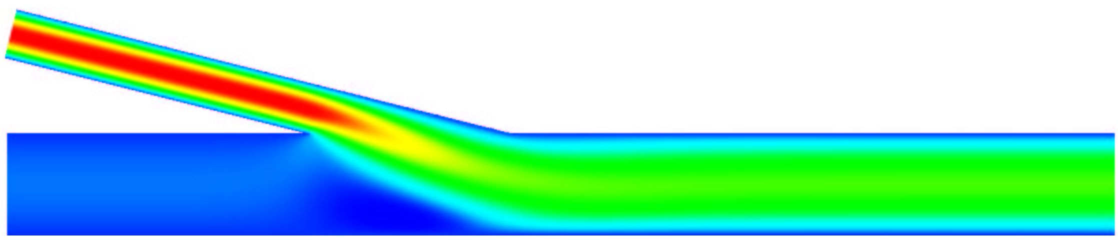


**Figure.** Estimated solution

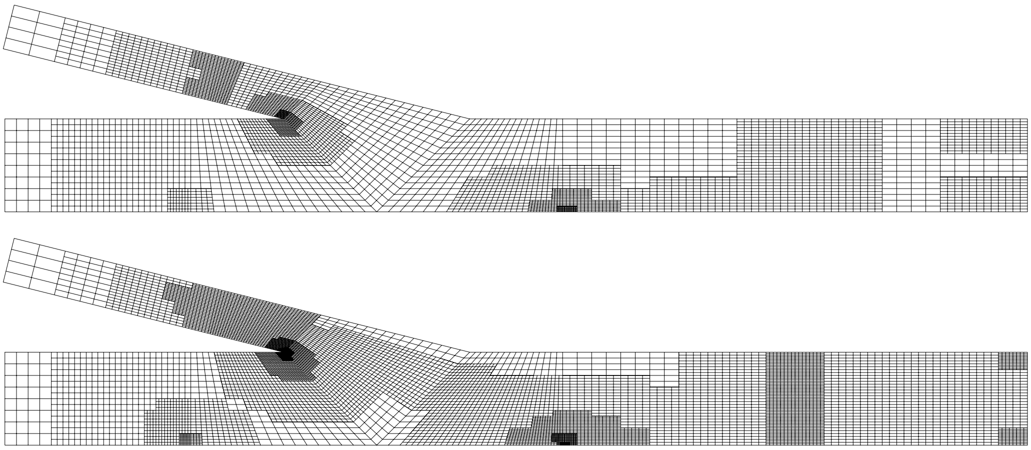


**Figure.** Locally refined meshes

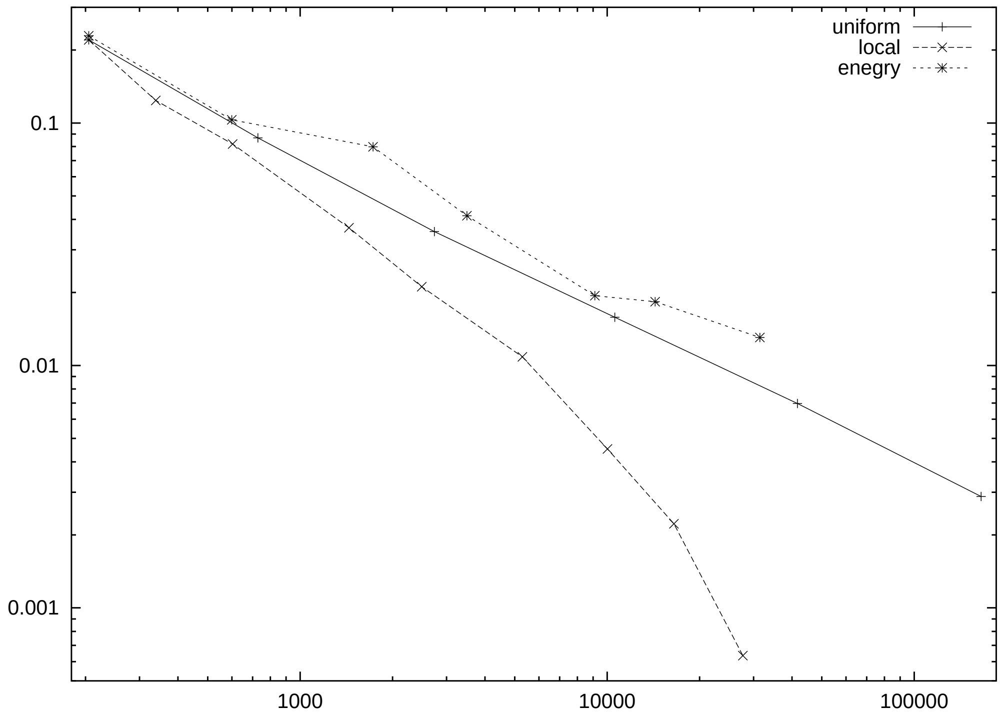



**Figure.** Quality of generated meshes