

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

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# Guaranteed accurate and efficient bounds

The finite element method is a basic tool in engineering design and is crucial to certify the quality of the results.

A lot of work has been done to provide **certificates** of the approximate solution, i.e. obtain **guaranteed bounds** in which the exact solution lies (either in energy norm or in QoI).

**GOAL:**  $|||e||| \leq \eta$  or  $s^- \leq \ell^0(e) \leq s^+$

The desired qualities of a posteriori estimators are:

- **CERTIFICATION:** they should provide **guaranteed/strict** bounds
- **ACCURACY:** they should be **accurate** (good effectivities)
- **COST:** they should be **cheap** (involve small local problems)

# Guaranteed accurate and efficient bounds

## CERTIFICATION

complementary energy  
dual formulation for the error

+

implicit error estimators  
involving only local problems

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Hybrid-flux estimators  
equilibrated

**CHEAPER**

Flux-free estimators  
stars/subdomain [PDH2006]

**MORE ACCURATE**

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Flux-free estimators  
stars/subdomain [PDH2006]

**MORE ACCURATE**



**CHEAP + ACCURATE**

EXPLICIT Flux-free estimator

# Model problem

Reaction-diffusion equation: 
$$\begin{aligned}
 -\Delta u + \kappa^2 u &= f && \text{in } \Omega, \\
 u &= u_D && \text{on } \Gamma_D, \\
 \nabla u \cdot \mathbf{n} &= g_N && \text{on } \Gamma_N.
 \end{aligned}$$

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

$$\underbrace{\int_{\Omega} (\nabla u \cdot \nabla v + \kappa^2 uv) \, d\Omega}_{a(u,v)} = \underbrace{\int_{\Omega} f v \, d\Omega + \int_{\Gamma_N} g_N v \, d\Gamma}_{\ell(v)} \quad \forall v \in \mathcal{V}.$$

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

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

triangular mesh + linear elements

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

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

# Guaranteed error bounds

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

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

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

new error unknowns

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**new error unknowns**

## Dual formulation:

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

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

provide an upper bound for the energy norm of the error

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

**complementary energy**



# Guaranteed error bounds

Optimal choice:  $(\mathbf{q}, r) = (\nabla e, e)$

$$\|e\|^2 = \int_{\Omega} (\mathbf{q} \cdot \mathbf{q} + \kappa^2 r^2) d\Omega$$

Very accurate but expensive:

compute **piecewise polynomial**  $(\mathbf{q}, r)$  solving a **GLOBAL** problem

Accurate but cheaper:

compute **piecewise polynomial**  $(\mathbf{q}, r)$  solving **LOCAL** problems

Global problem

$\implies$

domain decomposition!

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

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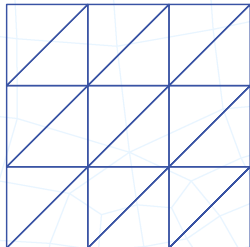
$$\int_{\Omega} (\mathbf{q} \cdot \nabla v + \kappa^2 r v) d\Omega = R(v)$$

Hybrid-flux / Flux-free

# Guaranteed error bounds

Global problem

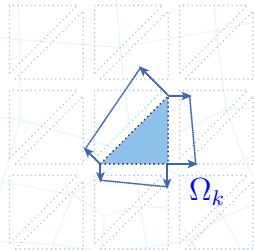
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# Guaranteed error bounds

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Hybrid-flux

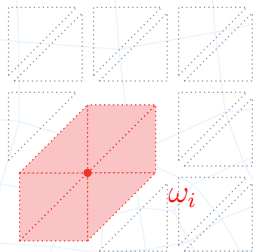
$$\int_{\Omega_k} (\mathbf{q}_k \cdot \nabla v + \kappa^2 r_k v) d\Omega = R_k(v) + \int_{\Omega_k} g_k v d\Gamma$$

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

# Guaranteed error bounds

Global problem

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



Hybrid-flux

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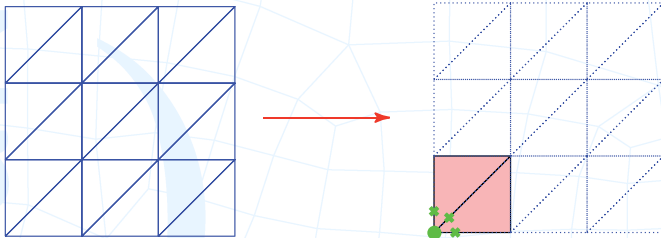
Flux-free

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

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

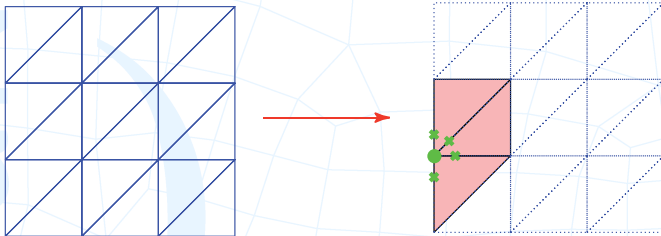
# Hybrid-flux / equilibrated error estimates

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



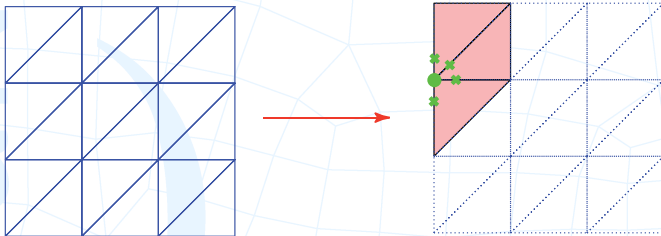
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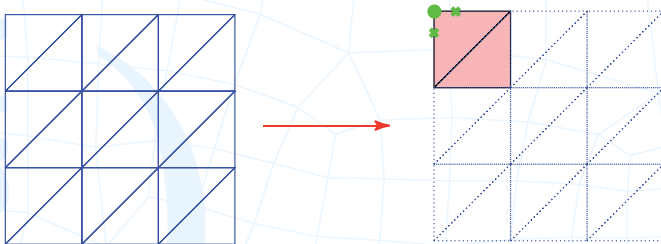
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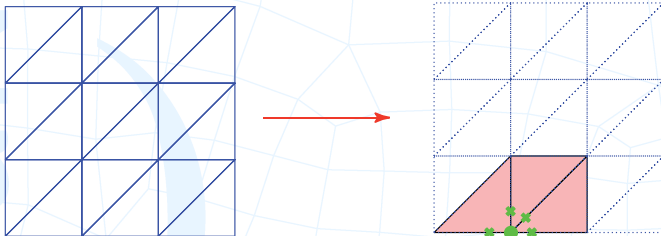
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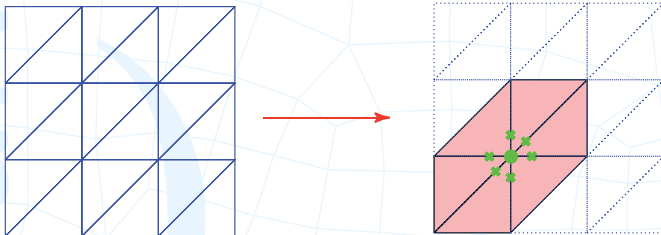
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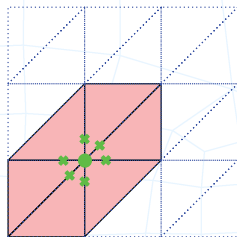
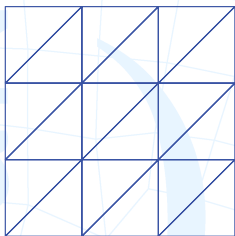
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# Hybrid-flux / equilibrated error estimates

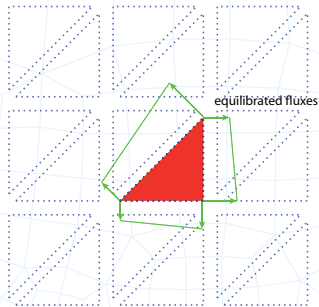
STEP 1: loop in nodes to compute the equilibrated tractions  $g_k$



STEP 2: loop in elements to compute the dual fluxes

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

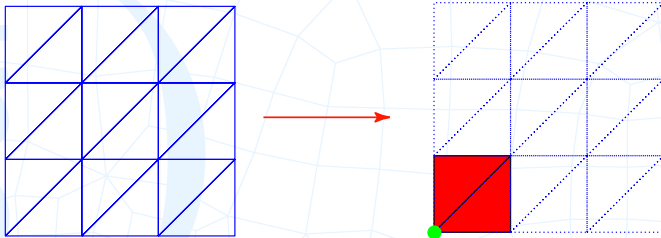
at each element  $\Omega_k$   
independently



# Flux-free error estimates

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

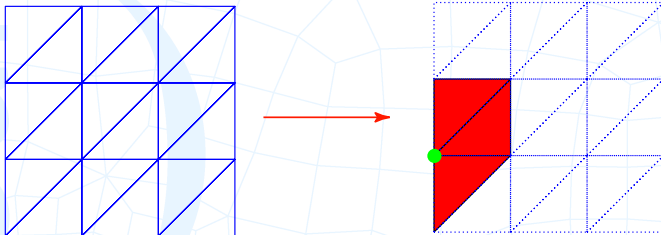
$(q^i, r^i)$  in  $\omega_i$  (patch of elements)



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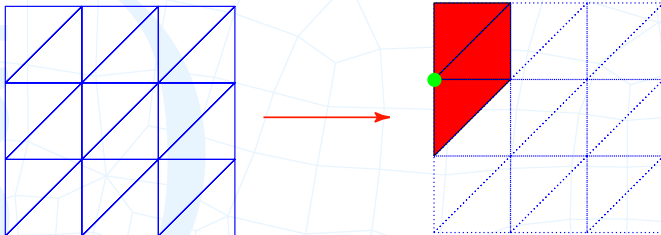
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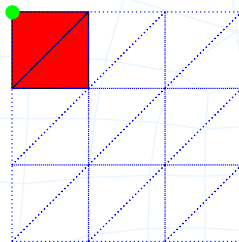
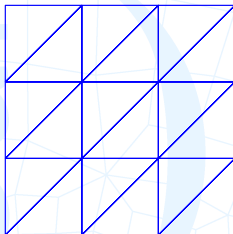
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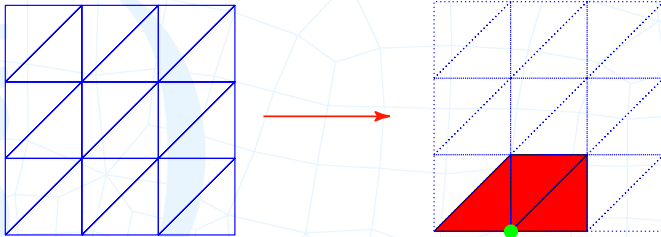




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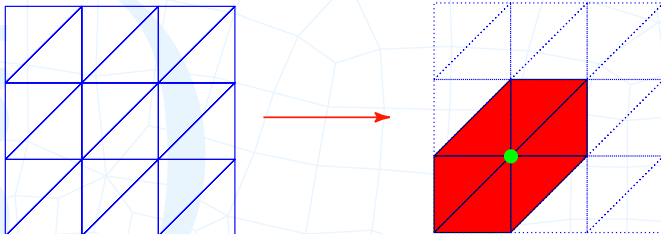
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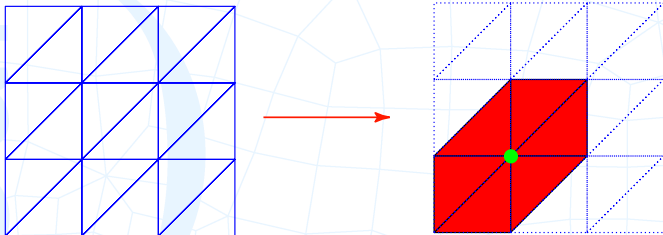
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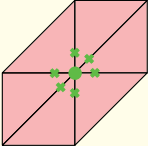
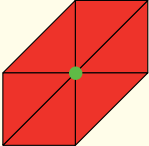
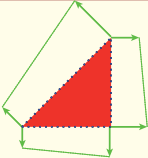
$(\mathbf{q}^i, r^i)$  in  $\omega_i$  (patch of elements)



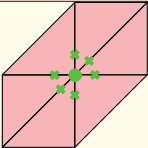
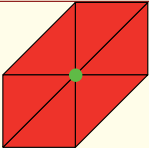
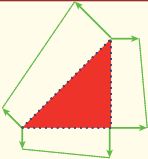
STEP 2: add all the local contributions and compute the norm

$$\mathbf{q} = \sum_{i=1}^{n_{\text{np}}} \mathbf{q}^i \quad , \quad r = \sum_{i=1}^{n_{\text{np}}} r^i$$

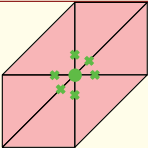
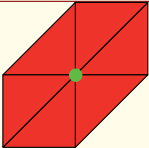
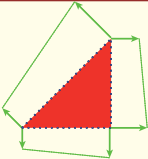
## Computational cost overview

	Equilibrated	Flux-free
Loop on nodes	 <p>DOF: one per edge of <math>\omega_i</math></p>	 <p>DOF: dof of <math>(\mathbf{q}_k^i, r_k^i)</math> × elements of <math>\omega_i</math></p>
Loop on elements	 <p>DOF: dof of <math>(\mathbf{q}_k, r_k)</math></p>	

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Loop on nodes	 <p>DOF: one per edge of <math>\omega_i</math></p>	 <p>DOF: dof of <math>(\mathbf{q}_k^i, r_k^i)</math> <math>\times</math> elements of <math>\omega_i</math></p>
Loop on elements	 <p>DOF: dof of <math>(\mathbf{q}_k, r_k)</math></p>	<div style="border: 2px solid red; padding: 5px; background-color: blue; color: white;"> <p>2D , <math>q=2 \rightarrow 18</math> 2D , <math>q=3 \rightarrow 30</math></p> </div>

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# New guaranteed, accurate and cheap error estimate (EE)

**Goal:** decompose the global problem into stars  $\omega_i$

$$\int_{\Omega} (\mathbf{q} \cdot \nabla v + \kappa^2 r v) d\Omega = R(v) \quad \forall v \in \mathcal{V}$$

minimizing the global complementary energy

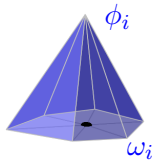
$$\int_{\Omega} (\mathbf{q} \cdot \mathbf{q} + \kappa^2 r^2) d\Omega$$

**Local problems:**  $\mathbf{q} = \sum_{i=1}^{n_{np}} \mathbf{q}^i$ ,  $r = \sum_{i=1}^{n_{np}} r^i$

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

minimizing the local complementary energy

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



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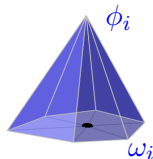
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## KEY POINT

Find a closed  
EXPLICIT solution  
for  $\mathbf{q}^i$  and  $r^i$

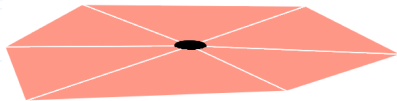




# New guaranteed, accurate and cheap EE

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

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

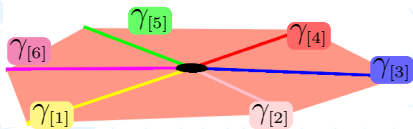


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From star  $\omega_i$  to elements  $\Omega_k \subset \omega_i$

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

The explicit solution is found introducing the linear tractions on the edges of the star  $\{g_{\gamma[m]}^i\}$

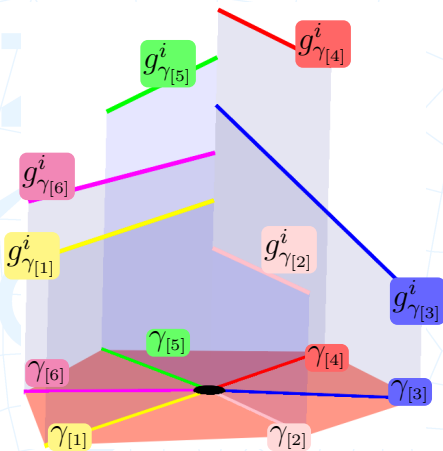


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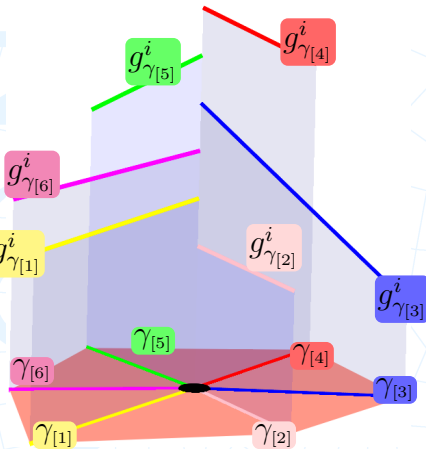


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Neumann BC

Divergence

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

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



for every  $\Omega_k \subset \omega_i$

# New guaranteed, accurate and cheap EE

Strong form of the elementary problems:

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

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

**ASSUMPTION:** for simplicity of presentation we assume that

- $f$  is piecewise linear and
- $g_N$  is piecewise constant

otherwise we need to introduce data oscillation terms

# New guaranteed, accurate and cheap EE

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

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

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

**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)

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

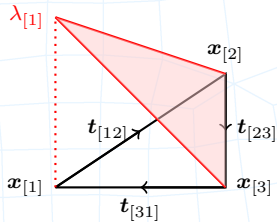
$$\mathbf{q}_k^i \cdot \mathbf{n}_k^\gamma = \sigma_k^\gamma \mathbf{g}_\gamma^i - \phi_i \nabla u_h \cdot \mathbf{n}_k^\gamma := \mathcal{R}_\gamma \quad \text{on } \partial\Omega_k$$

Explicit solution of the elementary problems:

$$\mathbf{q}_k^i = \mathbf{q}_k^{iL} + \mathbf{q}_k^{iC}$$

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

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



# New guaranteed, accurate and cheap EE

Strong form of the elementary problems:

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

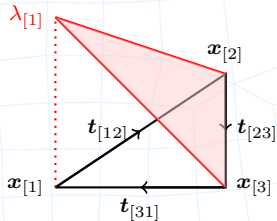
$$\mathbf{q}_k^i \cdot \mathbf{n}_k^\gamma = \sigma_k^\gamma \mathbf{g}_\gamma^i - \phi_i \nabla u_h \cdot \mathbf{n}_k^\gamma := \mathcal{R}_{|\gamma} \quad \text{on } \partial\Omega_k$$

Explicit solution of the elementary problems:

$$\mathbf{q}_k^i = \mathbf{q}_k^{iL} + \mathbf{q}_k^{iC}$$

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

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



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

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



# New guaranteed, accurate and cheap EE

Strong form of the elementary problems:

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

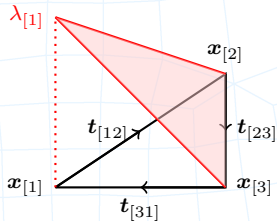
$$\mathbf{q}_k^i \cdot \mathbf{n}_k^\gamma = \sigma_k^\gamma g_\gamma^i - \phi_i \nabla u_h \cdot \mathbf{n}_k^\gamma := \mathcal{R}_{|\gamma}^F \quad \text{on } \partial\Omega_k$$

Explicit solution of the elementary problems:

$$\mathbf{q}_k^i = \mathbf{q}_k^{iL} + \mathbf{q}_k^{iC}$$

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

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



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

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

# New guaranteed, accurate and cheap EE

Explicit solution of the elementary problems:

$$\mathbf{q}_k^i = \mathbf{q}_k^{iL} + \mathbf{q}_k^{iC}$$

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

$$\mathbf{q}_k^{iC} = \frac{1}{3} \sum_{n=1}^3 \sum_{\substack{m=2 \\ m > n}}^3 \lambda_{[n]} \lambda_{[m]} \mathbf{t}_{[nm]} \mathbf{t}_{[nm]}^T$$

**FREE DOF**  $g_\gamma^i$

minimize  
compl. energy

subject to

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

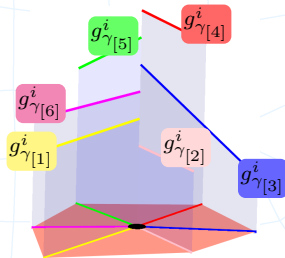
Complementary energy

$$\int_{\Omega_k} \mathbf{q}_k^i(g_\gamma^i) \cdot \mathbf{q}_k^i(g_\gamma^i) d\Omega$$

# New guaranteed, accurate and cheap EE

LOCAL QUADRATIC CONSTRAINED OPTIMIZATION PROBLEM:

find  $\{g_{\gamma[m]}^i\}$  solution of



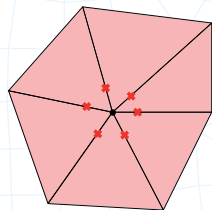
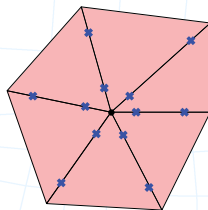
$$\begin{aligned}
 & \text{Minimize}_{g_{\gamma}^i} \sum_{\Omega_k \subset \omega_i} \int_{\Omega_k} \mathbf{q}_k^i(g_{\gamma}^i) \cdot \mathbf{q}_k^i(g_{\gamma}^i) d\Omega && \swarrow \text{two dof per edge} \\
 & \text{Subject to} \int_{\Omega_k} [\phi_i (f - \kappa^2 u_h) - \nabla u_h \cdot \nabla \phi_i] d\Omega \\
 & \text{one restriction per element} \nearrow + \sum_{\gamma \subset \partial \Omega_k} \int_{\gamma} \sigma_k^{\gamma} g_{\gamma}^i d\Gamma = 0
 \end{aligned}$$

# Hybrid-flux vs. Explicit Flux-free

## Explicit Flux-free

Minimize  $g_\gamma^i$   $\sum_{\Omega_k \subset \omega_i} \int_{\Omega_k} \mathbf{q}_k^i(g_\gamma^i) \cdot \mathbf{q}_k^i(g_\gamma^i) d\Omega$

two dof per edge



## Hybrid-flux / equilibrated

Minimize  $g_\gamma$   $[[\nabla u_h \cdot n]]_{\text{ave}}$

one dof per edge

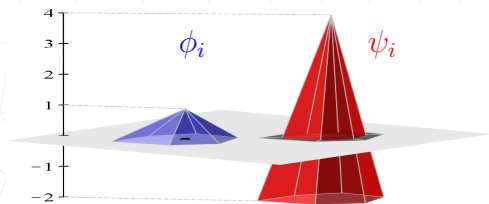
# Hybrid-flux vs. Explicit Flux-free

## Explicit Flux-free

$$\text{Minimize } \sum_{\Omega_k \subset \omega_i} \int_{\Omega_k} \mathbf{q}_k^i(g_\gamma^i) \cdot \mathbf{q}_k^i(g_\gamma^i) d\Omega$$

two dof per edge

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



## Hybrid-flux / equilibrated

$$\text{Minimize } g_\gamma - [[\nabla u_h \cdot \mathbf{n}]]_{\text{ave}}$$

one dof per edge

$$\text{s.t. } \int_{\Omega_k} [\psi_i (f - \kappa^2 u_h) - \nabla u_h \cdot \nabla \psi_i] d\Omega + \sum_{\gamma \subset \partial\Omega_k} \int_{\gamma} \sigma_k^\gamma g_\gamma \psi_i d\Gamma = 0$$

# 2D example

Uniformly forced square domain

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

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

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

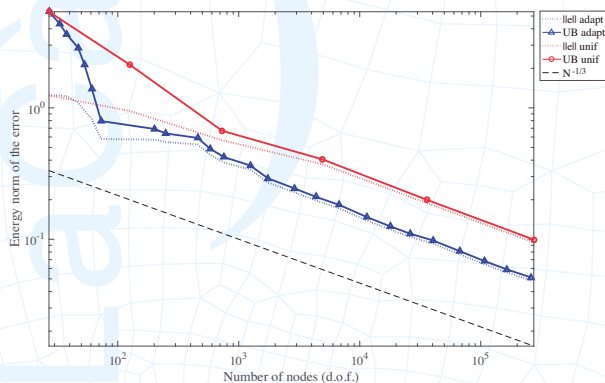
$n_{el}$	$\ e\ $	FLUX-FREE			EQUILIBRATED
		$\rho^{st}$	explicit		$\rho^{eq}$
			$\rho$	$\rho^q$	
8	0.34331271	1.00036	1.09131	1.01545	1.20880
32	0.27603795	1.04611	1.05288	1.03831	1.48894
128	0.15288301	1.04314	1.04621	1.03889	1.51749
512	0.07856757	1.04088	1.04470	1.03938	1.52104
2048	0.03955958	1.03948	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

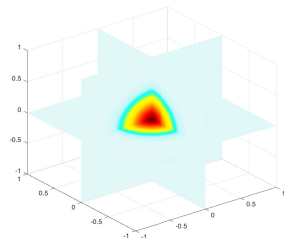
3D diffusion problem with data oscillation

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

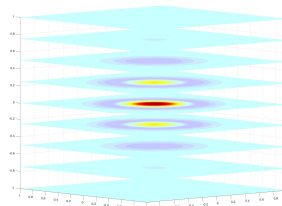
$$u(x, y, z) = e^{-20(x^2+y^2+z^2)}$$



Exact solution



Source term

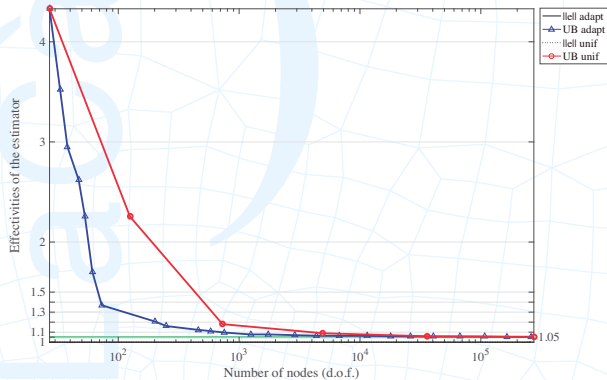


# 3D example

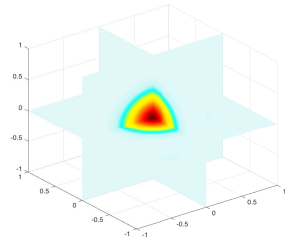
3D diffusion problem with data oscillation

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

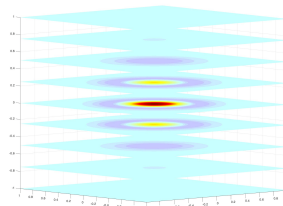
$$u(x, y, z) = e^{-20(x^2+y^2+z^2)}$$



Exact solution



Source term





# 3D example

3D diffusion problem with data oscillation

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

# 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 efficient 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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