Balancing Act: Stopping Criteria for the Conjugate Gradient Algorithm in High-order Finite Element Methods

Yichen Guo, Eric de Sturler, Tim Warburton

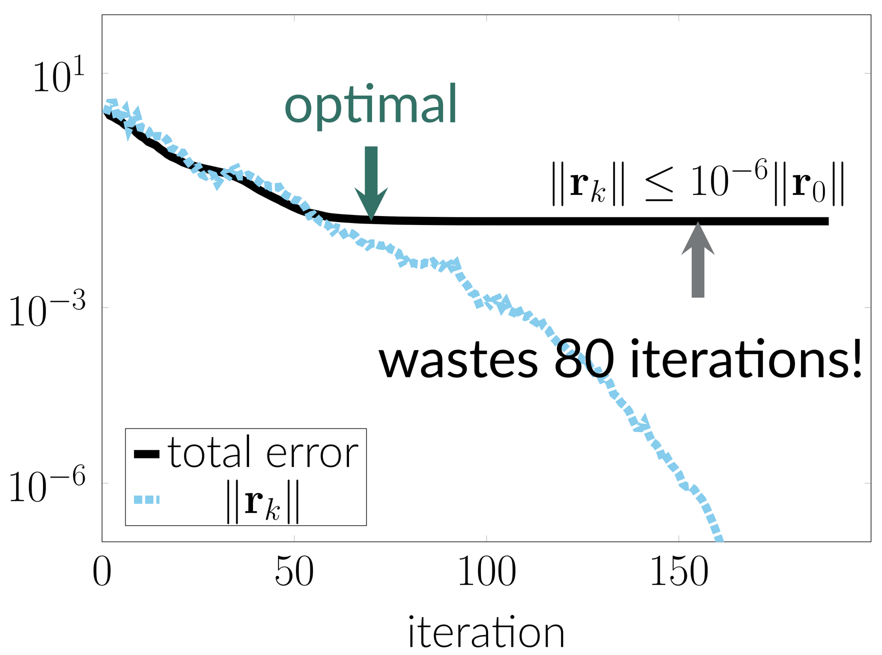
VIRGINIA TECH

Paper

1. Challenge: when to stop iterating FEM solutions

- Consider the Poisson equation $-\nabla \cdot (\kappa(x)\nabla u(x)) = f(x)$ on Ω.
- High-order finite elements **discretization** yields $\mathbf{Ax} = \mathbf{b}$.
- Using conjugate gradient (CG), obtain a sequence $\mathbf{x}_0, \mathbf{x}_1, \cdots, \mathbf{x}_k$ to **approximate** the solution $\mathbf{x}$. The associated residual is $\mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k$.
- Under the energy norm,

$$\underbrace{\|u-u_h^k\|_E}_{\text{total error}} = \underbrace{\|u-u_h\|_E}_{\text{discretization error}} + \underbrace{\|u_h-u_h^k\|_E}_{\text{algebraic error} = \|\mathbf{x}-\mathbf{x}_k\|_\mathbf{A}}$$



What is a good stopping criterion?

- Maintaining solution **accuracy**
- **Terminating** CG **earlier**
- **Robust** to h, N, mesh distortion, and $\kappa(x)$
- **Cost-effective** in computation and storage

2. Existing stopping criteria

A commonly adopted stopping criterion [2, 3]

estimated algebraic error $\ll$ estimated total error

Error estimation for CG (algebraic error) [4]

Choose the delay parameter d such that $\|\mathbf{x}-\mathbf{x}_{k+d}\|_\mathbf{A} \ll \|\mathbf{x}-\mathbf{x}_k\|_\mathbf{A}$.

$$\eta_{\text{alg}} := \|\mathbf{x}_{k+d} - \mathbf{x}_k\|_\mathbf{A}.$$

A posteriori error estimation for FEM (total error)

Define the element residual, r_E and the edge residual r_J by

$$r_E\big|_K = f + \nabla\cdot\left(\kappa(x)\nabla u_h^k\right), \quad r_J\big|_\ell = -\left[\left(\kappa(x)\nabla u_h^k\right)\cdot \mathbf{n}_\ell\right].$$

- **Residual a posteriori estimator [5]**

$$\eta_R^2 = \sum_{K\in\mathcal{T}_h} \frac{h_K^2}{\kappa_K N^2}\|r_E\|_K^2 + \sum_{\ell\in\mathcal{E}} \frac{h_\ell}{\kappa_\ell N}\|r_J\|_\ell^2, \quad \text{(C1)}\ \eta_{\text{alg}} \le \tau\,\eta_R.$$

- **Flux recovery-based estimator [6, 7]** Reconstructing the numerical flux $\boldsymbol{\sigma_K}$ by projecting $\kappa(x)\nabla u_h^k(x)$ onto H(div) space.

$$\eta_{\text{BDM}}^2 := \sum_{K\in\mathcal{T}_h} \left\|\kappa(x)^{-1/2}\left(\boldsymbol{\sigma_K} - \kappa(x)\nabla u_h^k(x)\right)\right\|^2, \quad \text{(C2)}\ \eta_{\text{alg}} \le \tau\,\eta_{\text{BDM}}.$$

3. Stopping criterion derived from residual

The n-th component of the linear residual is

$$(\mathbf{r}_k)_n = (\phi_n, f) - \sum_{K\in\mathcal{T}_h}\left(\kappa(x)\nabla\phi_n, \nabla u_h^k\right)_K.$$

Integrating the last term by parts, we obtain

$$(\mathbf{r}_k)_n = \textstyle\sum_{K\in\mathcal{T}_h}(\phi_n, r_E)_K - \sum_{\ell\in\mathcal{E}}(\phi_n, r_J)_\ell = (\mathbf{R}_k)_n + (\mathbf{F}_k)_n.$$

Introducing the weighted L_2 norm $\|\cdot\|_\mathbf{w}$ relevant to $\kappa(x)$, we define the indicator η_{RF}

$$\eta_{\text{RF}} := \|\mathbf{R}_k\|_\mathbf{w} + \|\mathbf{F}_k\|_\mathbf{w},$$

with the associated stopping criterion:

$$\text{(C3)} \quad \|\mathbf{r}_k\|_\mathbf{w} \le \tau\,\eta_{\text{RF}}.$$

For **highly variable piecewise constant coefficients** $\kappa(x)$, where the good preconditioner is not available and CG converges slowly, we partition the domain Ω into subdomains Ω_p, $p = 1, \dots, P$, based on the value of $\kappa(x)$.

We propose a subdomain-based stopping criterion by restricting $\mathbf{R}_k$, $\mathbf{F}_k$, and $\mathbf{r}_k$ to Ω_p

$$\text{(C4)} \quad \|\mathbf{r}_k^p\|_\mathbf{w} \le \tau\,\eta_{\text{RF}}^p, \quad \forall p = 1,\dots,P.$$

4. Numerical results

Define the quality ratio of a criterion as

$$\text{quality ratio} := \frac{\|u-u_h^{k^*}\|_E}{\|u-u_h\|_E},$$

with $u_h^{k^*}$ as the first solution that satisfies the stopping condition. Set $\tau = 1/20$.

Highly anisotropic mesh

Solve the Poisson problem on $[-1,1]^2$ with $\kappa(x)=1$, using a highly anisotropic mesh of triangles, as shown in fig. 1.

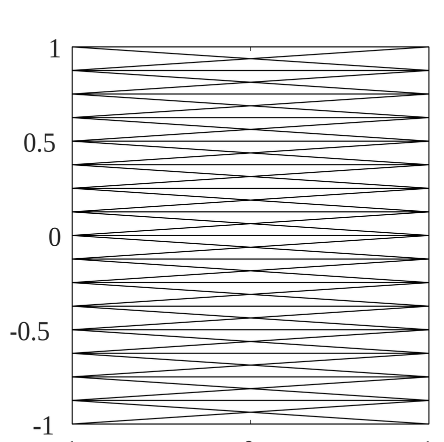


Figure 1. Mesh with minimal angles near $\pi/50$.

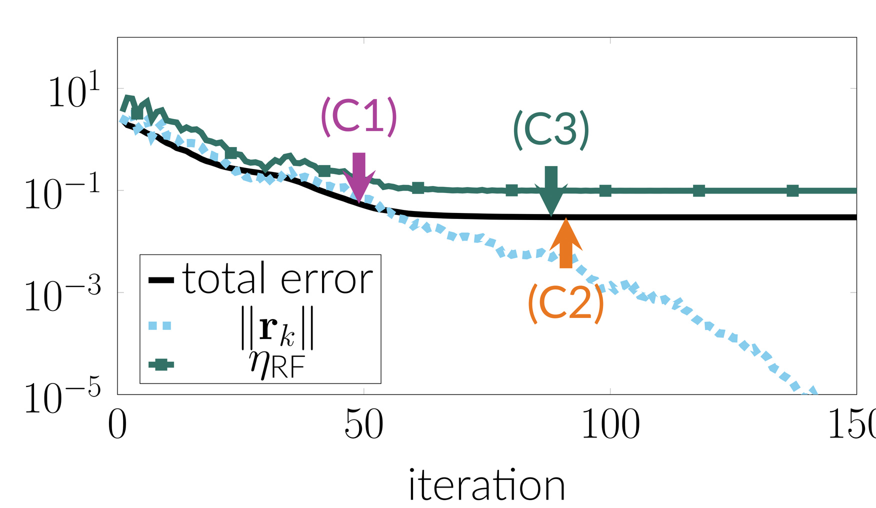


Figure 2. Arrows mark the criteria-suggested termination points for $N=6$. (C1) leads to early termination.

Criterion	$N=4$ iter	$N=4$ qual.	$N=6$ iter	$N=6$ qual.	$N=8$ iter	$N=8$ qual.
(C1) $\eta_{\text{alg}} \le \tau\eta_R$	7	1.60	49	1.84	141	4.78
(C2) $\eta_{\text{alg}} \le \tau\eta_{\text{BDM}}$	31	1.00	91	1.00	198	1.00
(C3) $\|\mathbf{r}_k\|_\mathbf{w} \le \tau\eta_{\text{RF}}$	28	1.00	88	1.01	199	1.00
$\|\mathbf{r}_k\| \le 10^{-6}\|\mathbf{r}_0\|$	87	1.00	155	1.00	235	1.00

Table 1. Numbers of iterations (iter) and quality ratios (qual.). The criterion (C3) consistently exhibits the best performance for almost all polynomial degrees.

Highly variable coefficient

Consider the Poisson equation on an L-shaped domain with $\kappa(x)$ shown in fig. 3. In fig. 5, criteria (C1)-(C3) lead to premature termination, while only (C4) ensures reliable termination. Referring to the domain partition in fig. 4, termination behavior is distinct in each subdomain, with the interior subdomain requiring more iterations.

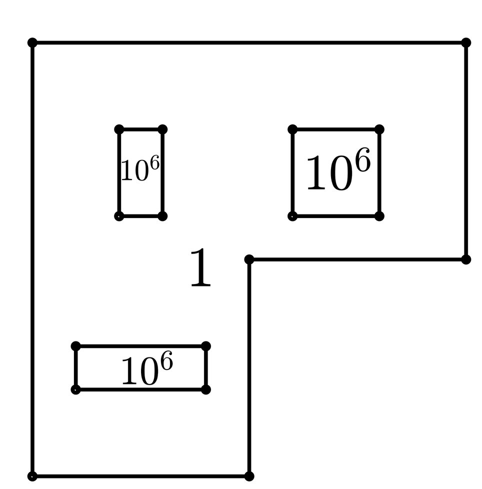


Figure 3. Mesh and $\kappa(x)$

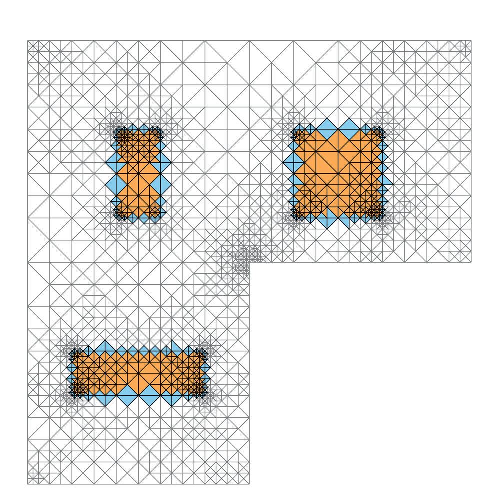


Figure 4. Partition for (C4) showcasing interior (orange), interface (blue), and exterior (white) subdomains.

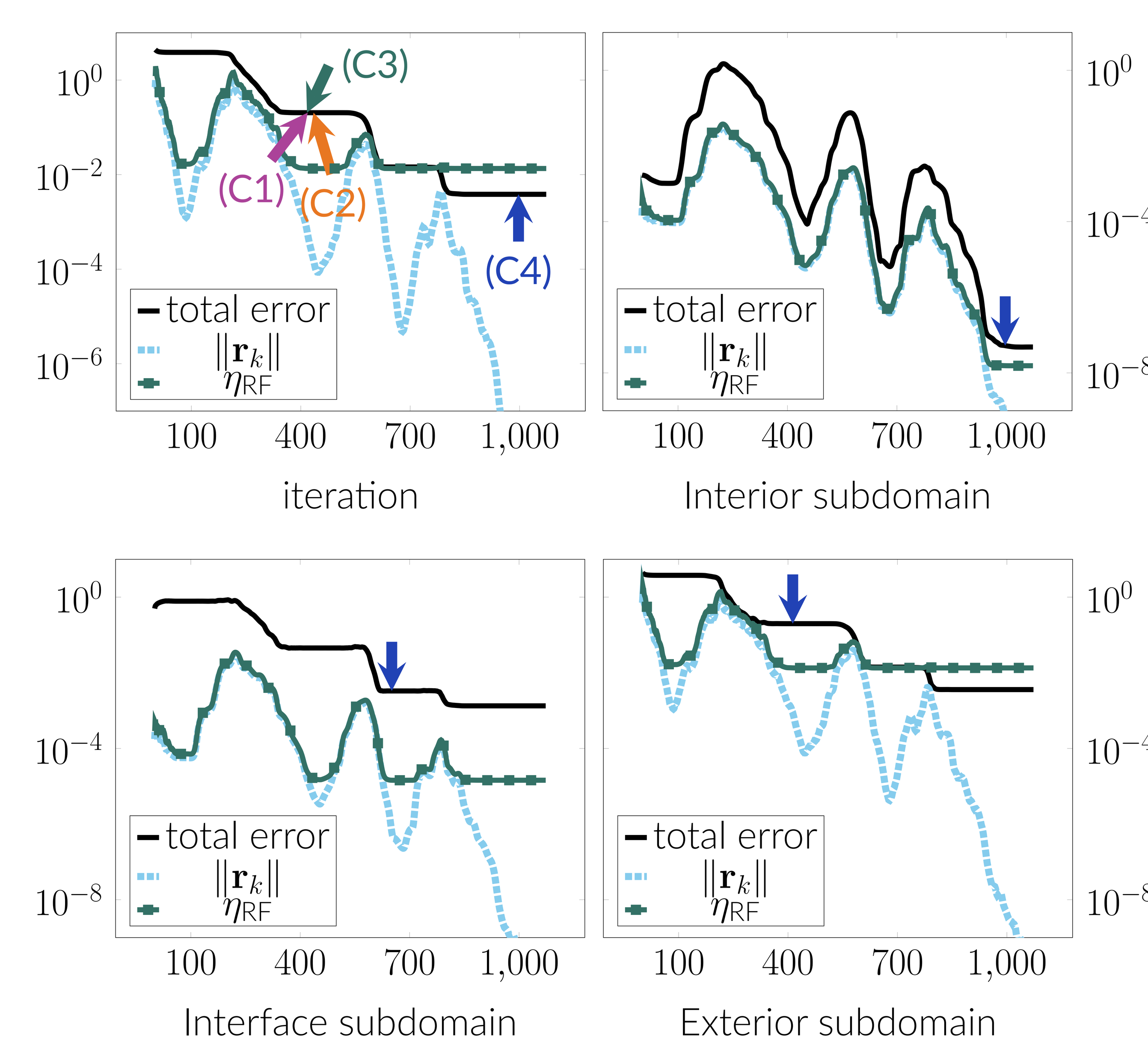


Figure 5. Convergence history in the whole domain and its subdomains

5. Summary

robust to	h,N	distortion	$\kappa(x)$	inexpensive
$\|\mathbf{r}_k\| \le 10^{-6}\|\mathbf{r}_0\|$	✗	✗	✗	✓
(C1) $\eta_{\text{alg}} \le \tau\eta_R$	✓	✗	✗	✓
(C2) $\eta_{\text{alg}} \le \tau\eta_{\text{BDM}}$	✓	✓	✗	✗
(C3) $\|\mathbf{r}\|_\mathbf{w} \le \tau\eta_{\text{RF}}$	✓	✓	✗	✓
(C4) subdomain-based	✓	✓	✓	✓

Reference

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ycguo@vt.edu