SAND2006-4593C

Integration Techniques for Extended Finite Element Methods

David R. Noble and David J. Holdych

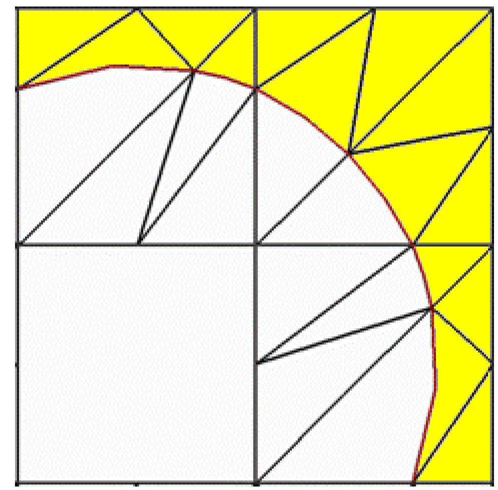
Sandia National Laboratories

Albuquerque, New Mexico

This work was performed at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

Sandia National Laboratories

XFEM Integration - Motivation



Modified Element Quadrature
- Basis and trial functions are now discontinuous
- For XFEM-Level set methods, functions become generalized functions of the level set variable
  - Heaviside and Dirac delta functions

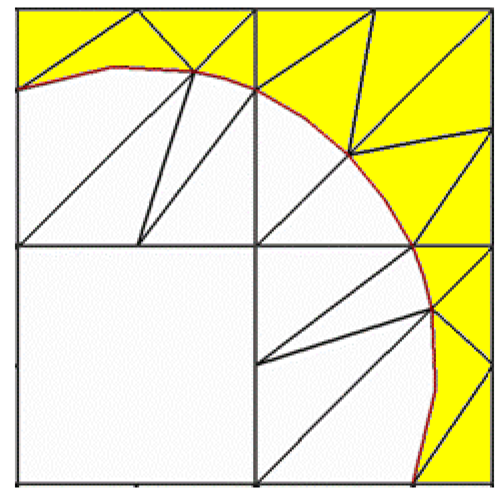
Moderately Invasive Feature in XFEM Codes
- Quadrature rule depends on level set variable
- Coupling issues, time derivative evaluation

Several Solutions
- Diffuse integration
  - Smoothed generalized functions
- Subelement integration
  - Subdivide elements into conformal subelements
  - Implementation issues
- Develop new integration rules for generalized functions
  - Derive new integration rules that account for generalized functions

XFEM Subelement Integration - Issues

Basics

- Decompose non-conformal element into conformal subelements
- Perform standard Gauss integration over subelements



Important Implementation Details

- What is definition of subelements?
  - Option 1: Coordinates of subelements are parametric coordinates for owning element
  - Option 2: Coordinates of subelements are real coordinates
- Consequences
  - Option 1
    - Gauss point locations in parent element are directly known
    - Pathological errors for low order subelements
  - Option 2
    - Gauss point locations are unknown and must be solved for using nonlinear iteration
    - Optimal accuracy obtained for low order subelements

Integration Rules for Elements with Generalized Functions - Motivation

Philosophical

- Integration rules designed to exactly integrate finite element functions
  - Enriched functions need modified quadrature rules

Pragmatic When Compared with Alternatives

- Diffuse methods
  - Simple but inaccurate, inconsistent
- Subelement methods
  - Must be carefully implemented
  - Can be expensive when having to solve nonlinear system for parametric coordinates
  - Must specifically account for degenerate cases

Allows Advanced Capabilities

- Provides analytical Jacobian information
  - Required by full Newton codes
  - Make interfacial optimization possible

Possible Disadvantages

- Possibly increases number of quadrature points for same element
- Difficult, if not impossible to derive for higher order elements

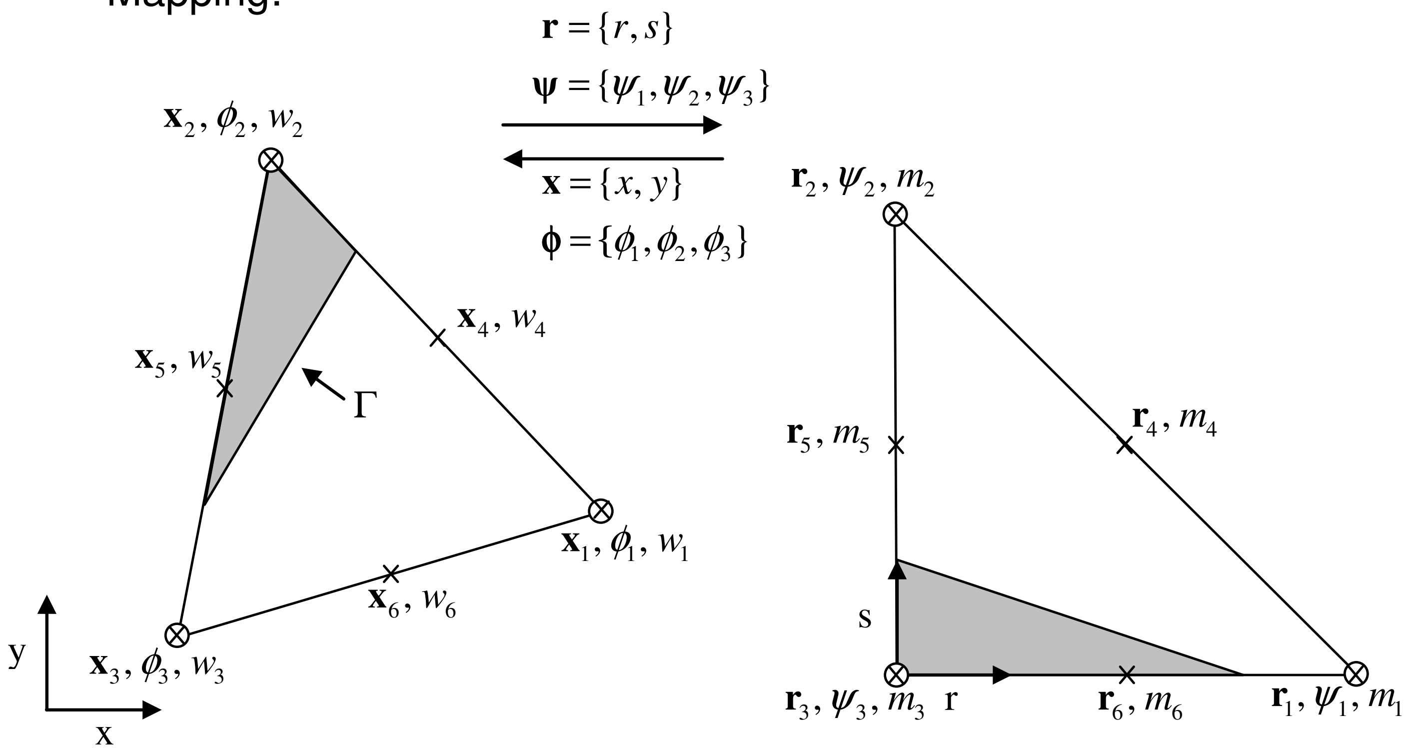
Generalized Quadrature - Method

Approach

- Develop quadrature rules capable of exactly integrating finite element functions including a generalized function of the level set variable
  - Piecewise polynomial times Heaviside or Dirac delta function
- Form:

$$\int_{\Omega^+} g(\mathbf{x})\, d\Omega_{\mathbf{x}} = \sum_{i=1}^{6} w_i^+(\boldsymbol{\phi})\, g(\mathbf{x}_i)\, J(\mathbf{x}_i) \qquad \int_{\Gamma} g\, d\Gamma_{\mathbf{x}} = \sum_{i=1}^{6} w_i^{\Gamma}(\boldsymbol{\phi}) \left|\nabla \phi(\mathbf{x}_i)\right| g(\mathbf{x}_i) J(\mathbf{x}_i)$$

- Mapping:



Sandia National Laboratories

Generalized Quadrature - Method

- Form linear system for weights

$$I_f^{\Delta}(\boldsymbol{\psi}) \equiv \int_{\Delta} f(\mathbf{r})\,d\Omega_{\mathbf{r}} = \sum_{i=1}^{6} m_i^{\Delta}(\boldsymbol{\phi}) f(\mathbf{r}_i)$$

$$\mathbf{A}\,\mathbf{m}^{\Delta}(\boldsymbol{\psi}) = \mathbf{I}^{\Delta}(\boldsymbol{\psi})$$

  - Require all monomials in a quadratic function be exactly integrated

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ r_1 & r_2 & r_3 & r_4 & r_5 & r_6 \\ s_1 & s_2 & s_3 & s_4 & s_5 & s_6 \\ r_1 s_1 & r_2 s_2 & r_3 s_3 & r_4 s_4 & r_5 s_5 & r_6 s_6 \\ r_1^2 & r_2^2 & r_3^2 & r_4^2 & r_5^2 & r_6^2 \\ s_1^2 & s_2^2 & s_3^2 & s_4^2 & s_5^2 & s_6^2 \end{bmatrix} \begin{bmatrix} m_1^{\Delta}(\boldsymbol{\psi}) \\ m_2^{\Delta}(\boldsymbol{\psi}) \\ m_3^{\Delta}(\boldsymbol{\psi}) \\ m_4^{\Delta}(\boldsymbol{\psi}) \\ m_5^{\Delta}(\boldsymbol{\psi}) \\ m_6^{\Delta}(\boldsymbol{\psi}) \end{bmatrix} = \begin{bmatrix} I_1^{\Delta}(\boldsymbol{\psi}) \\ I_r^{\Delta}(\boldsymbol{\psi}) \\ I_s^{\Delta}(\boldsymbol{\psi}) \\ I_{rs}^{\Delta}(\boldsymbol{\psi}) \\ I_{r^2}^{\Delta}(\boldsymbol{\psi}) \\ I_{s^2}^{\Delta}(\boldsymbol{\psi}) \end{bmatrix}$$

  - Select quadrature point locations
    - Valid quadrature rules yield nonsingular matrix,
    - Normally quadrature point locations considered unknowns select so that integration achieves desired order with minimal number of points
    - Arbitrary interface location makes fortuitous point selection impossible
    - Simplest valid quadrature rules involve points on the nodes and edges

Generalized Quadrature - Method

- Form linear system for weights, cont'd
  - Analytically evaluate integrals as function of nodal level set values

$$I_1^{\Delta}(\psi)=\frac{\psi_3^2}{2\Delta_{31}\Delta_{32}} \quad I_{rs}^{\Delta}(\psi)=\frac{\psi_3^4}{24\Delta_{31}^2\Delta_{32}^2}$$

$$I_r^{\Delta}(\psi)=\frac{\psi_3^3}{6\Delta_{31}^2\Delta_{32}} \quad I_{r^2}^{\Delta}(\psi)=\frac{\psi_3^4}{12\Delta_{31}^3\Delta_{32}}$$

$$I_s^{\Delta}(\psi)=\frac{\psi_3^3}{6\Delta_{31}^2\Delta_{32}} \quad I_{s^2}^{\Delta}(\psi)=\frac{\psi_3^4}{12\Delta_{31}\Delta_{32}^3}$$

$$\Delta_{31} \equiv \psi_3-\psi_1$$

$$\Delta_{32} \equiv \psi_3-\psi_2$$

- Solve for weights as functions of nodal level set values

$m_i^{\Delta}(\psi)$	functional form
$m_1^{\Delta}(\psi)$	$-I_r^{\Delta}(\psi)+2I_{r^2}^{\Delta}(\psi)$
$m_2^{\Delta}(\psi)$	$-I_s^{\Delta}(\psi)+2I_{s^2}^{\Delta}(\psi)$
$m_3^{\Delta}(\psi)$	$I_1^{\Delta}(\psi)-3I_r^{\Delta}(\psi)-3I_s^{\Delta}(\psi)+4I_{rs}^{\Delta}(\psi)+2I_{r^2}^{\Delta}(\psi)+2I_{s^2}^{\Delta}(\psi)$
$m_4^{\Delta}(\psi)$	$4I_{rs}^{\Delta}(\psi)$
$m_5^{\Delta}(\psi)$	$4(I_s^{\Delta}(\psi)-I_{rs}^{\Delta}(\psi)-I_{s^2}^{\Delta}(\psi))$
$m_6^{\Delta}(\psi)$	$4(I_r^{\Delta}(\psi)-I_{rs}^{\Delta}(\psi)-I_{r^2}^{\Delta}(\psi))$

Results

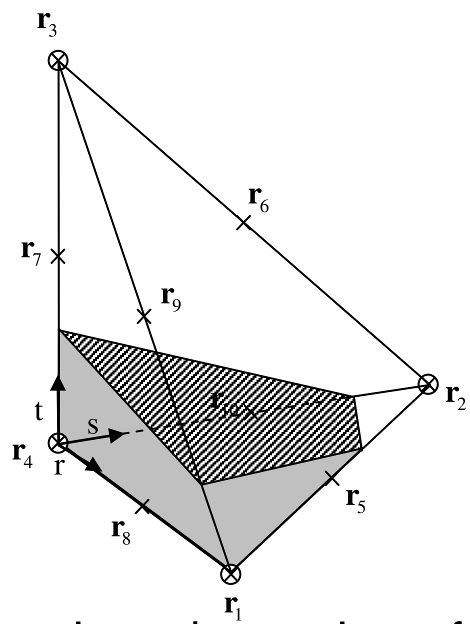
- Weights are continuous functions of nodal level set values
  - Allows analytical Jacobian formation
  - All degenerate cases handled without special consideration
- Weights are not positive definite

Sandia National Laboratories

Generalized Quadrature – Other Elements

3D Tetrahedra

- Mapping:



- Analytically evaluate integrals as function of nodal level set values
  - Case 1: 1 node on opposite side from other 3
  - Case 2: 2 nodes on opposite side from other 2

Higher Order Elements (Including quads/hexes)

- Analytically evaluate integrals as function of nodal level set values
  - Integrals difficult, if not impossible, to evaluate in general

Sandia National Laboratories

Generalized Quadrature – Test Problem

Conduction in Annulus and Spherical Shell

- Poisson equation, $k = 1$, $q = 1$

  $$\nabla \cdot k\nabla T + q = 0$$

- Boundary conditions
  - Insulated inner surface
  - Robin-type output surface, $h = 10$

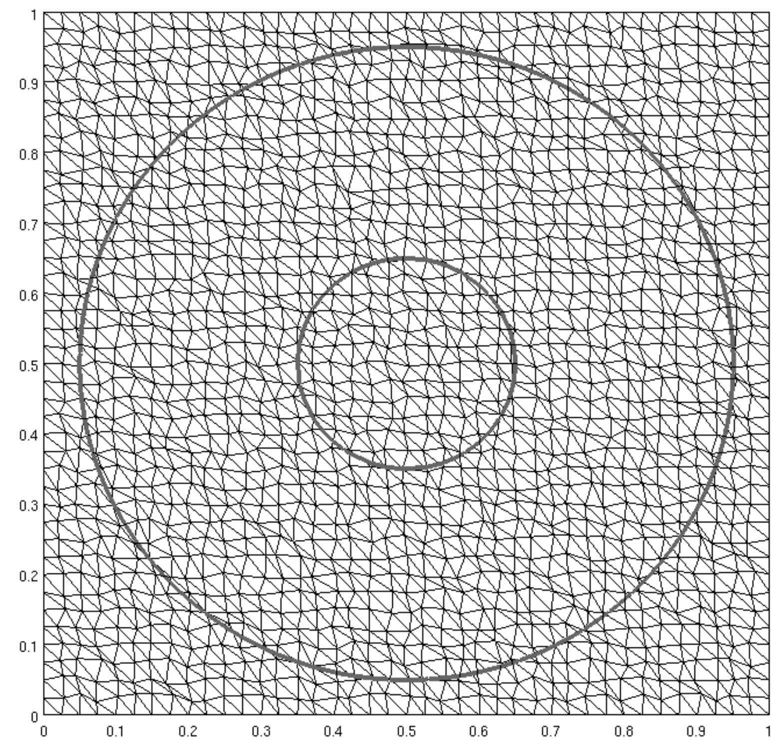
    $$-\mathbf{n}_{outer} \cdot k\nabla T = h(T-0)$$

Discretization

- Linear triangle and tetrahedral elements, linear temperature, linear level set function
- Randomly perturbed nodes of structured mesh
  - Rigorous test for deformed meshes

Validation

- Compare against exact solutions



$$T^{2D}(r) = \frac{q}{4k}\left(R_o^2 - r^2\right) + \frac{q}{2hR_o}\left(R_o^2 - R_i^2\right) - \frac{qR_i^2}{2k}\left(\log\left(R_o\right) - \log\left(r\right)\right)$$

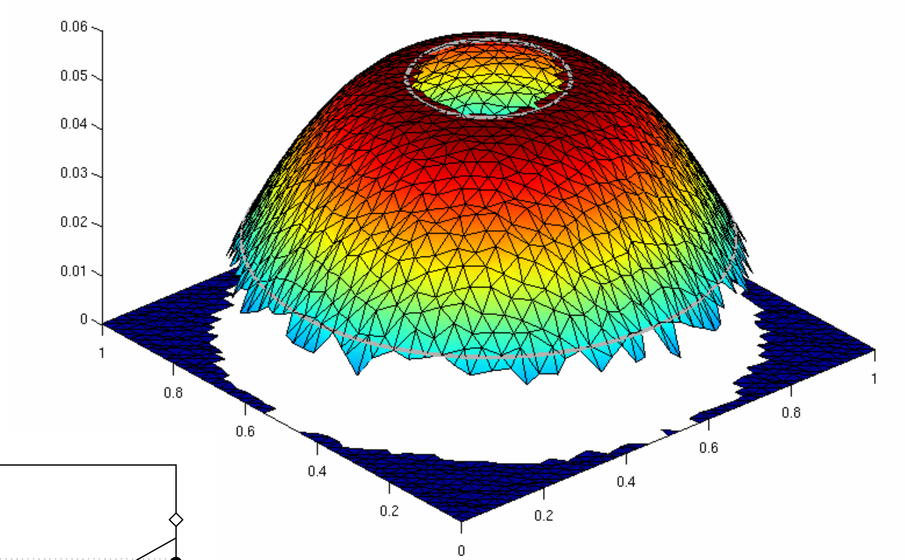
$$T^{3D}(r) = \frac{q}{3hR_o^2}\left(R_o^3 - R_i^3\right) - \frac{q}{6kr}\left(r^3 + 2R_i^3\right) + \frac{q}{6kR_o}\left(R_o^3 + 2R_i^3\right)$$

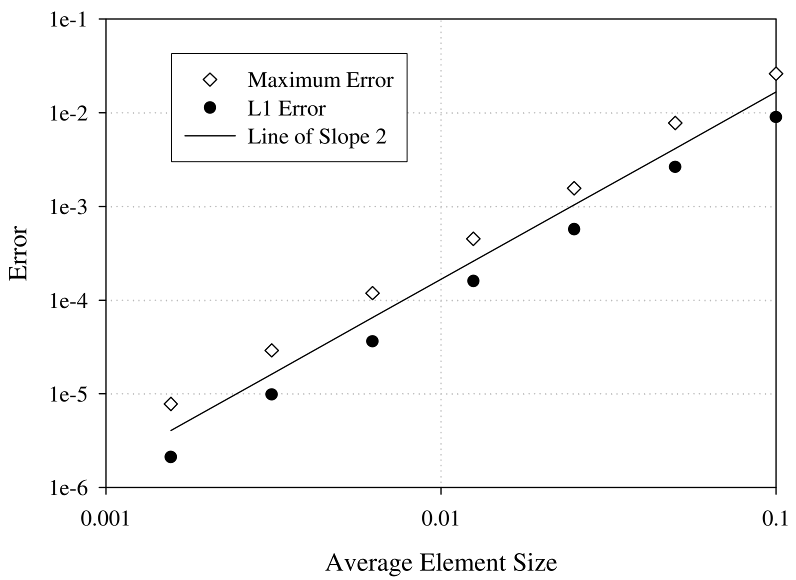
Sandia National Laboratories

Generalized Quadrature – 2D Test

Results

- Visualization - Elements that use ghost nodes and exterior nodes are removed
- Sharp discontinuities captured along inner and outer surfaces
- 2^{nd} order accuracy demonstrated over multiple decades



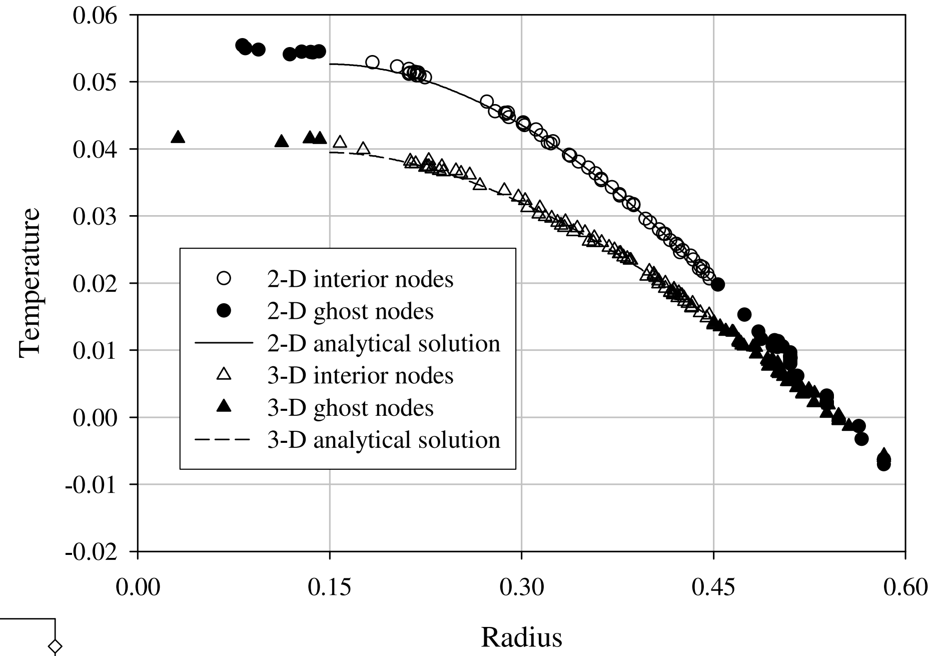


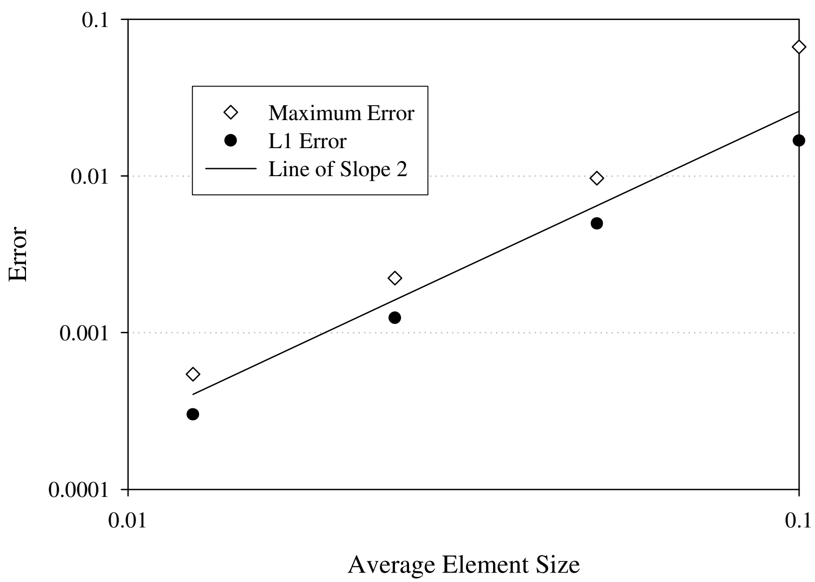
Sandia National Laboratories

Generalized Quadrature – 3D Test

Results

- 2^{nd} order accuracy
- Successfully integrates discontinuous function using fixed gauss point quadrature rule
- Successfully handles degenerate cases without special consideration





Sandia National Laboratories

Summary and Conclusions

Care Must be Taken When Using Subelement Integration

- Definition of subelements – Parametric or real coordinates?
- Performance issues – Quadrature point location inversion
- Low order subelements can lead to suboptimal convergence

Analytic Integration with Generalized Functions

- Can be used to formulate fixed point integration rules with weights that depend continuously on nodal level set values
- Provides analytic Jacobian information
- Handles degenerate cases smoothly without special consideration

Hybrids are Possible

- Subelement methods could be used to form fixed point integration rules

$$I_f^{\Delta}(\boldsymbol{\psi}) \equiv \int_{\Delta} f(\mathbf{r})\,d\Omega_{\mathbf{r}} = \sum_{i=1}^{6} m_i^{\Delta}(\boldsymbol{\phi})\, f(\mathbf{r}_i)$$

$$\mathbf{A}\,\mathbf{m}^{\Delta}(\boldsymbol{\psi}) = \mathbf{I}^{\Delta}(\boldsymbol{\psi})$$

Sandia National Laboratories

Implementation – Applying XFEM to Laser Welding

Problem Discretization

- Fixed unstructured mesh
- Solid-liquid interface described by enthalpy method
  - Specific heat is temperature dependent to account for latent heat
  - Viscosity sharp function of temperature around between solidus and liquidus
- Liquid-vapor interface described by level set method

Variable Enrichment

- Variables allowed to be discontinuous across liquid-vapor interface

Subelement Integration

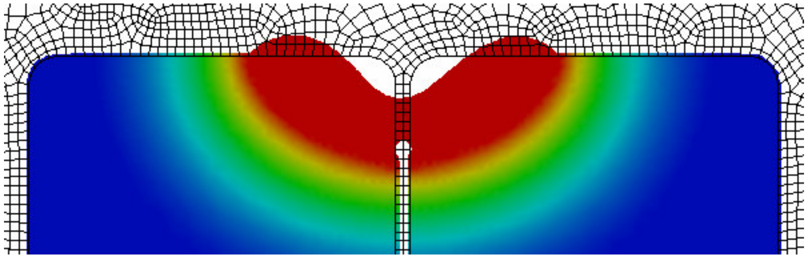
- Required to integrate discontinuous quantities resulting from discontinuous variables and trial functions

Interfacial conditions

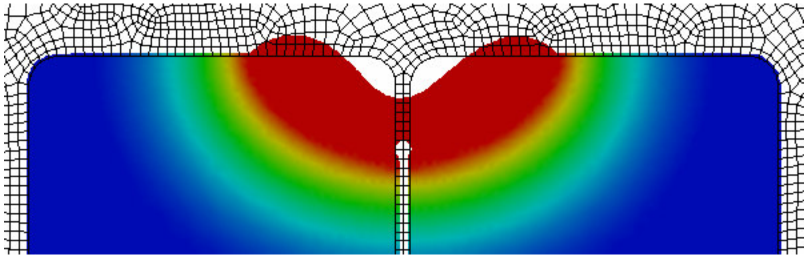
- XFEM approach produces natural mechanism for applying interfacial fluxes
- Several options discussed in literature for handling surface tension

Coupling

- Implemented in code designed for fully coupled, Newton's method
- Choice of surface tension application made this impossible
  - Final algorithm involves loosely coupling the level set evolution to the mass, momentum, and energy evolution



Implementation – Interfacial Conditions



Complex Interfacial Conditions

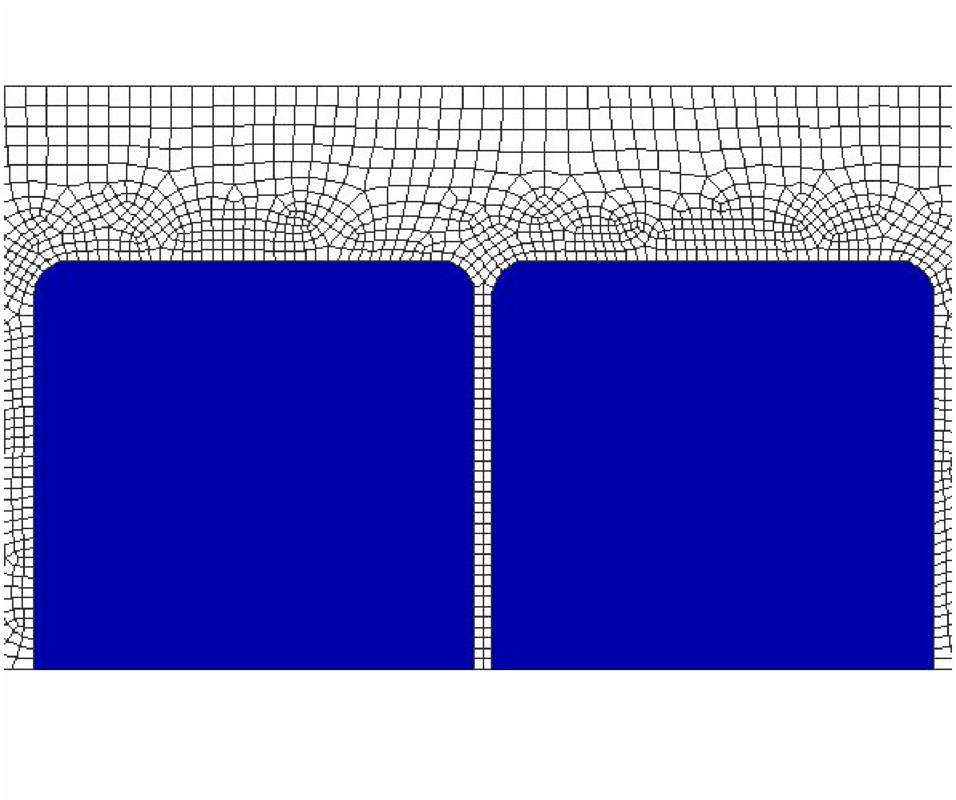
- Laser heat flux
  - Gaussian or flat radial distribution
  - Highly dependent on surface normal
  - Weakly applied to energy equation along interface
- Radiative heat flux
  - Highly dependent on surface temperature
  - Weakly applied to energy equation along interface
- Latent heat due to vaporization
  - Vaporization rate assumed to be function of surface superheat
  - Highly dependent on surface temperature
  - Weakly applied to energy equation along interface
- Vapor recoil pressure
  - Vaporization rate assumed to be function of surface superheat
  - Highly dependent on surface temperature
  - Weakly applied to momentum equation along interface
- Surface tension
  - Weakly applied to momentum equation along interface

Sandia National Laboratories

Results – XFEM Simulations of Laser Welding

Full physics simulations in realistic geometries

- Previous ALE capability limited to non-joining simulations of welding
- XFEM capturing important surface discontinuities
- XFEM framework amenable to varied interface conditions
- Not just prettier pictures, revealing new insight into process and failure mechanisms



Sandia National Laboratories

Implementation – Applying eXtended Finite Elements (XFEM) to Foam Decomposition

Problem Discretization

- Fixed unstructured mesh
- Solid-liquid interface described by enthalpy method
  - Specific heat is temperature dependent to account for latent heat
  - Viscosity sharp function of temperature around between solidus and liquidus
- Liquid-vapor interface described by level set method
  - Level set evolution described by evolution equation
  - 2 components of interfacial motion: flow and reaction

Variable Enrichment

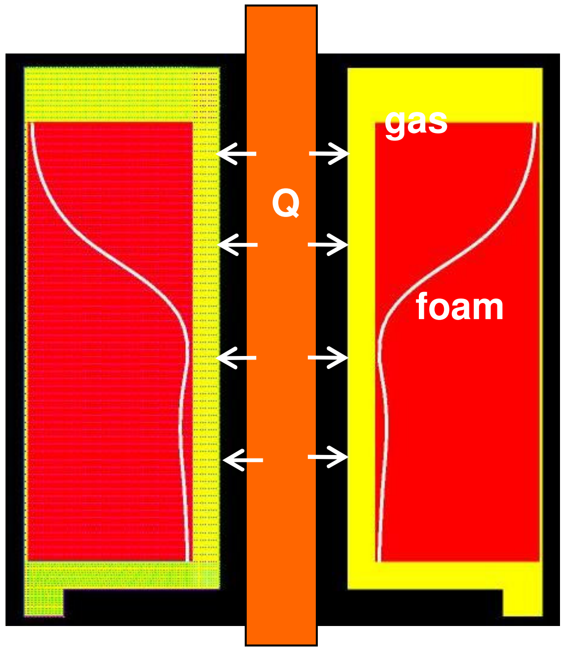
- Variables allowed to be discontinuous across liquid-vapor interface

Subelement Integration

- Required to integrate discontinuous quantities resulting from discontinuous variables and trial functions

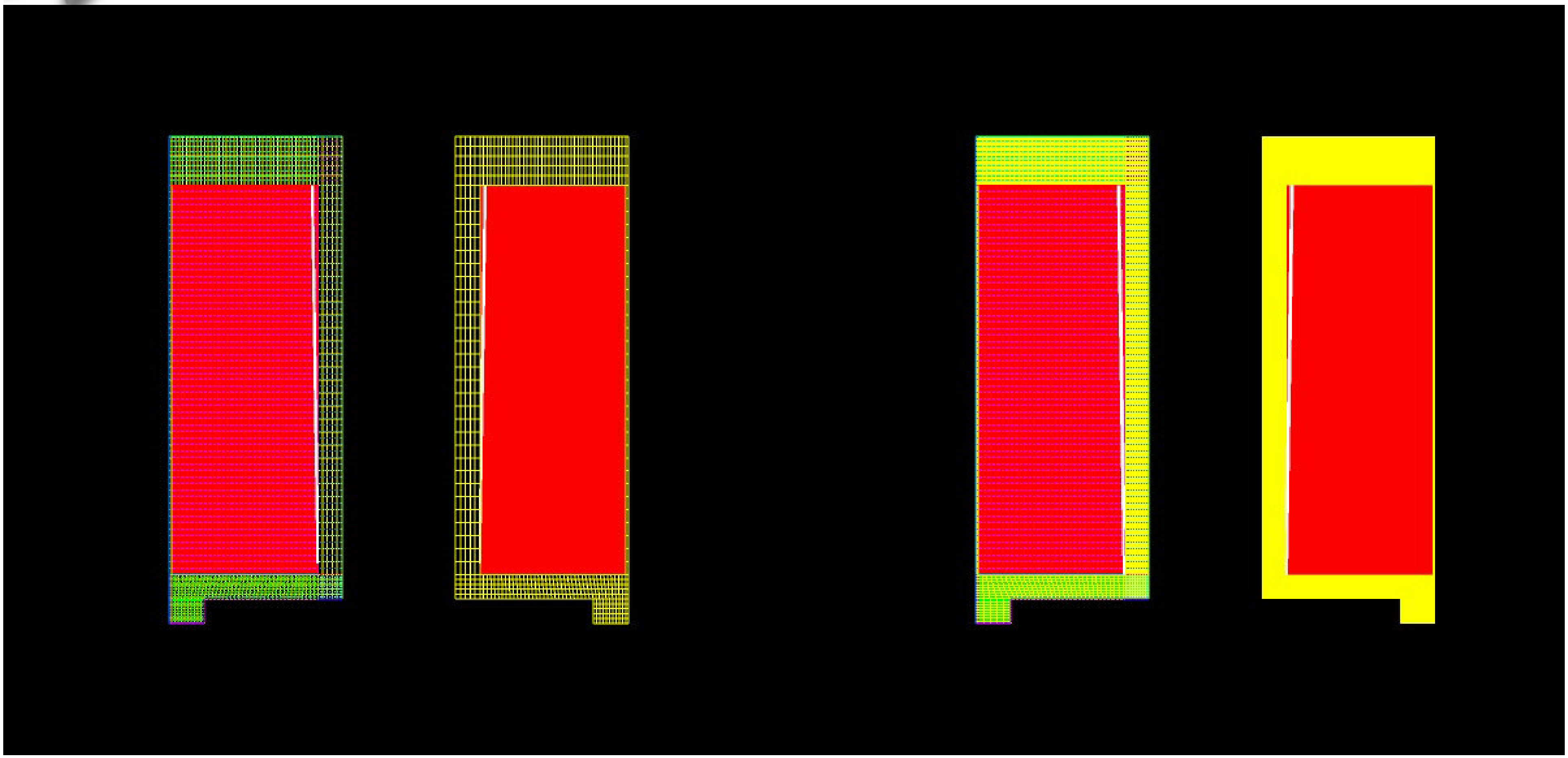
Interfacial Conditions

- XFEM approach produces natural mechanism for applying interfacial fluxes including surface reaction and surface tension



Sandia National Laboratories

Results – XFEM Simulations



- XFEM capturing important surface discontinuities, fluxes
- As expected, viscosity of fluid phase plays critical role in dynamics
  - Experimental effort to determine viscosity of decomposing foam

Sandia National Laboratories