Introduction to A Posteriori Error Estimation based on Duality

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Outline

Overview of tools and applications of computational mathematical modeling.

- Review of FEM
- A posteriori Error Estimation based on duality
- Examples

Contributors

Presentation based on work by:

- Rickard Bergström
- Don Estep
- Georgios Foufas
- Johan Hoffman
- Mike Holst
- Claes Johnson
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The finite element method

The Finite Element Method is a general method for computer solution of differential equations based on:

- Weak formulation of the differential equation.
- Piecewise polynomial approximation of the solution.

Applications include: solids, fluids, electromagnetics, heat conduction, etc.

Poisson equation: strong form

Find u such that

$$\begin{aligned} -\nabla \cdot A\nabla u &= f && \text{in } \Omega, \\ n \cdot A\nabla u &= g_N && \text{on } \Gamma_N, \\ u &= g_D && \text{on } \Gamma_D, \end{aligned}$$

with Ω a domain in $\mathbf{R}^d$ with boundary $\Gamma = \Gamma_D \cup \Gamma_N$.

Poisson equation: weak form

Find $u \in V_{g_D}$ such that

$$\boxed{a(u,v) = l(v) \quad \text{for all } v \in V_0,}$$

with $V_g = \{v \in H^1 : v = g \text{ on } \Gamma_D\}$ and

$$a(u,v) = \int_\Omega A\nabla u \cdot \nabla v dx,$$

$$l(v) = \int_{\Gamma_N} g_N v ds.$$

Poisson equation: FEM

FEM: Find $u_h \in V_h$ such that

$$\boxed{a(u_h, v) = l(v) \quad \text{for all } v \in V_h,}$$

where $V_h \subset V$ is a finite element space of piecewise polynomials de£ned on a triangulation $\mathcal{K}$ of Ω.

Abstract setting

Model problem: Find $u \in V$ such that

$$\boxed{a(u,v) = l(v) \quad \text{for all } v \in V,}$$

where $a(\cdot,\cdot)$ is an elliptic bilinear form and $l(\cdot)$ is a linear functional.

FEM: Find $u_h \in V_h$ such that

$$\boxed{a(u_h,v) = l(v) \quad \text{for all } v \in V_h,}$$

where $V_h \subset V$ is a £nite element space of piecewise polynomials de£ned on a triangulation $\mathcal{K}$.

What do we want to compute ?

The goal of a computation could be:

- a globally accurate solution.
- values of a number of quantities of particular interest, for instance the lift and drag in a ¤ow computation.

Corresponds to estimating the error in a:

- Global norm
- Set of functionals $m(\cdot)$ of the solution.

Goal oriented error estimates

Objective: Let $m(\cdot)$ be a linear functional on V. We seek to estimate the error

$$m(u) - m(u_h)$$

in the functional in terms of the computed solution.

Examples of functionals

- Average of error in subdomain

$$m(e) = \int_\omega e\psi dx$$

- Average of error in derivative in subdomain

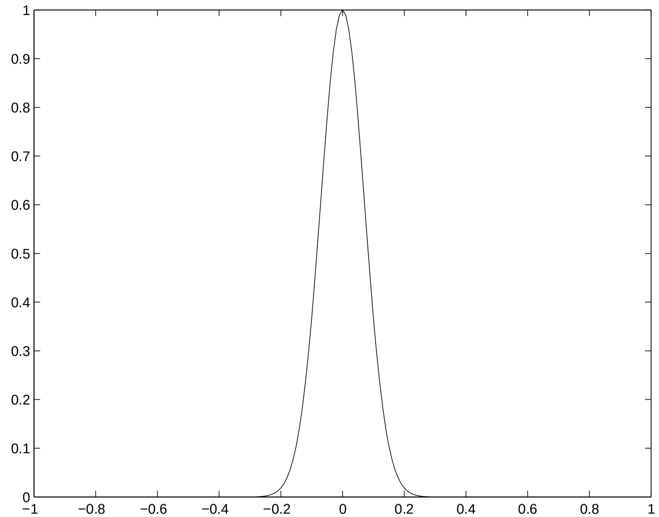
$$m(e) = -\int_\omega e\partial_x \psi dx$$

- Average of integrated ¤ux

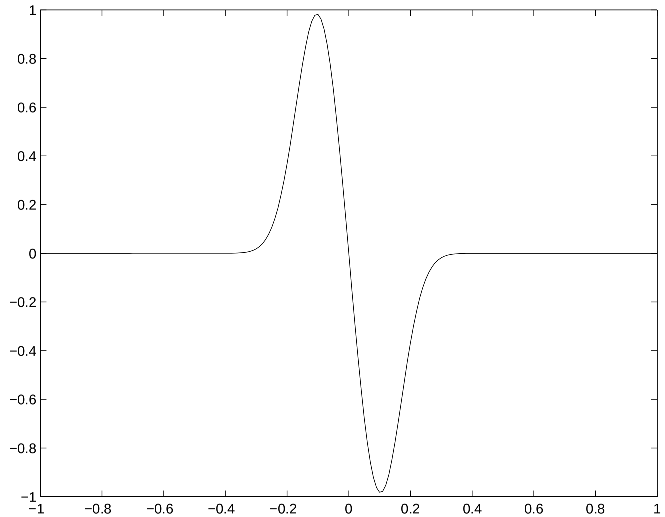
$$m(e) = -\int_\gamma n \cdot \nabla e\psi dx$$

- Use linearization for nonlinear functionals.

Data to dual problem



(a) Point value



(b) Derivative point value

Dual problem

To represent the error in the given linear functional $m(\cdot)$ we introduce the dual problem: Find $\phi \in V$ such that

$$m(v) = a(v, \phi) \quad \text{all } v \in V.$$

Remark: Note that the dual problem is continuous.

Error representation formula

Setting $v = e = u - u_h$ in the dual problem we get

$$
\begin{aligned}
\boxed{m(u) - m(u_h)} &= m(e) \\
&= a(e, \phi) \\
&= a(e, \phi - \pi\phi) \\
&= l(\phi - \pi\phi) - a(u_h, \phi - \pi\phi) \\
&= \boxed{\sum_{K \in \mathcal{K}} (r_K(u_h), \phi - \pi\phi)}
\end{aligned}
$$

Here we used the linearity of $a(\cdot,\cdot)$ and $m(\cdot)$ and orthogonality to subtract an interpolant $\pi\phi \in V_h$ of ϕ.

Residual based error estimates

$$
\begin{aligned}
|m(u) - m(u_h)| &= \left| \sum_{K \in \mathcal{K}} (r_K(u_h), \phi - \pi\phi) \right| && \text{Est. 1} \\
&\leq \sum_{K \in \mathcal{K}} \left| (r_K(u_h), \phi - \pi\phi) \right| && \text{Est. 2} \\
&\leq \sum_{K \in \mathcal{K}} R_K(u_h) \cdot W_K(\phi) && \text{Est. 3}
\end{aligned}
$$

Note: The *first* inequality prevents cancelation between elements. The *second* inequality prevents cancelation between different parts of the residual on an element level.

Poisson: residual

Let $v = \phi - \pi\phi$ we have

$$
\begin{aligned}
&(f, v) - (\nabla u_h, \nabla v) \\
&= \sum_{K \in \mathcal{K}} (f + \Delta u_h, v)_K + ([n \cdot \nabla u_h], v)_{\partial K}/2 \\
&= \sum_{K \in \mathcal{K}} (r_K(u_h), v).
\end{aligned}
$$

With the weak residual

$$\boxed{(r_K(u_h), v) = (f + \Delta u_h, v)_K + ([n \cdot \nabla u_h], v)_{\partial K}/2}$$

Poisson: residual and weight

The following estimate holds

$$\boxed{|(r_K(u_h), \phi - \pi\phi)| \leq R_K(u_h) \cdot W_K(\phi)}$$

with

$$R_K(u_h) = \begin{bmatrix} \|\Delta u_h + f\|_K \\ h_K^{-1/2} \|[n \cdot \nabla u_h]\|_{\partial K}/2 \end{bmatrix}$$

$$W_K(\phi) = \begin{bmatrix} \|\phi - \pi\phi\|_K \\ h_K^{1/2} \|\phi - \pi\phi\|_{\partial K} \end{bmatrix}$$

Poisson: residual and weight

Let $v = \phi - \pi\phi$. Then we have

$$\begin{aligned}(r_K(u_h), v) &= (f + \Delta u_h, v)_K + ([n \cdot \nabla u_h], v)_{\partial K}/2 \\ &\leq \|f + \Delta u_h\|_K \|v\|_K \\ &\qquad + h_K^{1/2}\|[n \cdot \nabla u_h]\|_{\partial K} h_K^{-1/2}\|v\|_{\partial K} \\ &= R_K(u_h) \cdot W_K(v).\end{aligned}$$

Remark: Note that the scaling with h_K in the boundary contribution is necessary for the two contributions to the residual and weight to scale in the same way.

The residual and weight

Based on approximation theory we expect that

$$|R_K(u_h)| \sim C h_K^{\alpha-2} |u|_{\alpha,K}$$
$$|W_K(\phi)| \sim C h_K^{\beta} |\phi|_{\beta,K}$$

with $1 \leq \alpha, \beta \leq p+1$, where is the order of polynomials used in the approximation.

- There are powers of h in both the residual and weight !

Stability factor for functional

Continuing the estimates we get:

$$
\begin{aligned}
|m(u) - m(u_h)| &\leq \sum_{K \in \mathcal{K}} R_K(u_h) \cdot W_K(\phi) \quad \text{Est. 3} \\
&\leq \left(\sum_{K \in \mathcal{K}} h_K^{2\beta} R_K^2(u_h) \right)^{1/2} \left(\sum_{K \in \mathcal{K}} h_K^{-2\beta} W_K^2(\phi) \right)^{1/2} \\
&\leq \mathcal{S}_m \left(\sum_{K \in \mathcal{K}} h_K^{2\beta_K} |R_K(u_h)|^2 \right)^{1/2} \qquad \text{Est. 4}
\end{aligned}
$$

where

$$
\boxed{\mathcal{S}_m^2 = \sum_{K \in \mathcal{K}} h_K^{-2\beta} W_K^2(\phi)}
$$

is the **stability factor** of the computation of $m(\cdot)$.

Computing the error estimate

- $R_K(u_h)$ directly computable.
- $W_K(\phi)$ can be approximated by solving the dual problem numerically. Note that derivative information is necessary here.

Important research topic: Construct ef£cient adaptive methods using only rough knowledge of ϕ.

Computing the error estimate

We consider the following techniques:

- Solve the dual with higher order elements or on a finer mesh.
- Solve the dual on the same or a coarser mesh and use postprocessing.
- Use interpolation error estimates theory to estimate the weight.

How can we use the error estimates?

There are two **different uses** for error estimates:

- To estimate the error (expensive)
- To construct an adaptive method (not expensive)

Estimates based on local problems

There is an alternative strategy for computing the a posteriori error estimate which is based on:

- Start from the same error representation formula.
- Use the parallelogram law to write the error representation formula as a difference of two energy like products.
- Employ upper and lower energy norm error estimates based on local problems to bound the difference.
- Results in upper and lower bounds on the functional.
- Developed by: Babuska, Oden, Pereira, and others.

Estimates based on local problems

Setting $v = e = u - u_h$ in the dual problem we get

$$\begin{aligned} m(u) - m(u_h) &= m(e) \\ &= a(e, \phi) \\ &= a(e, \phi - \phi_h) \\ &= a(e, \epsilon) \end{aligned}$$

Here we used the linearity of $a(\cdot, \cdot)$ and $m(\cdot)$ and orthogonality to subtract the finite element approximation $\phi_h \in V_h$.
We thus conclude:

$$\boxed{m(u) - m(u_h) = a(e, \epsilon)}$$

Estimates based on local problems

Starting from the error representation formula

$$(e, \psi) = a(e, \epsilon)$$

where

$$e = u - u_h, \qquad \epsilon = \phi - \phi_h$$

and using the identity

$$4ab = (a+b)(a+b) - (a-b)(a-b)$$

we obtain the alternative error representation formula

$$4(e, \psi) = a(e+\epsilon, e+\epsilon) - a(e-\epsilon, e-\epsilon)$$

Estimates based on local problems

Recall that there are upper and lower estimators

$$\rho_\pm^2 = \sum_K \rho_{\pm,K}^2, \qquad \eta_\pm^2 = \sum_K \eta_{\pm,K}^2$$

$\rho_\pm$ and $\eta_\pm$ such that

$$\eta_\pm^2 \le a(e \pm \epsilon, e \pm \epsilon) \le \rho_\pm^2$$

For the Poisson equation these estimators correspond to standard energy norm estimators for the problems

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

Estimates based on local problems

Combing the estmators and the error representation formula

$$4(e, \psi) = a(e + \epsilon, e + \epsilon) - a(e - \epsilon, e - \epsilon)$$

We obtain the upper and lower bounds

$$\boxed{\eta_+^2 - \rho_-^2 \leq 4(e, \psi) \leq \rho_+^2 - \eta_-^2}$$

Remarks:

- Upper and lower bounds with no constants in the estimate.
- More complicated and less general technique.

Extension to nonlinear problems

Assume that the forms $m(\cdot)$ and $a(\cdot,\cdot)$ are nonlinear then we may introduce linearized forms with the properties

$$m(u) - m(u_h) = \overline{m}(u, u_h)(u - u_h) \tag{1}$$

$$a(u, v) - a(u_h, v) = \overline{a}(u, u_h; u - u_h, v) \tag{2}$$

We then introduce the dual problem: Find $\phi \in V$ such that

$$\overline{m}(v) = \overline{a}(v, \phi) \quad \text{all } v \in V.$$

Remark: Note that the dual problem is continuous.

Error representation formula

Setting $v = e = u - u_h$ in the dual problem we get

$$\begin{aligned}
\boxed{m(u) - m(u_h)} &= \overline{m}(e) \\
&= \overline{a}(e, \phi) \\
&= a(u, \phi) - a(u_h, \phi) \\
&= l(\phi) - a(u_h, \phi) \\
&= l(\phi - \pi\phi) - a(u_h, \phi - \pi\phi) \\
&= \boxed{\sum_{K \in \mathcal{K}} (r_K(u_h), \phi - \pi\phi)}
\end{aligned}$$

Here we used the linearity of $a(\cdot, \cdot)$ and $m(\cdot)$ and orthogonality to subtract an interpolant $\pi\phi \in V_h$ of ϕ.

Adaptive methods

- Compute a solution on a coarse grid
- Evaluate element indicator (compute $R_K(u_h) \cdot W_K(\phi)$)
- Refine mesh, h or p, based on element error indicator
- Compute an improved solution
- Repeat until satisfactory accuracy is achieved (time, memory,...)

Refinement criteria: h-method

Refine

- 30% of the elements with largest indicator.
- refine all elements K with

$$R_K(u_h) \cdot W_K(\phi) \geq \kappa \max_K R_K(u_h) \cdot W_K(\phi)$$

  with $0 \leq \kappa \leq 1$.

Only coarse information on element indicator necessary to get roughly the same mesh.

Remark: $h - p$ methods much more delicate !

Examples

- Poisson’s equation
- Helmholtz equation
- Navier-Stokes
- Elasticity

Poisson's equation

We consider

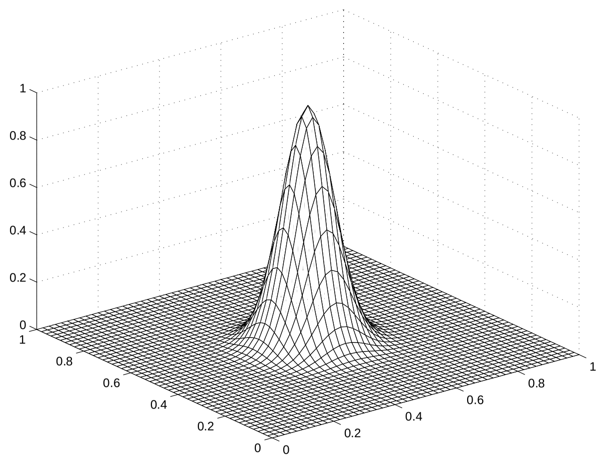
$$-\Delta u = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega$$

with f chosen so that

$$u = \sin \pi x \sin \pi y e^{-(r_1/R_1)^2}$$

with $r_1 = \sqrt{(x-0.5)^2 + (y-0.5)^2}$, $R_1 = 0.1$

Poisson's equation



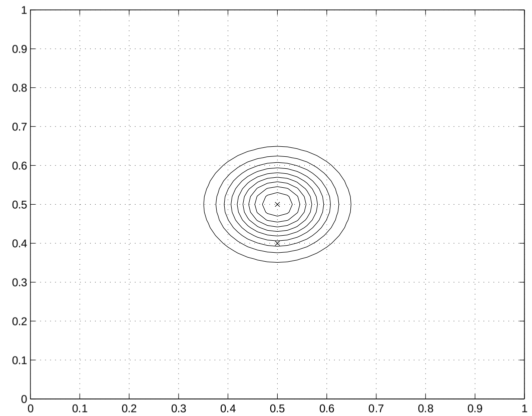
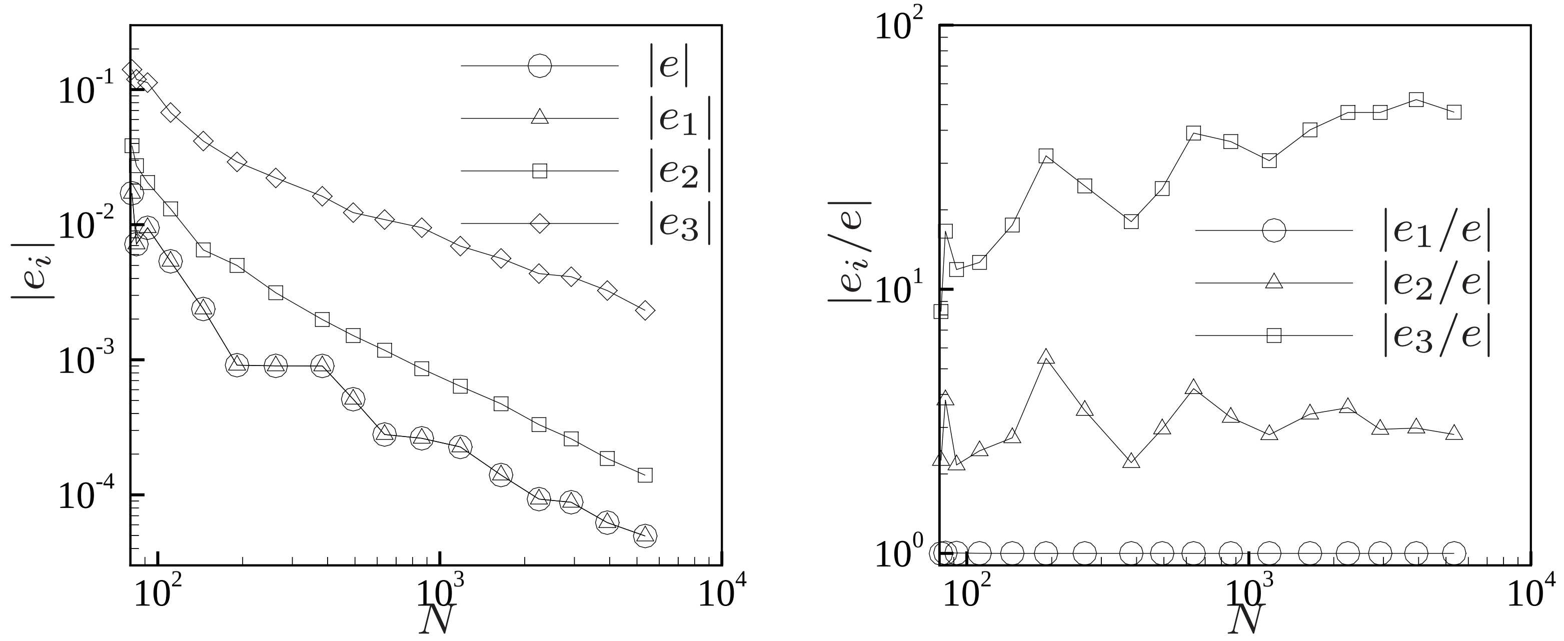


Figure 1: The exact solution for the 2D problem and two points where the error could be measured

Poisson's equation



(a) The error.

(b) The error indicators.

Figure 2: The error is measured in $(0.5, 0.4)$, linears, adaptive algorithm based on estimate 2.

The Helmholtz equation

find u such that

$$-\Delta u - k^2 u = 0,$$

together with suitable boundary conditions.

Helmholtz: Plane wave solution

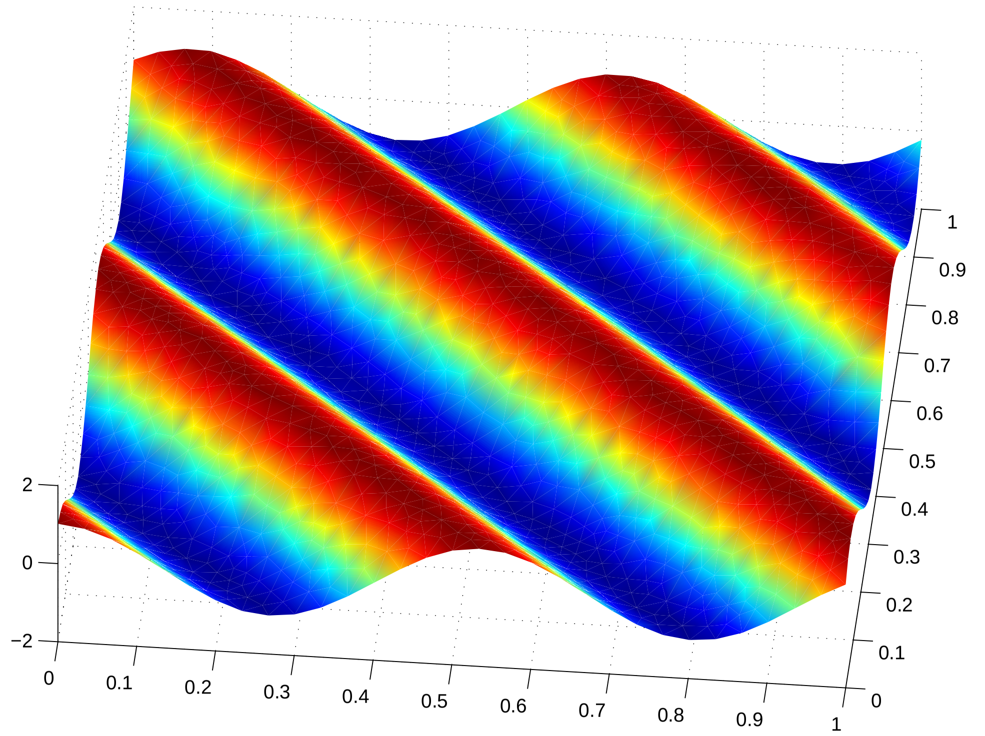


Figure 3: $k = 16.56$, $\theta = \pi/4$

Helmholtz: The dual problem

To control the error in a point x_0 we consider

$$-\triangle\phi - k^2\phi = \delta_{x_0}.$$

Helmholtz: Dual solution

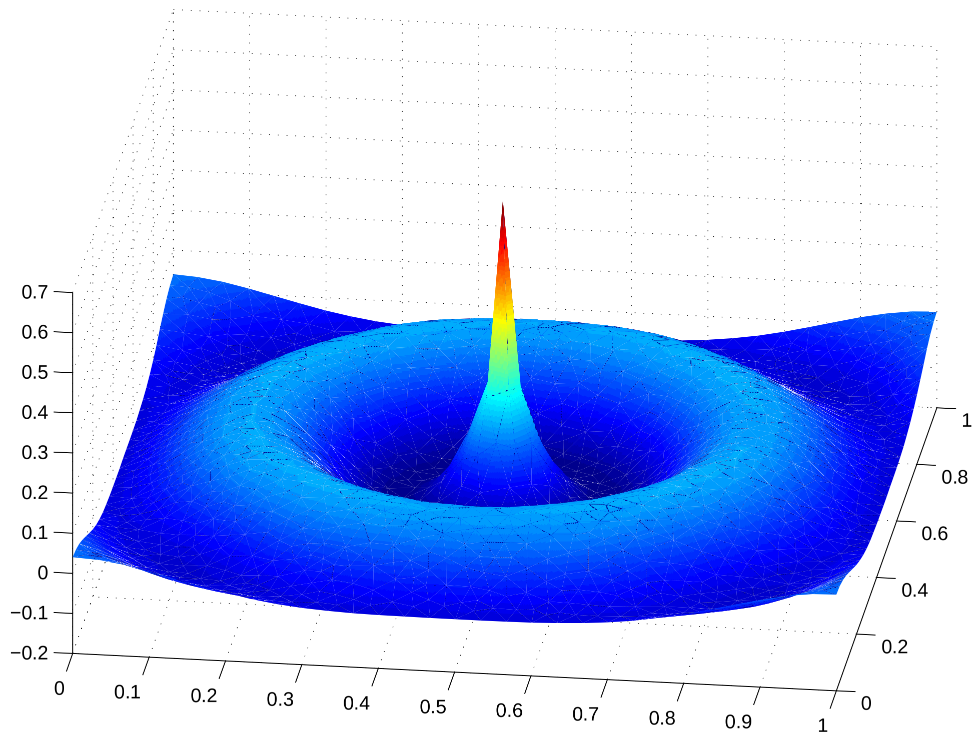


Figure 4: $k = 16.56$, $z = [0.5, 0.5]$

Here $\psi = \delta_{x_0}$ to control the error in the point x_0.

Navier-Stokes

Incompressible Navier-Stokes equations (NS)

$$\dot{u} + u \cdot \nabla u = \nu \Delta u - \nabla p \qquad \text{(Newton's 2:nd law)}$$

$$\nabla \cdot u = 0 \qquad \text{(incompressibility)}$$

Computational methods use NS to construct rules for how ¤uid particles in a simulation move with resp. to each other

NS: dual problem

The sensitivity of different error measures (e, ψ) is contained in the dual solution φ through the data ψ.

The linearized dual Navier-Stokes equations

$$\begin{aligned} -\dot{\varphi} - (u \cdot \nabla)\varphi + \nabla U \cdot \varphi + \nabla \theta - \nu \Delta \varphi &= \psi \\ \nabla \cdot \varphi &= 0 \end{aligned}$$

Information is transported backwards in space and time by the exact solution u through the term $-\dot{\varphi} - (u \cdot \nabla)\varphi$

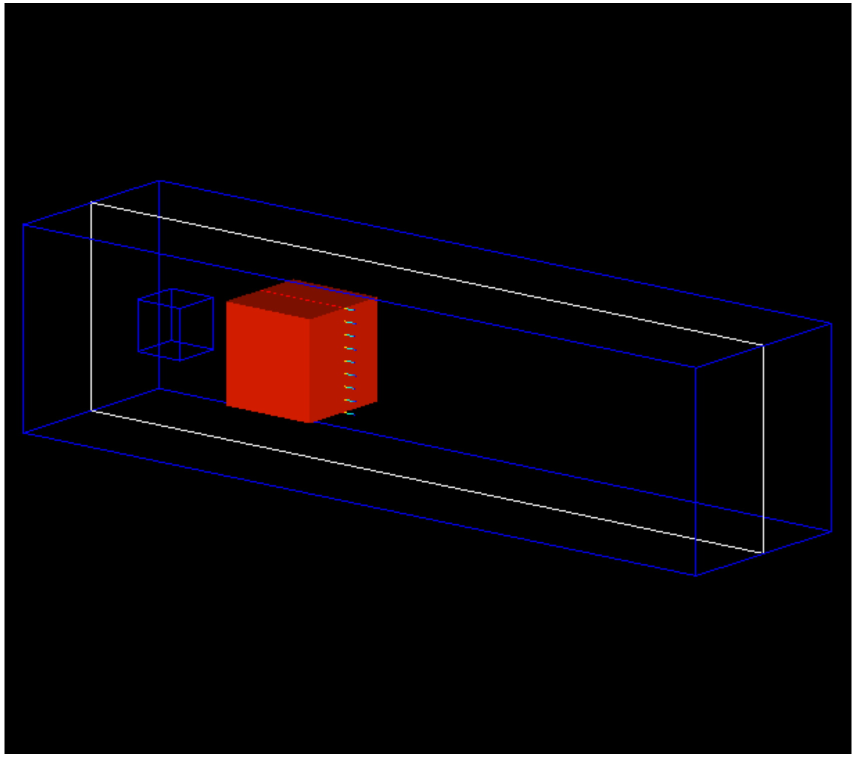
We have growth due to the reaction term $\nabla U \cdot \varphi$
(which in laminar ¤ow is dominated by diffusion effects)

NS: Example

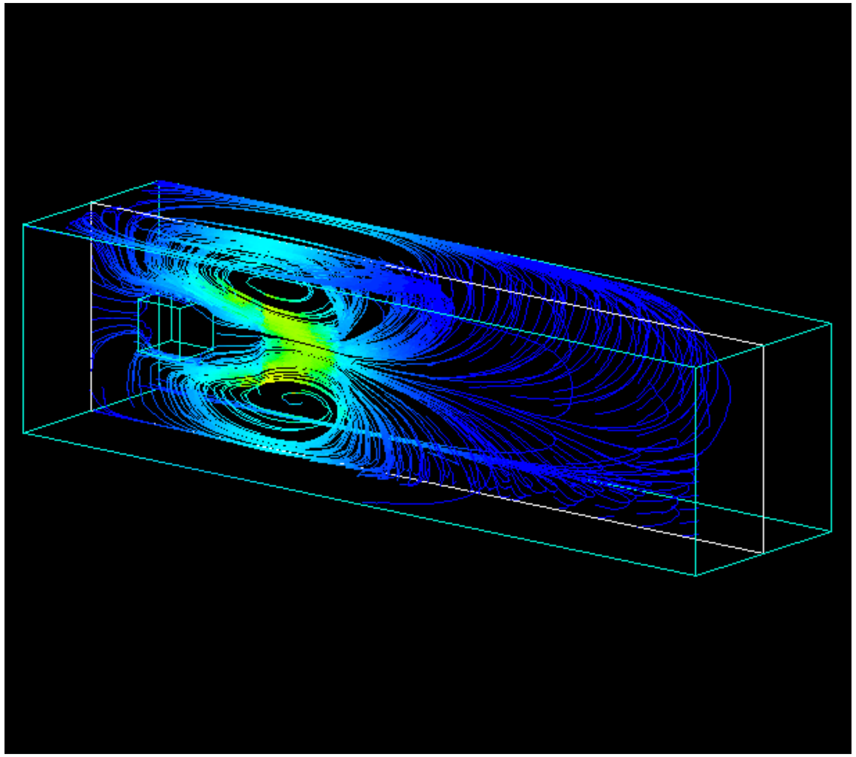
Estimate the error in space-time averages over a spatial cube ω with side $d(\omega)$, corresponds to a force ψ acting on ω over a time interval $I = [T - d(\omega), T]$:

$$\psi = \frac{\chi_{\omega\times I}}{|\chi_{\omega\times I}|} \Rightarrow (e, \psi) = \frac{1}{d(\omega)^4} \int_I \int_\omega e \, dx \, dt$$

NS: Bluff body dual solution

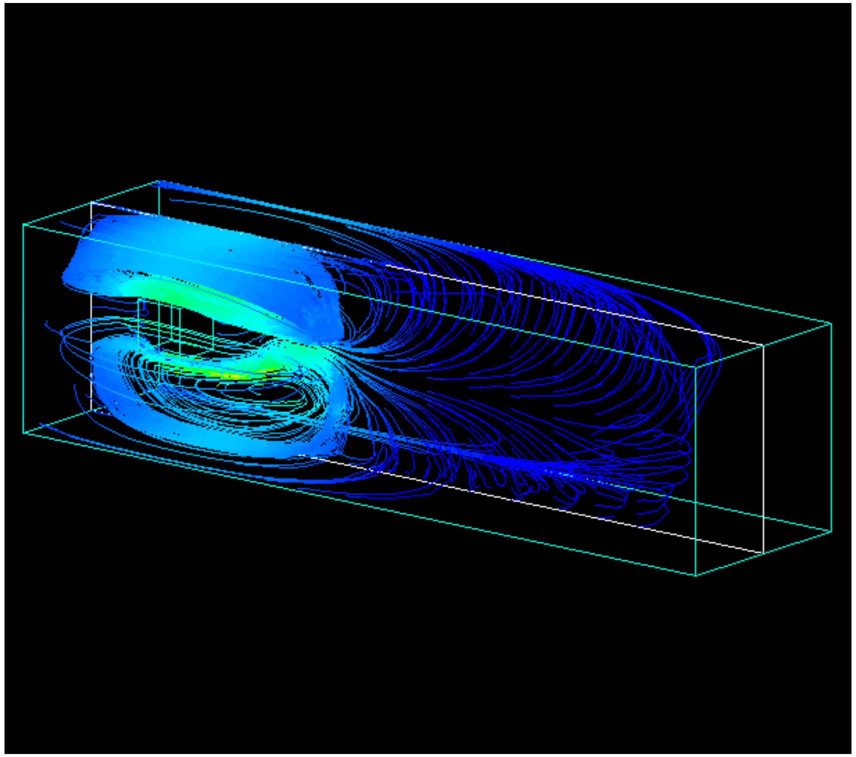


$t = 2.0$

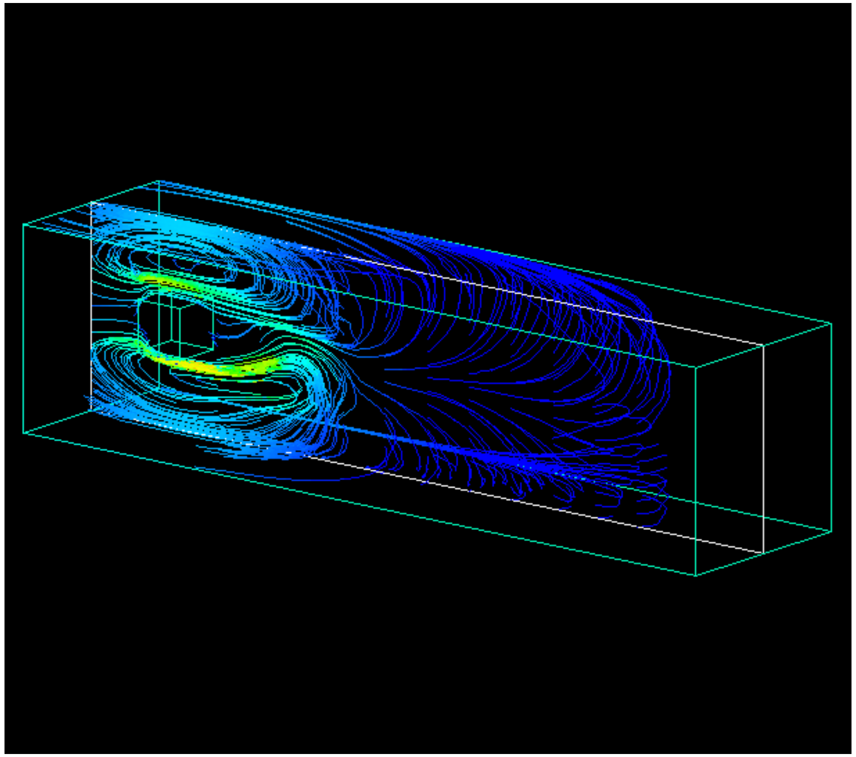


$t = 1.75$

NS: Bluff body dual solution

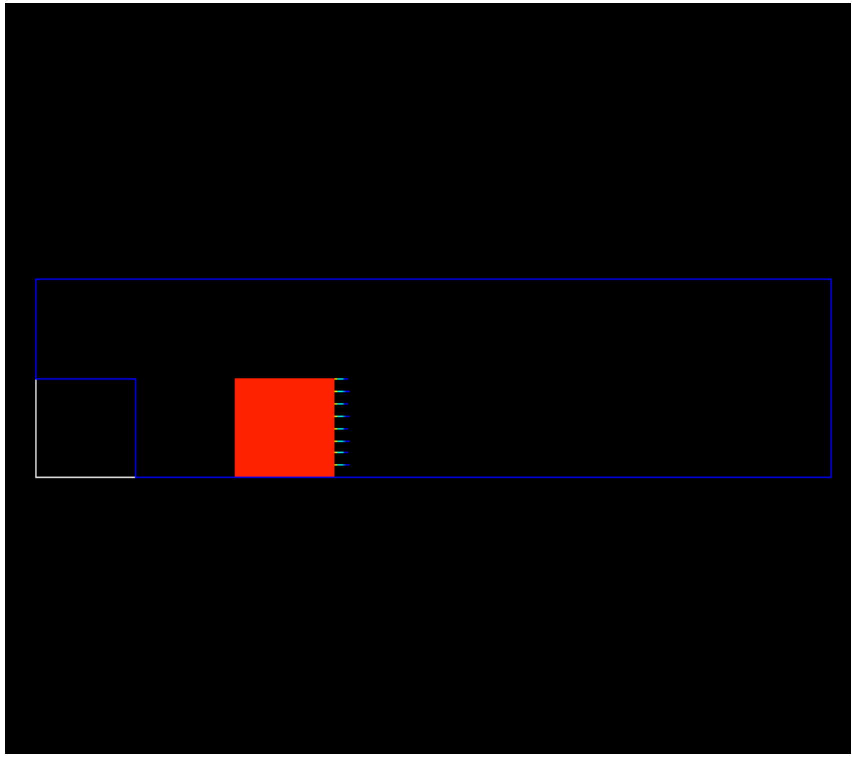


$t = 1.5$

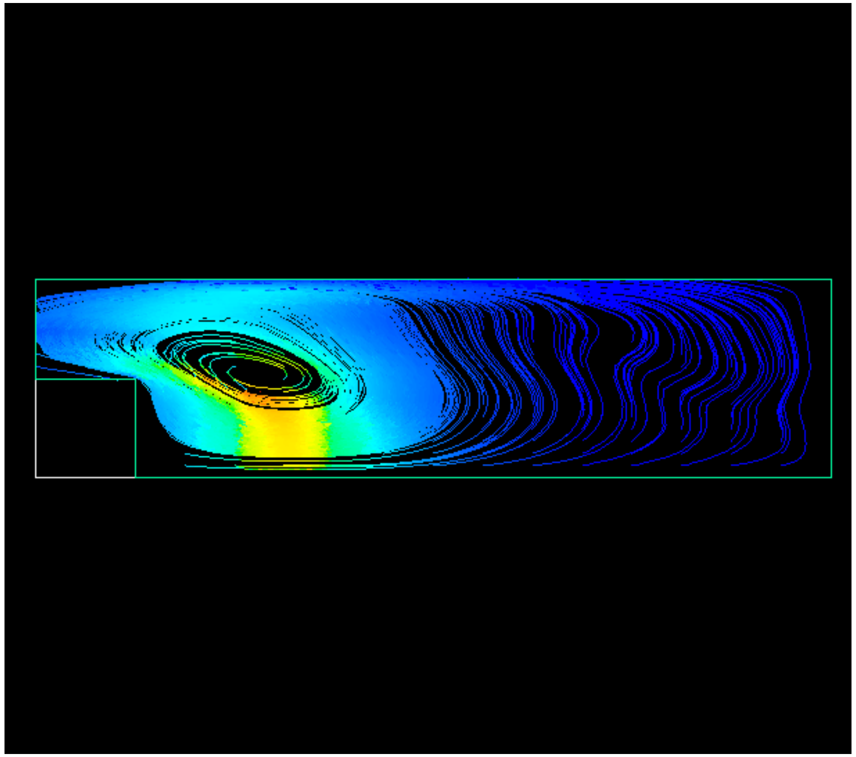


$t = 1.25$

NS: Step down dual solution

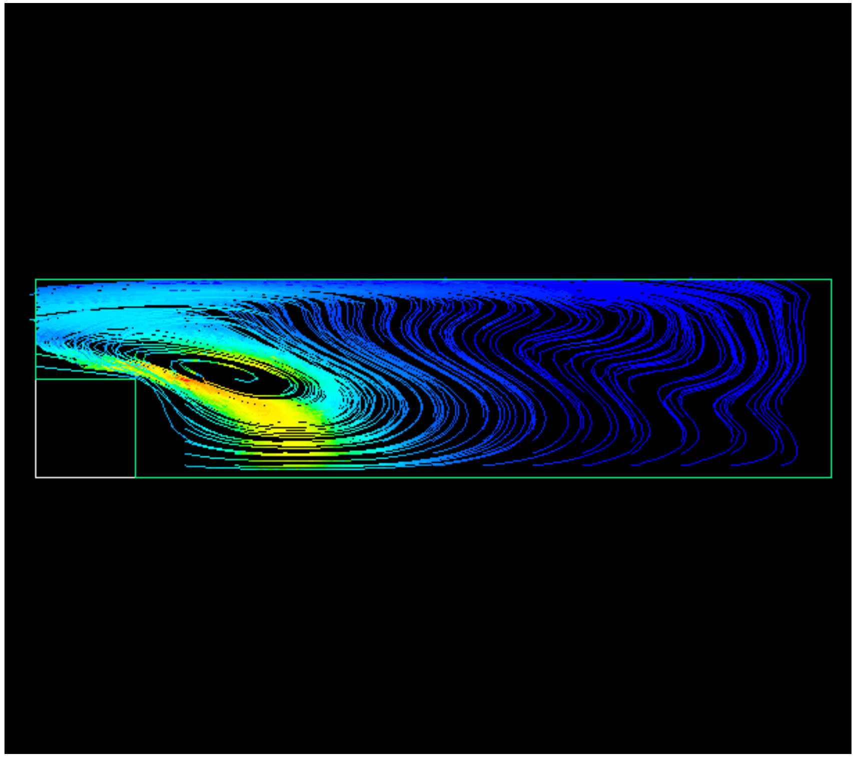


$t = 2.0$

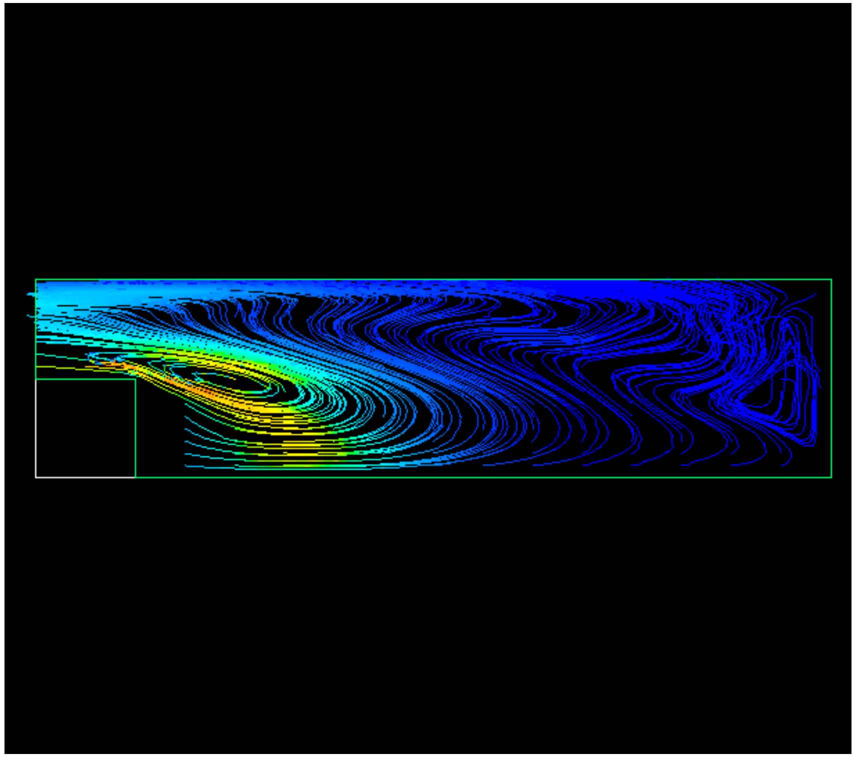


$t = 1.5$

NS: Step down dual solution



$t = 1.0$



$t = 0.5$

Elasticity

find $u : \Omega \to \mathbf{R}^3$ such that

$$\begin{aligned} -\nabla \cdot \sigma = f \quad & \text{in } \Omega, \\ \sigma = \lambda \nabla \cdot u I + 2\mu\epsilon(u) \quad & \text{in } \Omega, \\ u = g_D \quad & \text{on } \Gamma_\mathrm{D}, \\ n \cdot \sigma = g_N \quad & \text{on } \Gamma_\mathrm{N}. \end{aligned}$$

where $\epsilon(u) = (\nabla u + \nabla u^T)/2$ is the strain and λ and μ are the Lame parameters.

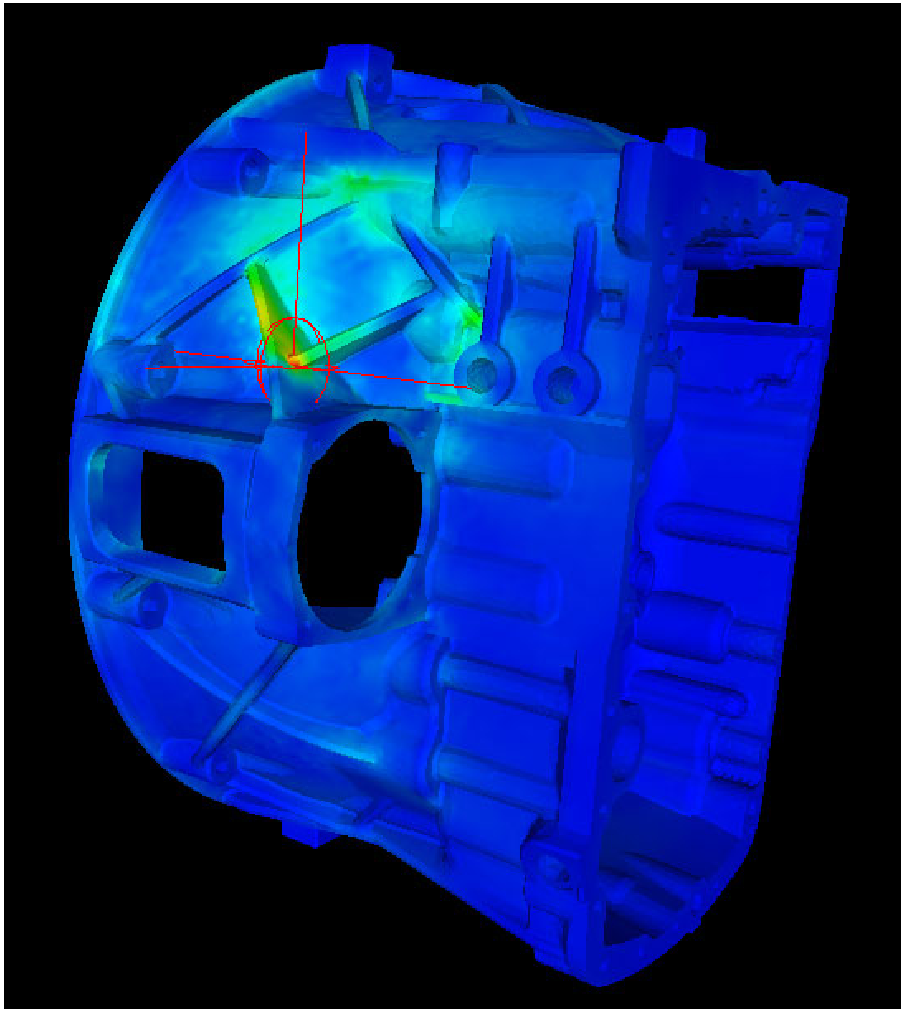
Elasticity: dual problem

find $\phi : \Omega \to \mathbf{R}^3$ such that

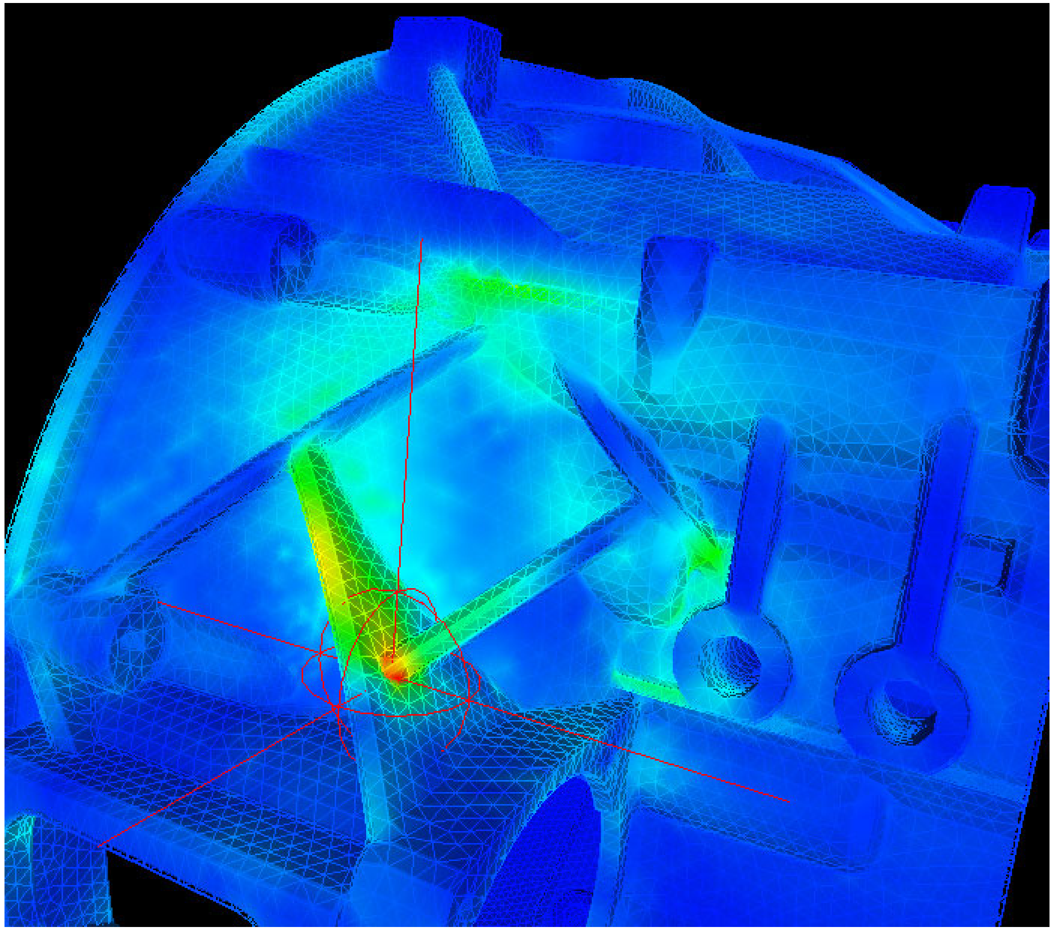
$$\begin{aligned} -\nabla \cdot \sigma = \psi \quad & \text{in } \Omega, \\ \sigma = \lambda \, \nabla \cdot \phi I + 2\mu\epsilon(\phi) \quad & \text{in } \Omega, \\ \phi = 0 \quad & \text{on } \Gamma_{\mathrm{D}}, \\ n \cdot \sigma = 0 \quad & \text{on } \Gamma_{\mathrm{N}}. \end{aligned}$$

Taking $\psi = \delta_{x_0} m$ controls the displacement error $(u - U)(x_0) \cdot m$.

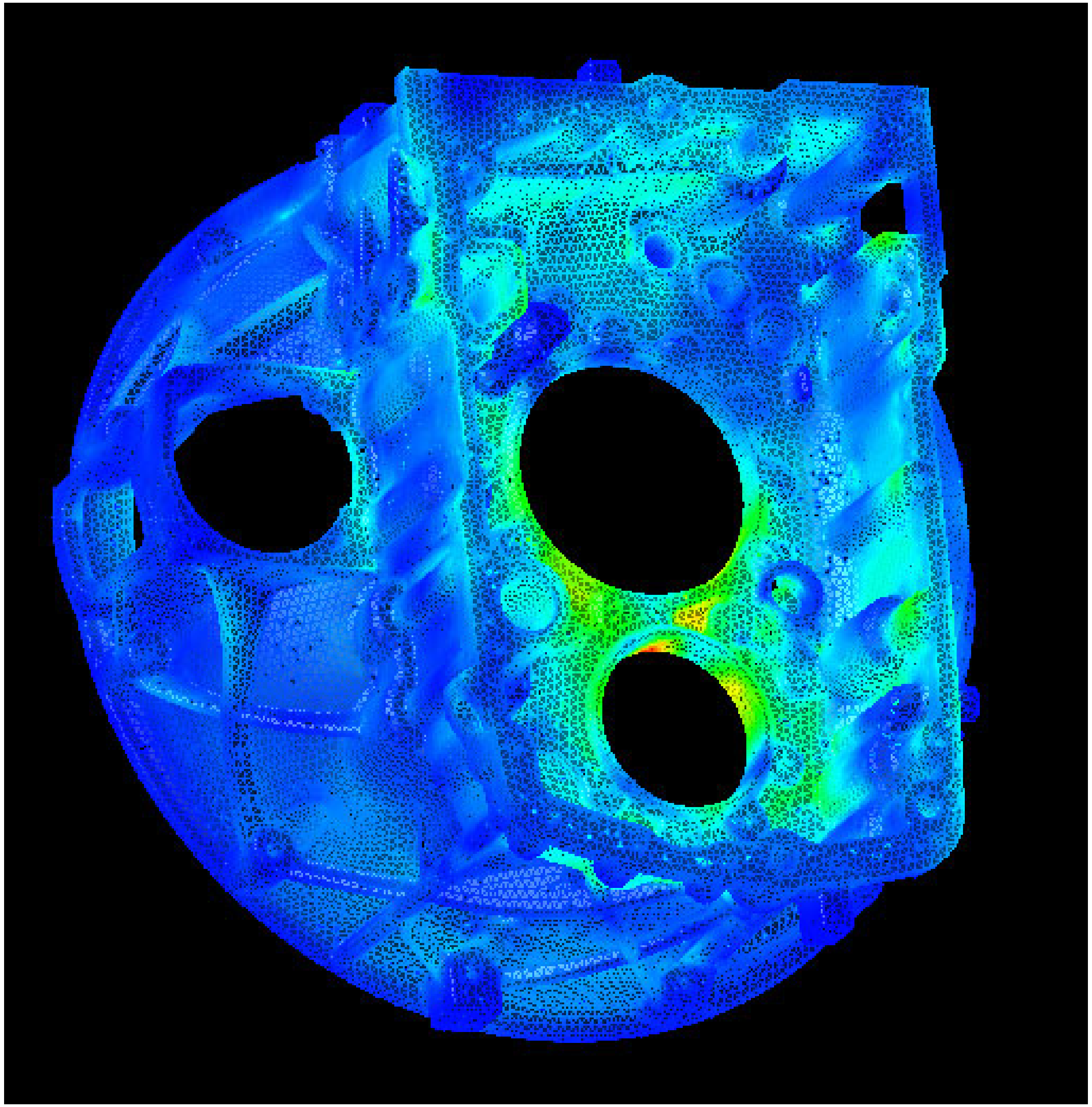
Elasticity: solution to dual



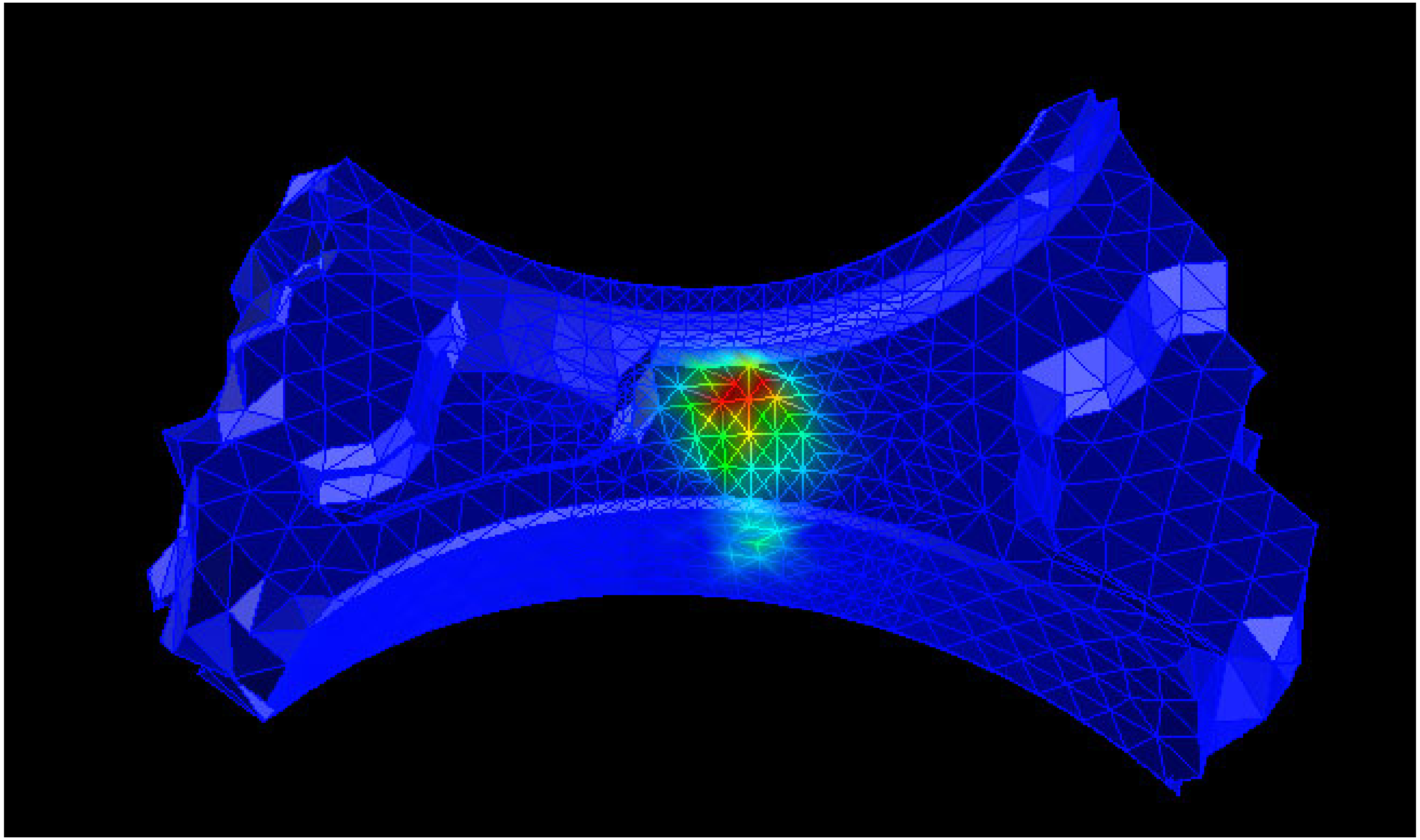
Elasticity: solution to dual



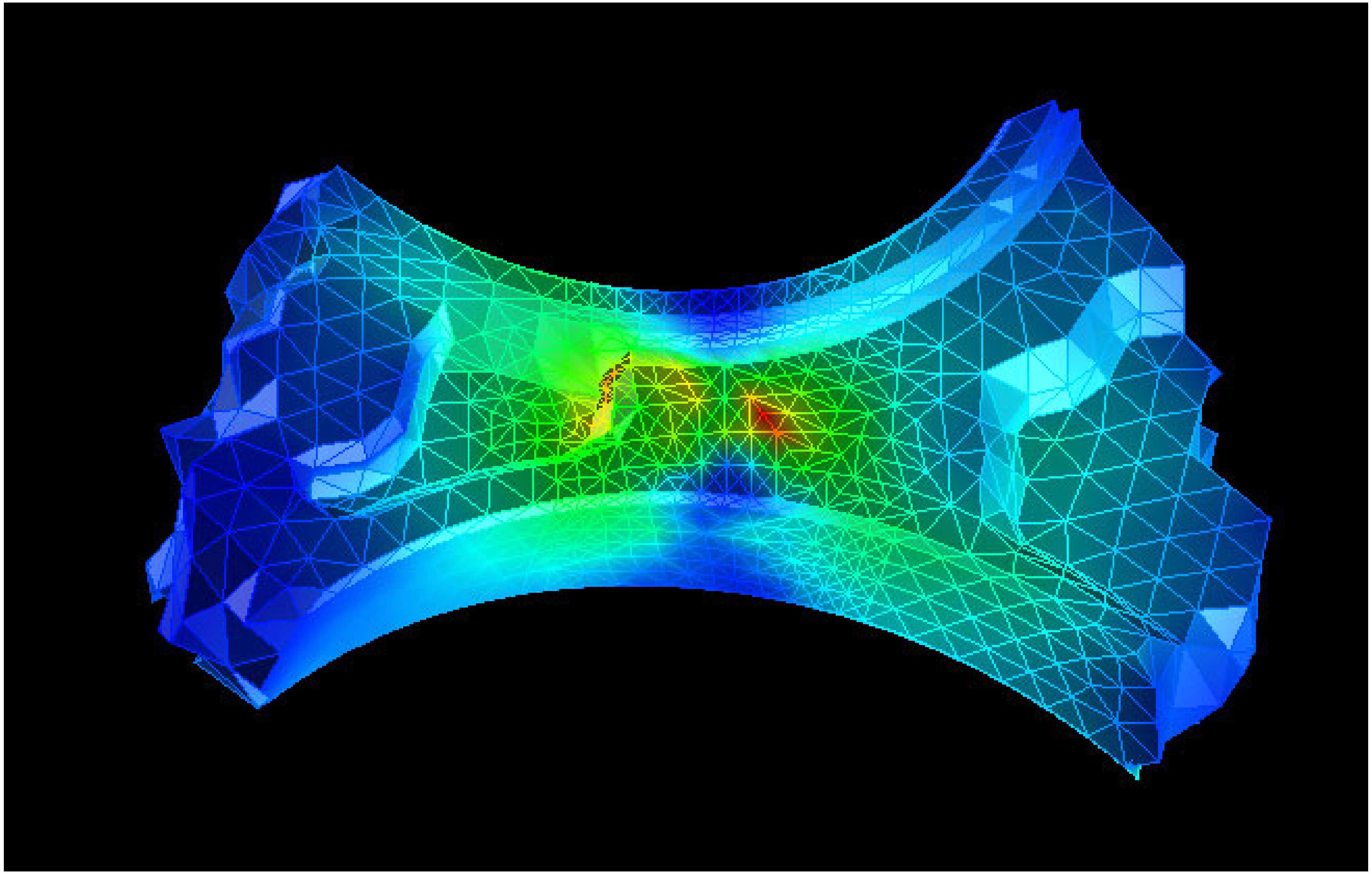
Elasticity: solution to primal



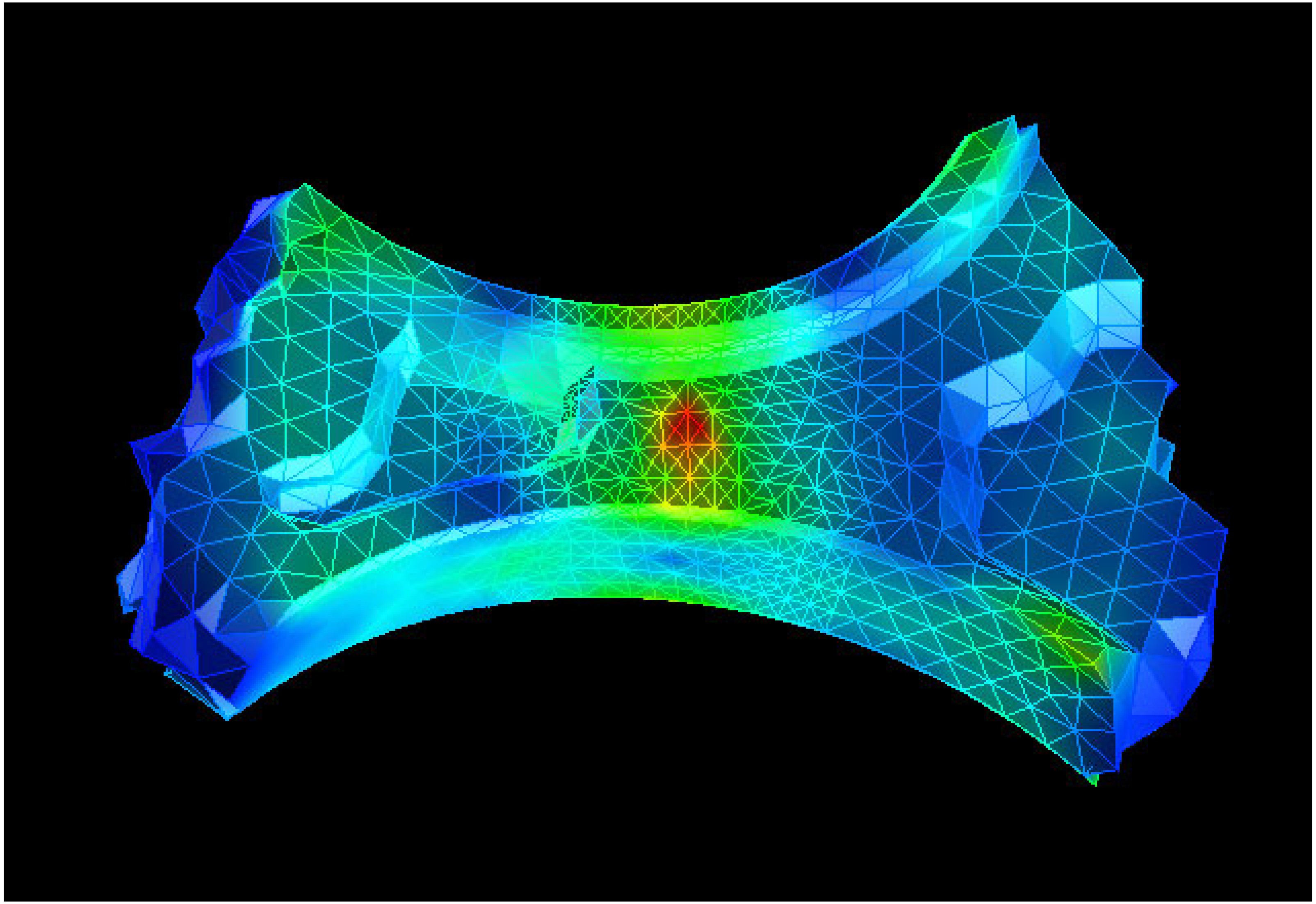
Elasticity: solution to local dual



Elasticity: solution to local dual



Elasticity: solution to local dual



Go to: **Grid** or **Multiscale**

Linear Elasticity: solution to dual

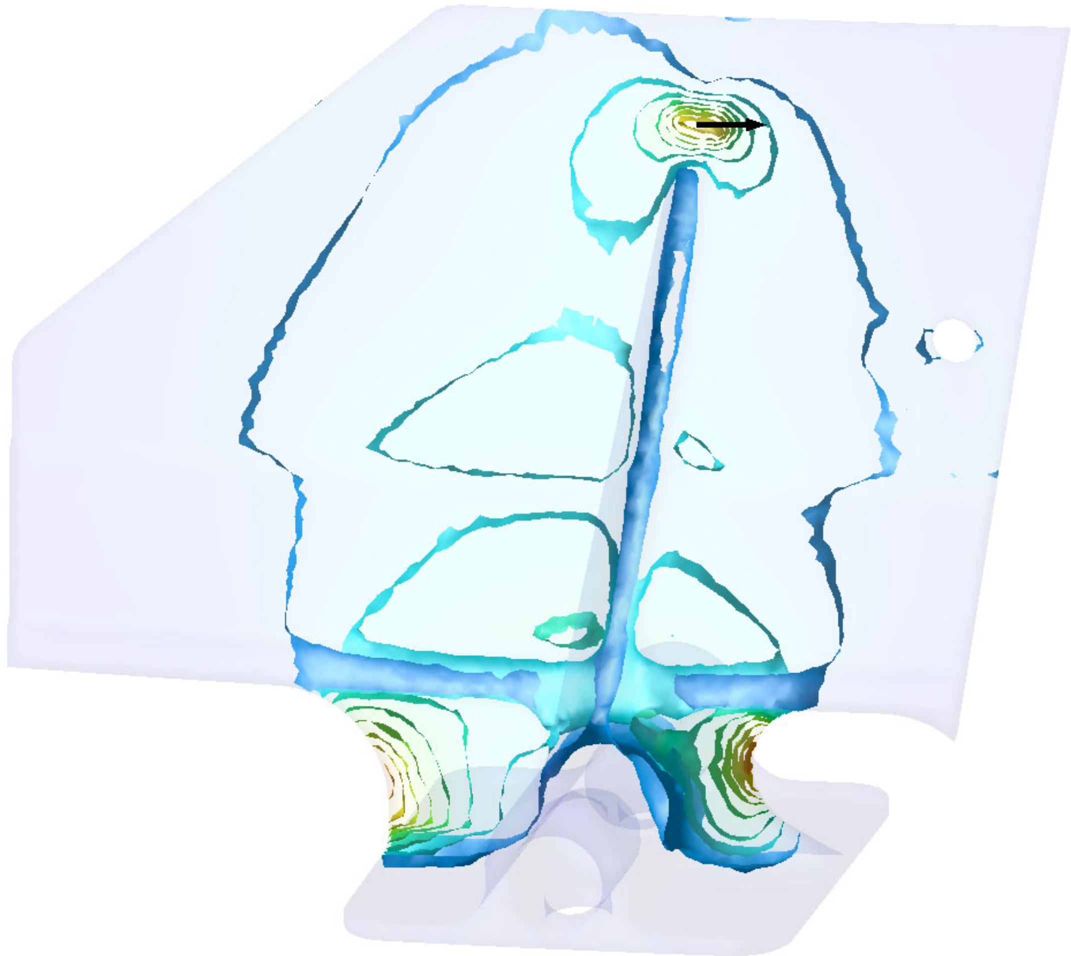


Figure: von Mises stress contours in a hoist£tting.

Extrapolation

Error estimate: From the error estimate using a discrete dual solution Φ

$$e_{est} = l(\Phi) - a(u_h, \Phi)$$

we get a value with sign !

Extrapolation: we have

$$\boxed{m_{extra} = m(u_h) + e_{est}}$$

If the estimate of the error is sharp we get an improved value.

Extrapolation

Let V_1 and V_2 be two finite element spaces.
Discrete dual problem: find $\phi_2 \in V_2$ such that

$$m(v) = a(v, \phi_2) \quad \text{all } v \in V_2.$$

Assume that $V_1 \subset V_2$, e.g. V_2 is an h- or p-refinement of V_1, then

$$\boxed{m(u_2) = m(u_1) + l(\phi_2) - a(u_1, \phi_2)}$$

where u_1 and u_2 are the solutions of the primal £nite element problem using the spaces V_1 and V_2, respectively.

Extrapolation

If nested spaces are used, then the functional could be computed by either

- Solving the coarse primal problem and fine dual problem and using the error representation formula.

$$\boxed{m(u_2) = m(u_1) + l(\phi_2) - a(u_1, \phi_2)}$$

or

- Solving the fine primal problem and evaluating the functional.

Solving PDEs on Networks

Computation of several functionals can be done in parallel:

- Each computer is assigned the computation of one functional.
- Each computer solves a dual problem and calculates on its own adapted grid and finally delivers only the value of the functional.
- Approximate solutions where each computer calculates an approximation to the solution in a subdomain using its own grid.

Paper: Estep-Holst-Larson: *Generalized Green's Functions and the Effective Domain of In¤uence*

Parallel: Examples

$$\begin{cases} -\frac{1}{\pi^2}\Delta u = 2 + 4e^{-5((x-.5)^2+(y-2.5)^2)}, & (x,y) \in \Omega, \\ u(x,y) = 0, & (x,y) \in \partial\Omega, \end{cases}$$

where Ω is the “square annulus” $\Omega = [0,3] \times [0,3] \setminus [1,2] \times [1,2]$.

One computer: initial and final mesh

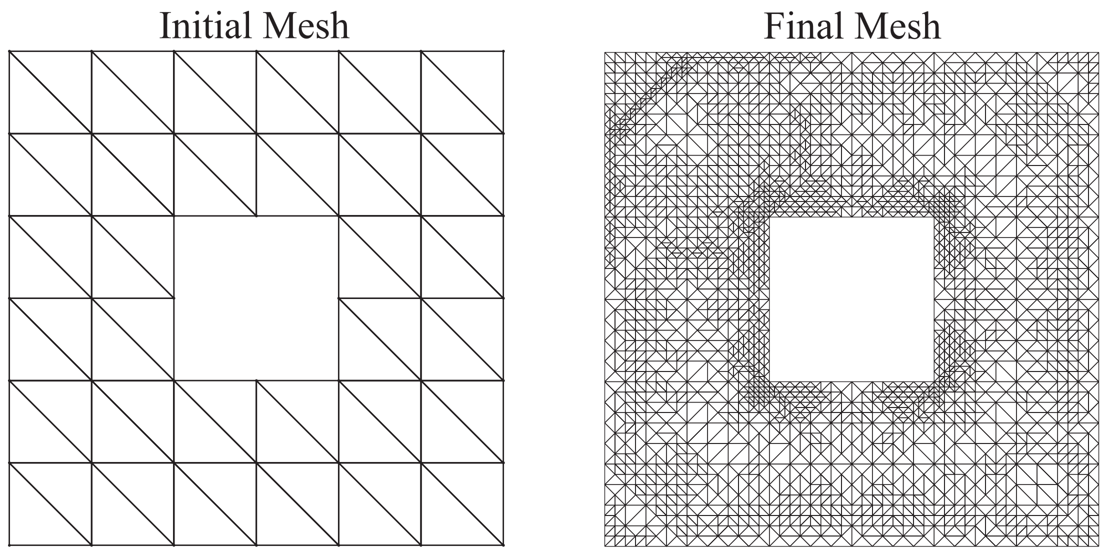
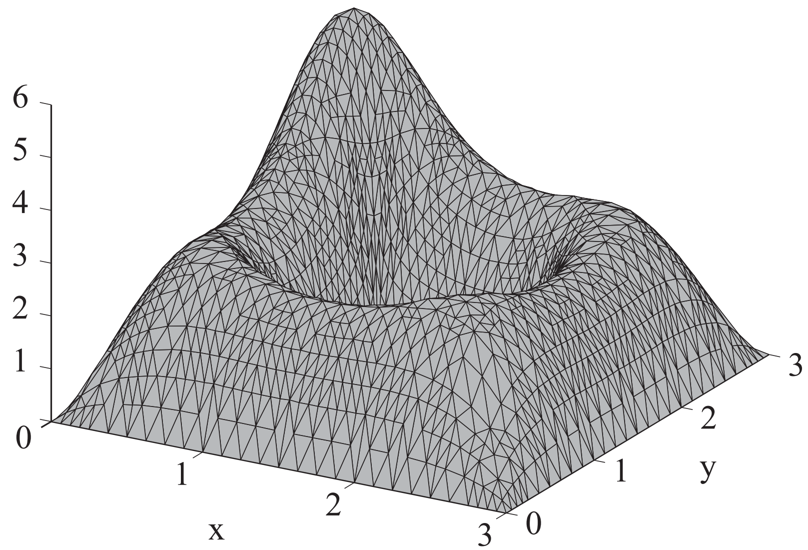


Figure 5: Plots of the initial (left) and £nal (right) meshes with data ψ giving the average error.

One computer: solution



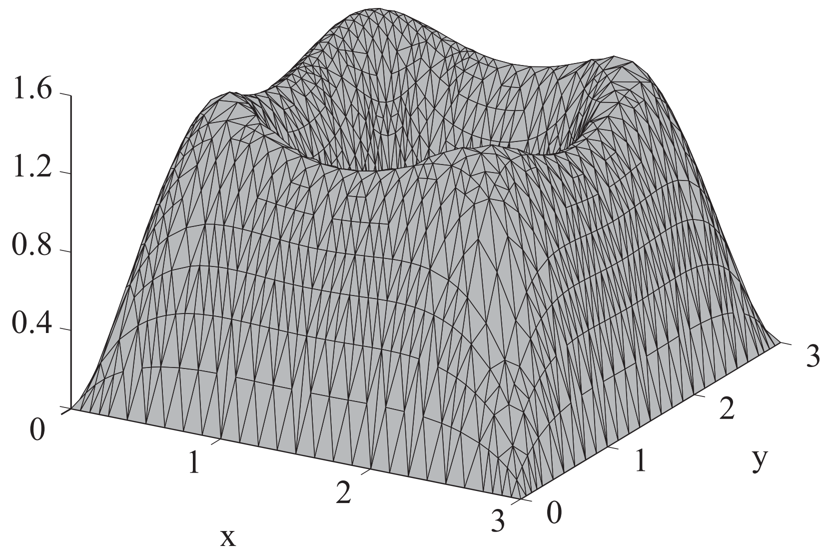


Figure 6: Plots of the £nal solution (left) and dual solution (right) with data ψ giving the average error.

Several computers: decomposition

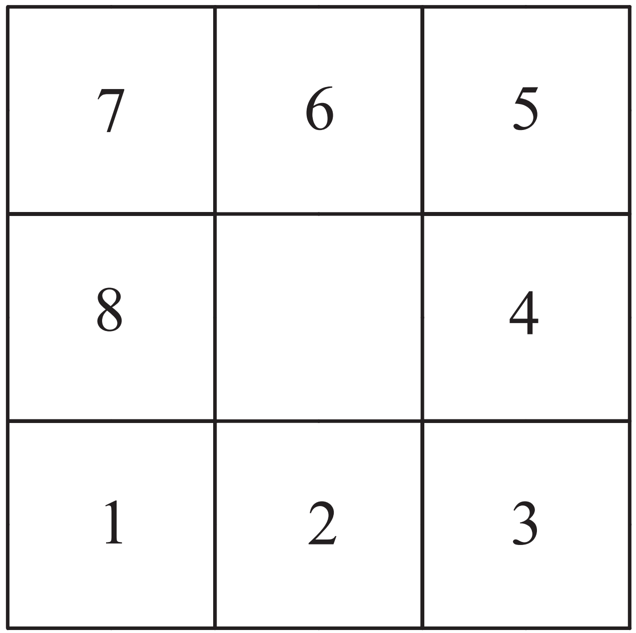
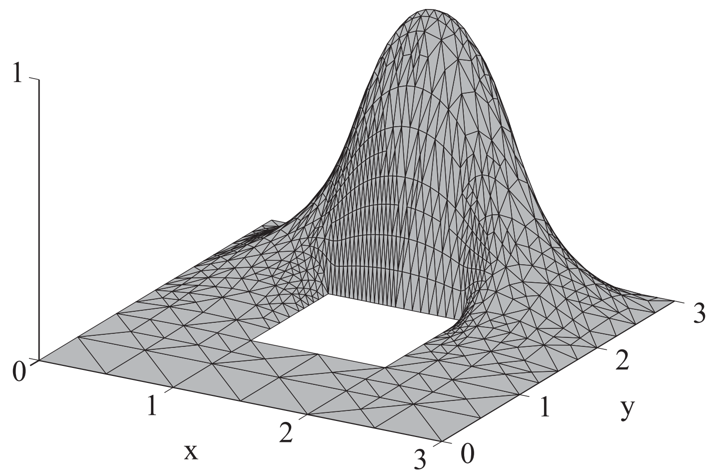


Figure 7: Domains for the partition of unity.

Several computers: dual solutions



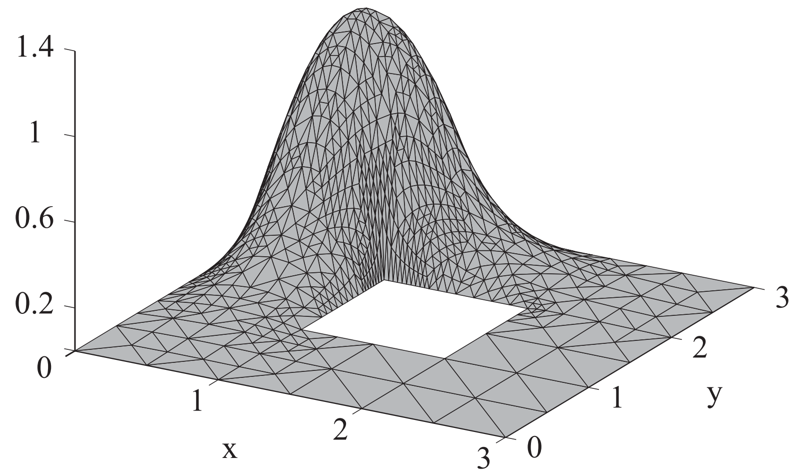


Figure 8: Plots of the dual solutions corresponding to ψ_6 (left) and ψ_7 (right) for the partition of unity decomposition.

Several computers: final meshes

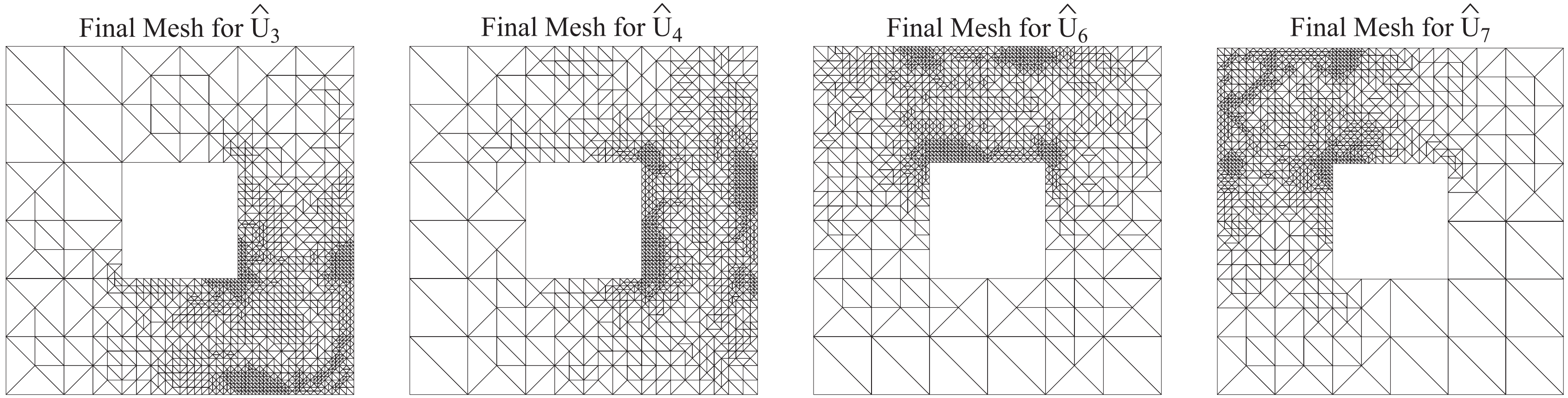


Figure 9: Plots of the final meshes for the localized solutions $\hat{U}_3$, $\hat{U}_4$, $\hat{U}_6$, and $\hat{U}_7$.