EXACT BOUNDS FOR LINEAR OUTPUTS OF THE CONVECTION-DIFFUSION-REACTION EQUATION USING FLUX-FREE ERROR ESTIMATORS

N. PARES, Y. VIDAL, P. DIEZ and A. HUERTA

- Laboratori de Càlcul Numèric (LaCàN)
- Universitat Politècnica de Catalunya (Spain)
  http://www-lacan.upc.es

LABORATORI DE CÀLCUL NUMÈRIC UNIVERSITAT POLITÈCNICA DE CATALUNYA

Motivation: assessing the error in QoI

- Numerical modeling (FEA) is currently a basic tool for engineering design
- In practice, the FE users seek values of some Quantities of Interest (QoI): local displacements or stresses, average fluxes…
- Numerical modeling must provide to the designer reliable approximations for these QoI
- Ideally, the answer of the numerical model is a narrow interval where this QoI lies…

without a shadow of a doubt!

→ **certified range for the QoI**

- Goal:
  - produce certified bounds (upper and lower)
  - adapt the mesh to reduce the interval

Outline of the presentation

- Basics on output oriented error estimation in Finite Elements
  - **Asymptotic versus guaranteed error bounds**
    - Asymptotic error estimates
    - Guaranteed error estimates (complementary energy approach)
  - **Domain decomposition strategy**
    - Hybrid-flux estimates
    - Flux-free error estimators
- Guaranteed bounds using flux-free error estimators
- Extension to stabilized finite element approximations
- Numerical examples

Generalities on Error assessment

Three conceptual steps to find bounds for the error in a QoI

1. Assessing the QoI in terms of energy: **error representation** using an adjoint problem (extractor)
   - Bounds of energy → bounds of QoI
2. Solving error equation piecewise: **Domain decomposition**
   - hybrid fluxes → one local problem per element
   - flux-free → one local problem per vertex node
3. **Local solver**
   - asymptotic → solving with a finer discretization
   - guaranteed → solving with a dual approach

Model problem

- Convection-diffusion-reaction equation:

$$-\nu \boldsymbol{\nabla}^2 u + \boldsymbol{\alpha} \cdot \boldsymbol{\nabla} u + \sigma u = f \quad \text{in } \Omega$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\alpha} = 0 \qquad\qquad u = 0 \quad \text{on } \partial\Omega$$

- Weak form: find $u \in \mathcal{H}_0^1(\Omega)$ such that $\forall v \in \mathcal{H}_0^1(\Omega)$

$$\int_\Omega \left[\nu \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v + \sigma u v + (\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} u) v \right] \mathrm{d}\Omega = \int_\Omega v f \, \mathrm{d}\Omega$$

- GOAL: bound the output

ex.: $\ell^{\mathcal{O}}(u) := \int_\Omega f^{\mathcal{O}} u \, \mathrm{d}\Omega + \int_{\Gamma_\mathrm{N}} g^{\mathcal{O}} u \, \mathrm{d}\Gamma$

Model problem

- Convection-diffusion-reaction equation:

$$-\nu \boldsymbol{\nabla}^2 u + \boldsymbol{\alpha} \cdot \boldsymbol{\nabla} u + \sigma u = f \quad \text{in } \Omega$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\alpha} = 0 \qquad u = 0 \quad \text{on } \partial\Omega$$

- Weak form: find $u \in \mathcal{H}_0^1(\Omega)$ such that $\forall v \in \mathcal{H}_0^1(\Omega)$

$$a(u, v) = l(v)$$

- GOAL: bound the output

ex.: $\ell^{\mathcal{O}}(u) := \int_{\Omega} f^{\mathcal{O}} u \, \mathrm{d}\Omega + \int_{\Gamma_{\mathrm{N}}} g^{\mathcal{O}} u \, \mathrm{d}\Gamma$

Estimating bounds of functional outputs

- Finite element approximation: $u^H \in \mathcal{V}^H \subset \mathcal{H}_0^1(\Omega)$

$$a(u^H, v) = l(v) \quad \forall v \in \mathcal{V}^H$$

- Estimate of the output: $\ell^{\mathcal{O}}(u^H)$

- GOAL: bound the error in the QoI $\ell^{\mathcal{O}}(u) - \ell^{\mathcal{O}}(u^H) = \ell^{\mathcal{O}}(e)$

$$e = u - u^H$$

$$s^- \leq s := \ell^{\mathcal{O}}(e) \leq s^+$$

$$\ell^{\mathcal{O}}(u^H) + s^- \leq \ell^{\mathcal{O}}(u) \leq \ell^{\mathcal{O}}(u^H) + s^+$$

Estimating bounds of functional outputs

ADJOINT PROBLEM:

- Adjoint infinite dimensional problem: [Babuska & Miller IJNME 1982]
  find $\psi \in \mathcal{H}_0^1(\Omega)$

$$a(v,\psi) = \ell^{\mathcal{O}}(v) \quad \forall v \in \mathcal{H}_0^1(\Omega)$$

- Finite dimensional approximation: find $\psi^H \in \mathcal{V}^H$

$$a(v,\psi^H) = \ell^{\mathcal{O}}(v) \quad \forall v \in \mathcal{V}^H$$

- Error of adjoint problem: $\varepsilon = \psi - \psi^H \in \mathcal{H}_0^1(\Omega)$

SYMMETRIZATION:

$$a^{\mathrm{s}}(w,v) = \int_\Omega \Big(\nu \boldsymbol{\nabla} w \cdot \boldsymbol{\nabla} v + \sigma w v \Big) d\Omega$$

Error representation: from QoI to energy

- For NON-SYMMETRIC FORMS [Paraschivoiu, Peraire & Patera, CMAME97]

- SYMMETRIZED ERROR EQUATIONS:

$$a^{\mathrm{s}}(e^{\mathrm{s}}, v) = l(v) - a(u^H, v) \quad \forall v \in \mathcal{H}_0^1(\Omega)$$
$$a^{\mathrm{s}}(v, \varepsilon^{\mathrm{s}}) = \ell^{\mathcal{O}}(v) - a(v, \psi^H) \quad \forall v \in \mathcal{H}_0^1(\Omega)$$

REMARK:

- e^{s} and ε^{s} are found solving diffusion-reaction problems

- BOUNDS:

$$-\frac{1}{4}\|\kappa e^{\mathrm{s}} - \frac{1}{\kappa}\varepsilon^{\mathrm{s}}\|_{\mathrm{UB}} \leq s \leq \frac{1}{4}\|\kappa e^{\mathrm{s}} + \frac{1}{\kappa}\varepsilon^{\mathrm{s}}\|_{\mathrm{UB}} \qquad \kappa \in \mathbb{R}$$

LABORATORI DE CÀLCUL NUMÈRIC UNIVERSITAT POLITÈCNICA DE CATALUNYA

- GOAL: compute upper bounds for the energy norm for diffusion-reaction problems

- For simplicity, the computation of upper bounds for $\|e^{\mathrm{s}}\|$ is presented.

Applying the same strategy to $\kappa e^{\mathrm{s}} \pm \frac{1}{\kappa}\varepsilon^{\mathrm{s}}$ yields the desired bounds for the output.

Asymptotic vs guaranteed implicit error bounds for diffusion (no reaction term)

- Equation of the primal symmetrized error

$$a^{\mathrm{s}}(e^{\mathrm{s}}, v) = l(v) - a(u^H, v) =: R^{\mathrm{P}}(v) \quad \forall v \in \mathcal{H}_0^1(\Omega)$$

- Obtain the norm $\|e^{\mathrm{s}}\|$ from the Primal formulation:

$$\|e^{\mathrm{s}}\|^2 = \max_{v \in \mathcal{H}_0^1(\Omega)} R^{\mathrm{P}}(v) - \frac{1}{2} a^{\mathrm{s}}(v, v) \geq \underbrace{\max_{v \in \mathcal{V}^h} R^{\mathrm{P}}(v) - \frac{1}{2} a^{\mathrm{s}}(v, v)}$$

The maximization problem induces

$$a^{\mathrm{s}}(e^{\mathrm{s},h}, v) = \ell(v) - a(u^H, v) \quad \forall v \in \mathcal{V}^h$$

$$\|e^{\mathrm{s}}\|^2 \geq \|e^{\mathrm{s},h}\|^2$$

A finite-dimensional problem induces a **lower bound** !

Guaranteed error bounds for diffusion (no reaction term)

Complementary energy allows to overestimate $\|e^{\mathrm{s}}\|$, approach introduced by Fraeijs de Veubeke in 1964.

$$\int_\Omega \nu \underbrace{\nabla e^{\mathrm{s}}}_{\boldsymbol{q}} \cdot \nabla v \, d\Omega = R^{\mathrm{P}}(v) \quad \Longleftarrow \quad \underbrace{\int_\Omega \nu \boldsymbol{q} \cdot \nabla v \, d\Omega}_{\bar{a}^{\mathrm{s}}(\boldsymbol{q}, \nabla v)} = R^{\mathrm{P}}(v)$$

- Dual formulation:

complementary energy $\bar{a}^{\mathrm{s}}(\boldsymbol{q}, \boldsymbol{p}) = \int_\Omega \nu \boldsymbol{q} \cdot \boldsymbol{p} \, \mathrm{d}\Omega$

$$\|e^{\mathrm{s}}\|^2 = \bar{a}^{\mathrm{s}}(\boldsymbol{p}, \boldsymbol{p}) = \min_{\bar{a}^{\mathrm{s}}(\boldsymbol{q}, \nabla v) = R^{\mathrm{P}}(v) \quad \forall v \in \mathcal{H}_0^1(\Omega)} \bar{a}^{\mathrm{s}}(\boldsymbol{q}, \boldsymbol{q})$$

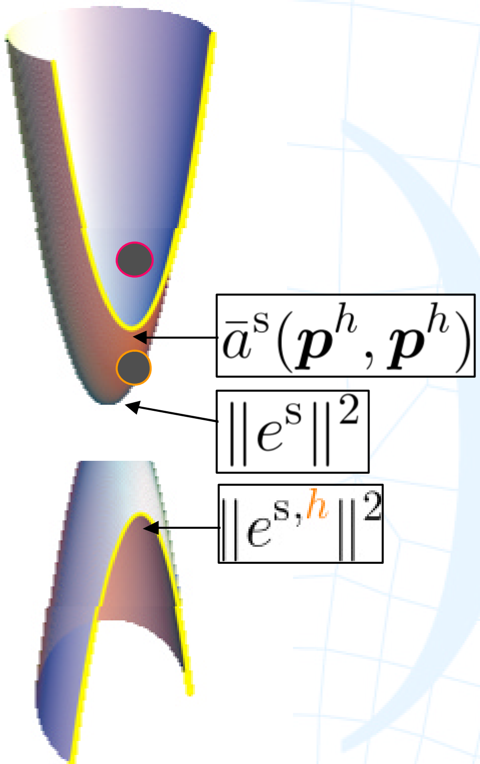
$$\leq \bar{a}^{\mathrm{s}}(\boldsymbol{q}, \boldsymbol{q}) \;\; \forall \boldsymbol{q} \text{ s.t. } \bar{a}^{\mathrm{s}}(\boldsymbol{q}, \nabla v) = R^{\mathrm{P}}(v)$$

Asymptotic vs guaranteed error bounds summary

- Asymptotic:

$$a^{\mathrm{s}}(e^{\mathrm{s},h}, v) = \ell(v) - a(u^H, v) \quad \forall v \in \mathcal{V}^h$$

$$\|e^{\mathrm{s}}\|^2 \geq \|e^{\mathrm{s},h}\|^2$$



- Guaranteed:

$$\bar{a}^{\mathrm{s}}(\boldsymbol{p}^h, \boldsymbol{\nabla} v) = \ell(v) - a(u^H, v) \quad \forall v \in \mathcal{H}^1_0(\Omega)$$

$$\bar{a}^{\mathrm{s}}(\boldsymbol{p}^h, \boldsymbol{p}^h) \geq \|e^{\mathrm{s}}\|^2$$

Global problems ➡ **domain decomposition** !

the domain decomposition technique introduces overestimation

Subdomain flux-free guaranteed error estimates

- Guaranteed subdomain flux-free error estimates:
  - Objective: decompose the global problem

$$\bar{a}^{\mathrm{s}}(\boldsymbol{p}^h, \boldsymbol{\nabla} v) = R^P(v) \qquad \forall v \in \mathcal{H}^1_0(\Omega)$$

    into local computations

  - Main idea: use a partition of unity defined by vertex nodes.

    That is, given $\{\phi^i\}_{i=1\ldots\mathrm{n_{np}}}$ such that $\sum_{i=1}^{\mathrm{n_{np}}} \phi^i = 1$

    Introduce in the residual $R^P(\cdot)$,

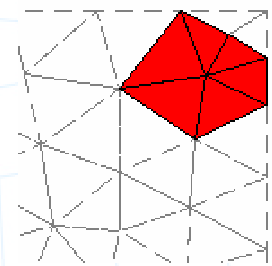
$$R^P(v) = R^P\Big(\sum_{i=1}^{\mathrm{n_{np}}} \phi^i v\Big) = \sum_{i=1}^{\mathrm{n_{np}}} R^P(\phi^i v)$$

Subdomain flux-free guaranteed error estimates

✓ Define n_{np} global problems: min. complementary energy s.t.

$$\forall v \in \mathcal{H}^1_0(\Omega) \;\; \bar{a}^{\mathrm{s}}(\boldsymbol{p}_i, \boldsymbol{\nabla} v) = R^{\mathrm{P}}(\phi^i v)\,, \quad \text{then } \boldsymbol{\nabla} e^{\mathrm{s}} = \boldsymbol{p} = \sum_{i=1}^{n_{\mathrm{np}}} \boldsymbol{p}_i.$$

✓ **LOCALIZATION:** Restrict the problems to a star



$$\int_\Omega \longrightarrow \int_{\omega^i}$$

Thus, impose $\bar{a}^{\mathrm{s}}_{w^i}(\tilde{\boldsymbol{p}}_i, v) = R^{\mathrm{P}}(\phi^i v)$

Then: $\tilde{\boldsymbol{p}}_i \approx \boldsymbol{p}_i$ and $\tilde{\boldsymbol{p}} := \sum_{i=1}^{n_{\mathrm{np}}} \tilde{\boldsymbol{p}}_i \approx \boldsymbol{p} = \boldsymbol{\nabla} e^{\mathrm{s}}$

and6 $\bar{a}^{\mathrm{s}}(\tilde{\boldsymbol{p}}, \tilde{\boldsymbol{p}}) \geq \|e^{\mathrm{s}}\|^2$

extension of [Pares, Diez, Huerta CMAME 06]

EXTENSION TO STABILIZED FE METHODS

- STABILIZED SUPG FE APPROXIMATION:

$$a(u^H, v) + \boxed{\sum_{k=1}^{n_{\rm el}} \int_{\Omega_k} \tau_k^P \mathcal{R}^P(u^H) \boldsymbol{\alpha} \cdot \boldsymbol{\nabla} v \, d\Omega} = \ell(v) \quad \forall v \in \mathcal{V}^H$$

stabilization term

- MAIN DIFFICULTY: the Galerkin orthogonality does not hold

$$R^{\rm P}(v) = l(v) - a(u^H, v) \text{ is not necessarily zero } \forall v \in \mathcal{V}^H$$

- New terms in the error representation

$$\boxed{R^P(\psi^H)} - \frac{1}{4}\|\kappa e^s - \frac{1}{\kappa}\varepsilon^s\|^2_{ub} \leq s \leq \boxed{R^P(\psi^H)} + \frac{1}{4}\|\kappa e^s + \frac{1}{\kappa}\varepsilon^s\|^2_{ub}$$

- New term in the local equations

$$\bar{a}^{\mathrm{s}}_{w^i}(\tilde{\boldsymbol{p}}_i, v) = R^{\mathrm{P}}(\phi^i v) + \boxed{\sum_{k=1}^{n_{\mathrm{el}}} \int_{\Omega_k} \tau_k^P \mathcal{R}^P(u^H)\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} \phi^i \, v \, d\Omega}$$

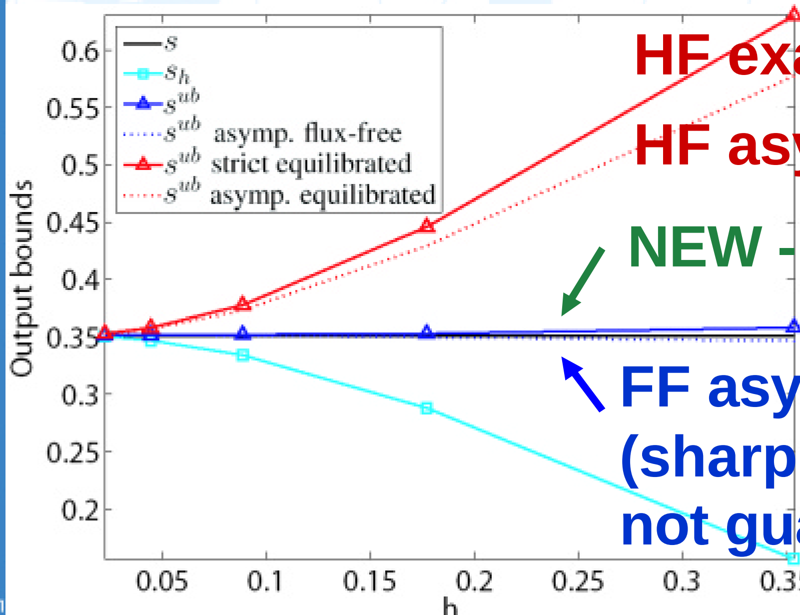
ensures solvability
while retaining upper bound property

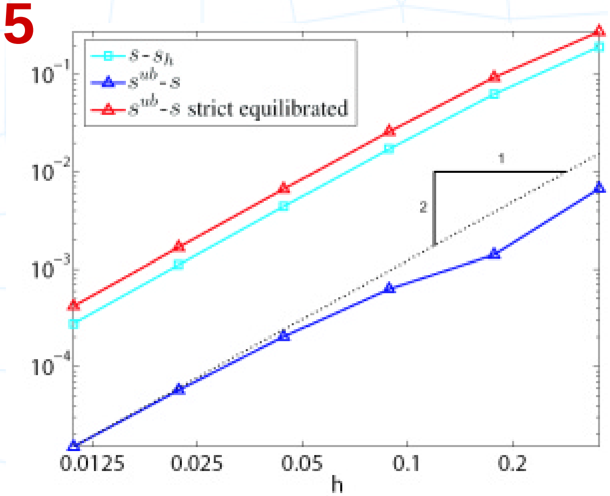
POISSON EQUATION

$-\Delta u = f \quad \text{in } [0,1]^2$ with homogeneous Dirichlet BC

$$f = \sqrt{10}$$

$$\ell^{\mathcal{O}}(u) = \int_\Omega \sqrt{10}\, u(x,y)\, \mathrm{d}\Omega = \|u\|^2$$





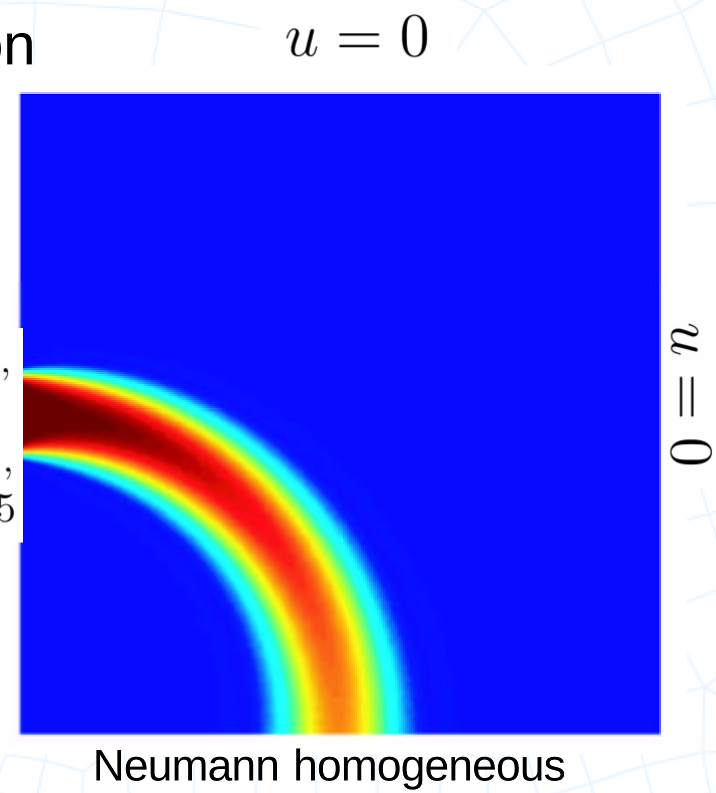
Solution with inner layers

$$-\nu\nabla^2 u + \boldsymbol{\alpha}\cdot\nabla u = 0 \quad \text{in } \Omega$$
$$\boldsymbol{\alpha} = (y, -x)$$

Two different values for the diffusion parameter are considered

$$\nu = 10^{-2} \quad \nu = 10^{-3}$$

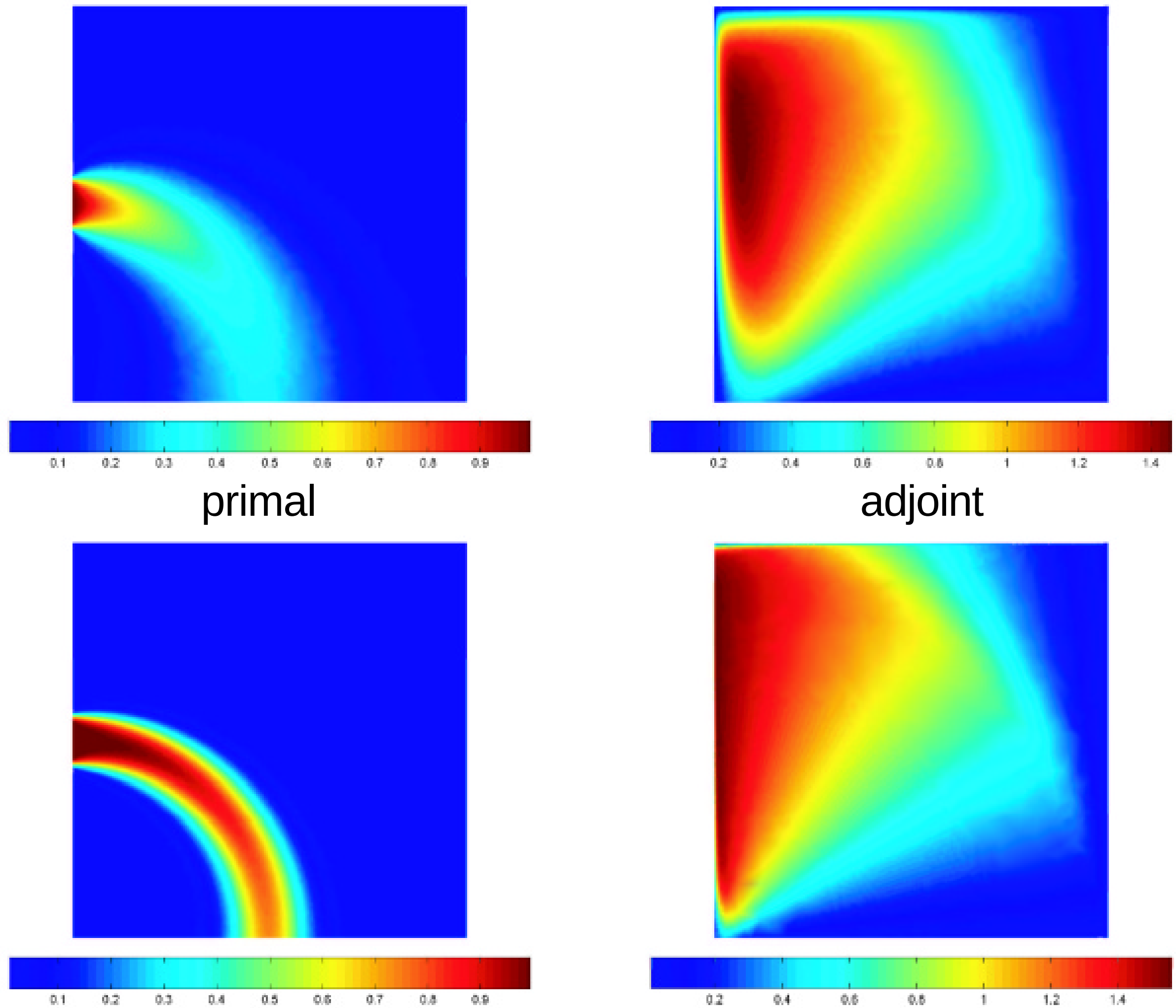
$$u(0,y) = \begin{cases} 0 & \text{for} \quad |y-0.5| > 0.075\,, \\ 1 & \text{for} \quad |y-0.5| < 0.05\,, \\ 40(y-0.425) & \text{for} \quad 0.425 \le y \le 0.45\,, \\ 40(0.575-y) & \text{for} \quad 0.455 \le y \le 0.575 \end{cases}$$



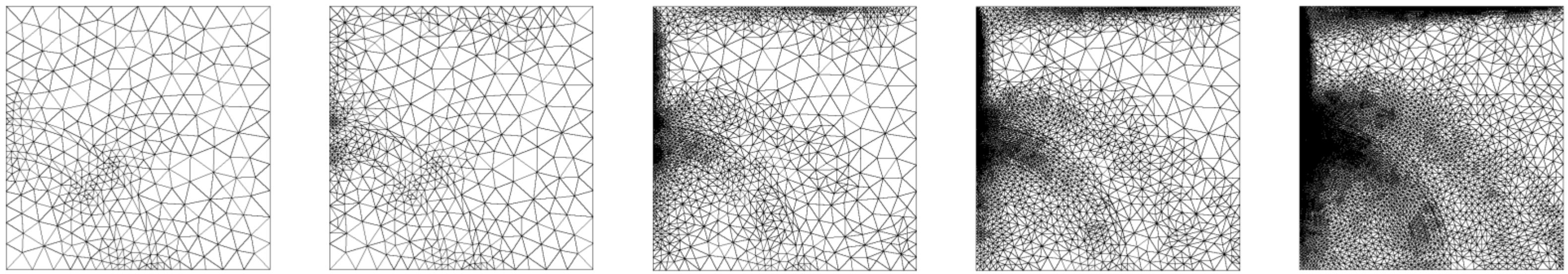
$$\ell^{\mathcal{O}}(u) = \int_\Omega u(x,y)\,\mathrm{d}\Omega$$

$\nu = 10^{-2}$

$\nu = 10^{-3}$



$\nu = 10^{-2}$

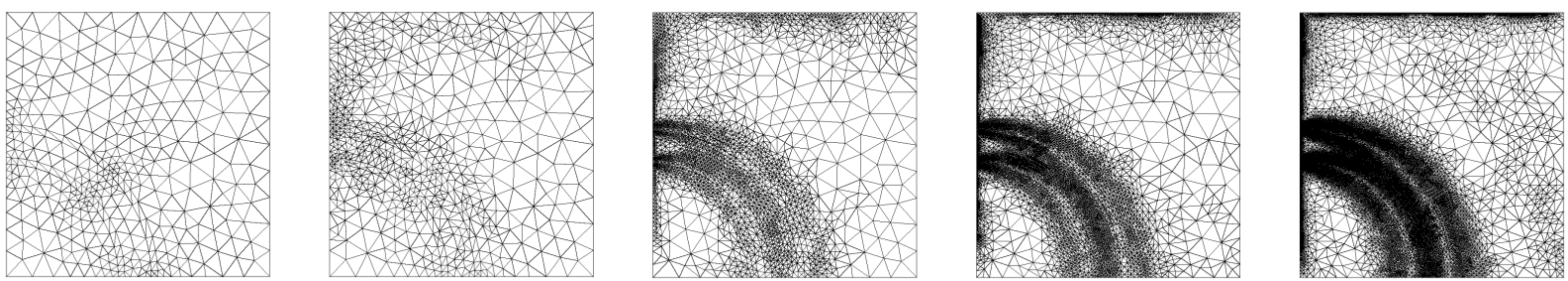


Final mesh
36285 elem.

Flux-free: $s = 0.097694 \pm 0.11\%$

Hybrid-flux bounds: $s = 0.097689 \pm 3.32\%$

$\nu = 10^{-3}$



Final mesh
37807 elem.

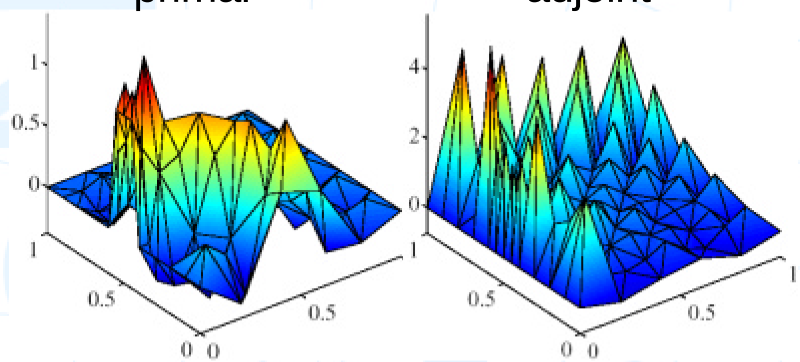
Flux-free: $s = 0.098175 \pm 0.38\%$

Hybrid-flux bounds: $s = 0.098182 \pm 8.11\%$

$\nu = 10^{-3}$

209 elements
119 nodes

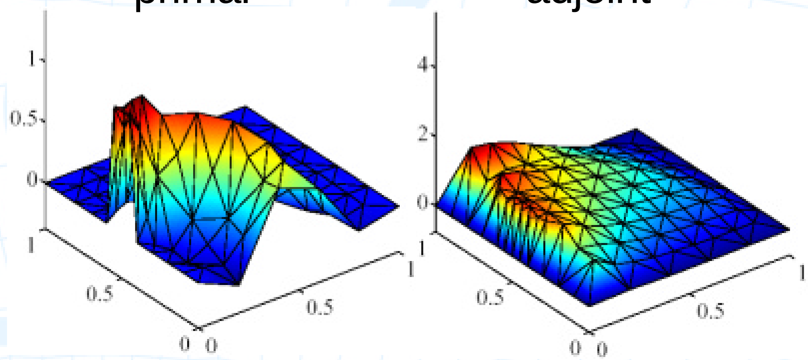
standard FE approximations



FF: $s = -0.5061 \pm 4.9568$

HF: $s = -0.8528 \pm 9.0653$

stabilized FE approximations



FF: $s = 0.1189 \pm 0.6605$

HF: $s = 0.1499 \pm 2.8003$

EXACT BOUNDS FOR LINEAR OUTPUTS OF THE CONVECTION-DIFFUSION-REACTION EQUATION USING FLUX-FREE ERROR ESTIMATORS

N. PARES, Y. VIDAL, P. DIEZ and A. HUERTA

- Laboratori de Càlcul Numèric (LaCàN)
- Universitat Politècnica de Catalunya (Spain)
  http://www-lacan.upc.es

Thank you for your attention