

1 **A DISCRETIZATION-ACCURATE STOPPING CRITERION FOR**
2 **ITERATIVE SOLVERS FOR FINITE ELEMENT APPROXIMATION***

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4 **Abstract.** This paper introduces a discretization-accurate stopping criterion of symmetric iter-
5 ative methods for solving systems of algebraic equations resulting from the finite element approxima-
6 tion. The stopping criterion consists of the evaluations of the discretization and the algebraic error
7 estimators, that are based on the respective duality error estimator and the difference of two consecu-
8 tive iterates. Iterations are terminated when the algebraic estimator is of the same magnitude as the
9 discretization estimator. Numerical results for multigrid $V(1,1)$ -cycle and symmetric Gauss-Seidel
10 iterative methods are presented for the linear finite element approximation to the Poisson equa-
11 tions. A large reduction in computational cost is observed compared to the standard residual-based
12 stopping criterion.

13 **1. Introduction.** Consider the Dirichlet boundary value problem in a bounded
14 polygonal/polyhedral domain $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) for the diffusion equation as follows:

15 (1.1)
$$\begin{cases} -\nabla \cdot (A \nabla u) = f, & \text{in } \Omega, \\ u = g, & \text{on } \partial\Omega, \end{cases}$$

16 where A is a scalar diffusion coefficient, and the data $f \in L^2(\Omega)$ and $g \in L^2(\partial\Omega)$.

17 In practice, the system of algebraic equations resulting from the finite element
18 approximation to (1.1) is often solved by iterative methods, e.g., Gauss-Seidel, conju-
19 gate gradient, multigrid methods, etc. Instead of having the exact solution u_τ of the
20 algebraic system at hand, $\bar{u}_\tau := u_\tau^{(k)}$ is the current output from an iterative solver,
21 where k is the number of iterations. The total energy error of \bar{u}_τ to the solution u
22 of the continuous problem in (1.1) consists of both discretization and algebraic errors
23 as follows:

24 (1.2)
$$\underbrace{\|u - \bar{u}_\tau\|_A^2}_{\text{total error}} = \underbrace{\|u_\tau - \bar{u}_\tau\|_A^2}_{\text{algebraic error}} + \underbrace{\|u - u_\tau\|_A^2}_{\text{discretization error}},$$

25 where $\|\cdot\|_A$ is the energy norm associated with the problem in (1.1) (for the norm
26 notations, see section 2).

27 The goal of this paper is to propose a stopping criterion for iterative solvers. To
28 do so, we need to develop two error estimators for the respective discretization and
29 algebraic errors. Since the discretization error is fixed for a given finite element space,
30 (1.2) clearly indicates that the stopping criterion of the iterative solver is when the
31 algebraic estimator is of the same magnitude as the discretization estimator, provided
32 that both represent their error counterparts reliably.

33 Discretization error estimators for the exact finite element approximations have
34 been intensively studied during the past four decades (see books [1, 26] and references

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35 therein). In the context of stopping criterion for iterative solvers, the residual-based a
 36 posteriori error estimator was employed for the conforming finite element approxima-
 37 tion by several researchers (see, e.g., [5, 24, 3, 2, 4]); recovery-based estimators were
 38 used by Vohralik and his collaborators in [20] for the finite volume discretization and
 39 in [17] for the discontinuous finite element approximation on non-matching grids.

40 In this paper, we will adopt the equilibrated flux error estimator (see, e.g., [8,
 41 16, 21, 25, 13]) for the discretization error. This is because the reliability bound of
 42 estimators of this type is constant free. Using this technique, a locally post-processed
 43 flux based on the iterate $\bar{u}_\mathcal{T}$ will be constructed. Unlike the exact finite element
 44 approximation $u_\mathcal{T}$, the local problems based on the current iterate $\bar{u}_\mathcal{T}$ on vertex
 45 patches are not consistent. To overcome this difficulty, we modify the local problems
 46 by adding back the algebraic errors. The resulting discretization error estimator
 47 plus the algebraic error is proved to be reliable and the reliability bound for the
 48 discretization estimator component is constant free (see Theorem 4).

49 To construct the algebraic error estimator, we first bound $\|u_\mathcal{T} - u_\mathcal{T}^{(k)}\|_A$ above
 50 by the energy norm of the difference of consecutive iterates, and the constant in the
 51 upper bound depends on the spectral radius of the error propagation operator (see
 52 Theorem 5). The unknown spectral radius is further approximated by the ratio of
 53 the l^2 norms of the residuals of consecutive iterates. The resulting algebraic error
 54 estimator is then shown to be reliable when sufficiently many iterations have been
 55 performed.

56 Lastly, in Section 6, based on the discretization and algebraic estimators, a new
 57 stopping criterion for a given linear solver is verified numerically by some test prob-
 58 lems. The numerics shows promising results in that the bounds are independent of
 59 the coefficient jump ratio even without the quasi-monotonicity assumption [6, 18, 23]
 60 for the distribution of the diffusion coefficient A .

61 **2. Finite element method and iterative solver.** In this section, all prelim-
 62 inaries are presented. Denote $H^1(\Omega)$ with a specified boundary value as $H_g^1(\Omega) :=$
 63 $\{v \in H^1(\Omega) : v = g \text{ on } \partial\Omega\}$, and then the variational problem of (1.1) is

64 (2.1) Find $u \in H_g^1(\Omega)$ such that $(A\nabla u, \nabla v) = (f, v), \quad \forall v \in H_0^1(\Omega),$

65 where (\cdot, \cdot) denotes the L^2 -inner product on the whole domain.

66 Let $\mathcal{T} = \{K\}$ be a triangulation of Ω using simplicial element, where \mathcal{T} is assumed
 67 to be quasi-uniform and regular. For each $K \in \mathcal{T}$, $h_K := \text{diam}(K) = O(|K|^{1/d})$. The
 68 set of all the vertices of this triangulation is denoted by \mathcal{N} . Throughout this paper,
 69 the term ‘‘face’’ is used to refer to the $(d-1)$ -facet of a d -simplex in this triangulation
 70 ($d = 2, 3$). For the $d = 2$ case, a face actually represents an edge. The set of all the
 71 interior faces is denoted by \mathcal{F} . For any $F \in \mathcal{F}$, $h_F := \text{diam}(F) = O(|F|^{1/(d-1)})$. Each
 72 face $F \in \mathcal{F}$ is associated with a fixed unit normal \mathbf{n}_F globally. For any function or
 73 distribution v well-defined on the two elements sharing a face F respectively, define
 74 $\llbracket v \rrbracket_F = v^- - v^+$ on an interior face. The v^- and v^+ are defined in the limiting sense
 75 of $v^\pm = \lim_{\epsilon \rightarrow 0^\pm} v(\mathbf{x} + \epsilon \mathbf{n}_F)$. If F is a boundary face, the function v is extended by zero
 76 outside the domain to compute $\llbracket v \rrbracket_F$. For every geometrical object D and for every
 77 integer $k \geq 0$, $P_k(D)$ denotes the set of polynomials of degree $\leq k$ on D .

78 For the purpose of constructing the local error estimation procedure for the finite
 79 element approximation, notations of the following local geometric objects are used in
 80 this paper. First, denote by \mathcal{N}_K the set of all the vertices of $K \in \mathcal{T}$. For any vertex

81 $\mathbf{z} \in \mathcal{N}$, denote by

$$82 \quad \omega_{\mathbf{z}} := \bigcup_{\{K \in \mathcal{T} : \mathbf{z} \in \mathcal{N}_K\}} K$$

83 as the vertex patch, which is the union of all elements sharing \mathbf{z} as a common vertex.

84 Now $\mathcal{T}_{\mathbf{z}}$ stands for the triangulation of this patch such that $\mathcal{T}_{\mathbf{z}} := \{K : K \subset \omega_{\mathbf{z}}\}$.

85 Denote

$$86 \quad \omega_K := \bigcup_{\mathbf{z} \in \mathcal{N}_K} \omega_{\mathbf{z}}$$

87 as the element patch for K that contains all the elements sharing a vertex with K .

88 For a face $F \in \mathcal{F}$, denote the face patch as

$$89 \quad \omega_F := \bigcup_{F \cap \partial K \neq \emptyset} K,$$

90 which contains the elements sharing F as a common face. The L^2 -inner product and
91 norm on $\omega = \cup K \subset \Omega$ are denoted by

$$92 \quad (u, v)_{\omega} := \sum_{K \subset \omega} (u, v)_K \quad \text{and} \quad \|v\|_{0, \omega}^2 := (v, v)_{\omega},$$

93 respectively. These notations carry through for vector-valued functions. The “energy”
94 seminorm associated with the problem (2.1) is (with slight abuse of notation, because
95 the local seminorm is denoted as a norm):

$$96 \quad (2.2) \quad \|v\|_A^2 := (A \nabla u, \nabla v) \quad \text{and} \quad \|v\|_{A, \omega}^2 := (A \nabla u, \nabla v)_{\omega}.$$

97 Let \mathcal{F}_K be the set of faces of an element $K \in \mathcal{T}$. Denote the set of the interior
98 faces within $\omega_{\mathbf{z}}$ as:

$$99 \quad \mathcal{F}_{\mathbf{z}} := \{F \in \mathcal{F} : F \in \mathcal{F}_K \text{ for } K \subset \omega_{\mathbf{z}}, F \cap \partial \omega_{\mathbf{z}} = \emptyset\}.$$

100 Denote the H^1 -conforming linear finite element space by

$$101 \quad (2.3) \quad \mathcal{S}^1 := \{v \in H^1(\Omega) : v|_K \in P_1(K), \forall K \in \mathcal{T}\},$$

102 and the piecewise constant space with respect to the triangulation \mathcal{T} by

$$103 \quad (2.4) \quad \mathcal{S}^0 := \{v \in L^2(\Omega) : v|_K \in P_0(K), \forall K \in \mathcal{T}\},$$

104 Then the finite element approximation to (2.1) is

$$105 \quad (2.5) \quad \begin{cases} \text{Find } u_{\mathcal{T}} \in \mathcal{S}^1 \cap H_g^1(\Omega) \text{ such that} \\ (A \nabla u_{\mathcal{T}}, \nabla v) = (f, v), \quad \forall v \in \mathcal{S}^1 \cap H_0^1(\Omega). \end{cases}$$

106 For the presentation purpose, here it is assumed that both the diffusion coefficient
107 A and the data f are in \mathcal{S}^0 , and denote $A|_K = A_K, f|_K = f_K$. Additionally, the
108 Dirichlet boundary data g can be represented by the trace of a function in \mathcal{S}^1 . In this
109 setting, no data oscillation term will be present in the final error estimate bounds.

110 Let $\phi_{\mathbf{z}_i}$ be the Lagrange nodal basis function of \mathcal{S}^1 associated with an interior
111 vertex $\mathbf{z}_i \in \mathcal{N}$. Using these nodal basis functions, the discrete problem in (2.5) may
112 be written as the following system of linear equations:

$$113 \quad (2.6) \quad \mathbf{A} \mathbf{u} = \mathbf{f},$$

114 where the stiffness matrix \mathbf{A} is $\mathbf{A}[i, j] = a_{ij}$ with $a_{ij} = (A\nabla\phi_{z_j}, \nabla\phi_{z_i})$; the \mathbf{u} is the
 115 vector representation of the exact solution $u_{\mathcal{T}}$; and the \mathbf{f} is the vector representation
 116 of the right hand side with i -th row $\mathbf{f}[i]$ of \mathbf{f} being (f, ϕ_{z_i}) . For a given initial guess
 117 $\mathbf{u}^{(0)}$, an iterative solver for problem (2.6) has the following form

$$118 \quad (2.7) \quad \mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \mathbf{B}(\mathbf{f} - \mathbf{A}\mathbf{u}^{(k)}),$$

119 where $\mathbf{u}^{(l)}$ is the vector representation of the l -th iterate $u_{\mathcal{T}}^{(l)}$ for $l = 0, 1, \dots$. Our
 120 attention in this paper is restricted to symmetric iterative methods, i.e., the matrix
 121 \mathbf{B} in (2.7) is symmetric.

122 Next we define the norms for vectors and matrices: with the help of the context,
 123 the usual 2-norm $\|\cdot\|_2$ for a vector $\mathbf{v} \in \mathbb{R}^n$ and a non-singular symmetric matrix
 124 $\mathbf{M} \in \mathbb{R}^{n \times n}$ is defined by:

$$125 \quad (2.8) \quad \|\mathbf{v}\|_2 := \sqrt{\mathbf{v} \cdot \mathbf{v}} \text{ and } \|\mathbf{M}\|_2 := \sup_{\|\mathbf{v}\|_2=1} \|\mathbf{M}\mathbf{v}\|_2 = \rho(\mathbf{M}),$$

126 respectively, where $\rho(\mathbf{M})$ is the spectral radius of \mathbf{M} equaling its largest eigenvalue.

127 The stiffness matrix \mathbf{A} is symmetric positive definite for the Dirichlet boundary
 128 value problem. As a result, $\mathbf{A}^{1/2}$ is non-singular and can be used to induce a norm:

$$129 \quad (2.9) \quad \|\mathbf{v}\|_{\mathbf{A}} := \sqrt{\mathbf{A}\mathbf{v} \cdot \mathbf{v}} = \|\mathbf{A}^{1/2}\mathbf{v}\|_2 \text{ and } \|\mathbf{M}\|_{\mathbf{A}} := \sup_{\|\mathbf{v}\|_{\mathbf{A}}=1} \|\mathbf{M}\mathbf{v}\|_{\mathbf{A}}.$$

130 By definition it is straightforward to verify that:

$$131 \quad (2.10) \quad \|\mathbf{M}\|_{\mathbf{A}} = \sup_{\|\mathbf{A}^{1/2}\mathbf{v}\|_2=1} \|\mathbf{A}^{1/2}\mathbf{M}\mathbf{v}\|_2 = \|\mathbf{A}^{1/2}\mathbf{M}\mathbf{A}^{-1/2}\|_2.$$

132 For a finite element function v and its vector representation \mathbf{v} , the following equiva-
 133 lence between vector norm and Sobolev norm holds as well:

$$134 \quad (2.11) \quad \|v\|_A = \|\mathbf{v}\|_{\mathbf{A}}.$$

135 **3. Discretization error estimator using an equilibrated flux.** In this sec-
 136 tion, firstly the duality theory for the error estimation is introduced. Then a locally
 137 post-processed flux based on the iterate $\bar{u}_{\mathcal{T}} := u_{\mathcal{T}}^{(k)}$ for a fixed $k \geq 1$ is constructed.
 138 Lastly the reliability of the estimator based on this recovered flux is proved in order
 139 that a stopping criterion can be designed for the iterative solver.

140 **3.1. Duality theory.** It is known that the variational problem in (2.1) can be
 141 rewritten as a functional minimization problem, where the primal functional is:

$$142 \quad (3.1) \quad \mathcal{J}(v) := \frac{1}{2} (A\nabla v, \nabla v) - (f, v)$$

143 Then problem (2.1) is equivalent to the following minimization problem:

$$144 \quad (3.2) \quad \text{Find } u \in H_g^1(\Omega) \text{ such that } \mathcal{J}(u) = \min_{v \in H_g^1(\Omega)} \mathcal{J}(v).$$

145 The dual functional with respect to (3.1) is:

$$146 \quad (3.3) \quad \mathcal{J}^*(\boldsymbol{\tau}) := -\frac{1}{2} (A^{-1}\boldsymbol{\tau}, \boldsymbol{\tau}).$$

147 The dual problem is then to maximize $\mathcal{J}^*(\boldsymbol{\tau})$ in the following space:

$$148 \quad (3.4) \quad \boldsymbol{\Sigma} := \{\boldsymbol{\tau} \in \mathbf{H}(\operatorname{div}; \Omega) : \nabla \cdot \boldsymbol{\tau} = f\},$$

149 and can be phrased as:

$$150 \quad (3.5) \quad \text{Find } \boldsymbol{\sigma} \in \boldsymbol{\Sigma} \text{ such that } \mathcal{J}^*(\boldsymbol{\sigma}) = \max_{\boldsymbol{\tau} \in \boldsymbol{\Sigma}} \mathcal{J}^*(\boldsymbol{\tau}).$$

151 The foundation to use the dual problem in constructing a posteriori error estima-
152 tor is that the minimum of the primal functional $\mathcal{J}(\cdot)$ coincides with the maximum
153 of the dual functional $\mathcal{J}^*(\boldsymbol{\sigma})$ (see [19] Chapter 3):

$$154 \quad (3.6) \quad \mathcal{J}(u) = \mathcal{J}^*(\boldsymbol{\sigma}) \text{ and } \boldsymbol{\sigma} = -A\nabla u.$$

155 Now that (3.6) is satisfied, then a guaranteed upper bound can be obtained as follows:
156 for any $\boldsymbol{\sigma}_\tau \in \boldsymbol{\Sigma}_\tau := \boldsymbol{\Sigma} \cap \mathcal{RT}^0$ being a subspace of $\boldsymbol{\Sigma}$, where \mathcal{RT}^0 is the lowest order
157 Raviart-Thomas element (e.g., see [9]),

$$158 \quad (3.7) \quad \|u - \bar{u}_\tau\|_A^2 = 2\left(\mathcal{J}(\bar{u}_\tau) - \mathcal{J}(u)\right) = 2\left(\mathcal{J}(\bar{u}_\tau) - \mathcal{J}^*(\boldsymbol{\sigma})\right) \leq 2\left(\mathcal{J}(\bar{u}_\tau) - \mathcal{J}^*(\boldsymbol{\sigma}_\tau)\right).$$

159 One of the main goals of this paper is to locally construct such $\boldsymbol{\sigma}_\tau$ based on the
160 current iterate \bar{u}_τ , so that the global reliability bound in (3.7) is automatically met.

161 **3.2. Localized flux recovery.** Let $\boldsymbol{\sigma}^\Delta$ be the correction from the numerical
162 flux $\bar{\boldsymbol{\sigma}}_\tau := -A\nabla\bar{u}_\tau$ to the true flux $\boldsymbol{\sigma} := -A\nabla u$:

$$163 \quad (3.8) \quad \boldsymbol{\sigma}^\Delta := \boldsymbol{\sigma} - \bar{\boldsymbol{\sigma}}_\tau$$

164 Decompose $\boldsymbol{\sigma}^\Delta$ by a partition of unity $\{\phi_z\}_{z \in \mathcal{N}}$, which is the set of the nodal basis
165 functions for the linear finite element space \mathcal{S}^1 , as follows:

$$166 \quad (3.9) \quad \boldsymbol{\sigma}^\Delta = \sum_{z \in \mathcal{N}} \boldsymbol{\sigma}_z^\Delta \text{ with } \boldsymbol{\sigma}_z^\Delta := \phi_z \boldsymbol{\sigma}^\Delta.$$

167 Denote the element residual on an element K and the jump of the normal component
168 of the numerical flux on a face F by

$$169 \quad (3.10) \quad r_K := \{f + \nabla \cdot (A\nabla\bar{u}_\tau)\}_K = f_K$$

$$170 \quad (3.11) \text{ and } j_F := -\llbracket A\nabla(u - \bar{u}_\tau) \cdot \mathbf{n}_F \rrbracket_F = \begin{cases} \llbracket A\nabla\bar{u}_\tau \cdot \mathbf{n}_F \rrbracket_F, & \text{if } F \in \mathcal{F}_z, \\ A\nabla(u - \bar{u}_\tau) \cdot \mathbf{n}_F, & \text{if } F \subset \partial\Omega, \end{cases}$$

171 respectively. Note that r_K and j_F are constants in K and on F if F is an interior
172 face, respectively. When $z \notin \partial\Omega$ is an interior vertex, $\boldsymbol{\sigma}_z^\Delta$ satisfies the following local
173 problem:

$$174 \quad (3.12) \quad \begin{cases} \nabla \cdot \boldsymbol{\sigma}_z^\Delta = \phi_z r_K - \nabla \phi_z \cdot \nabla(u - \bar{u}_\tau), & \text{on } K \subset \omega_z, \\ \llbracket \boldsymbol{\sigma}_z^\Delta \cdot \mathbf{n}_F \rrbracket_F = \phi_z j_F, & \text{on } F \in \mathcal{F}_z, \\ \boldsymbol{\sigma}_z^\Delta \cdot \mathbf{n}_F = 0, & \text{on } F \subset \partial\omega_z. \end{cases}$$

175 If $z \in \partial\Omega$, then the first equation in (3.12) is unchanged, and the flux jump equations
176 change to

$$177 \quad (3.13) \quad \begin{cases} \llbracket \boldsymbol{\sigma}_z^\Delta \cdot \mathbf{n}_F \rrbracket_F = \phi_z j_F, & \text{on } F \in \mathcal{F}_z \text{ and } F \not\subset \partial\omega_z \cap \partial\Omega, \\ \boldsymbol{\sigma}_z^\Delta \cdot \mathbf{n}_F = 0, & \text{on } F \subset \partial\omega_z \setminus \partial\Omega. \end{cases}$$

178 To approximate problem (3.12), an approximated correction flux $\sigma_{z,\tau}^\Delta$ is sought
 179 in the following broken lowest-order Raviart-Thomas space:

$$180 \quad (3.14) \quad \mathcal{RT}_{-1,\omega_z}^0 := \left\{ \tau \in L^2(\omega_z) : \tau|_K \in \mathcal{RT}^0(K), \forall K \subset \omega_z \right\},$$

181 where $\mathcal{RT}^0(K)$ denotes the local lowest-order Raviart-Thomas space on K (see [9]).

182 An explicit procedure called the hypercircle method or equilibration (see [7, 8])
 183 is used to construct $\sigma_{z,\tau}^\Delta$. The correction flux $\sigma_{z,\tau}^\Delta$ satisfies the following problem on
 184 an interior vertex patch ω_z ($z \notin \partial\Omega$):

$$185 \quad (3.15) \quad \begin{cases} \nabla \cdot \sigma_{z,\tau}^\Delta = \bar{r}_{K,z} + c_z, & \text{on } K \subset \omega_z, \\ \llbracket \sigma_{z,\tau}^\Delta \cdot \mathbf{n}_F \rrbracket_F = \bar{j}_{F,z}, & \text{on } F \in \mathcal{F}_z, \\ \sigma_{z,\tau}^\Delta \cdot \mathbf{n}_F = 0, & \text{on } F \subset \partial\omega_z, \end{cases}$$

186 where $\bar{r}_{K,z}$ and $\bar{j}_{F,z}$ are defined as the L^2 -projection of $\phi_z r_K$ and $\phi_z j_F$ onto the
 187 constant space of K and interior F , respectively, for $d = 2, 3$:

$$188 \quad (3.16) \quad \begin{aligned} \bar{r}_{K,z} &:= \Pi_K(\phi_z r_K) = \frac{1}{d+1} f_K = \frac{1}{d+1} r_K, \\ \bar{j}_{F,z} &:= \Pi_F(\phi_z j_F) = \frac{1}{d} \llbracket (A \nabla \bar{u}_\tau) \cdot \mathbf{n}_F \rrbracket_F = \frac{1}{d} j_F. \end{aligned}$$

189 When $z \in \partial\Omega$, $c_z = 0$, and the normal fluxes in (3.15) are modified accordingly by
 190 (3.13).

191 Note that, without c_z , the compatibility condition for (3.15) is not automatically
 192 satisfied, that is,

$$193 \quad \sum_{K \subset \omega_z} (\bar{r}_{K,z}, 1)_K - \sum_{F \in \mathcal{F}_z} (\bar{j}_{F,z}, 1)_F \neq 0,$$

194 which implies that (3.15) does not have a solution. To guarantee the existence of
 195 a solution to (3.15), an element-wise compensation term c_z is added on the right
 196 hand side of the divergence equation in (3.15). Notice that the normal fluxes are
 197 kept unchanged so that the final recovered flux can still fulfill the $\mathbf{H}(\text{div})$ -continuity
 198 condition of the space in (3.4). The c_z is defined as a constant on this vertex patch
 199 ω_z enforcing the compatibility condition for (3.15):

$$200 \quad (3.17) \quad \sum_{K \subset \omega_z} (\bar{r}_{K,z} + c_z, 1)_K - \sum_{F \in \mathcal{F}_z} (\bar{j}_{F,z}, 1)_F = 0,$$

201 which, together with (3.16), yields for an interior vertex z

$$202 \quad (3.18) \quad \begin{aligned} c_z &:= \frac{1}{|\omega_z|} \left(\sum_{F \in \mathcal{F}_z} (\bar{j}_{F,z}, 1)_F - \sum_{K \subset \omega_z} (\bar{r}_{K,z}, 1)_K \right) \\ &= \frac{1}{|\omega_z|} \left(\sum_{F \in \mathcal{F}_z} (j_F, \phi_z)_F - \sum_{K \subset \omega_z} (r_K, \phi_z)_K \right) \\ &= \frac{1}{|\omega_z|} (A \nabla(u - \bar{u}_\tau), \nabla \phi_z)_{\omega_z}. \end{aligned}$$

203 With c_z , the solution to (3.15) exists since the compatibility condition (3.17) is met
 204 (see [8, 13]). We note that if \bar{u}_τ solves (2.5) exactly, i.e., $\bar{u}_\tau = u_\tau$, then $c_z = 0$ for
 205 an interior vertex by (3.18), and this is a consequence of the Galerkin orthogonality.

206 In the case that \bar{u}_τ is not an exact solution to problem (2.5), we emphasize
 207 again that problem (3.15) is not solvable without the presence of c_z . The Galerkin
 208 orthogonality, which occurs as the compatibility condition for (3.15) if $z \notin \partial\Omega$, is
 209 violated if \bar{u}_τ is not the exact finite element approximation.

210 We also note that if $z \in \partial\Omega$, the Galerkin orthogonality does not hold either,
 211 $(A\nabla u_\tau, \nabla\phi_z) \neq (f, \phi_z) = (A\nabla u, \nabla\phi_z)$, since the nodal basis ϕ_z is not in the test
 212 function space for the discretized problem in (2.5). A direct usage of (3.18) implies
 213 $c_z \neq 0$, yet, the degrees of freedom for $\sigma_{z,\tau}^\Delta$ on the faces on $\partial\omega_z \cap \partial\Omega$ are treated as
 214 unknowns in (3.19), and c_z is not needed in (3.15) on a boundary vertex $z \in \partial\Omega$.

215 The flux correction is postprocessed by a minimization procedure locally on ω_z :

$$216 \quad (3.19) \quad \left\| A^{-1/2} \sigma_{z,\tau}^\Delta \right\|_{0,\omega_z} = \min_{\tau \in \Sigma_{z,\tau}} \left\| A^{-1/2} \tau \right\|_{0,\omega_z},$$

217 where $\Sigma_{z,\tau} := \{ \tau \in \mathcal{RT}_{-1,\omega_z}^0 : \tau \text{ satisfies (3.15)} \}$. The element-wise and the global
 218 flux corrections are then:

$$219 \quad (3.20) \quad \sigma_{K,\tau}^\Delta := \sum_{z \in \mathcal{N}_K} \sigma_{z,\tau}^\Delta \quad \text{and} \quad \sigma_\tau^\Delta := \sum_{z \in \mathcal{N}} \sigma_{z,\tau}^\Delta.$$

220 Lastly, a compensatory flux σ_τ^c , which is in the globally $\mathbf{H}(\text{div})$ -conforming \mathcal{RT}^0
 221 space, is then sought using c_z defined in (3.18) as data:

$$222 \quad (3.21) \quad \nabla \cdot \sigma_\tau^c = - \sum_{z \in \mathcal{N}_K} c_z, \quad \text{in any } K \in \mathcal{T},$$

223 By the surjectivity of the divergence operator from \mathcal{RT}^0 to \mathcal{S}^0 , the above problem
 224 has a solution (e.g., [9, ?]). If σ_τ^c is sought by minimizing a weighted L^2 -norm, with
 225 (3.21) being a constraint, then it is equivalent to seeking the solution to a mixed
 226 finite element approximation problem in the \mathcal{RT}^0 - \mathcal{S}^0 pair. The energy estimate in
 227 a weighted L^2 -norm for σ_τ^c , which bridges it with the algebraic error, will be shown
 228 later in Lemma 3.

229 The recovered flux based on the \bar{u}_τ is defined as:

$$230 \quad (3.22) \quad \sigma_\tau := -A\nabla\bar{u}_\tau + \sigma_\tau^\Delta + \sigma_\tau^c.$$

231 In practice, only σ_τ^Δ is explicitly computed. For explicit local constructions of σ_τ^Δ ,
 232 we refer the readers to [13, 8]. The σ_τ^c is here to compensate the change in divergence
 233 caused by the correction term c_z , and is not needed, nor explicitly computed for the
 234 estimator defined in (3.23).

235 **LEMMA 1.** *The recovered flux σ_τ is in the conforming finite element subspace of*
 236 *the duality space: $\sigma_\tau \in \Sigma_\tau := \Sigma \cap \mathcal{RT}^0$.*

237 *Proof.* Using (3.15) and (3.21), together with the fact that $A\nabla\bar{u}_\tau$ is a constant
 238 vector on each element K , we have:

$$239 \quad \nabla \cdot \sigma_\tau|_K = \nabla \cdot \sigma_\tau^\Delta + \nabla \cdot \sigma_\tau^c = \sum_{z \in \mathcal{N}_K} \bar{r}_{K,z} = f_K.$$

240 On $F \in \mathcal{F}$, the continuity of the normal component implies $\sigma_\tau^c \in \mathbf{H}(\text{div}; \Omega)$

$$241 \quad \llbracket \sigma_\tau \cdot \mathbf{n} \rrbracket_F = \llbracket \sigma_\tau^\Delta \cdot \mathbf{n} \rrbracket_F - \llbracket A\nabla\bar{u}_\tau \cdot \mathbf{n} \rrbracket_F = \sum_{z \in \mathcal{N}(F)} \bar{j}_{F,z} - j_F = 0. \quad \square$$

242 **3.3. Discretization error estimator and reliability.** With the recovered flux
 243 correction defined in (3.20), we define the discretization error estimator η_d as:

$$244 \quad (3.23) \quad \eta_{d,K} = \|A^{-1/2} \boldsymbol{\sigma}_{K,\tau}^\Delta\|_{0,K}, \quad \text{and} \quad \eta_d = \|A^{-1/2} \boldsymbol{\sigma}_\tau^\Delta\|_0.$$

245 The reliability we show in this section is: the total error $\|u - \bar{u}_\tau\|_A$ is bounded by
 246 the error estimator η_d plus the algebraic error.

247 In (3.18), the representation of $c_{\mathbf{z}}$ uses $u - \bar{u}_\tau$. Nevertheless, inserting the Galerkin
 248 orthogonality into (3.18), which reads $(A\nabla(u - u_\tau), \nabla\phi_{\mathbf{z}})_{\omega_{\mathbf{z}}} = 0$ for any interior
 249 vertex \mathbf{z} , we have

$$250 \quad (3.24) \quad c_{\mathbf{z}} = \frac{1}{|\omega_{\mathbf{z}}|} (A\nabla(u_\tau - \bar{u}_\tau), \nabla\phi_{\mathbf{z}})_{\omega_{\mathbf{z}}} = \frac{1}{|\omega_{\mathbf{z}}|} \sum_{K \subset \omega_{\mathbf{z}}} (A\nabla(u_\tau - \bar{u}_\tau), \nabla\phi_{\mathbf{z}})_K.$$

251 Now the compatibility compensation term $c_{\mathbf{z}}$ can be decomposed as follows:

$$252 \quad (3.25) \quad c_{\mathbf{z}} = \sum_{K \subset \omega_{\mathbf{z}}} c_{\mathbf{z},K}, \quad \text{with} \quad c_{\mathbf{z},K} := \frac{1}{|\omega_{\mathbf{z}}|} (A\nabla(u_\tau - \bar{u}_\tau), \nabla\phi_{\mathbf{z}})_K.$$

253 **LEMMA 2** (Nodal estimate for the compensation term). *For any interior vertex*
 254 *$\mathbf{z} \in \mathcal{N}_K$, on $K \subset \omega_{\mathbf{z}}$, $c_{\mathbf{z},K}$ satisfies the following L^2 -estimate with C depending on*
 255 *the shape regularity of the patch $\omega_{\mathbf{z}}$:*

$$256 \quad (3.26) \quad h_K A_K^{-1/2} \|c_{\mathbf{z},K}\|_{0,K} \leq C \|u_\tau - \bar{u}_\tau\|_{A,K},$$

257 *Proof.* By the representation in (3.25), it follows from the Cauchy-Schwarz in-
 258 equality, the fact that $\|\nabla\phi_{\mathbf{z}}\|_{0,K} \leq C h_K^{\frac{d}{2}-1}$, and the shape regularity of the patch
 259 that

$$260 \quad |c_{\mathbf{z},K}| = \frac{1}{|\omega_{\mathbf{z}}|} |(A\nabla(u - \bar{u}_\tau), \nabla\phi_{\mathbf{z}})_K| \leq \frac{1}{|\omega_{\mathbf{z}}|} \|u - \bar{u}_\tau\|_{A,K} \|\phi_{\mathbf{z}}\|_{A,K}$$

$$261 \quad \leq C h_K^{-\frac{d}{2}-1} A_K^{1/2} \|u - \bar{u}_\tau\|_{A,K}.$$

262 Since $c_{\mathbf{z},K}$ is a constant on K , $\|c_{\mathbf{z}}\|_{0,K} \leq h_K^{\frac{d}{2}} |c_{\mathbf{z},K}|$, the validity of (3.26) is then
 263 verified. \square

264 To bridge the energy estimate for $\boldsymbol{\sigma}_\tau^c$ with the algebraic error, the following norms
 265 are need: let $A_F := \max_{K \subset \omega_F} A_K$, for $p \in \mathcal{S}^0$, and $f \in L^2(\Omega)$

$$266 \quad (3.27) \quad \|f\|_{-1,h} := \sup_{q \in \mathcal{S}^0} \frac{(f, q)}{\|q\|_{1,h}}, \quad \text{and} \quad \|p\|_{1,h} := \left(\sum_{F \in \mathcal{F}} h_F^{-1} A_F \left\| \llbracket p \rrbracket \right\|_{0,F}^2 \right)^{1/2}.$$

267 **LEMMA 3** (A discrete energy estimate for $\boldsymbol{\sigma}_\tau^c$). *If $\boldsymbol{\sigma}_\tau^c$ is obtained by*

$$268 \quad (3.28) \quad \left\| A^{-1/2} \boldsymbol{\sigma}_\tau^c \right\|_0 = \min_{\substack{\boldsymbol{\tau} \in \mathcal{RT}^0 \\ \nabla \cdot \boldsymbol{\tau} = f^c}} \left\| A^{-1/2} \boldsymbol{\tau} \right\|_0,$$

269 *where f^c is defined as follows on an element K using (3.21),*

$$270 \quad (3.29) \quad f^c|_K := - \sum_{\mathbf{z} \in \mathcal{N}_K} c_{\mathbf{z}}$$

271 then the following estimate holds:

$$272 \quad (3.30) \quad \left\| A^{-1/2} \boldsymbol{\sigma}_\tau^c \right\|_0 \leq C_A \|u_\tau - \bar{u}_\tau\|_A,$$

273 in which C depends on the shape regularity of the triangulation, the maximum number
274 of elements in each ω_K , and the diffusion coefficient A .

275 *Proof.* The minimizer of problem (3.28) satisfies the following global mixed prob-
276 lem: find $(\boldsymbol{\sigma}_\tau^c, p) \in \mathcal{RT}^0 \times \mathcal{S}^0$

$$277 \quad (3.31) \quad \begin{cases} (A^{-1} \boldsymbol{\sigma}_\tau^c, \boldsymbol{\tau}) - (p, \nabla \cdot \boldsymbol{\tau}) = 0, & \forall \boldsymbol{\tau} \in \mathcal{RT}^0, \\ (\nabla \cdot \boldsymbol{\sigma}_\tau^c, q) = (f^c, q), & \forall q \in \mathcal{S}^0. \end{cases}$$

278 By the inf-sup stability of discrete H^1 - L^2 analysis of the mixed problem when the
279 shape regularity of the mesh is assumed ($h_F \approx h_K$ for F 's neighboring elements) ([7,
280 Chapter 3 §5.7]), problem (3.31) has a unique solution satisfying the following energy
281 estimate: letting $\boldsymbol{\tau} = \boldsymbol{\sigma}_\tau^c$, $q = p$, we have

$$282 \quad (3.32) \quad \begin{aligned} & \left\| A^{-1/2} \boldsymbol{\sigma}_\tau^c \right\|_0^2 \leq \|f^c\|_{-1,h} \|p\|_{1,h} \leq \|f^c\|_{-1,h} \sup_{\boldsymbol{\tau} \in \mathcal{RT}^0} \frac{(p, \nabla \cdot \boldsymbol{\tau})}{\left\| A^{-1/2} \boldsymbol{\tau} \right\|_0} \\ & = \|f^c\|_{-1,h} \sup_{\boldsymbol{\tau} \in \mathcal{RT}^0} \frac{(A^{-1} \boldsymbol{\sigma}_\tau^c, \boldsymbol{\tau})}{\left\| A^{-1/2} \boldsymbol{\tau} \right\|_0} \leq \|f^c\|_{-1,h} \left\| A^{-1/2} \boldsymbol{\sigma}_\tau^c \right\|_0. \end{aligned}$$

283 Now, to prove the validity of the lemma, by (3.27), it suffices to show that for $q \in \mathcal{S}^0$

$$284 \quad (3.33) \quad (f^c, q) \leq C \|u_\tau - \bar{u}_\tau\|_A \|q\|_{1,h}.$$

285 To this end, first denote $q_K := q|_K$, and f_c is written out explicitly using (3.29),

$$286 \quad (3.34) \quad (f^c, q) = - \sum_{K \in \mathcal{T}} \left(\sum_{\mathbf{z} \in \mathcal{N}_K} c_{\mathbf{z}, K} \right)_K = - \sum_{K \in \mathcal{T}} \sum_{\mathbf{z} \in \mathcal{N}_K} c_{\mathbf{z}, K} q_K |K|.$$

287 Using $c_{\mathbf{z}} = \sum_{K \subset \omega_{\mathbf{z}}} c_{\mathbf{z}, K}$ in (3.25) for interior vertices and $c_{\mathbf{z}} = 0$ for $\mathbf{z} \in \partial\Omega$ yields,

$$288 \quad (3.35) \quad (f^c, q) = - \sum_{K \in \mathcal{T}} \sum_{\mathbf{z} \in \mathcal{N}_K, \mathbf{z} \notin \partial\Omega} \left(\sum_{T \subset \omega_{\mathbf{z}}} c_{\mathbf{z}, T} \right) q_K |K|.$$

289 We switch the order of the summation, by summing up the inner terms $c_{\mathbf{z}, T}$ last, then
290 the above equation becomes

$$291 \quad (3.36) \quad \begin{aligned} & - \sum_{K \in \mathcal{T}} \sum_{\mathbf{z} \in \mathcal{N}_K, \mathbf{z} \notin \partial\Omega} \left(\sum_{T \subset \omega_{\mathbf{z}}} c_{\mathbf{z}, T} \right) q_K |K| \\ & = - \sum_{K \in \mathcal{T}} \sum_{\mathbf{z} \in \mathcal{N}_K, \mathbf{z} \notin \partial\Omega} \left\{ c_{\mathbf{z}, K} \left(\sum_{T \subset \omega_{\mathbf{z}}} q_T |T| \right) \right\} =: -(*), \end{aligned}$$

292 in which for each vertex $\mathbf{z} \in \mathcal{N}_K$, the term $c_{\mathbf{z}, K}$ is only summed against $q_T |T|$ for
293 $T \subset \omega_{\mathbf{z}}$. The reason is that among the terms in the original summation in (3.35), a
294 term involving $c_{\mathbf{z}, T}$ is summed up multiplying $q_K |K|$ only when $\omega_{\mathbf{z}} \subset \omega_K$.

295 Now on each K not touching $\partial\Omega$, we have the following weighted average of $c_{z,K}$,
 296 using $|\omega_z|m_K$ as weights, being zero for any m_K that is a constant on the patch ω_K :

$$297 \quad (3.37) \quad \sum_{z \in \mathcal{N}_K, z \notin \partial\Omega} c_{z,K}(|\omega_z|m_K) = m_K \sum_{z \in \mathcal{N}_K, z \notin \partial\Omega} (A\nabla(u_\tau - \bar{u}_\tau), \nabla\phi_z)_K = 0.$$

298 As a result, $|\omega_z|m_K$ can be inserted into (3.36), and m_K is chosen as the average of
 299 q on ω_K , i.e., $m_K := (\sum_{P \subset \omega_K} q_P|P|)/|\omega_K|$, thus (*) in (3.36) becomes
 (3.38)

$$300 \quad \sum_{K \in \mathcal{T}} \sum_{z \in \mathcal{N}_K, z \notin \partial\Omega} \left\{ c_{z,K} \left(\sum_{T \subset \omega_z} q_T|T| - \frac{|\omega_z|}{|\omega_K|} \sum_{P \subset \omega_K} q_P|P| \right) \right\}$$

$$= \sum_{K \in \mathcal{T}} \sum_{z \in \mathcal{N}_K, z \notin \partial\Omega} \left\{ c_{z,K} \sum_{T \subset \omega_z} \left(\frac{|T|}{|\omega_K|} \sum_{P \subset \omega_K} (q_T - q_P)|P| \right) \right\} =: \sum_{K \in \mathcal{T}} \sum_{z \in \mathcal{N}_K, z \notin \partial\Omega} \beta_{z,K}.$$

301 For any $T \subset \omega_z$, if T and $P \subset \omega_K$ have a common face $F = \partial T \cap \partial P$, $|q_T - q_P| = \llbracket q \rrbracket_F$
 302 on F ; otherwise, there always exists a path consisting of finite many elements $K_i \subset \omega_K$
 303 ($i = 1, \dots, n_{TP}$) starting from $K_1 := T$ to $K_{n_{TP}} := P$, such that K_i and K_{i-1} share
 304 a face F_i , then

$$305 \quad (3.39) \quad |q_T - q_P| = |q_{K_1} - q_{K_2} + q_{K_2} - q_{K_3} \dots| \leq \sum_{i=1}^{n_{TP}} \left| \llbracket q \rrbracket_{F_i} \right| \leq \sum_{F \in \mathcal{F}_{\omega_K}} \left| \llbracket q \rrbracket_F \right|.$$

306 Applying above on the innermost summation for P of (3.38), exploiting the local
 307 shape regularity on every element in ω_K , and using the fact that $c_{z,K}$ and $\llbracket q \rrbracket_F$
 308 are constants on K and F , respectively, yields:

$$309 \quad (3.40) \quad \beta_{z,K} \leq |c_{z,K}| \left| \sum_{T \subset \omega_z} \left(\frac{|T|}{|\omega_K|} \sum_{P \subset \omega_K} (q_T - q_P)|P| \right) \right| \leq |c_{z,K}| \left(\sum_{T \subset \omega_z} |T| \sum_{F \in \mathcal{F}_{\omega_K}} \left| \llbracket q \rrbracket_F \right| \right)$$

$$\leq CA_K^{-1/2} h_K \|c_{z,K}\|_{0,K} \cdot A_K^{1/2} h_K^{-1} |K|^{1/2} \left(\sum_{F \in \mathcal{F}_{\omega_K}} \left\| \llbracket q \rrbracket_F \right\|_{0,F} |F|^{-1/2} \right).$$

310 Using the Cauchy-Schwarz inequality and the shape regularity of the triangulation,
 311 (*) can be estimated as follows:

$$312 \quad (3.41) \quad (*) \leq C \left(\sum_{K \in \mathcal{T}} \sum_{z \in \mathcal{N}_K, z \notin \partial\Omega} A_K^{-1} h_K^2 \|c_{z,K}\|_{0,K}^2 \right)^{1/2}$$

$$\left(\sum_{K \in \mathcal{T}} \sum_{z \in \mathcal{N}_K, z \notin \partial\Omega} A_K \sum_{F \in \mathcal{F}_{\omega_K}} h_F^{-1} \left\| \llbracket q \rrbracket_F \right\|_{0,F}^2 \right)^{1/2}.$$

313 Finally, the lemma follows from Lemma 2 and definition (3.27). \square

314 **THEOREM 4.** *There exists a positive constant C_A , depending on the shape regu-*
 315 *larity of the mesh and the coefficient A , such that*

$$316 \quad (3.42) \quad \|u - \bar{u}_\tau\|_A \leq \eta_d + C_A \|u_\tau - \bar{u}_\tau\|_A.$$

317 *Proof.* The proof of (3.42) starts from (3.7)

$$318 \quad \|u - \bar{u}_\tau\|_A^2 \leq 2\left(\mathcal{J}(\bar{u}_\tau) - \mathcal{J}^*(\boldsymbol{\sigma}_\tau)\right) = \left\|A^{1/2}\nabla\bar{u}_\tau\right\|_0^2 - 2(f, \bar{u}_\tau) + (A^{-1}\boldsymbol{\sigma}_\tau, \boldsymbol{\sigma}_\tau).$$

319 With $\boldsymbol{\sigma}_\tau = -A\nabla\bar{u}_\tau + \boldsymbol{\sigma}_\tau^\Delta + \boldsymbol{\sigma}_\tau^c$ defined in (3.22), we have

$$320 \quad (A^{-1}\boldsymbol{\sigma}_\tau, \boldsymbol{\sigma}_\tau) = \left\|A^{-1/2}(\boldsymbol{\sigma}_\tau^\Delta + \boldsymbol{\sigma}_\tau^c)\right\|_0^2 - 2(\boldsymbol{\sigma}_\tau, \nabla\bar{u}_\tau) - \left\|A^{1/2}\nabla\bar{u}_\tau\right\|_0^2,$$

321 which, together with the above inequality, implies

$$322 \quad \|u - \bar{u}_\tau\|_A^2 \leq \left\|A^{-1/2}(\boldsymbol{\sigma}_\tau^\Delta + \boldsymbol{\sigma}_\tau^c)\right\|_0^2 - 2(\boldsymbol{\sigma}_\tau, \nabla\bar{u}_\tau) - 2(f, \bar{u}_\tau)$$

$$323 \quad = \left\|A^{-1/2}(\boldsymbol{\sigma}_\tau^\Delta + \boldsymbol{\sigma}_\tau^c)\right\|_0^2.$$

324 The last equality uses the fact that $(\boldsymbol{\sigma}_\tau, \nabla\bar{u}_\tau) + (f, \bar{u}_\tau) = 0$, which follows from
325 integration by parts element-wise and Lemma 1. By the triangle inequality, we have

$$326 \quad \|u - \bar{u}_\tau\|_A \leq \left\|A^{-1/2}\boldsymbol{\sigma}_\tau^\Delta\right\|_0 + \left\|A^{-1/2}\boldsymbol{\sigma}_\tau^c\right\|_0 = \eta_d + \left\|A^{-1/2}\boldsymbol{\sigma}_\tau^c\right\|_0.$$

327 Now, the theorem simply follows from estimate (3.30) in Lemma 3. \square

328 **4. Algebraic error estimator.** The upper bound in (3.42) contains the al-
329 gebraic error $\|u_\tau - \bar{u}_\tau\|_A$. This section introduces an algebraic error estimator in
330 terms of the energy norm of two consecutive iterates with a constant depending on
331 an approximation of the spectral radius of the error propagation matrix.

332 Recall the stiffness matrix \mathbf{A} introduced in Section 2 and the iteration in (2.7).
333 Denote the algebraic iteration error at the k -th iteration by

$$334 \quad (4.1) \quad \mathbf{e}^{(k)} := \mathbf{u}_\tau - \mathbf{u}_\tau^{(k)},$$

335 then the error propagation can be verified to be:

$$336 \quad (4.2) \quad \mathbf{e}^{(k+1)} = (\mathbf{I} - \mathbf{BA})\mathbf{e}^{(k)}.$$

337 Let $e^{(k)}$ be the function in the finite element space having $\mathbf{e}^{(k)}$ as its vector represen-
338 tation in the nodal basis. Define the spectral radius of the error propagation matrix
339 $\mathbf{I} - \mathbf{BA}$ as ρ_{err} :

$$340 \quad (4.3) \quad \rho_{\text{err}} := \rho(\mathbf{I} - \mathbf{BA}) = \|\mathbf{I} - \mathbf{BA}\|_2.$$

341 **THEOREM 5** (Upper bound of the algebraic error). *Let $\{\mathbf{u}^{(k)}\}$ be the sequence*
342 *generated by (2.7), then the algebraic error $\mathbf{e}^{(k)}$ defined in (4.1) satisfies the following*
343 *estimate:*

$$344 \quad (4.4) \quad \left\|\mathbf{e}^{(k+1)}\right\|_{\mathbf{A}} \leq \frac{\rho_{\text{err}}}{1 - \rho_{\text{err}}} \left\|\mathbf{u}^{(k+1)} - \mathbf{u}^{(k)}\right\|_{\mathbf{A}},$$

345 *or in the finite element function form:*

$$346 \quad (4.5) \quad \left\|u_\tau - u_\tau^{(k+1)}\right\|_A \leq \frac{\rho_{\text{err}}}{1 - \rho_{\text{err}}} \left\|u_\tau^{(k+1)} - u_\tau^{(k)}\right\|_A.$$

347 *Proof.* By the norm equivalence in (2.10) and the fact that $(\mathbf{I} - \mathbf{A}^{1/2}\mathbf{B}\mathbf{A}^{-1/2})$ is
 348 similar to $(\mathbf{I} - \mathbf{B}\mathbf{A})$ (they have the same eigenvalues), we have

$$349 \quad (4.6) \quad \|\mathbf{I} - \mathbf{B}\mathbf{A}\|_{\mathbf{A}} = \left\| \mathbf{A}^{1/2}(\mathbf{I} - \mathbf{B}\mathbf{A})\mathbf{A}^{-1/2} \right\|_2 = \rho(\mathbf{I} - \mathbf{A}^{1/2}\mathbf{B}\mathbf{A}^{-1/2}) = \rho_{\text{err}}.$$

350 Hence, $\|\mathbf{e}^{(k+1)}\|_{\mathbf{A}} \leq \rho_{\text{err}} \|\mathbf{e}^{(k)}\|_{\mathbf{A}}$, and the result follows from a standard contraction
 351 mapping convergence theorem (see, e.g., [22, Theorem 12.1.2]). \square

352 In Theorem 5, ρ_{err} is the true rate of convergence of the solver. However, in
 353 practice, ρ_{err} is not available during any iteration of the solver, unless an eigenvalue
 354 problem is solved for the error propagation matrix $\mathbf{I} - \mathbf{B}\mathbf{A}$. What we have access to
 355 is the following quantity:

$$356 \quad (4.7) \quad \rho_{\text{err}}^{(k)} := \frac{\|\mathbf{r}_k\|_2}{\|\mathbf{r}_{k-1}\|_2},$$

357 where $\mathbf{r}_k := \mathbf{A}\mathbf{e}^{(k)}$ with j -th entry given by $(f, \phi_{z_j}) - (A\nabla u_{\tau}^{(k)}, \nabla \phi_{z_j})$. The fol-
 358 lowing lemma describes the convergence of $\rho_{\text{err}}^{(k)}$ provided that the iterative solver is
 359 convergent.

360 **LEMMA 6** (Convergence of $\rho_{\text{err}}^{(k)}$). *Assuming the error propagation matrix $\mathbf{I} - \mathbf{B}\mathbf{A}$
 361 has eigenvalues $1 > \rho_{\text{err}} = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_N > 0$, then $\rho_{\text{err}}^{(k)} \rightarrow \rho_{\text{err}}$ as $k \rightarrow \infty$.*

362 *Proof.* First notice that, by applying (4.2) from 0 to k in a cascading fashion,

$$363 \quad \mathbf{r}_k = \mathbf{A}\mathbf{e}^{(k)} = \mathbf{A}(\mathbf{I} - \mathbf{B}\mathbf{A})^k \mathbf{e}^{(0)} = (\mathbf{I} - \mathbf{A}\mathbf{B})^k \mathbf{A}\mathbf{e}^{(0)} = (\mathbf{I} - \mathbf{A}\mathbf{B})^k \mathbf{r}_0.$$

364 Since $\mathbf{A}^{-1}(\mathbf{I} - \mathbf{A}\mathbf{B})\mathbf{A} = \mathbf{I} - \mathbf{B}\mathbf{A}$, $\mathbf{I} - \mathbf{A}\mathbf{B}$ and $\mathbf{I} - \mathbf{B}\mathbf{A}$ share the same eigenvalues
 365 and eigenvectors. Suppose that $\{\mathbf{v}_i\}_{i=1}^N$ are the set of orthonormal eigenvectors in the
 366 ℓ^2 -sense corresponding to the eigenvalue set $\{\lambda_i\}_{i=1}^N$. Let $c_i = \mathbf{r}_0 \cdot \mathbf{v}_i$ be the coefficient
 367 of the eigen-expansion of \mathbf{r}_0 . Without loss of generality, assume the multiplicity of
 368 the largest eigenvalue λ_1 is 1. Then we have:

$$369 \quad (4.8) \quad \begin{aligned} \rho_{\text{err}}^{(k)} &= \frac{\|(\mathbf{I} - \mathbf{A}\mathbf{B})^k \mathbf{r}_0\|_2}{\|(\mathbf{I} - \mathbf{A}\mathbf{B})^{k-1} \mathbf{r}_0\|_2} = \frac{\left\| \sum_{i=1}^N \lambda_i^k c_i \mathbf{v}_i \right\|_2}{\left\| \sum_{i=1}^N \lambda_i^{k-1} c_i \mathbf{v}_i \right\|_2} \\ &= \lambda_1 \frac{\left\| \sum_{i=1}^N \left(\frac{\lambda_i}{\lambda_1}\right)^k c_i \mathbf{v}_i \right\|_2}{\left\| \sum_{i=1}^N \left(\frac{\lambda_i}{\lambda_1}\right)^{k-1} c_i \mathbf{v}_i \right\|_2} = \lambda_1 \frac{1 + \sum_{i=2}^N b_i \gamma_i^k}{1 + \sum_{i=2}^N b_i \gamma_i^{k-1}}, \end{aligned}$$

370 where $b_i := (c_i/c_1)^2$, and $\gamma_i := (\lambda_i/\lambda_1)^2$. The lemma follows from letting $k \rightarrow \infty$.
 371 When the multiplicity of λ_1 is $m \geq 2$, factoring out the first m terms and i starts
 372 from $(m+1)$ in the eigen-expansion in (4.8) yields the same result. \square

373 **LEMMA 7** (Monotonicity of $\rho_{\text{err}}^{(k)}$). *Under the same assumption as in Lemma 6,
 374 $\rho_{\text{err}}^{(k)} \leq \rho_{\text{err}}^{(k+1)}$, for any fixed $k \in \mathbb{R}^+$.*

375 *Proof.* By (4.8), to prove the validity of the lemma, it suffices to show that:

$$376 \quad (4.9) \quad \left(1 + \sum_{i=2}^N b_i \gamma_i^k \right)^2 \leq \left(1 + \sum_{i=2}^N b_i \gamma_i^{k-1} \right) \left(1 + \sum_{i=2}^N b_i \gamma_i^{k+1} \right),$$

377 which is equivalent to
 (4.10)

$$378 \quad 2 \sum_{i=2}^N b_i \gamma_i^k + \left(\sum_{i=2}^N b_i \gamma_i^k \right)^2 \leq \sum_{i=2}^N b_i (\gamma_i^{k-1} + \gamma_i^{k-1}) + \left(\sum_{i=2}^N b_i \gamma_i^{k-1} \right) \left(\sum_{i=2}^N b_i \gamma_i^{k+1} \right).$$

379 Since $b_i \geq 0$, $\lambda_i \geq 0$, and $2\gamma_i \leq 1 + \gamma_i^2$, we have

$$380 \quad 2 \sum_{i=2}^N b_i \gamma_i^k \leq \sum_{i=2}^N b_i (\gamma_i^{k-1} + \gamma_i^{k-1}),$$

381 Then it suffices to show the following inequality:

$$382 \quad (4.11) \quad a := \left(\sum_{i=2}^N b_i \gamma_i^k \right)^2 - \left(\sum_{i=2}^N b_i \gamma_i^{k-1} \right) \left(\sum_{i=2}^N b_i \gamma_i^{k+1} \right) \leq 0,$$

383 which will be proved by a standard inductive argument. To this end, let $N = 2$, it is
 384 easy to see that (4.11) holds with equality. Next, assume that (4.11) holds for $N = n$.
 385 For $N = n + 1$: we have

$$(4.12) \quad \begin{aligned} a &= \left(\sum_{i=2}^n b_i \gamma_i^k + b_{n+1} \gamma_{n+1}^k \right)^2 - \left(\sum_{i=2}^n b_i \gamma_i^{k-1} + b_{n+1} \gamma_{n+1}^{k-1} \right) \left(\sum_{i=2}^n b_i \gamma_i^{k+1} + b_{n+1} \gamma_{n+1}^{k+1} \right) \\ 386 \quad &\leq \left(\sum_{i=2}^n b_i \gamma_i^k \right)^2 - \left(\sum_{i=2}^n b_i \gamma_i^{k-1} \right) \left(\sum_{i=2}^n b_i \gamma_i^{k+1} \right) - b_{n+1} \gamma_{n+1}^{k-1} \sum_{i=2}^n b_i (\gamma_{n+1} - \gamma_i)^2 \gamma_i^{k-1}. \end{aligned}$$

387 Now (4.11) is a direct consequence of the induction hypothesis. This completes the
 388 proof of the lemma. \square

389 After the preparation, now we define the algebraic error estimator as follows at
 390 the $(k + 1)$ -th iteration of the solver: for $k \geq 1$

$$391 \quad (4.13) \quad \eta_a^{(k+1)} := e^{1/k} \frac{\rho_{\text{err}}^{(k)}}{1 - \rho_{\text{err}}^{(k)}} \|\mathbf{u}^{(k+1)} - \mathbf{u}^{(k)}\|_{\mathbf{A}} = e^{1/k} \frac{\rho_{\text{err}}^{(k)}}{1 - \rho_{\text{err}}^{(k)}} \|u_{\tau}^{(k+1)} - u_{\tau}^{(k)}\|_A.$$

392 The $e^{1/k}$ factor is added to remedy the fact that $\rho_{\text{err}}^{(k)}$ converges to ρ_{err} from below.
 393 Without it, the solver might stop too early, before a good estimate of ρ_{err} is obtained.

394 **THEOREM 8** (Reliability of the algebraic error estimator). *Under the same set-*
 395 *ting with Theorem 5 and Lemma 6, there exists an $N \in \mathbb{R}^+$ such that for all $k \geq N$,*

$$396 \quad (4.14) \quad \|\mathbf{e}^{(k+1)}\|_{\mathbf{A}} = \|u_{\tau} - u_{\tau}^{(k+1)}\|_A \leq \eta_a^{(k+1)}.$$

397 *Proof.* Denote $p(k) := \rho_{\text{err}}^{(k)}$, $\xi(k) := p(k)/(1 - p(k))$, and $\xi := \rho_{\text{err}}/(1 - \rho_{\text{err}})$. By
 398 Theorem 5, it suffices to show that: there exists an N such that for $k \geq N$

$$399 \quad (4.15) \quad \xi \leq e^{1/k} \xi(k).$$

400 It is straightforward to verify that $\xi(k) \rightarrow \xi$ from below as $p(k) \rightarrow \rho_{\text{err}}$. Moreover,
 401 $e^{1/k} \xi(k) \rightarrow \xi$ as $k \rightarrow \infty$. Now it suffices to show that when k is sufficiently large,

402 $e^{1/k}\xi(k)$ is a decreasing function of k . Recalling from (4.8) in Lemma 6 that if k is
 403 sufficiently large,

$$404 \quad (4.16) \quad p(k) = \rho_{\text{err}}^{(k)} \simeq \rho_{\text{err}} \frac{1 + b\gamma^k}{1 + b\gamma^{k-1}},$$

405 where $\gamma := (\lambda_{m+1}/\lambda_1)^2 < 1$, and $b := (c_{m+1}/c_1)^2 \geq 0$ where m is the multiplicity of
 406 the largest eigenvalue. Taking the derivative of $e^{1/k}\xi(k)$ with respect to k leads to:

$$407 \quad (4.17) \quad \frac{d}{dk}(e^{1/k}\xi(k)) = e^{1/k} \frac{-k^{-2}p(k)(1-p(k)) + p'(k)}{(1-p(k))^2}.$$

408 By (4.16), we have

$$409 \quad (4.18) \quad p'(k) \simeq \rho_{\text{err}} \frac{b(\gamma-1)\gamma^{k-1} \ln \gamma}{(1+b\gamma^{k-1})^2} = O(\gamma^{k-1}).$$

410 Using (4.18) in (4.17) and noting that k^{-2} decreases at a slower rate than γ^{k-1} , then
 411 for sufficiently large k , $\frac{d}{dk}(e^{1/k}\xi(k)) < 0$, and the theorem follows. \square

412 **REMARK 9** (Speed up of the rate of convergence estimate). *We notice that without*
 413 *the correction factor in (4.13), the closer $\rho_{\text{err}}^{(k)}$ is to ρ_{err} , the more accurate the algebraic*
 414 *estimator is. The convergence of $\rho_{\text{err}}^{(k)}$ can be accelerated in the following way:*

$$415 \quad \rho_{\text{err}}^{(k)} \approx \rho_{\text{err}} \frac{1 + b\gamma^k}{1 + b\gamma^{k-1}} \quad , \quad \text{and} \quad \rho_{\text{err}}^{(k-1)} \approx \rho_{\text{err}} \frac{1 + b\gamma^{k-1}}{1 + b\gamma^{k-2}}.$$

416 Now we define for $k \geq 2$:

$$417 \quad (4.19) \quad \widehat{\rho}_{\text{err}}^{(k)} := \rho_{\text{err}}^{(k)} \frac{\rho_{\text{err}}^{(k)}}{\rho_{\text{err}}^{(k-1)}}.$$

418 And $\widehat{\rho}_{\text{err}}^{(k)}$ converges to ρ_{err} faster than the original $\rho_{\text{err}}^{(k)}$. To see this, taking derivative
 419 of $\widehat{\rho}_{\text{err}}^{(k)}$ with respect to k gives,

$$420 \quad \frac{d}{dk}(\widehat{\rho}_{\text{err}}^{(k)}) = O(\gamma^{k-2}),$$

421 which is an order faster than the convergence of $\rho_{\text{err}}^{(k)}$ in (4.18).

422 **5. Discretization-accurate stopping criterion.** Identity (1.2) clearly indi-
 423 cates that the iterative solver should be stopped when the algebraic error is of the
 424 same magnitude as the discretization error. This observation suggests the following
 425 stopping criterion: let $\eta_d^{(k)}$ be η_d from (3.23) computed using the iterate $u_{\mathcal{T}}^{(k)}$, the
 426 iterative solver shall stop when

$$427 \quad (5.1) \quad \eta_a^{(k)} < \varepsilon^{-1} \cdot \eta_d^{(k)} \quad \text{and} \quad \left| \rho_{\text{err}}^{(k)} / \rho_{\text{err}}^{(k-1)} - 1 \right| < \varepsilon_\rho,$$

428 where $\varepsilon = \eta_d / \|u - u_{\mathcal{T}}\|_A$ is the effectivity index. In light of the proof of Theorem 8,
 429 the second condition implies that $\rho_{\text{err}}^{(k)}$ is a good approximation to ρ_{err} and, hence,
 430 $\eta_a^{(k)}$ is an accurate representation of the algebraic error $\|u_{\mathcal{T}} - u_{\mathcal{T}}^{(k)}\|_A$ at the k -th
 431 iteration. Together with the first condition, the estimated algebraic error is of the
 432 same magnitude in the discretization error.

433 **6. Numerical examples.** In this section, several examples are presented to
 434 verify the reliability of the estimators proposed, as well as the stopping criterion. The
 435 error estimator η_d , using a localized equilibrated flux to solve (3.15), is implemented
 436 in *i*FEM [14]. The initial guess for all examples presented in this section is a random
 437 guess with each entry of $\mathbf{u}^{(0)}$ satisfying a uniform distribution in $[-1, 1]$ using a fixed
 438 seed. An effectivity index of $\varepsilon = 1.5$ or $\varepsilon^{-1} = 2/3 \approx 0.67$ is used in (5.1). This is
 439 similar to typical values used in practice when $u_{\mathcal{T}}$ is computed with a direct solver.

440 The first test problem is the Poisson equation

$$441 \quad -\Delta u = f, \text{ in } \Omega = (-1, 1)^2$$

442 with Dirichlet boundary conditions and the exact solution is given by

$$443 \quad u = \alpha \left(\sin(\pi x) \sin(\pi y) + 0.5 \sin(4\pi x) \sin(4\pi y) \right),$$

444 where the constant α is chosen such that $\|u\|_A = 1$. This problem is discretized by
 445 the continuous piecewise linear finite element method on a uniform triangular mesh
 446 with mesh size $h = 1/32$.

447 The resulting system of algebraic equations is first solved by a multigrid method
 448 with $V(1, 1)$ -cycle. Convergence of the multigrid solver in the energy norm along
 449 with the algebraic estimator are depicted in Figure 1a (see the red and blue dot-circle
 450 lines), which numerically verify Theorem 8 for the algebraic estimator η_a being an
 451 upper bound of the algebraic error. The total and the discretization errors along with
 452 the discretization estimator are also depicted in Figure 1a (see the red solid-diamond,
 453 the red dot, and the blue solid-diamond lines, respectively). Estimated convergence
 454 rates based on both $\rho_{\text{err}}^{(k)}$ and $\hat{\rho}_{\text{err}}^{(k)}$ are presented to numerically verify Remark 9.

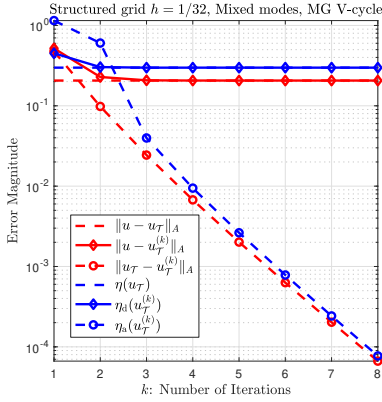
455 Using the first stopping criterion in (5.1) with $\varepsilon^{-1} = 0.67$, the multigrid iteration
 456 stops after merely two iterations, and Figure 1a shows that the algebraic error
 457 already drops below the discretization error. For a conventional stopping criterion
 458 using the relative residual measured in the ℓ^2 -norm: $\|\mathbf{Ae}^{(k)}\|_0 / \|\mathbf{Ae}^{(0)}\|_0 \leq 10^{-7}$,
 459 the multigrid iteration stops after fifteen iterations. For a slower iterative solver, we
 460 also implement symmetric Gauss-Seidel iterative method. The first stopping criterion
 461 in (5.1) with $\varepsilon^{-1} = 0.67$ requires only thirty-one iterations, while the conventional
 462 stopping criterion with the tolerance 10^{-5} needs more than two hundred eighty itera-
 463 tions. These results show a dramatic reduction in computational cost when using the
 464 discretization-accurate stopping criterion introduced in this paper. The numbers of
 465 iterations for the multigrid and the symmetric Gauss-Seidel iterative methods with
 466 both the stopping criteria as well as the total and the algebraic errors are sum-
 467 marized in Table 1. As observed from Table 1, additional iterations needed by the
 468 conventional stopping criterion significantly decrease the algebraic errors but not the
 469 total errors. Figure 2 compares the solution u_h obtained by a direct solver with that
 470 of a multigrid solver after 2 iterations.

471 The second test problem tests the stopping criterion on a non-uniform mesh for
 472 the Kellogg intersecting interface problem. The Kellogg problem with a checkerboard
 473 coefficient distribution [10] is a commonly used benchmark for testing the efficiency
 474 and robustness of a posteriori error estimators ([13, 11, 12, 15, 23]):

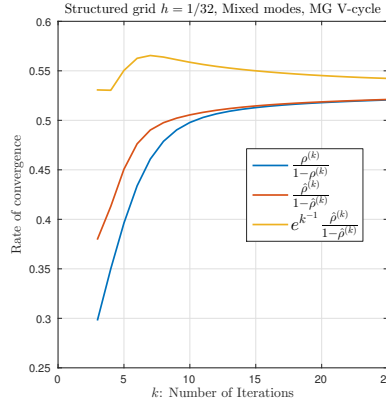
$$475 \quad (6.1) \quad -\nabla \cdot (A \nabla u) = 0, \text{ in } \Omega = (-1, 1)^2$$

Table 1: The number of iterations and the total and algebraic errors for the Poisson problem.

	Stopping	# Iter	$\ u - u_{\mathcal{T}}^{(k)}\ _A$	$\ u_{\mathcal{T}} - u_{\mathcal{T}}^{(k)}\ _A$
MG V(1,1)	$\eta_a \leq 0.67\eta_d$	2	0.0821	3.5×10^{-1}
MG V(1,1)	$\ \mathbf{r}_k\ _2/\ \mathbf{r}_0\ _2 \leq 10^{-7}$	15	0.0741	3.4×10^{-8}
Sym GS	$\eta_a \leq 0.67\eta_d$	31	0.1051	7.5×10^{-1}
Sym GS	$\ \mathbf{r}_k\ _2/\ \mathbf{r}_0\ _2 \leq 10^{-5}$	289	0.0741	2.7×10^{-4}



(a) The convergence of the V(1,1)-cycles.



(b) The convergence of the estimated rate of convergence

Fig. 1: The convergence results for the Poisson problem: the solution has mixed modes, the problem is discretized on a uniform triangular mesh, and the linear system is approximated using V(1,1)-cycle iterations.

476 with Dirichlet boundary condition, where the diffusion coefficient A is given by

$$477 \quad A = \begin{cases} R & \text{in } (0, 1)^2 \cup (-1, 0)^2, \\ 1 & \text{in } \Omega \setminus ((0, 1)^2 \cup (-1, 0)^2). \end{cases}$$

478 The exact solution u of (6.1) is given in polar coordinates (r, θ) :

$$479 \quad u = r^\gamma \psi(\theta) \in H^{1+\gamma-\epsilon}(\Omega) \text{ for any } \epsilon > 0,$$

480 where the definition of $\psi(\theta)$ is given in, e.g., [15]. Here the parameters are:

$$481 \quad \gamma = 0.5, \quad R \approx 5.8284271247461907, \quad \rho = \pi/4, \quad \text{and } \sigma \approx -2.3561944901923448.$$

482 For this example, \mathcal{T} is a graded mesh on which the relative error for the direct
 483 solve $\|u - u_{\mathcal{T}}\|_A / \|u\|_A \approx 10\%$, in addition, we choose $\varepsilon^{-1} = 0.67$ and $\varepsilon_\rho = 0.1$ for the
 484 stopping criterion. The stopping criterion (5.1) is checked every three V(1,1)-cycles.
 485 The local error distribution is shown in Figure 3.

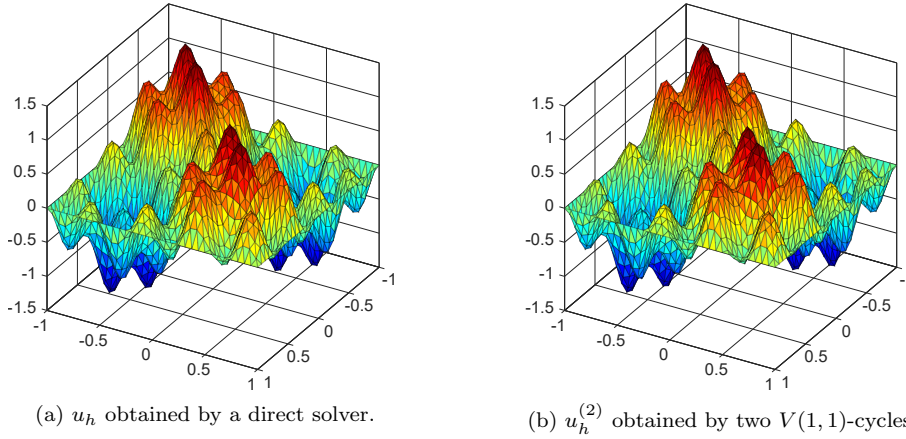


Fig. 2: The comparison of the direct-solved approximation u_h and the multigrid iterate $u_h^{(2)}$ in the first test problem.

Table 2: The number of iterations and the total and algebraic errors for the Kellogg problem.

	Stopping	# Iter	$\ u - u_\tau^{(k)}\ _A$	$\ u_\tau - u_\tau^{(k)}\ _A$
MG V(1,1)	$\eta_a \leq 0.67\eta_d$	2	0.05141	1.577×10^{-3}
MG V(1,1)	$\ \mathbf{r}_k\ _2 / \ \mathbf{r}_0\ _2 \leq 10^{-7}$	6	0.05139	8.026×10^{-8}

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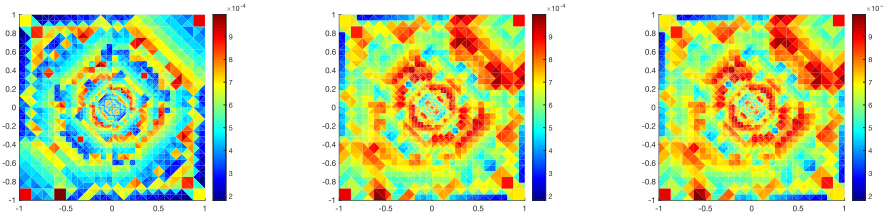
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(a) $\|u - u_{\mathcal{T}}\|_{A,K}$, the local energy error. (b) The local error indicator $\eta_{d,K}$ in (3.23) using direct solve $u_{\mathcal{T}}$. (c) The local error indicator $\eta_{d,K}$ using iterate $\bar{u}_{\mathcal{T}}$.

Fig. 3: The comparison the local error and the error indicator distributions.

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