Hierarchical Unstructured Meshes for Accurate and Efficient Numerical PDE Solvers

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Computational Challenges in PDE Discretizations

- Geometry and Grid Generation
  - ... “remains one of the most important bottlenecks for large-scale complex simulations”
  - “Curved mesh elements for higher order methods”, “tight CAD coupling and production adaptive mesh refinement (AMR)”

- Numerical Algorithms
  - “Discretization techniques such as higher-order accurate methods offer the potential for better accuracy and scalability, although robustness and cost considerations remain”
  - “Linear and nonlinear solvers ... that are ... near optimal”, including extension of “Krylov methods, highly parallel multigrid methods”

These two areas are intimately related, at both theoretical and practical levels, and require a holistic approach.

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Survey Results on Simulation Chain from IMR 2015

- Make solvers more robust to lesser quality meshes
- Evolve solvers to support other element types
- Improve or introduce mesh adaptation coupled to solvers
Overview of Our Approach

1. Achieve element-quality independence by weighted least squares
2. Improve efficiency of linear solvers using hierarchical meshes
3. Accurate geometric algorithms

Representative Publications

Outline

1. Element-Quality Independent PDE Discretizations
   - Unified Formulation of PDE Discretizations
   - Robust, Easy-to-Use Finite Elements
   - Implications on Geometry and Meshing

2. Hierarchical Mesh Generation for Efficiency

3. WLS-Based High-Order Surface Reconstruction

4. Conclusions
Unified Weighted-Residual Formulation for PDEs

- Consider abstract but general form of linear, time-independent PDE

\[ \mathcal{P} u(x) = f(x), \]

with boundary conditions, where \( \mathcal{P} \) is linear differential operator

- In a *weighted residual method*, given a set of test functions \( \Psi(x) = \{\psi_j(x)\} \), we obtain one equation for each \( \psi_j \) as

\[ \int_\Omega \mathcal{P} u(x) \psi_j \, dx = \int_\Omega f(x) \psi_j \, dx. \]

- Boundary conditions are applied by modifying the linear system
- In *Galerkin finite elements*, \( \psi_j \) are finite-element shape functions
- In *(generalized)* *finite differences*, \( \psi_j \) are Dirac delta functions at nodes
- In *finite volumes*, \( \psi_j \) are step functions over control volume
Algebraic Equations from Weighted-Residual Methods

- Introduce basis functions $\Phi(\mathbf{x}) = \{\phi_i(\mathbf{x})\}$ to approximate $u$ and $f$
- Suppose $\Phi = [\phi_1, \phi_2, \ldots, \phi_n]^T$ and $\Psi = [\psi_1, \psi_2, \ldots, \psi_n]^T$
- Let $u \approx \mathbf{u}^T \Phi = \sum_i u_i \phi_i$, and similarly $f(\mathbf{x}) \approx \sum_i f_i \phi_i$
- PDE leads to linear system $\mathbf{A}\mathbf{u} = \mathbf{b}$, where

$$A_{ij} = \int_{\Omega} \psi_i(\mathbf{x}) \mathcal{P} \phi_j(\mathbf{x}) d\mathbf{x} \quad \text{and} \quad b_i = \int_{\Omega} f(\mathbf{x}) \psi_i(\mathbf{x}) d\mathbf{x}$$

- In FEM, $\int_{\Omega} \psi_i(\mathbf{x}) \mathcal{P} \phi_j(\mathbf{x}) d\mathbf{x}$ is often transformed to $\int_{\Omega} \mathcal{L}_1 \psi_i(\mathbf{x}) \cdot (\mathcal{L}_2 \phi_i(\mathbf{x}))^T d\mathbf{x}$ via integration by parts

We use WLS-based basis functions, and in turn generalize finite difference, finite element, and finite volume methods.
Overcoming Element-Quality Dependency of FEM

- FEM is workhorse in engineering, but its accuracy, stability, and efficiency heavily depends on element shapes, so engineers often spend > 60% of time on meshing.

Examples of poor-shaped elements in 2-D and 3-D.

- This dependency is due to interpolation-based basis functions.
- We propose *Adaptive Extended-Stencil FEM* to overcome this issue.
Overview of Adaptive Extended-Stencil FEM

- Basic Idea of Adaptive Extended-Stencil FEM (AES-FEM)\(^2\)
  - Preserve overall framework, including weak form, test functions, quadrature rules, ways to enforce boundary conditioners, etc.
  - Replace Lagrange basis functions in FEM with generalized Lagrangian polynomial (GLP) basis functions constructed using WLS over adaptive, extended neighborhood at each node

Definition

Given a set of degree-\(d\) polynomial basis functions \(\{\phi_i\}\), we say it is a set of degree-\(d\) generalized Lagrange polynomial (GLP) basis functions if:

1. \(\sum_i f(x_i) \phi_i\) approximates a function \(f\) to \(O(h^{d+1})\) in a neighborhood of the stencil, where \(h\) is some characteristic length measure, and
2. \(\sum_i \phi_i = 1\).

Examples of Adaptive, Extended Stencils

- In 2-D, use 1, 1.5, 2 & 2.5 rings for degree-2, 3, 4 & 5, respectively
- In 3-D, define rings at 1/3 increments for better granularity
- Adaptively enlarge stencils if WLS is ill-conditioned
Properties of AES-FEM

**Theorem**

Suppose $u$ is smooth and thus $\|\nabla u\|$ is bounded. Then, when solving the Poisson equation using AES-FEM with degree-$d$ GLP basis functions, for each $\psi_i$ the weak form is approximated to $O(h^d)$, where $h$ is some characteristic length measure of the mesh.

- With similar sparsity pattern, AES-FEM allows higher-order basis functions than those of FEM, and hence enables better accuracy.
- For its extended stencil, AES-FEM is insensitive to element shapes.
Comparison of Accuracy of AES-FEM vs. FEM

Poisson equation
\[-\nabla^2 u = f \quad \text{in } \Omega\]
\[u = g \quad \text{on } \partial \Omega\]

Convection-diffusion equation
\[-\nabla^2 u + c \cdot \nabla u = f \quad \text{in } \Omega\]
\[u = g \quad \text{on } \partial \Omega\]

- AES-FEM is about 10 times more accurate than classical FEM
Comparison of Stability of AES-FEM vs. FEM

Condition numbers as function of min angles in 3-D

Numbers of solver iterations as function of min angles in 3-D

- Stability (and accuracy) of AES-FEM is independent of element quality
Comparison of Efficiency of AES-FEM vs. FEM

Error vs. runtime for 2D convection-diffusion equation

- AES-FEM is about 2–10 times faster than classical FEM.

Error vs. runtime for 3D convection-diffusion equation
High-Order AES-FEM with Linear Elements

$L_\infty$ errors of AES-FEM and FEM for 2-D Poisson equation

$L_2$ errors of AES-FEM and FEM for 3-D convection-diffusion equation

- AES-FEM delivers high-order accuracy (up to sixth order in this example) with only linear elements, even poorly shaped elements\(^3\)

\(^3\)Submitted to *SIAM J. Sci. Comput. (SISC).*

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Robust AES-FEM Over Tangled Meshes

Example mesh with inverted elements

- AES-FEM is accurate and stable even over tangled meshes
- This requires adapting stencil and test functions near tangled regions

Convergence results of FEM and AES-FEM

\[ L^\infty \text{Error} \]

<table>
<thead>
<tr>
<th>Number of Vertices</th>
<th>AES-FEM</th>
<th>FEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10^3)</td>
<td>(10^{-3})</td>
<td>(10^{-2})</td>
</tr>
<tr>
<td>(10^4)</td>
<td>(10^{-1})</td>
<td>(10^{-2})</td>
</tr>
</tbody>
</table>

2nd order
Are Geometry and Mesh Generation Important?

- AES-FEM change how we look at meshing
  - Element shapes should not be as important for **stability**
  - Isoparametric elements are not necessary for high-order **accuracy**
  - Mesh generation for FEM should not be as hard as it has been

- Geometry and mesh generation remain for efficiency and accuracy!
  - **Hierarchical meshes** can lead to nearly optimal linear solvers
  - **Geometric accuracy** is critical for overall accuracy of PDE solutions
  - Other issues that remain important include adaptive mesh refinement and semi-structured meshes
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Motivation of Hierarchical Meshes

- Simple approach for generating large-scale meshes is to refine an intermediate scale mesh.

- Geometric multigrid, which is optimal solver for large-scale linear systems from PDEs, requires hierarchical meshes.

Geometric multigrid (GMG) is desirable as the linear solver of numerical PDEs for its efficiency and it requires a hierarchical mesh.

Goal: generate large-scale hierarchical mesh accurately and efficiently through uniform refinement and support linear solvers with GMG.
Multi-Degree Refinement of Tetrahedral Meshes

- Partition each tetrahedron into congruent sub-tetrahedra and octahedra
- Each octahedron is divided into 4 sub-tetrahedra with shortest diagonal strategy, resulting $k^3$ sub-tetrahedra for degree-$k$ refinement

degree 2, 3 refinement of a tetrahedron
Basic Hierarchical Data Structure

Level

0/Initial Mesh

1

2

Degree

N/A

2

3

L_p

Mesh Storage

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Generalized Hierarchical Data Structure

Coordinates for all vertices

<table>
<thead>
<tr>
<th>vertices on $L_1$</th>
<th>new vertices by refinement</th>
</tr>
</thead>
</table>

v2pe: new vertex to one of its parents

Hierarchical Mesh

conn: connectivity of original mesh

sibhfs: Data in AHF for adjacency queries

e2pe: NULL

e2ce: element to its first child element

conn: connectivity of new elements in $L_2$

sibhfs: update AHF data for refined elements, optional

e2pe: new element to its parent elements, optional

e2ce: element to its first child element

- Support conformal and non-conformal adaptive mesh refinement
- In parallel, we resolve shared vertex and ghost layers
Hybrid Geometric+Algebraic Multigrid Method

- Hybrid approach combining geometric and algebraic multigrid methods
- Full-multigrid cycle
- V-cycles
- Mesh refinement
- Graph coarsening
- Krylov-subspace coarse-grid solvers
- Semi-iterative smoothers
- Restriction
- Prolongation

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Multigrid Method with Hierarchical Meshes

Solve Poisson equation using FEM on a mesh with 5k vertices and 2.5k tetrahedra, with further 2 levels refinement for GMG.

HyGA converges twice as fast as AMG for degree-2 refinements, and about three times as fast in the presence of a degree-3 refinement.

(a) degrees-2+2 refinement. (b) degrees-2+3 refinement.
Effectiveness of Hierarchical Meshes for Multigrid Solvers

Timing results (in seconds) for FEM, with PCG as reference.

<table>
<thead>
<tr>
<th>test case</th>
<th>AMG((L + 1))</th>
<th>GMG</th>
<th>HyGA: Hybrid Multigrid</th>
<th>PCG (ichol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>verts</td>
<td>setup</td>
<td>solve</td>
<td>solve</td>
<td>(2,(L)-2)</td>
</tr>
<tr>
<td>36K</td>
<td>5</td>
<td>0.15</td>
<td>0.74</td>
<td>0.16</td>
</tr>
<tr>
<td>147K</td>
<td>6</td>
<td>0.63</td>
<td>3.68</td>
<td>0.65</td>
</tr>
<tr>
<td>32K</td>
<td>3</td>
<td>0.37</td>
<td>1.79</td>
<td><strong>0.38</strong></td>
</tr>
<tr>
<td>292K</td>
<td>4</td>
<td>3.98</td>
<td>24.5</td>
<td><strong>5.66</strong></td>
</tr>
<tr>
<td>2.5M</td>
<td>5</td>
<td>28.5</td>
<td>509</td>
<td><strong>58.3</strong></td>
</tr>
</tbody>
</table>

- We use hybrid geometric+algebraic multigrid solvers
- With 2–3 levels of mesh hierarchy, multigrid solver can be sped up more than 10 times
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An important issue in hierarchical meshing is treatment of curved boundaries and sharp features.
Importance of Geometric Accuracy

- Overall solution error may be dominated by geometric error, independently of order of PDE solvers
- We use WLS-based high-order reconstruction of surfaces to ensure geometry has sufficient accuracy relative to PDE discretization
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Concluding Remarks

- Meshing should not be responsible for stability of PDE discretizations
- Meshing will still have significant impact of accuracy (point density) and efficiency (point distribution and mesh hierarchy)
- Weighted-least square offers a unified mathematical framework
  - Numerical discretizations of PDEs without mesh-quality dependency
  - High-order geometry for meshing
- Hybrid geometric+algebraic multigrid with small number of levels of mesh hierarchy can enable near optimal and scalable linear solvers
- Tighter integration of geometry, meshing, discretization methods and linear/nonlinear solvers may be fruitful