A Posteriori Error Analysis for a Cut Cell Finite Volume Method

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Introduction
Elliptic Problems with Discontinuous Coefficients

We solve

\[-\nabla \cdot (a \nabla p) = f, \quad x \in \Omega\]

\[p = g, \quad x \in \partial \Omega,\]

where $\Omega \in \mathbb{R}^2$ is a convex domain with boundary $\partial \Omega$ separating two materials with different properties.
Elliptic Problems with Discontinuous Coefficients

Such problems pose well known challenges for accurate numerical solution.

There is a strong preference towards the use of locally conservative methods, e.g. finite volume, Ghost Fluid Method, etc.

Locally conservative schemes are generally easier to construct and implement on regularly-shaped discretizations.

In such methods, an interface cuts through the discretization cells, yielding a "cut-cell" problem.

The difficulties are magnified when the interface has complex geometry that is not aligned with a discretization mesh and when the coefficient is not piecewise constant.
Error Estimation

There is usually loss of accuracy due to the discontinuity and numerical error is always significant.

We derive an accurate computational error estimate for a quantity of interest.

We use adjoint-based variational a posteriori error analysis.

To apply this to finite volume methods, we formulate the method as an equivalent mixed finite element method + special quadrature.

A cut-cell problem makes the use of quadrature (eq. finite differences) problematic in the cells around the interface.

We develop a systematic approach to discretization that applies to general cut-cell problems and allows a posteriori error analysis.
Discretization by a cut-cell finite element method has two steps

1. The diffusion coefficient is modeled by a continuous piecewise polynomial function in a small region $\Omega_d$. This spreads the discontinuity to the boundary of $\Omega_d$, which is aligned with the mesh.

2. A mixed finite element method + quadrature is used to obtain a finite volume scheme that is equivalent to the powerful Ghost Fluid Method in simple cases.

The key point is that the Ghost Fluid Method involves both a modeling step and a discretization step.

Hence, both modeling and discretization error affects results.

An a posteriori error estimate has to quantify both sources.
Construction of the Model Problem
The Model Problem

We introduce the model problem

$$-\nabla \cdot (a_m \nabla p) = f, \quad x \in \Omega$$

$$p = g, \quad x \in \partial \Omega.$$ 

where

$$a_m \approx a$$

We use the weighted harmonic average to compute $a_m$.
Weighted Harmonic Average

Consider a canonical linear interval $\Omega$

Assume

- Assume $\Omega$ has been discretized using a partition
  \[
  \{[x_{j-1/2}, x_{j+1/2}], \ j = 1, 2, \ldots, N\}
  \]
- Cell boundaries are at $x_{j+1/2}$
- Cell centers are at $x_j$
- $\Omega = [x_{1/2}, x_{N+1/2}]$

The discontinuity is located at $x_* \in [x_i, x_{i+1}]$

The weighted harmonic average is

\[
a_{i+1/2}^* = \left( \frac{\gamma}{a_i} + \frac{1 - \gamma}{a_{i+1}} \right)^{-1},
\]

where $a_i = a(x_i)$, $a_{i+1} = a(x_{i+1})$ and $\gamma = (x_* - x_i)/(x_{i+1} - x_i)$
Weighted Harmonic Average

\[
\gamma = \frac{\frac{1}{a_i} - \frac{1}{a_{i+1/2}}}{\frac{1}{a_{i+1/2}} - \frac{1}{a_{i+1}}}
\]

\[
\gamma = \frac{1}{x_i - x_{i-1/2}} - \frac{1}{x_{i+1/2} - x_i}
\]

\[
\gamma = \frac{1}{x_{i+1} - x_{i+3/2}} - \frac{1}{x_{i+3/2} - x_{i+1}}
\]
Construction of Model in One Dimension

\( a_m(x) \) is a continuous piecewise linear approximation of \( a(x) \) that is different on \( \Omega_d = [x_{i-1/2}, x_{i+3/2}] \)

- \( a_m(x) \) interpolates \( a \) at \( x_{i-1/2} \) and \( x_{i+3/2} \)
- the value at \( x_{i+1/2} \) is the weighted harmonic average
- \( a_m = a \) outside \( \Omega_d \)

On \( \Omega_d \),

\[
\begin{align*}
\frac{(a_{i+1/2})^{-1} - (a_{i-1/2})^{-1}}{x_{i+1/2} - x_{i-1/2}} (x - x_{i-1/2}) + (a_{i-1/2})^{-1}, \\
\frac{(a_{i+3/2})^{-1} - (a^*_{i+1/2})^{-1}}{x_{i+3/2} - x_{i+1/2}} (x - x_{i+3/2}) + (a_{i+3/2})^{-1},
\end{align*}
\]

\[ x \in [x_{i-1/2}, x_{i+1/2}], \]

\[ x \in [x_{i+1/2}, x_{i+3/2}], \]
Construction of Model in One Dimension

\( (a_{i-1/2})^{-1} \)

\( (a_{i+1/2})^{-1} \)

\( (a_{i+3/2})^{-1} \)

\( x_{i-1/2} \)

\( x_i \)

\( x_{i+1/2} \)

\( x_* \)

\( x_{i+1} \)

\( x_{i+3/2} \)

\( a \)

\( a_m \)
Construction of Model in Two Dimensions

Geometric complexity significantly increases

The weighted harmonic average is applied on line segments connecting cell centers across a common cell boundary or diagonally across a common cell node

$\Omega$ is discretized by cells (finite volumes) $K_{ij}$

$= (x_{i-1/2}, x_{i+1/2}) \times (y_{j-1/2}, y_{j+1/2})$ on a grid

$0 = x_1 < x_2 < \cdots < x_k < x_{k+1/2} = 1$

$0 = y_1 < y_2 < \cdots < y_{\ell-1/2} < y_{\ell} < y_{\ell+1/2} = 1$

$\Omega_d$ uses cells containing the interface curve $\Gamma_d$ along with their immediate neighbors

$a_m$ is a continuous piecewise biquadratic function on $\Omega_d$
interpolating at the cell nodes, boundary centers, and cell centers
Construction of Model in Two Dimensions
We specify a systematic algorithm for computing $a_m$.

Beginning with an interface and a discretization:
- $\circ$ = average over cell
- $\square$ = harmonic average
- $\triangledown$ = standard average
- $\vartriangle$ = average of harmonic and standard averages
- $\bullet$ = interpolation
We specify a systematic algorithm for computing \( a_m \)

We identify \( \Omega_d \) and set values at cell centers

- \( \circ \) = average over cell
- \( \square \) = harmonic average
- \( \triangularright \) = standard average
- \( \heartsuit \) = average of harmonic and standard averages
- \( \bullet \) = interpolation
We specify a systematic algorithm for computing $a_m$.

We compute harmonic averages at cell boundary centers.

- $\circ$ = average over cell
- $\square$ = harmonic average
- $\triangledown$ = standard average
- $\blacksquare$ = average of harmonic and standard averages
- $\bullet$ = interpolation
We specify a systematic algorithm for computing $a_m$

We compute standard averages at other cell boundary centers

- $\circ$ = average over cell
- $\square$ = harmonic average
- $\triangledown$ = standard average
- $\boxdot$ = average of harmonic and standard averages
- $\bullet$ = interpolation
We specify a systematic algorithm for computing $a_m$

We average previously computed values at interior cell nodes

- $\bigcirc$ = average over cell
- $\square$ = harmonic average
- $\triangledown$ = standard average
- $\blacksquare$ = average of harmonic and standard averages
- $\bullet$ = interpolation
We specify a systematic algorithm for computing $a_m$

We use interpolation to assign remaining values

- $\bigcirc$ = average over cell
- $\Box$ = harmonic average
- $\triangledown$ = standard average
- $\blacklozenge$ = average of harmonic and standard averages
- $\bullet$ = interpolation
Examples of the Model in Two Dimensions

The discontinuity interface $\Gamma_d$ is the line $y + 0.45x - 0.73 = 0$

$a$ equals $10^3$ on one side of the line and 1 on the other
Examples of the Model in Two Dimensions

The discontinuity interface $\Gamma_d$ is the circle

$$(x - 0.5)^2 + (y - 0.5)^2 = 0.4^2$$

The diffusion coefficient $a$ equals $10^3$ outside the circle and 1 inside.
Discretization of the Model Problem
We discretize using a Raviart-Thomas mixed finite element method with a special quadrature that yields a cell-centered finite volume scheme.

The scheme is equivalent to the Ghost Fluid Method in special cases.

The variational formulation uses integrals over volumes that allows the finite element approximation to “see” the geometry of the diffusion interface inside each volume.
The Finite Element Method

We set \( u_m = -a_m \nabla p_m \)

Solve an equivalent first order system

\[
\left( a_m^{-1} u_m, v \right)_\Omega - (p_m, \nabla \cdot v)_\Omega = -\langle g, v \cdot n \rangle_{\partial\Omega},
\]

\[
(\nabla \cdot u_m, w)_\Omega = (f, w)_\Omega,
\]

for \((v, w) \in (V, W)\), where

\[
p_m \in W = L^2(\Omega)
\]

\[
u_m \in V = H(\text{div}; \Omega) = \{ v \in (L^2(\Omega))^2 : \text{div} \, v \in L^2(\Omega) \}
\]

\((\cdot, \cdot)_D\) is an inner product on \(D \subset \mathbb{R}^2\)

\langle \cdot, \cdot \rangle_{\gamma} \text{ is an inner product on } \gamma
The Finite Element Method

Finite element spaces:

- $W_h \subset W =$ piecewise constant functions
- $V_h \subset V =$ vector-valued functions whose $x$-components are continuous linear in $x$ and discontinuous constant in $y$ and whose $y$-components are discontinuous constant in $x$ and continuous linear in $y$

Quadratures:

- $T_x$ and $T_y$ are trapezoidal rules in the $x$ and $y$-directions
- $M_x$ and $M_y$ are midpoint rules in the $x$ and $y$-direction
- $M$ is the midpoint rule on cell edges
The Finite Element Method

Compute \((u_{m,h}, p_{m,h}) \in V_h \times W_h\) satisfying

\[
\begin{align*}
\left(a^{-1}_m u^x_{m,h}, v^x\right)_{T_x M_y} + \left(a^{-1}_m u^y_{m,h}, v^y\right)_{M_x T_y} - (p_{m,h}, \nabla \cdot v) &= -\langle g, v \cdot n \rangle_{M}, \\
(\nabla \cdot u_{m,h}, w) &= (f, w)_{M_x M_y}, 
\end{align*}
\]

for any \(v \in V_h, w \in W_h\), where \(u_{m,h} = (u^x_{m,h}, u^y_{m,h})\), \(v = (v^x, v^y)\)

Observations:

- This scheme is equivalent to a cell-centered finite volume scheme that is the Ghost Fluid Method for simple geometry
- The model diffusion coefficient is a convex interpolant
- The approximation preserves flux across cell boundaries at cell boundary centers
Error Analysis
Decomposition of the Error

We decompose the error as

\[ e_p = p - p_{m,h} = (p_m - p_{m,h}) + (p - p_m) = e_{p,h} + e_{p,m} \]
\[ e_u = u - u_{m,h} = (u_m - u_{m,h}) + (u - u_m) = e_{u,h} + e_{u,m} \]

- The first errors \( e_{p,h}, e_{u,h} \) are the approximation error due to numerical discretization. These can be analyzed by standard a posteriori techniques.
- The second errors \( e_{p,m}, e_{u,m} \) represent the difference between the analytic solutions of the original and model problems.

**Theorem**

The modeling errors converge as \( a_m \) converges to \( a \)

Depending on geometry, the modeling errors are typically \( O \left( h^{1/2} \right) \)
Adjoint Problems

Quantity of interest:

\[ Q(p, u) = (p, \psi_p) + (u, \psi_u), \]

Adjoint problem for the original equation: Find \( \phi_p \in H^1(\Omega) \) and \( \phi_u \in H(\text{div}; \Omega) \) such that

\[
a^{-1} \phi_u - \nabla \phi_p = \psi_u, \quad \text{in} \ \Omega,
\]

\[
-\nabla \cdot \phi_u = \psi_p, \quad \text{in} \ \Omega,
\]

\[
\langle \phi_p, v \cdot n \rangle = 0 \quad \text{on} \ \partial \Omega, \ \forall \ v \in H(\text{div}; \Omega).
\]

Adjoint problem for the model: Find \( \phi_{p,m} \in H^1(\Omega) \) and \( \phi_{u,m} \in H(\text{div}; \Omega) \) such that

\[
a_m^{-1} \phi_{u,m} - \nabla \phi_{p,m} = \psi_u, \quad \text{in} \ \Omega,
\]

\[
-\nabla \cdot \phi_{u,m} = \psi_p, \quad \text{in} \ \Omega,
\]

\[
\langle \phi_{p,m}, v \cdot n \rangle = 0 \quad \text{on} \ \partial \Omega, \ \forall \ v \in H(\text{div}; \Omega).
\]
A Posteriori Error Estimate

**Theorem**

\[(e_p, \psi_p) + (e_u, \psi_u) = \left\{ - \left( a_m^{-1} u_{m,h}, \phi_{u,m} - \Pi_h \phi_{u,m} \right) \right. \]

\[+ \left( f, \phi_{p,m} - \mathbb{P}_h \phi_{p,m} \right) - \left\langle g, \left( \phi_{u,m} - \Pi_h \phi_{u,m} \right) \cdot n \right\rangle \right\}

\[+ \text{QE1}(\Pi_h \phi_{u,m}) + \text{QE2}(\mathbb{P}_h \phi_{p,m}) - \left( (a^{-1} - a_m^{-1}) u_{m,h}, \phi_{u,m} \right), \]

\[\text{QE1}(v) = - \left( a_m^{-1} u_{m,h}, v \right) + \left( \left( a_m^{-1} u_{m,h}^x, v^x \right)_{T_x M_y} \right) \]

\[+ \left( a_m^{-1} u_{m,h}^y, v^y \right)_{M_x T_y} \right) - \left\langle g, v \cdot n \right\rangle + \left\langle g, v \cdot n \right\rangle_M, \]

\[\text{QE2}(w) = (f, w) - (f, w)_{M_x M_y}, \]

\(\Pi_h\) and \(\mathbb{P}_h\) are the lowest order Raviart-Thomas and \(L^2\) projections.
Modeling Error Term

The actual modeling error term is $((a^{-1} - a_m^{-1})u_m, \phi_u)$, which is not computable.

We show that it can be approximated by $((a^{-1} - a_m^{-1})u_{m,h}, \phi_{u,m})$ plus a remainder that is higher order.

The modeling error term is zero outside $\Omega_d$.

If the quantity of interest is located away from the interface $\Gamma_d$, modeling error has little effect.
Numerical Examples
Numerical Examples

We illustrate the accuracy of the a posteriori error estimates and the relative sizes of error contributions.

For most of the problems, we manufacture solutions so that we can compute a true error.

We stress the estimates by choosing problems with large discontinuities in $a$ and/or large scale difference in the solution across the interface.

We consider quantities of interest that are both located near and away from the discontinuous interface.

We show values of the error/estimate ratio $\nu$. 
A One Dimensional Example

\[ a(x) = \begin{cases} 
10^{-3}(x + 1), & x > 0.45 \\
x + 1, & x \leq 0.45,
\end{cases} \]

We compute \( f \) so that

\[ p(x) = \begin{cases} 
10^3 \sin(x - 0.45) + 2, & x > 0.45 \\
\sin(x - 0.45) + 2, & x \leq 0.45,
\end{cases} \]

Quantities of interest: the value of \( p \) near .45 and .95
A One Dimensional Example

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Quantity of interest \( p \) near .45
A One Dimensional Example

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Quantity of interest \( p \) near .95

Residual and quadrature contributions are larger at .95 because \( a^{-1} \) is larger

Modeling error contribution is less at .95
Discontinuity Across a Straight Line

\[ \Gamma_d \text{ is } y + 0.45x - 0.73 = 0 \]

\[ a = 10^3 \text{ on one side and } a = 1 \text{ on the other} \]

We compute \( f \) so that

\[
p(x, y) = \begin{cases} 
10^{-3} \exp(y + 0.45x - 0.73), & \text{on the left} \\
\exp((y + 0.45x - 0.73) - 1 + 10^{-3}), & \text{on the right}
\end{cases}
\]

Quantities of interest:

- the average error over the whole domain
- the average error in a small region close to the discontinuity
- the average error in a small region far away from the discontinuity
## Discontinuity Across a Straight Line

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Average over the domain
### Discontinuity Across a Straight Line

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Near the interface
## Discontinuity Across a Straight Line

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Away from the interface

Contributions from modeling are about the same as those from quadrature+residual
Adjoint solutions for the three quantities of interest reflect the decreasing impact of modeling error away from the interface.
Discontinuity Across a Circle

\( \Gamma_d \) is the circle of radius 0.4 centered at \((0.5, 0.5)\)

\( a = 10^3 \) inside and 1 outside

We compute \( f \) so

\[
p(x, y) = \begin{cases} 
    \exp((x - 0.5)^2 + (y - 0.5)^2 - 0.16), & (x - 0.5)^2 + (y - 0.5)^2 \leq 0.16 \\
    10^3(\exp((x - 0.5)^2 + (y - 0.5)^2 - 0.16) - 1 + 10^{-3}), & (x - 0.5)^2 + (y - 0.5)^2 > 0.16, 
\end{cases}
\]

We use the same three quantities of interest
<table>
<thead>
<tr>
<th>level</th>
<th>$\nu$</th>
<th>Discr.</th>
<th>Quad.</th>
<th>Model.</th>
</tr>
</thead>
<tbody>
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Average over the domain
## Discontinuity Across a Circle

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<tr>
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<th>Quad.</th>
<th>Model.</th>
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Average near the interface
### Discontinuity Across a Circle

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Average away from the interface
Cell Contributions to the Error

We show individual cell contributions to the error for a problem with a curved interface
A Complex Interface

\( \alpha \) is \( 10^3 \) inside a “cross” shaped region in the middle of the unit square and 1 outside

\( f \) is the sum of a Gaussian function of height 100 near \((1, 1)\) and a Gaussian of height -100 near \((0, 0)\)

The boundary conditions are homogeneous Dirichlet

The quantity of interest is the average error in a small region near the source
A Complex Interface

We consider two orientations
A Complex Interface

Cross aligned with the mesh
A Complex Interface

Cross aligned at an angle with the mesh
Conclusion
Conclusions

We have described a systematic approach to discretize elliptic problems with a diffusion coefficient that discontinuous across a complex interface

The discretization has two steps

- A modeling step
- A special finite element discretization

The resulting scheme is a cell-centered finite volume scheme

We also derive a posteriori error estimates that account for discretization and modeling error

We are also able to include errors in the location of the interface, e.g. due to measurement, in the analysis