Parallel Adaptive $C^1$ Macro-Elements for Nonlinear Thin Film and Non-Newtonian Flow Problems

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Dissertation Goals

- Parallel adaptive solution of fourth order problems
- Adaptive mesh refinement of $C^1$ macroelements
- Error estimation on conforming formulations of fourth order problems
- New weak formulations of thin film flow problems
- Numerical experiments of thin film flow phenomena
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Macroelement Spaces

Application Classes

Fourth Order Terms

- Streamfunction Viscosity
- Thin Film Surface Tension
- Material Interface Diffusion
In Galerkin approximations of fourth order problems we find integrated products of second derivatives of trial and test functions. Conforming finite element approximations require at least $H^2$ conforming functions. We can use $C^1$ continuous (and $W^{2,\infty}$ bounded, $W^{2,p}$ conforming) finite elements:

**Macroelement Types**

- Powell-Sabin 6-split triangle
- Powell-Sabin-Heindl 12-split triangle
- Clough-Tocher 3-split triangle
Constraining $C^1$ continuity on arbitrary meshes requires quintics, a higher degree than desired for many approximations. Instead, we subdivide each macroelement:
Constructing Macroelements

**Macroelement Basis Precalculation**

- Index the “raw” degrees of freedom
- “Write” all constraints as symbolic matrix rows
- Put constraint matrix in row reduced form
- Add boundary DoF equations (checking each for linear independence)
- If necessary, make matrix square with interior DOF equations (again checking for linear independence)
- Invert matrix, multiply by \( \hat{e}_i \) to get basis coefficients corresponding to the DOF on row \( i \)
Clough-Tocher 3-split
Powell-Sabin and Clough-Tocher macroelements can exactly reproduce quadratics and cubics \((k \equiv 2, 3)\), respectively. Standard interpolation, \(H^2\) approximation rules apply.

For \(w \in H^n(\Omega), n \leq k + 1\),

\[
P_h(f) \equiv \sum_{i=1}^{N} \sigma_i(f) \phi_i
\]

\[
\|w - P_h w\|_{H^m(\Omega)} \leq Ch^{n-m} |w|_{H^n(\Omega)}
\]

\[
\|u - u_h\|_{H^2(\Omega)} \leq Ch^{n-2} |u|_{H^n(\Omega)}
\]
\[ L_2 \text{ Approximation Convergence} \]

Clough-Tocher elements obtain an additional power of \( h \) over Powell-Sabin elements in \( H^2 \) norm. The difference is greater in \( L_2 \).

With \( \eta \equiv \min (2(k + 1 - m), k + 1 - r, n - r) \), for Galerkin approximation \( u_h \) to an elliptic problem on \( H^m(\Omega) \),

\[
||u - u_h||_{H^r(\Omega)} \leq Ch^\eta ||u||_{H^n(\Omega)}
\]

For \( k = 3 \), or \( k = 2, r \geq 1 \), this is familiar.

For fourth order problems \( (m = 2) \), quadratic elements \( (k = 2) \), in the \( L_2 \) norm \( (r = 0) \), \( \eta = 2(k + 1 - m) = 2 \).
\( h \) Adaptivity

- Macroelement splitting, adaptive refinement subdivision must match along element sides
- 12-split, 3-split triangles, 4-split tetrahedra are compatible
- 6-split triangles, 12-split tetrahedra are not
Maintaining function space continuity requires constraining some degrees of freedom on fine elements in terms of degrees of freedom on coarse neighbor elements.

\[ u^F = u^C \]
\[ \sum_i u^F_i \phi_i^F = \sum_j u^C_j \phi_j^C \]
\[ A_{ki} u_i = B_{kj} u_j \]
\[ u_i = A_{ki}^{-1} B_{kj} u_j \]

Integrated values (and fluxes, for $C^1$ continuity) give element-independent matrices:

\[ A_{ki} \equiv (\phi_i^F, \phi_k^F) \]
\[ B_{kj} \equiv (\phi_j^C, \phi_k^F) \]
Error Indicators

Integration by parts gives an upper error bound on subelements $S$ for the biharmonic problem:

$$
\| e \|_{H^2(\Omega)} \leq C_\Omega \sum_S \left[ \| f - \Delta^2 u_h \|_S h_S^2 + \frac{1}{2} \|[\partial_n \Delta u_h]\|_{\partial S} h_S^{3/2} + \frac{1}{2} \|[\Delta u_h]\|_{\partial S} h_S^{1/2} \right]
$$

The most significant term gives a simple indicator on elements $K$ for more general fourth order problems:

$$
\eta_K \equiv \sqrt{h_K} \|[\Delta u_h]\|_{\partial K}
$$
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Software Implementation

libMesh C++ Finite Element Library

Initial developers: Benjamin Kirk, John Peterson
Contributions from Michael Anderson, Bill Barth, Daniel Dreyer, Derek Gaston, David Knezevic, Hendrik van der Heijden, Steffen Petersen, Florian Prill, others

Key Features

- Mixed element geometries in unstructured grids
- Adaptive mesh h-refinement with hanging nodes
- Parallel system assembly and solution
- Integration w/ PETSc, LASPack, METIS, ParMETIS
- Export/import to common data formats

200 downloads/month, 100 current users, 20 papers
libMesh Usage

- libMesh library provides elements, linear algebra, common tools
- Application code implements physical equations, control loops
Finite Element Classes

Finite Element object computes data for each geometric Elem object

Application code is element independent
New Contributions to libMesh

Current chief software architect: Roy Stogner

Key Features Added

- Macroelement construction and quadrature
- $C^1$ macroelement, Hermite classes
- Hessian calculations
- Parallel adaptivity for general element types
- Parallel unstructured meshing
- Projection, interpolation for general elements
- New nonlinear solver, timestepping frameworks
- Additional error estimators, adaptivity strategies
Adaptive Time Stepping

- Trapezoidal integration to avoid extrapolation failures
- Truncation error compares $2\delta t$ to $\delta t$ in relative $H^r$ norm
Adaptive Time Stepping

- Time step length may be limited by random topological events at any time.
- Mean step lengths grow smoothly.

![Adaptive Time Step Lengths for Imposed Bias Magnitude Study](image)
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Solver Details

Newton-Krylov Nonlinear Solver

- Adaptively reduced linear residual reduction tolerance
- Inner GMRES iteration, Block Jacobi/ILU preconditioning

Reliability Improvements

- Brent’s Method line search to find residual reduction
- Feedback to adaptive time stepping or continuation solvers
Divergence-free Elements

- Curls of $C^1$ basis functions become div-free $C^0$ spanning functions
- Constraining kernel of $\nabla \times$ is simple in 2D
- Pressure term disappears from Navier-Stokes equations:

$$\int_{\Omega} \nabla P \cdot \vec{v} d\Omega = \int_{\partial \Omega} P \vec{v} \cdot \vec{n} dS - \int_{\Omega} P \nabla \cdot \vec{v} d\Omega = 0$$
Lid-Driven Cavity

The lid-driven cavity is a standard incompressible viscous flow benchmark:

- Extended Williamson Fluid
- $Re_0 = 500, \frac{\nu_0}{\nu_\infty} = 10$
- Thin shear layers
- Corner derivative singularities
- Vorticity convected to interior
Adapted meshes capture both corner singularities and interior
Thin Film Flow

Thin Film Flow Characteristics
- Microscale buoyancy effects vanish
- Long-wavelength thermocapillary effects dominate
Surfactant Transport

Flow Characteristics
- Temperature, surfactant distribution determine surface tension
- Temperature destabilizes, surfactant stabilizes
Thin Film Flow and Transport Equations

Taking only the dominant bulk fluid flow terms as $d/L \rightarrow 0$, depth integration derives the 2D thin film flow equations:

\[
\frac{\partial u}{\partial t} = \nabla \cdot \left( \frac{u^3}{B} \nabla \left( \left( 1 + \frac{Dud^2}{(1 + F - Fu) L^2} - D_s \frac{d^2}{L^2} c_s \right) \Delta u \right) \right) - \frac{3u^2}{2} \frac{D(1 + F)}{(1 + F - Fu)^2} \nabla u + \frac{u^2}{2} \nabla c_s + \frac{G u^3}{3} \nabla u
\]

\[
\frac{\partial c_s}{\partial t} = \nabla \cdot \left( \left( \frac{3u^2}{2B} \nabla \left( \left( 1 + \frac{Dud^2}{(1 + F - Fu) L^2} - D_s \frac{d^2}{L^2} c_s \right) \Delta u \right) \right) + \frac{D(1 + F)u}{(1 + F - Fu)^2} \nabla u - D_s u \nabla c_s \right) c_s
\]
Surfactant-Driven Flow

Adding a surfactant droplet to the corner of an initially flat film surface, local surface tension reduction pushes a fluid wave through the domain.

Surfactant concentration at $t = 0, 0.2$

Fluid depth at $t = 0.1, 0.2$
Microscale and Nanoscale Phenomena

Cahn-Hilliard Applications

- Tin-Lead solder aging
- Void lattice formation in irradiated semiconductors
- Self-assembly of thin film patterns
Cahn-Hilliard systems model material separation and interface evolution based on a weakly non-local free energy density.

\[ f(c, \nabla c) \equiv f_0(c) + f_\gamma(\nabla c) \]
\[ f_\gamma(\nabla c) \equiv \frac{\epsilon_c^2}{2} \nabla c \cdot \nabla c \]
\[ f_{0m}(c) \equiv \frac{1}{4} (c^2 - 1)^2 \]

\[ f_0(c) \equiv NkT \left[ c \ln(c) + (1 - c) \ln(1 - c) \right] + N\omega_c(1 - c) \]
A mobility coefficient $M_c$ defines the concentration flux $\vec{J}$. For positive definite $M_c$, the resulting Cahn-Hilliard equation gives globally non-increasing free energy.

\[
\vec{J} = M_c \nabla \frac{df}{dc} = M_c \nabla \left( f'_0(c) + f'_\gamma(c) \right)
\]

\[
\frac{\partial c}{\partial t} = \nabla \cdot M_c \nabla \left( f'_0(c) - \epsilon_c^2 \Delta c \right)
\]
Weak Cahn-Hilliard Equation

\[
\left( \frac{\partial c}{\partial t}, \phi \right)_\Omega = - \left( M_c \nabla f'_0(c), \nabla \phi \right)_\Omega - \epsilon_c^2 \left( \Delta c, \nabla \cdot M_c^T \nabla \phi \right)_\Omega \\
+ \left( \left( M_c \nabla \left( f'_0(c) - \epsilon_c^2 \Delta c \right) \right) \cdot \vec{n}, \phi \right)_{\partial \Omega} \\
+ \epsilon_c^2 \left( \Delta c, M_c^T \nabla \phi \cdot \vec{n} \right)_{\partial \Omega}
\]
Free Energy Decay

Non-increasing global free energy can be guaranteed for modified weak equations, and typically observed even with unmodified Galerkin
Initial Evolution

- Initial homogeneous blend quenched below critical T
- Random perturbations rapidly segregate into two distinct phases, divided by a labyrinth of sharp interfaces
- Rapid anti-diffusionary process
Spinodal Decomposition

Long-term Evolution

- Single-phase regions gradually coalesce
- Motion into curvature vector resembles surface tension
- Patterning may occur when additional stress, surface tropisms are applied
Cahn-Hilliard with AMR/C

Interface Tracking Problem
- Coarsening in single-phase regions is traded for refinement in sharp layers
- Equivalent accuracy achieved here with 75% fewer degrees of freedom
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Cahn-Hilliard Phase Decomposition

Cahn-Hilliard with AMR/C

Phase Decomposition Problem

- Adaptive Mesh Refinement / Coarsening reduces solver expense
- Laplacian Jump error indicator keeps up with moving interfaces
Thin Film Patterning

Material Self-Assembly

- Electrostatic or chemical surface treatment attracts one material component preferentially
- A spatially varying bias is added to the configurational free energy
Low surface potential energy biases are overwhelmed by random noise
Effects of Bias Strength

Higher surface potential energy biases form patterns with decreasing defect density
Effects of Bias Strength

Free Energy Evolution for Various Imposed Bias Magnitudes

Patterning locks system into stable local free energy minima
Postprocessing - Defect Count

Quantitative measure of pattern non-conformity
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Cahn-Hilliard Phase Decomposition

Postprocessing - Correlation Lengths

\[ r(\vec{y}) \equiv \langle c(\vec{x})c(\vec{x} + \vec{y}) \rangle - \langle c(\vec{x}) \rangle^2 \]
Effects of Film Thickness

- Thin films rapidly become uniform in $z$ direction
- Thick films show more connectivity, fewer defects
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Cahn-Hilliard Phase Decomposition

Effects of Interfacial Free Energy

- Small increases in gradient coefficient speed defect reduction
- Wide diffuse interfaces lead to pattern instability
Effects of Quench Temperature

- Less reliable patterning at low T
- Incomplete phase decomposition at high T

Concentration Rate of Change for Various Temperatures
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Contributions

Primary New Contributions

- Macroelement/generalized constraints for adaptive mesh refinement/coarsening
- “Laplacian jump” a posteriori error indicator
- Algorithms for automatic AMR/C on transient problems
- Adaptive div-free elements for non-Newtonian flow
- Conforming, fully coupled heat and surfactant driven thin film flow formulations, solvers
- Conforming Cahn-Hilliard solutions on 2D, 3D, adaptive meshes
- Parametric/Monte Carlo studies of directed pattern self-assembly in thin film phase decomposition
Published Work

**Reviewed Articles**

