UNIVERSITAT POLITÈCNICA DE CATALUNYA

LABORATORI DE CÀLCUL NUMÈRIC

A new equilibrated residual method: improving accuracy and efficiency of flux-free error estimates

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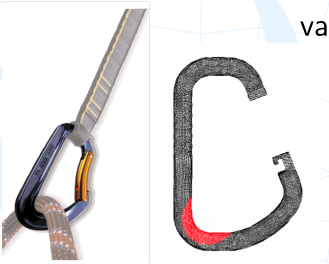
Certification of FE approximations

The finite element method is a basic tool in engineering design and since engineering decisions are based on approximations of the solution, it is crucial to certify the quality of the results.



GOAL: provide a guaranteed interval for the value of the QoI

$$\ell^{\mathcal{O}}(u) = \int_{\Gamma} \sigma_{VM}(u) d\Gamma$$

$$\boxed{\ell^{\mathcal{O}}(u) \in [L^-, L^+]}$$

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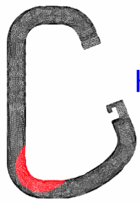

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HOW?

1. compute $\ell^{\mathcal{O}}(u_h)$
2. define $\ell^{\mathcal{O}}(e) = \ell^{\mathcal{O}}(u) - \ell^{\mathcal{O}}(u_h)$
3. bound $s^- \leq \ell^{\mathcal{O}}(e) \leq s^+$

$$\ell^{\mathcal{O}}(u) \in [\ell^{\mathcal{O}}(u_h) + s^-, \ell^{\mathcal{O}}(u_h) + s^+]$$

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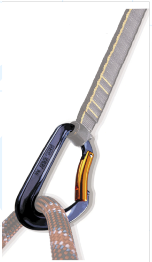

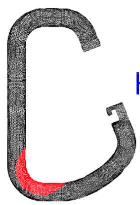

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We need a posteriori GUARANTEED/STRICT error bounds. They also have to be ACCURATE and CHEAP

Guaranteed, accurate and efficient bounds

CERTIFICATION

complementary energy	+	implicit error estimators
dual formulation for the error		involving only local problems

Guaranteed, accurate and efficient bounds

CERTIFICATION

complementary energy — dual formulation for the error

+

implicit error estimators — involving only local problems

Hybrid-flux estimators
equilibrated

CHEAPER

Flux-free estimators
stars/subdomain [PDH2006]

MORE ACCURATE

Guaranteed, accurate and efficient bounds

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CHEAPER

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MORE ACCURATE

CHEAP + ACCURATE

EXPLICIT Flux-free estimator

Model problem

Reaction-diffusion equation:

$$\begin{aligned} -\Delta u + \kappa^2 u &= f && \text{in } \Omega, \\ u &= u_{\mathrm{D}} && \text{on } \Gamma_{\mathrm{D}}, \\ \boldsymbol{\nabla} u \cdot \boldsymbol{n} &= g_{\mathrm{N}} && \text{on } \Gamma_{\mathrm{N}}. \end{aligned}$$

Weak form: find $u \in \mathcal{U}$ such that

$$\underbrace{\int_\Omega \left(\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v + \kappa^2 uv\right)\, d\Omega}_{a(u,v)} = \underbrace{\int_\Omega fv\, d\Omega + \int_{\Gamma_{\mathrm{N}}} g_{\mathrm{N}} v\, d\Gamma}_{\ell(v)} \quad \forall v \in \mathcal{V}.$$

Finite element approximation: find $u_h \in \mathcal{U}^h$ such that

$$a(u_h, v) = \ell(v) \qquad \text{for all } v \in \mathcal{V}^h.$$

triangular mesh + linear elements

Error equations: find $e = u - u_h \in \mathcal{V}$ such that

$$a(e, v) = \ell(v) - a(u_h, v) = R(v) \qquad \text{for all } v \in \mathcal{V}.$$

Guaranteed error bounds

The complementary energy approach allows to overestimate $|||e|||$
approach introduced by Fraeijs de Veubeke in 1964

$$a(e,v) = \int_\Omega \left(\boldsymbol{\nabla} e \cdot \boldsymbol{\nabla} v + \kappa^2 e v\right) d\Omega = R(v) \qquad \text{for all } v \in \mathcal{V}$$

$$\int_\Omega \left(\ \boldsymbol{q} \cdot \boldsymbol{\nabla} v + \kappa^2 r v\right) d\Omega = R(v) \qquad \text{for all } v \in \mathcal{V}$$

new error unknowns

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Dual formulation:

Any pair of dual estimates $(\boldsymbol{q}, r)$ such that

$$\int_\Omega \left(\boldsymbol{q} \cdot \nabla v + \kappa^2 r v\right) d\Omega = R(v) \qquad \text{for all } v \in \mathcal{V}$$

provide an upper bound for the energy norm of the error

$$|||e|||^2 = \int_\Omega \left(\nabla e \cdot \nabla e + \kappa^2 e^2\right) d\Omega \leq \int_\Omega \left(\boldsymbol{q} \cdot \boldsymbol{q} + \kappa^2 r^2\right) d\Omega$$

complementary energy

Guaranteed error bounds

Global problem: find $\boldsymbol{q}$ and r

s.t. $\displaystyle\int_\Omega \left(\boldsymbol{q}\cdot\boldsymbol{\nabla} v + \kappa^2 r v\right) d\Omega = R(v)$ TOO EXPENSIVE

minimizing the upper bound $\displaystyle\int_\Omega \left(\boldsymbol{q}\cdot\boldsymbol{q} + \kappa^2 r^2\right) d\Omega$

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⇩

SPLIT THE GLOBAL PROBLEM INTO LOCAL PROBLEMS

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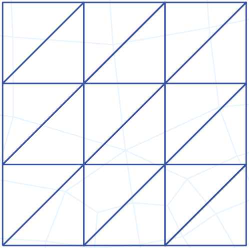
SPLIT THE GLOBAL PROBLEM INTO LOCAL PROBLEMS

Hybrid-flux estimators

Flux-free estimators

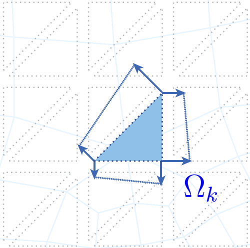
Guaranteed error bounds



Global problem

$$\int_{\Omega} \left(\boldsymbol{q} \cdot \boldsymbol{\nabla} v + \kappa^2 r v \right) d\Omega = R(v)$$

Guaranteed error bounds



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Hybrid-flux →

$$\int_{\Omega_k} \left(\boldsymbol{q}_k \cdot \boldsymbol{\nabla} v + \kappa^2 r_k v\right) d\Omega = R_k(v) + \int_{\Omega_k} g_k v \, d\Gamma$$

single element

$$\boldsymbol{q}|_{\Omega_k} = \boldsymbol{q}_k \quad , \quad r|_{\Omega_k} = r_k$$

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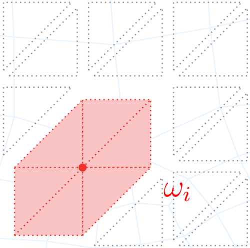

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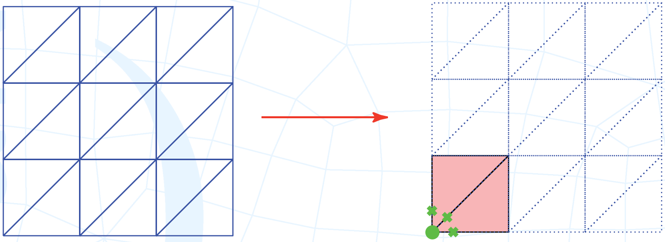
Flux-free →

$$\int_{\omega_i} \left(\boldsymbol{q}^i \cdot \boldsymbol{\nabla} v + \kappa^2 r^i v\right) d\Omega = R(\phi_i v)$$

patch of elements $\quad \boldsymbol{q} = \sum_{i=1}^{n_{\mathrm{np}}} \boldsymbol{q}^i \quad , \quad r = \sum_{i=1}^{n_{\mathrm{np}}} r^i$

Hybrid-flux / equilibrated error estimates

STEP 1: loop in nodes to compute the equilibrated tractions g_k



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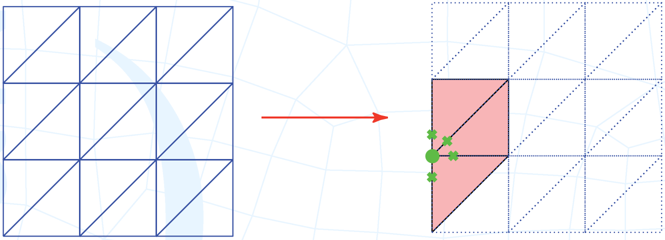

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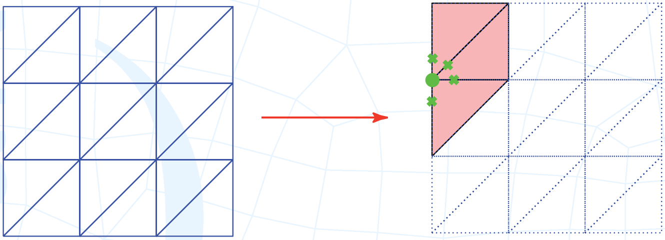

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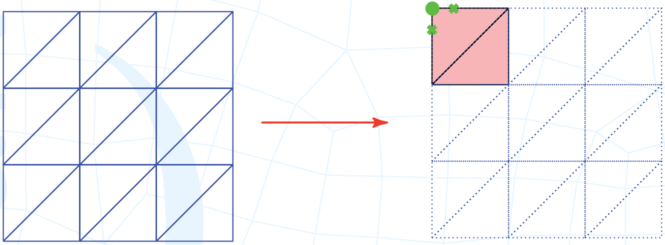

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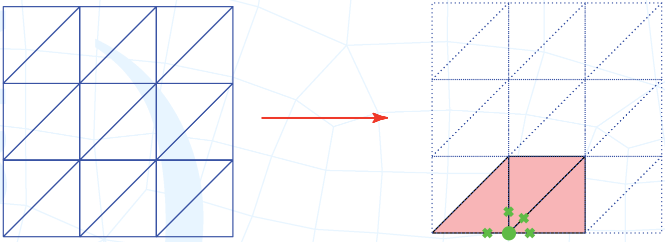

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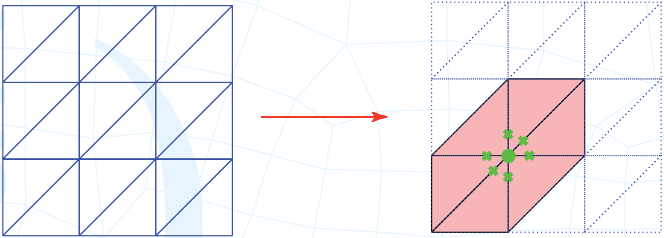

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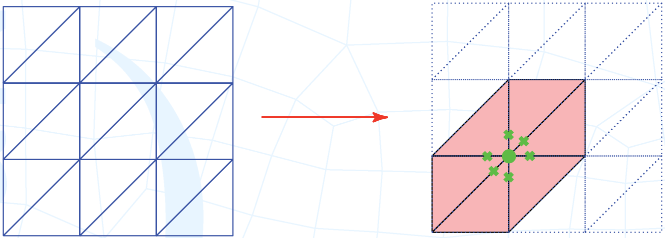
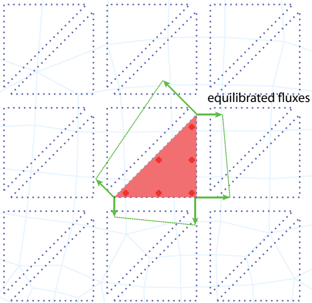


STEP 2: loop in elements to compute the dual fluxes

$$(\boldsymbol{q}_k, r_k)$$

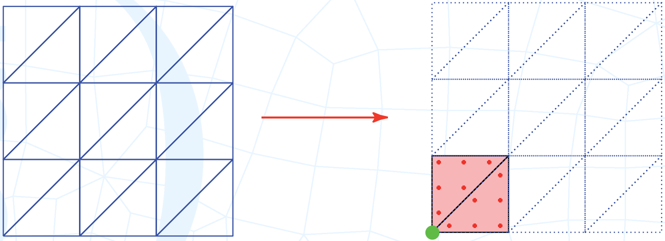
at each element Ω_k independently



Flux-free error estimates

STEP 1: loop in nodes to compute the dual fluxes in the stars

$$(\boldsymbol{q}^i, r^i) \quad \text{in} \quad \omega_i \quad \text{(patch of elements)}$$



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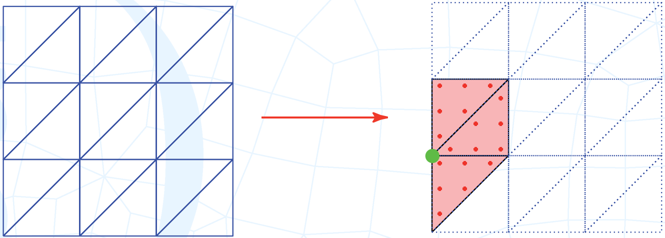

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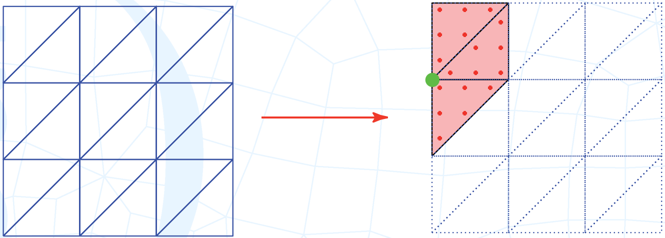

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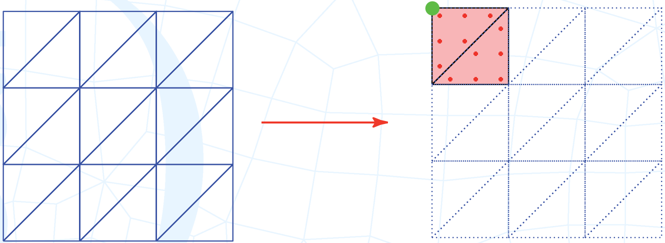

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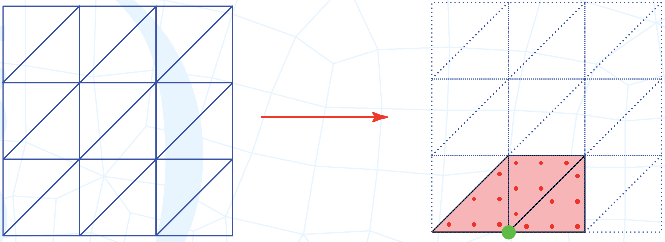

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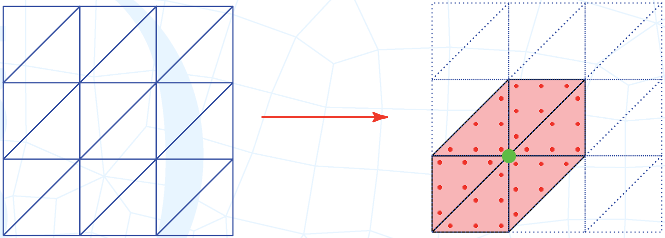

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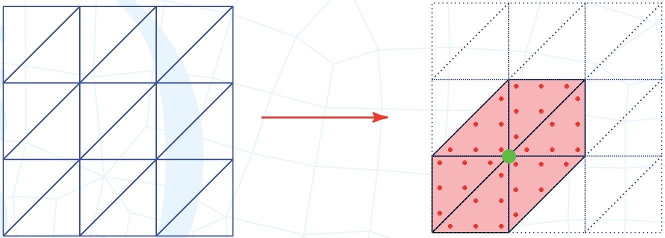
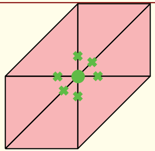
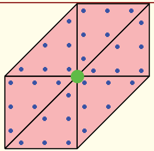
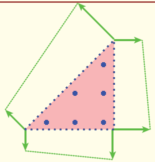


STEP 2: add all the local contributions and compute the norm

$$\boldsymbol{q} = \sum_{i=1}^{n_{\mathrm{np}}} \boldsymbol{q}^i \quad , \quad r = \sum_{i=1}^{n_{\mathrm{np}}} r^i$$

Computational cost overview

	Equilibrated	Flux-free
Loop on nodes	 DOF: one per edge of ω_i	 DOF: dof of $(\boldsymbol{q}_k^i, r_k^i)$ $\times$ elements of ω_i
Loop on elements	 DOF: dof of $(\boldsymbol{q}_k, r_k)$	

Computational cost overview

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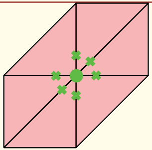
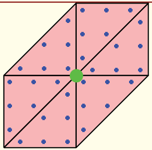
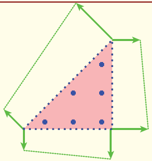
Loop on nodes	 DOF: one per edge of ω_i	 DOF: dof of $(\boldsymbol{q}_k^i, r_k^i)$ $\times$ elements of ω_i
Loop on elements	 DOF: dof of $(\boldsymbol{q}_k, r_k)$	higher cost better accuracy

Computational cost overview

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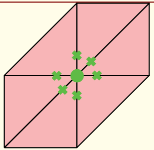
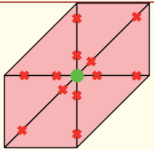
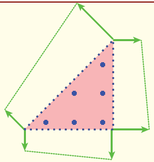
Loop on nodes	 DOF: one per edge of ω_i	 NEW!!! two per edge of ω_i
Loop on elements	 DOF: dof of $(\boldsymbol{q}_k, r_k)$	

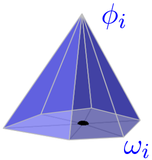
New guaranteed, accurate and cheap error estimate (EE)

Local problems: find $\boldsymbol{q}^i$ and r^i such that

$$\int_{\omega_i} \left(\boldsymbol{q}^i \cdot \boldsymbol{\nabla} v + \kappa^2 r^i v\right) d\Omega = R(\phi_i v) \quad \forall v \in \mathcal{V}(\omega_i)$$

minimizing the local complementary energy

$$\int_{\omega_i} \left(\boldsymbol{q}^i \cdot \boldsymbol{q}^i + \kappa^2 (r^i)^2\right) d\Omega$$



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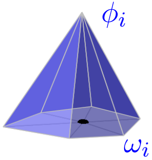

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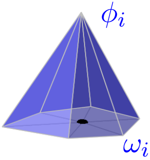
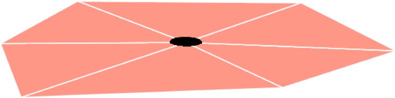


KEY POINT

Find a closed EXPLICIT solution for $\boldsymbol{q}^i$

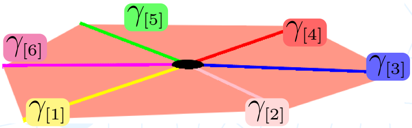
New guaranteed, accurate and cheap EE



From star ω_i to elements $\Omega_k \subset \omega_i$

$$\int_{\omega_i} \boldsymbol{q}^i \cdot \boldsymbol{\nabla} v d\Omega = R(\phi_i v)$$

New guaranteed, accurate and cheap EE



From star ω_i to elements $\Omega_k \subset \omega_i$

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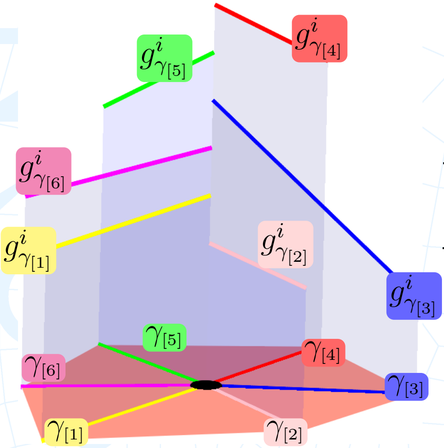
The explicit solution is found introducing the linear tractions on the edges of the star $\{g^i_{\gamma_{[m]}}\}$

New guaranteed, accurate and cheap EE



From star ω_i to elements $\Omega_k \subset \omega_i$

$$\int_{\omega_i} \boldsymbol{q}^i \cdot \boldsymbol{\nabla} v d\Omega = R(\phi_i v)$$

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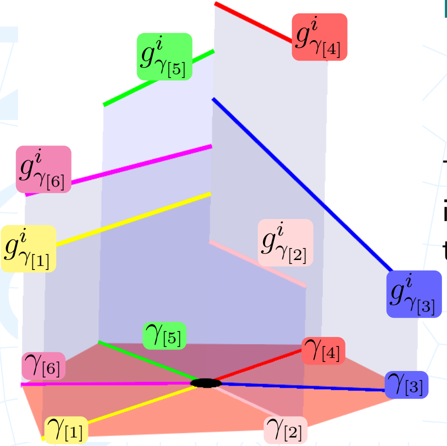

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The explicit solution is found introducing the linear tractions on the edges of the star $\{g^i_{\gamma_{[m]}}\}$

$$\Downarrow$$

for every $\Omega_k \subset \omega_i$

Neumann BC
$$(\boldsymbol{q}_k^i + \phi_i \boldsymbol{\nabla} u_h) \cdot \boldsymbol{n}_k^\gamma = \sigma_k^\gamma g_\gamma^i$$

Divergence
$$-\boldsymbol{\nabla} \cdot (\boldsymbol{q}_k^i + \phi_i \boldsymbol{\nabla} u_h) = \phi_i (f - \kappa^2 u_h) - \boldsymbol{\nabla} u_h \cdot \boldsymbol{\nabla} \phi_i$$

New guaranteed, accurate and cheap EE

Strong form of the elementary problems:

$$-\boldsymbol{\nabla}\cdot\left(\boldsymbol{q}_k^i+\phi_i\boldsymbol{\nabla}u_h\right)=\phi_i(\ f-\kappa^2u_h\ )-\boldsymbol{\nabla}u_h\cdot\boldsymbol{\nabla}\phi_i \quad \text{in } \Omega_k$$

$$\boldsymbol{q}_k^i\cdot\boldsymbol{n}_k^\gamma=\sigma_k^\gamma g_\gamma^i-\phi_i\boldsymbol{\nabla}u_h\cdot\boldsymbol{n}_k^\gamma:=\ \mathcal{R}_{|\gamma} \quad \text{on } \partial\Omega_k$$

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Explicit solution: $\boldsymbol{q}_k^i=\boldsymbol{q}_k^{iL}+\boldsymbol{q}_k^{iC}$ as long as

$$\int_{\Omega_k}\left[\phi_i\left(f-\kappa^2u_h\right)-\nabla u_h\cdot\nabla\phi_i\right]\ d\Omega+\sum_{\gamma\subset\partial\Omega_k}\int_\gamma\sigma_k^\gamma g_\gamma^i\ d\Gamma=0,$$

Details can be found in

N. Parés, P. Díez, *A new equilibrated residual method improving accuracy and efficiency of flux-free error estimates*, CMAME, Volume 313, Pages 785-816 (2017)

New guaranteed, accurate and cheap EE

Strong form of the elementary problems:

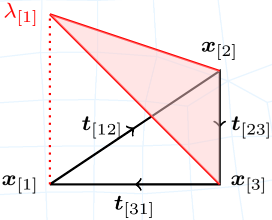
$$-\boldsymbol{\nabla}\cdot\left(\boldsymbol{q}_k^i+\phi_i\boldsymbol{\nabla}u_h\right)=\phi_i(\ f-\kappa^2u_h\ )-\boldsymbol{\nabla}u_h\cdot\boldsymbol{\nabla}\phi_i \quad \text{in } \Omega_k$$

$$\boldsymbol{q}_k^i\cdot\boldsymbol{n}_k^\gamma=\sigma_k^\gamma g_\gamma^i-\phi_i\boldsymbol{\nabla}u_h\cdot\boldsymbol{n}_k^\gamma:=\ \mathcal{R}_{|\gamma} \quad \text{on } \partial\Omega_k$$

Explicit solution of the elementary problems: $\boldsymbol{q}_k^i=\boldsymbol{q}_k^{iL}+\boldsymbol{q}_k^{iC}$

$$\boldsymbol{q}_k^{iL}=\frac{1}{2|\Omega_k|}\sum_{n=1}^{3}\sum_{\substack{m=1\\m\neq n}}\ell_{[m]}\ R|_{\gamma_{[m]}}(\boldsymbol{x}_{[n]})\ \boldsymbol{t}_{[mn]}\lambda_{[n]}$$

$$\boldsymbol{q}_k^{iC}=\frac{1}{3}\sum_{n=1}^{3}\sum_{\substack{m=2\\m>n}}^{3}\lambda_{[n]}\lambda_{[m]}\boldsymbol{t}_{[nm]}\boldsymbol{t}_{[nm]}^{\mathsf{T}}\quad\nabla v^Q$$



New guaranteed, accurate and cheap EE

Strong form of the elementary problems:

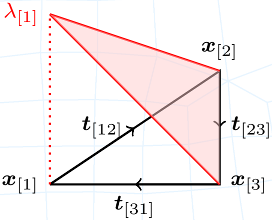
$$-\boldsymbol{\nabla}\cdot\left(\boldsymbol{q}_k^i+\phi_i\boldsymbol{\nabla}u_h\right)=\phi_i(\ f-\kappa^2u_h\ )-\boldsymbol{\nabla}u_h\cdot\boldsymbol{\nabla}\phi_i \quad \text{in } \Omega_k$$

$$\boldsymbol{q}_k^i\cdot\boldsymbol{n}_k^\gamma=\sigma_k^\gamma g_\gamma^i-\phi_i\boldsymbol{\nabla}u_h\cdot\boldsymbol{n}_k^\gamma:=\boxed{\mathcal{R}_{|\gamma}} \quad \text{on } \partial\Omega_k$$

Explicit solution of the elementary problems: $\boxed{\boldsymbol{q}_k^i=\boldsymbol{q}_k^{iL}+\boldsymbol{q}_k^{iC}}$

$$\boldsymbol{q}_k^{iL}=\frac{1}{2|\Omega_k|}\sum_{n=1}^{3}\sum_{\substack{m=1\\m\neq n}}\ell_{[m]}\boxed{R|_{\gamma_{[m]}}(\boldsymbol{x}_{[n]})}\boldsymbol{t}_{[mn]}\lambda_{[n]}$$

$$\boldsymbol{q}_k^{iC}=\frac{1}{3}\sum_{n=1}^{3}\sum_{\substack{m=2\\m>n}}^{3}\boxed{\lambda_{[n]}\lambda_{[m]}\boldsymbol{t}_{[nm]}\boldsymbol{t}_{[nm]}^{\mathsf{T}}}\nabla v^Q$$



$\boldsymbol{q}_k^{iL}$ imposes the tractions on the element

$\boldsymbol{q}_k^{iC}$ is traction free

New guaranteed, accurate and cheap EE

Strong form of the elementary problems:

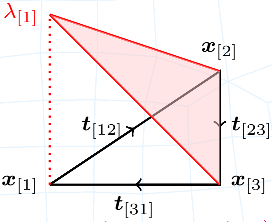
$$-\nabla\cdot\left(\boldsymbol{q}_k^i+\phi_i\nabla u_h\right)=\phi_i(\underbrace{f-\kappa^2 u_h}_{F})-\nabla u_h\cdot\nabla\phi_i \quad \text{in } \Omega_k$$

$$\boldsymbol{q}_k^i\cdot\boldsymbol{n}_k^\gamma=\sigma_k^\gamma g_\gamma^i-\phi_i\nabla u_h\cdot\boldsymbol{n}_k^\gamma := \mathcal{R}_{|\gamma} \quad \text{on } \partial\Omega_k$$

Explicit solution of the elementary problems: $\boldsymbol{q}_k^i=\boldsymbol{q}_k^{iL}+\boldsymbol{q}_k^{iC}$

$$\boldsymbol{q}_k^{iL}=\frac{1}{2|\Omega_k|}\sum_{n=1}^{3}\sum_{\substack{m=1\\m\neq n}}\ell_{[m]}\;R|_{\gamma_{[m]}}(\boldsymbol{x}_{[n]})\;\boldsymbol{t}_{[mn]}\lambda_{[n]}$$

$$\boldsymbol{q}_k^{iC}=\frac{1}{3}\sum_{n=1}^{3}\sum_{\substack{m=2\\m>n}}^{3}\lambda_{[n]}\lambda_{[m]}\boldsymbol{t}_{[nm]}\boldsymbol{t}_{[nm]}^{\mathsf{T}}\;\boxed{\nabla v^Q}$$



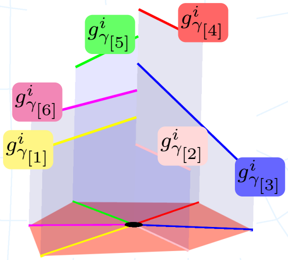
$$v^Q=\tfrac{3}{8}\phi_i F+\tfrac{1}{8}\left(4F_{[1]}\lambda_{[1]}-F_{[2]}\lambda_{[3]}-F_{[3]}\lambda_{[2]}\right)$$

$\boldsymbol{q}_k^{iC}$ imposes the divergence condition

New guaranteed, accurate and cheap EE

LOCAL QUADRATIC CONSTRAINED OPTIMIZATION PROBLEM:

find $\{g^i_{\gamma_{[m]}}\}$ solution of



Minimize g^i_γ
$$\sum_{\Omega_k \subset \omega_i} \int_{\Omega_k} \boldsymbol{q}^i_k(g^i_\gamma) \cdot \boldsymbol{q}^i_k(g^i_\gamma) d\Omega$$

↖ two dof per edge

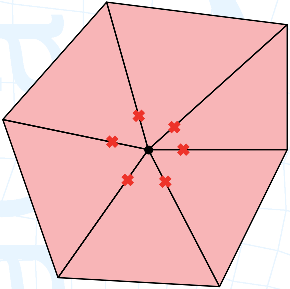
Subject to
$$\int_{\Omega_k} \left[\phi_i \left(f - \kappa^2 u_h\right) - \nabla u_h \cdot \nabla \phi_i\right] \, d\Omega + \sum_{\gamma \subset \partial\Omega_k} \int_\gamma \sigma^\gamma_k g^i_\gamma \, d\Gamma = 0$$

one restriction per element ↗

Hybrid-flux vs. Explicit Flux-free

Hybrid-flux/equilibrated

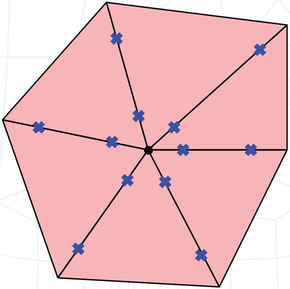
$$\min_{g_\gamma} \quad g_\gamma - [[\boldsymbol{\nabla} u_h \cdot n]]_{\text{ave}}$$



one dof per edge

Explicit Flux-free

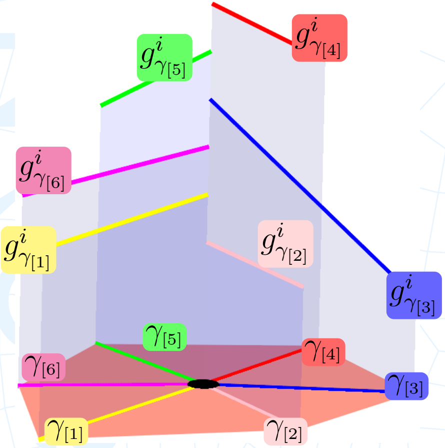
$$\min_{g^i_\gamma} \quad \sum_{\Omega_k \subset \omega_i} \int_{\Omega_k} \boldsymbol{q}^i_k(g^i_\gamma) \cdot \boldsymbol{q}^i_k(g^i_\gamma) d\Omega$$



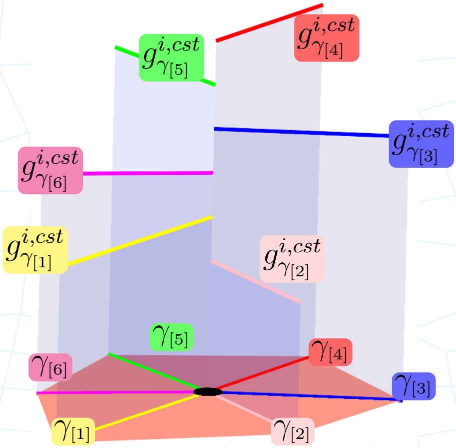
two dof per edge

+ one restriction per element in both cases

Constant Explicit Flux-free



two dof per edge



one dof per edge

$$g^i_\gamma = \phi_i g^{i,cst}_\gamma$$

2D example

Uniformly forced square domain

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

$$u(x,y) = \frac{1-x^2}{2} - \frac{16}{\pi^3} \sum_{\substack{k=1 \\ \text{odd}}}^{+\infty} \frac{\sin(k\pi(1+x)/2)(\sinh(k\pi(1+y)/2)+\sinh(k\pi(1-y)/2))}{k^3 \sinh(k\pi)}$$

$\rho = |||e|||_{ub}/|||e||| \approx 1$

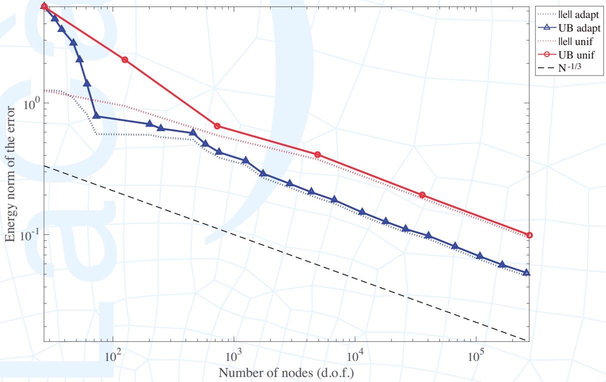
		FLUX-FREE			EQUILIBRATED
			explicit		
n_{el}	$\|\|\|e\|\|\|$	ρ^{st}	ρ	ρ^q	ρ^{eq}
8	0.34331271	1.00036	1.09131	1.01545	1.20880
32	0.27603795	1.04611	1.05288	1.03831	1.48894
128	0.15288301	1.04314	1.04621	1.03889	1.51749
512	0.07856757	1.04088	1.04470	1.03938	1.52104
2048	0.03955958	1.03948	1.04429	1.03962	1.51898
8192	0.01980831	1.03862	1.04420	1.03974	1.51641
32768	0.00990510	1.03813	1.04419	1.03982	1.51453

3D example

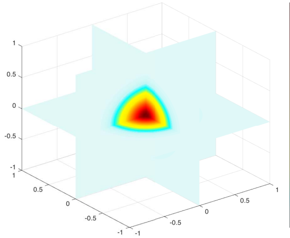
3D diffusion problem with data oscillation

$-\Delta u = f$ in $[-1,1]^3$ with Dirichlet BC

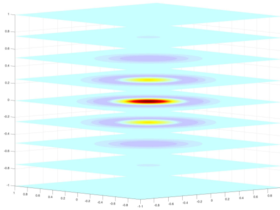
$u(x,y,z) = e^{-20(x^2+y^2+z^2)}$



Exact solution



Source term



3D example

3D diffusion problem with data oscillation

$$-\Delta u = f \quad \text{in } [-1,1]^3 \quad \text{with Dirichlet BC}$$

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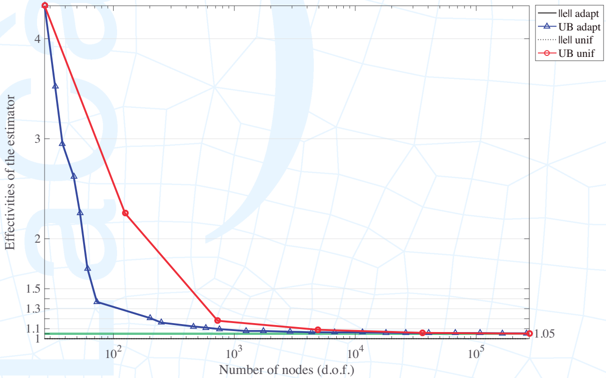
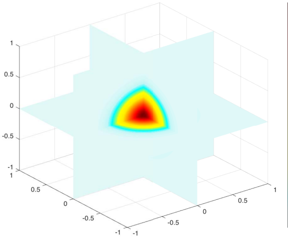
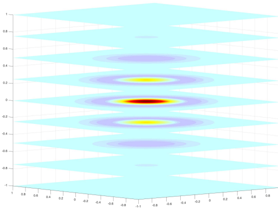


Exact solution



Source term



3D example

3D diffusion problem with data oscillation

$$|||e|||^2 \leq \sum_{k=1}^{n_{\text{el}}} \left(\underbrace{\|\boldsymbol{q}\|_{[\mathcal{L}^2(\Omega_k)]^3}}_{\text{dual error}} + \underbrace{\frac{h_k}{\pi}\|f - \Pi^1 f\|_{\mathcal{L}^2(\Omega_k)}}_{\text{data oscillation}} \right)^2$$

Conclusions

- We have developed a new technique to compute guaranteed upper bounds for the energy norm of the error (which can also be used to compute bounds for QoI)
- The proposed strategy may be seen as either:
  (1) an improved *cheap* version of the flux-free estimate
  (2) a new more *acurate* hybrid-flux equilibrated EE
- Alleviating the cost of the flux-free approach does not introduce a significant difference on accuracy
- The new equilibrated tractions yield sharper bounds than the original ones

A new equilibrated residual method: improving accuracy and efficiency of flux-free error estimates in two and three dimensions

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