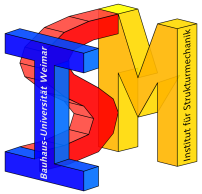

Institute of Structural Mechanics

The Three Dimensional Extended Bridging Domain Method (XBDM) for Modelling Dynamic Fracture

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ECCOMAS, 2012

Outline

- Motivation
- The eXtended Bridging Domain Method
- Setup and Implementation
- Verification and Validation
- Numerical Examples
- Discussion
- Conclusion and Future Work

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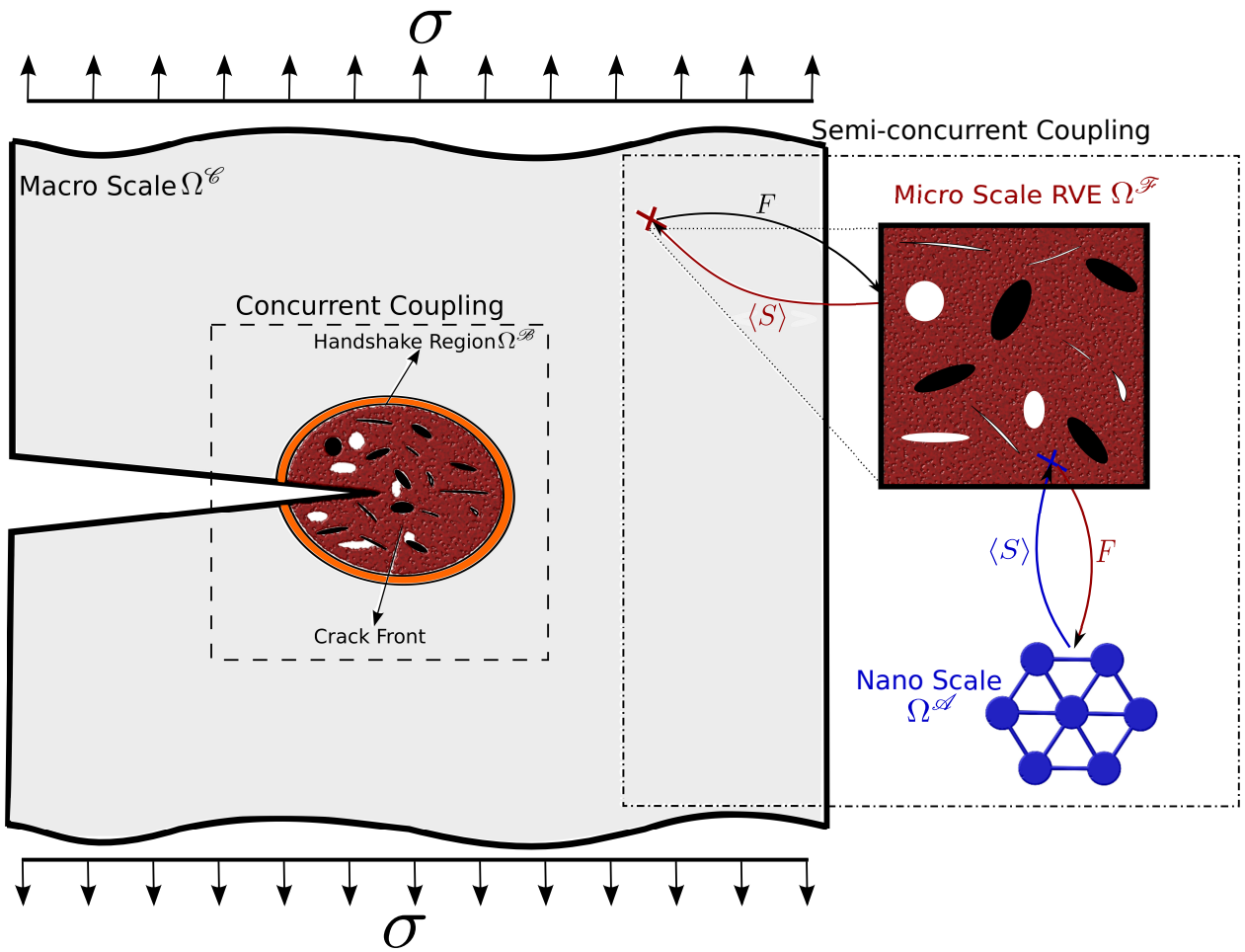
- Atomistic simulations – computationally expensive
- Multiscale methods to compute what actually matters
- In fracture simulation, crack and dislocation propagation should be confined around the crack tip
- We focus on the Arlequin type methods which is suitable for dynamic fracture
- For MD–XFEM coupling it is called *eXtended Bridging Domain Method (XBDM)*

Multiscale methods



Semi-concurrent and Concurrent multiscale methods

The XBDM method

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  ii. Wave reflection is minimum

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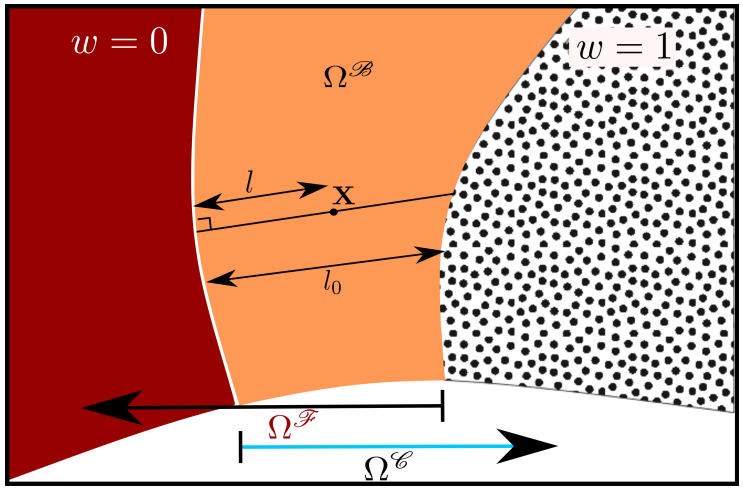
  ii. Wave reflection is minimum
- Coupling is enforced with the Lagrange multipliers
- Ghost atoms move with the continuum

The Coupling Method



weighting function

$$w(\boldsymbol{X}) = \begin{cases} 1 & \forall \boldsymbol{X} \in \Omega^{\mathscr{C}} \setminus \Omega^{\mathscr{F}} \\ [0,1] & \forall \boldsymbol{X} \in \Omega^{\mathscr{B}} \\ 0 & \forall \boldsymbol{X} \in \Omega^{\mathscr{F}} \setminus \Omega^{\mathscr{C}}. \end{cases}$$

$$w(\boldsymbol{X}) = \frac{l(\boldsymbol{X})}{l_0}$$

Governing Equations

The governing equations are derived from the Hamiltonian of both systems:

$$H = wH^{\mathscr{F}} + (1-w)H^{\mathscr{C}} = \sum_{\alpha}(w(\boldsymbol{X}_\alpha))\frac{\boldsymbol{P}_\alpha^{\mathscr{F}} \cdot \boldsymbol{P}_\alpha^{\mathscr{F}}}{2m_\alpha} +$$

$$(w)W^{\mathscr{F}} + \sum_{I}(1-w)(\boldsymbol{X}_I)\frac{\boldsymbol{P}_I^{\mathscr{C}} \cdot \boldsymbol{P}_I^{\mathscr{C}}}{2M_I} + (1-w)W^{\mathscr{C}}$$

In the Lagrange multipler method, the total Hamiltonian is:

$$H_L = H + \lambda^T \boldsymbol{g}$$

And g is the gap vector between the displacements.

Governing Equations

In explicit dynamics the semi-discrete equations are:

$$M_{IJ}\ddot{u}_{Ji} = f_{Ii}^{\text{ext}} - f_{Ii}^{int} + f_{Ii}^{\lambda\mathscr{C}}$$

$$m_{\alpha}^{\mathscr{F}}\ddot{d}_{\alpha i}^{\mathscr{F}} = f_{\alpha i}^{\mathscr{F}} + f_{\alpha i}^{\lambda\mathscr{F}}$$

$$M_{IJ} = \int_{\Omega_0^{\mathscr{C}}} (1-w)\,\rho_0 N_I N_J d\Omega_0^{\mathscr{C}} \quad ,$$

Internal forces in continuum:

$$f_{Ii}^{int} = \int_{\Omega_0^{\mathscr{C}}} (1-w)\,P_{ij}\frac{\partial N_I}{\partial X_j} d\Omega_0^{\mathscr{C}},$$

Governing Equations

The forces on each atom are determined from the interatomic potential W as:

$$f_{\alpha i}^{\mathscr{F}} = -\sum_{\beta} \frac{1}{2} \left(w\left(X_\alpha\right) + w\left(X_\beta\right) \right) \frac{\partial W\left(r_{\alpha\beta}\right)}{\partial d_{i\beta}^{\mathscr{F}}} \quad ,$$

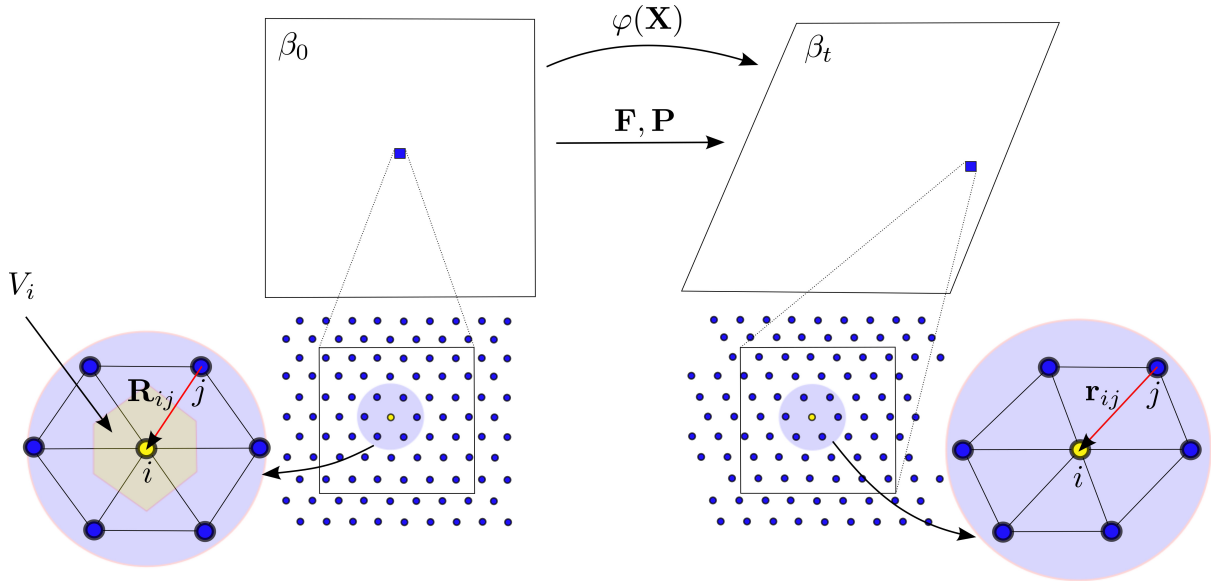
The coupling forces on the fine and coarse scales are:

$$f_{Ii}^{\lambda\mathscr{C}} = \sum_{\alpha \in \Omega_0^{\mathscr{B}}} \lambda_{\alpha i} N_I\left(X_\alpha\right), \quad f_{\alpha i}^{\lambda\mathscr{F}} = -\lambda_{\alpha i}$$

The displacement approximation with XFEM is

$$\boldsymbol{u}^h\left(\boldsymbol{X}\right) = \underbrace{\sum_{I \in \mathcal{N}} N_I\left(\boldsymbol{X}\right) \boldsymbol{u}_I}_{\mathbf{u}^{\text{cont}}} + \underbrace{\sum_{I \in \mathcal{N}_b} N_I\left(\boldsymbol{X}\right) H\left(f_I\left(\boldsymbol{X}\right)\right) \boldsymbol{a}_I}_{\mathbf{u}^{\text{discont}}}$$

Cauchy-Born Rule



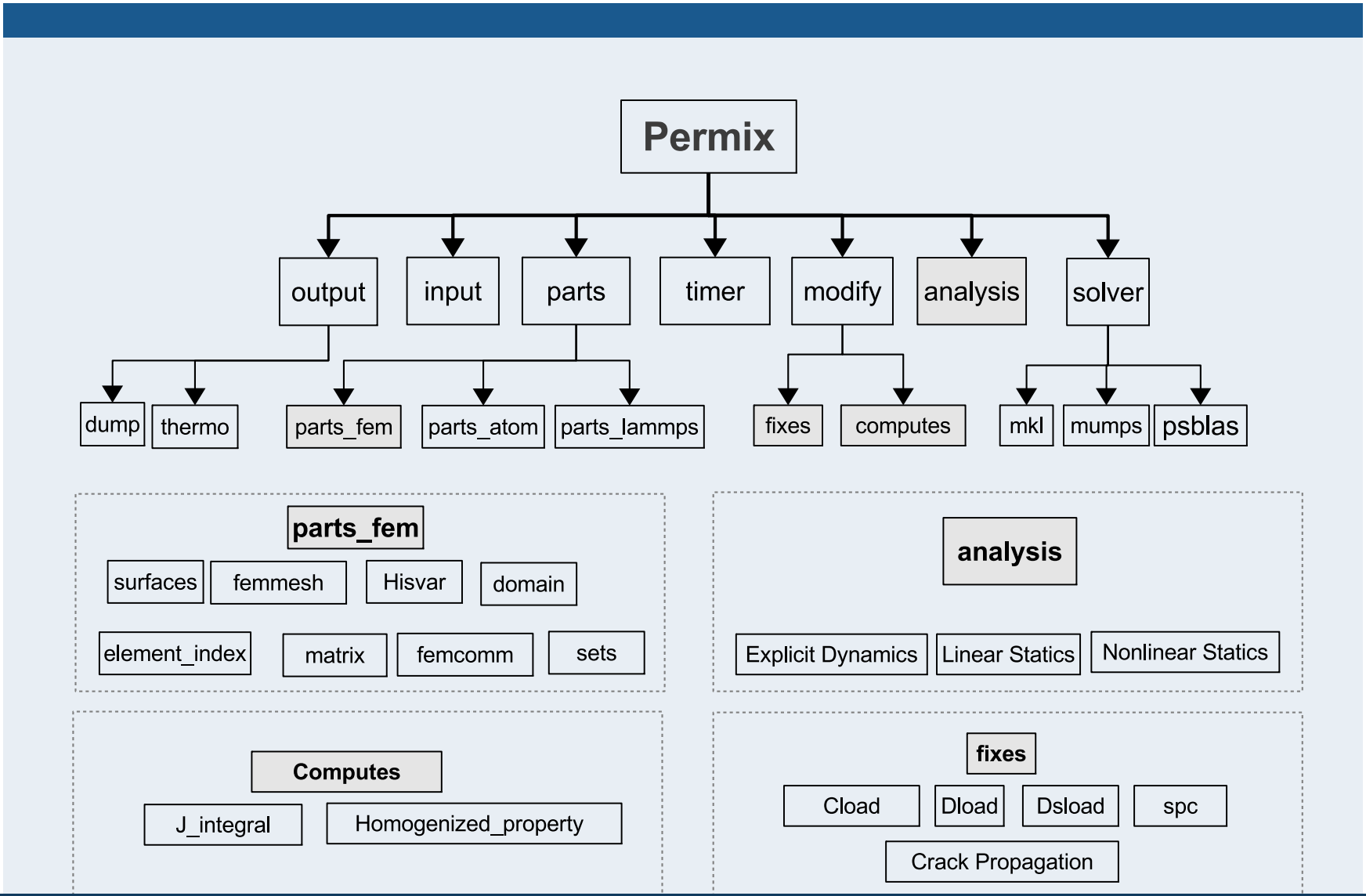
1^{st} Piola-Kirchhoff stress tensor and 4^{th} tangent operator

$$\mathbf{P}_i \doteq \frac{1}{2V_i} \sum_{j \neq i} \mathbf{f}_{ji} \otimes \mathbf{R}_{ij} \ , \ \mathbf{C} \doteq \frac{\partial^2 W_0}{\partial \mathbf{F} \otimes \partial \mathbf{F}}$$

Problem Setup

- 1. Read the coarse and fine scale model definitions
- 2. Minimize the potential energy of the atomistic part
- 3. Build the neighbor lists for the coarse scale
- 4. Find all the atoms in all elements
- 5. Find active elements, bridging elements and nodes
- 6. Compute the weights of the nodes and integration points
- 7. Find active atoms, bridging atoms and ghost atoms
- 8. Recompute coarse and fine scale masses
- 9. Set up the Lagrange multiplier points
- 10. Compute the coupling matrix

A Platform for Multiscale Analysis

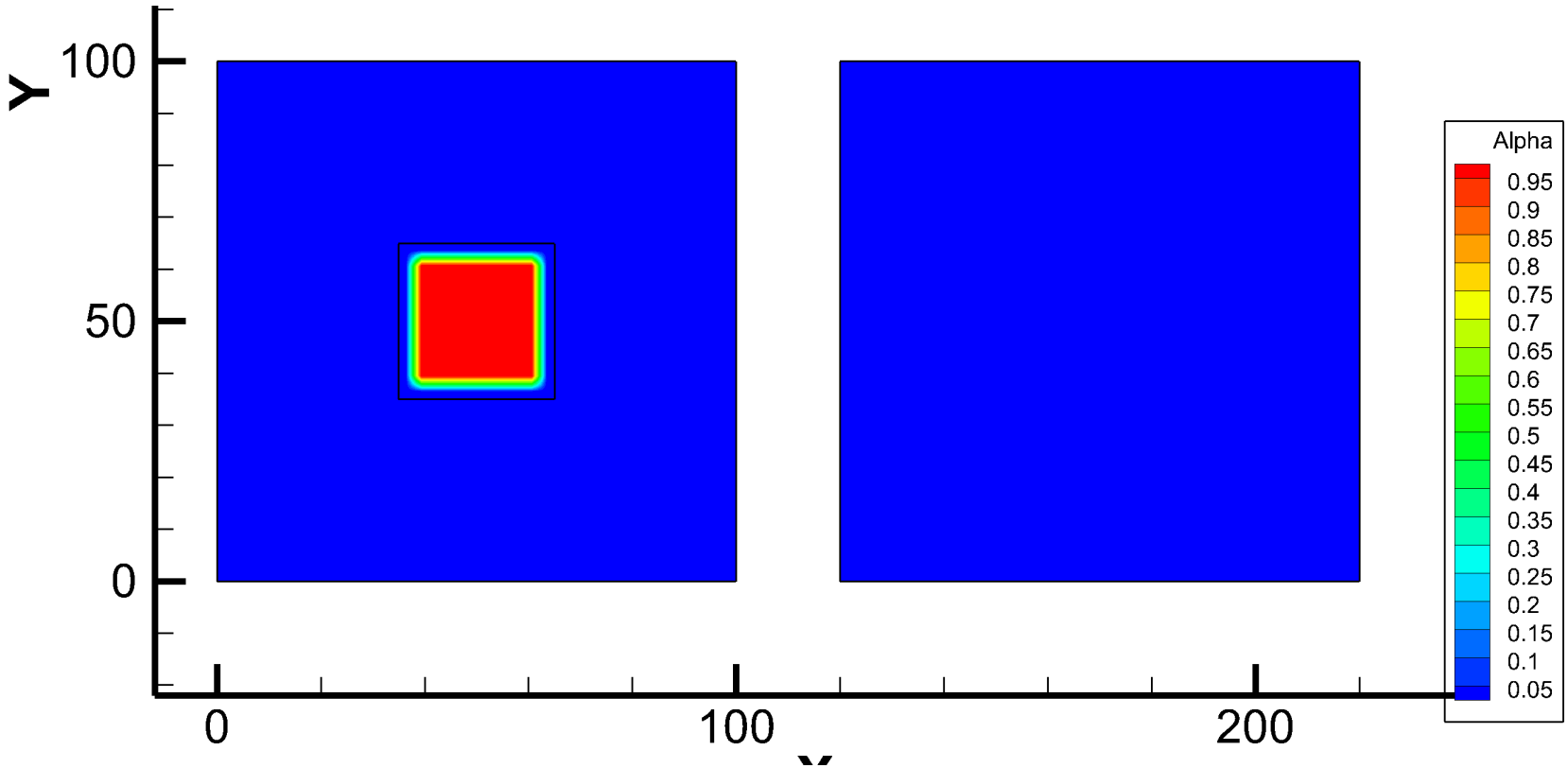


Major PERMIX Features

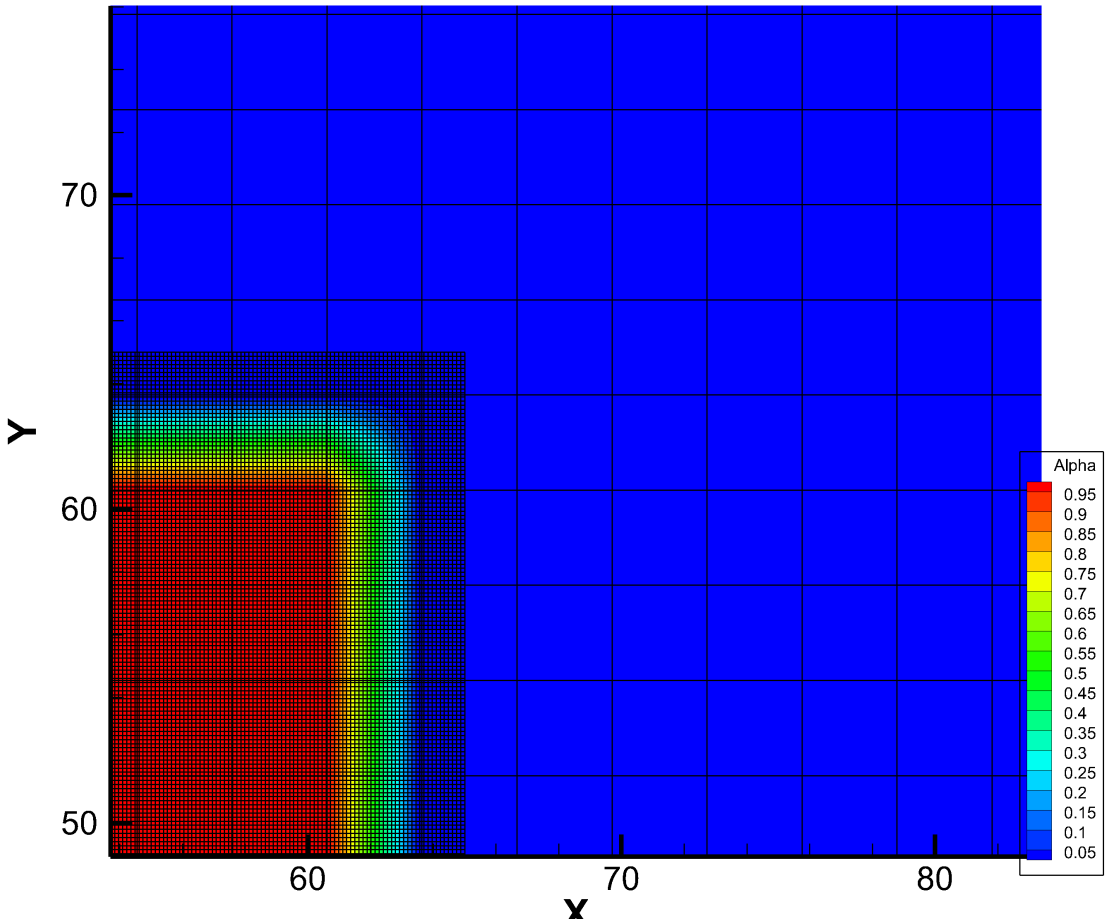
- Fully extensible object oriented Fortran 2003 compliant
- Parallel MD part (LJ, EAM, MEAM) based on WARP
- An F03 interface for LAMMPS (C++ version).
- 2 and 3 dimensional Extended Finite Elements.
- Explicit Dynamic and Nonlinear Static Solver
- Coupling FE–XFEM and XFEM–MD using Arlequin method
- Can handle semi-concurrent multiscale methods
- Material models, boundary conditions and loading types
- Interface to many libraries such as TETGEN, GEOMPACK, MUMPS, MKL, etc.

Verification Example 1

Dynamic FE-FE coupling



Verification Example 1: Zoom



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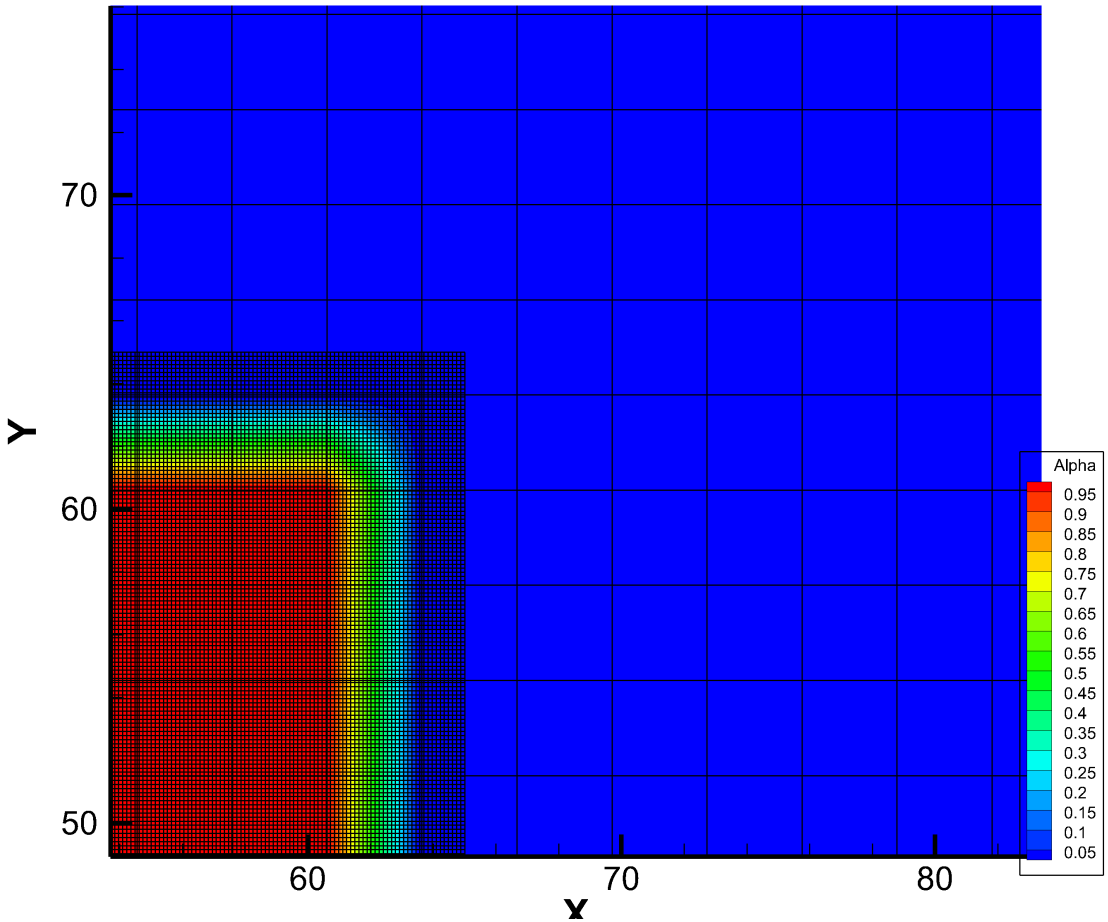
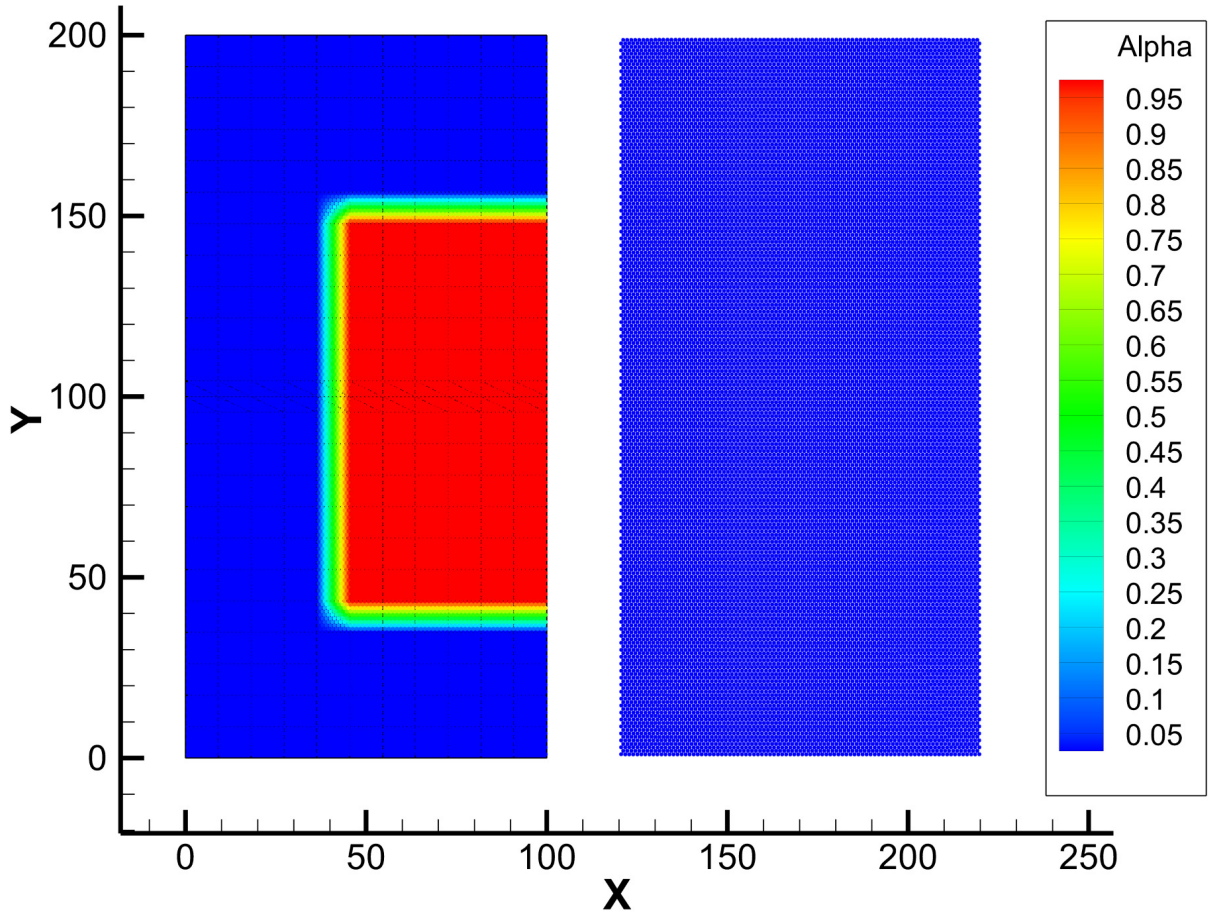


Results: Movie 1

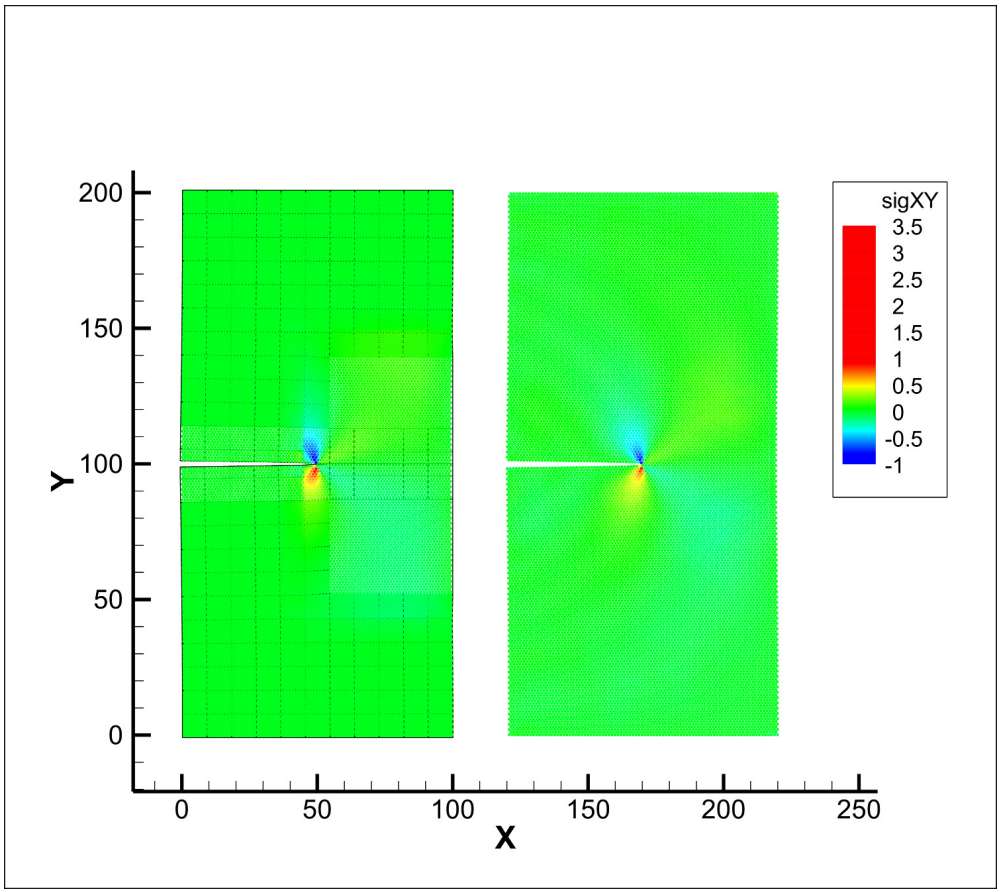
Verification Example 2

Dynamic XFEM-MD coupling in 2D



Verification Example 2

Results: Virial Stress is shown



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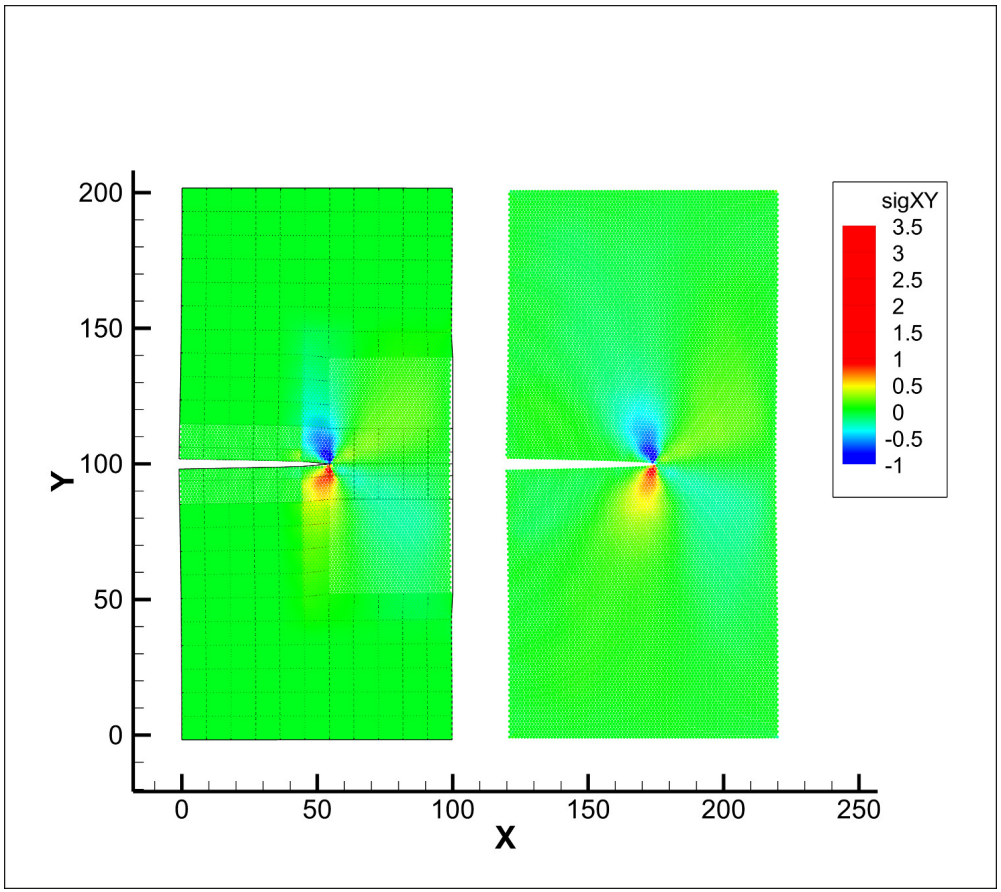

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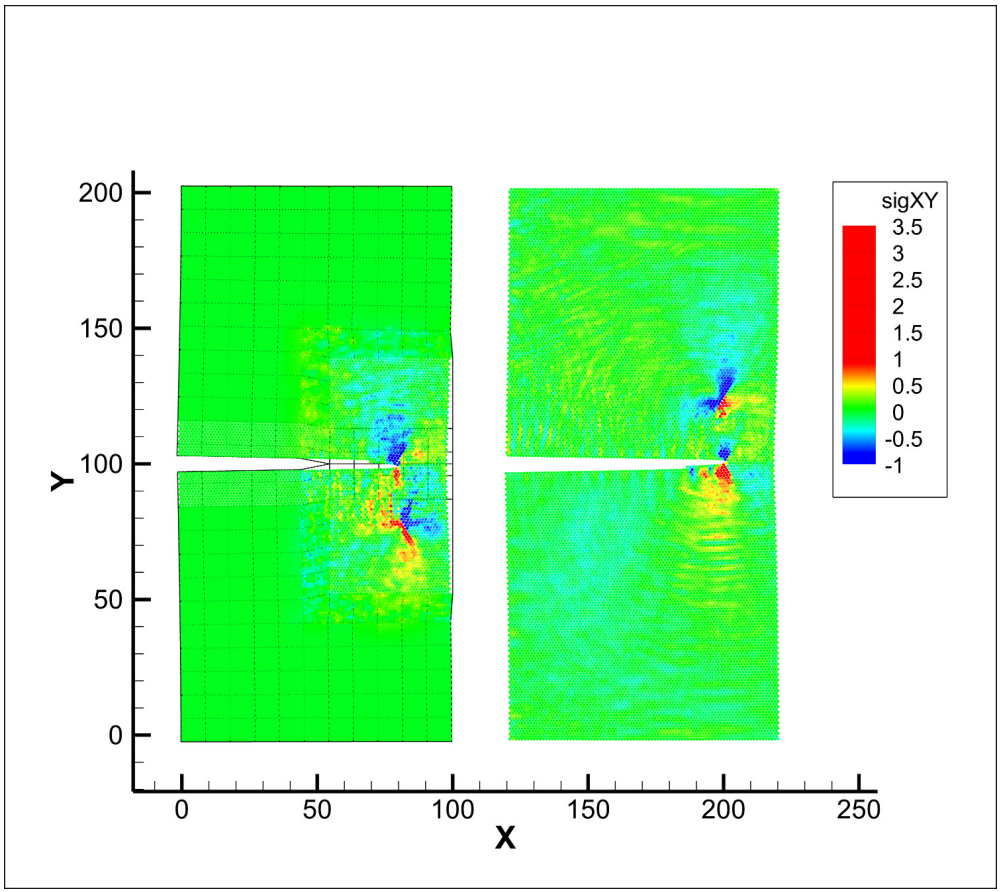
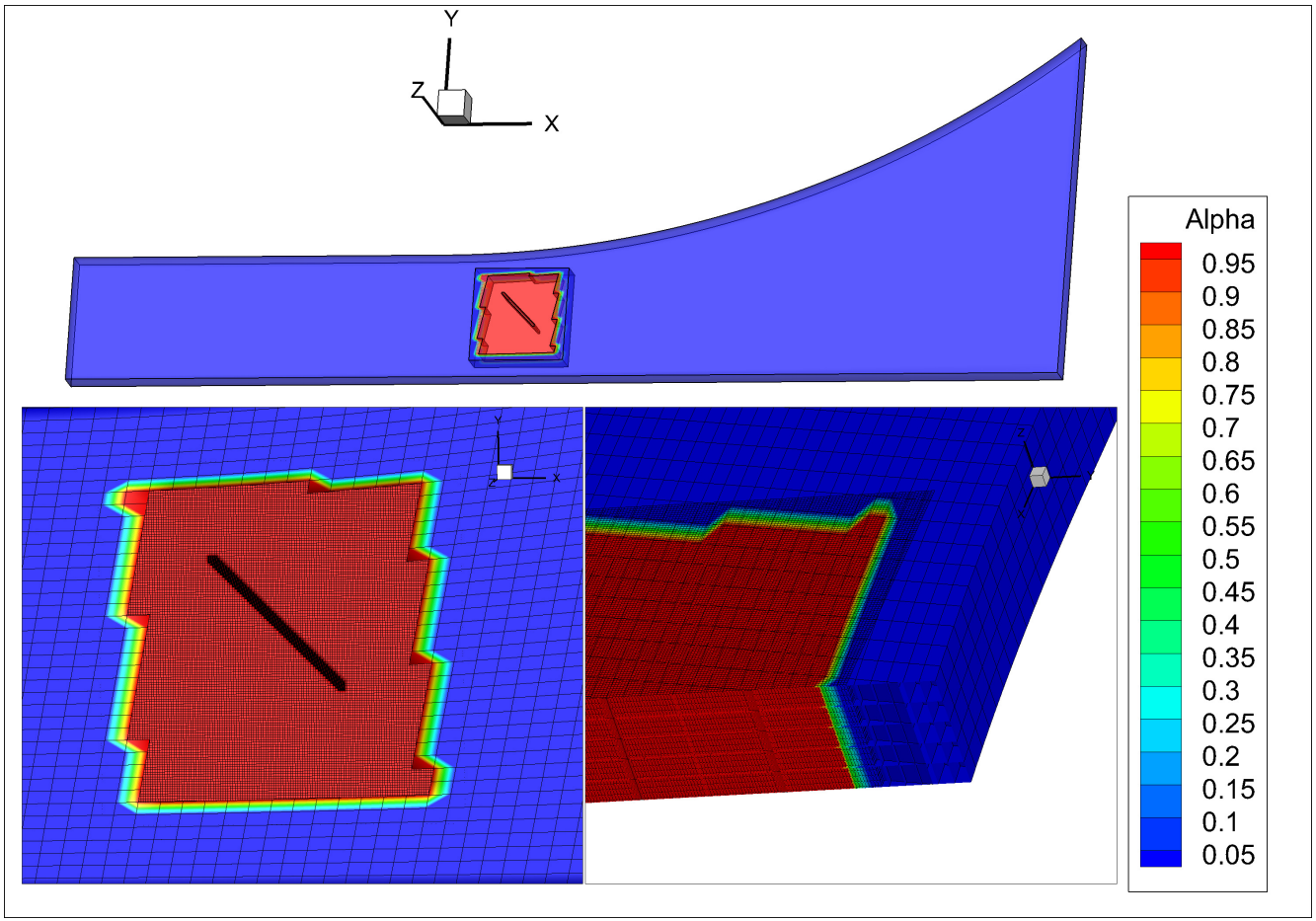


Example 1: 3D FE-XFEM Coupling

Initial Configuration



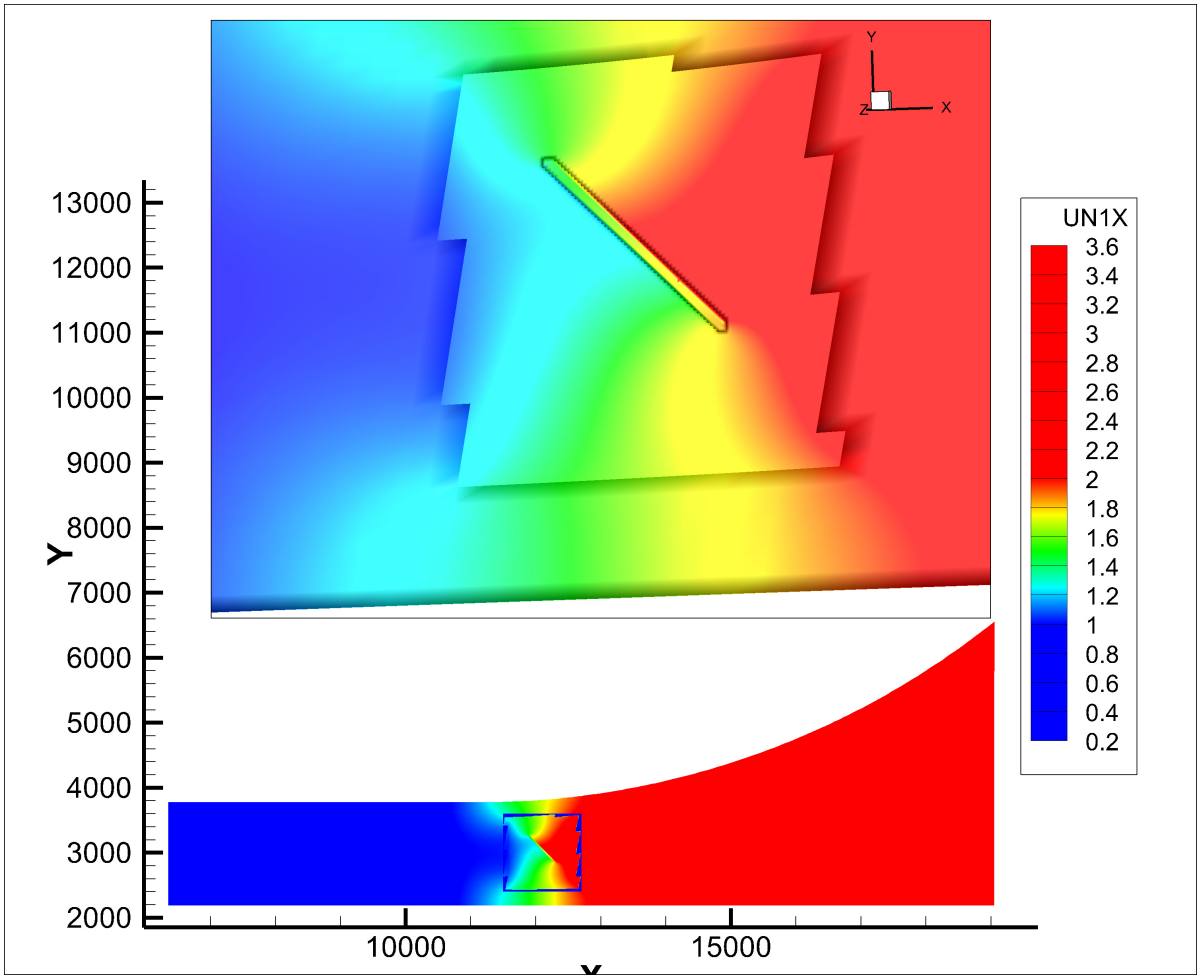
Example 1: 3D FE-XFEM Coupling

Simulation Details

- A 3D dogbone specimen in dynamic explicit
- Coarse scale has 33,735 elements and 41,760 nodes.
- Fine scale has 427,500 elements and 456,020 nodes.
- A linear elastic material model is used.
- The right hand side is loaded with pressure.
- Can be applied to multiscale problems.
- No complicated meshing-remeshing tools/algorithms are needed.

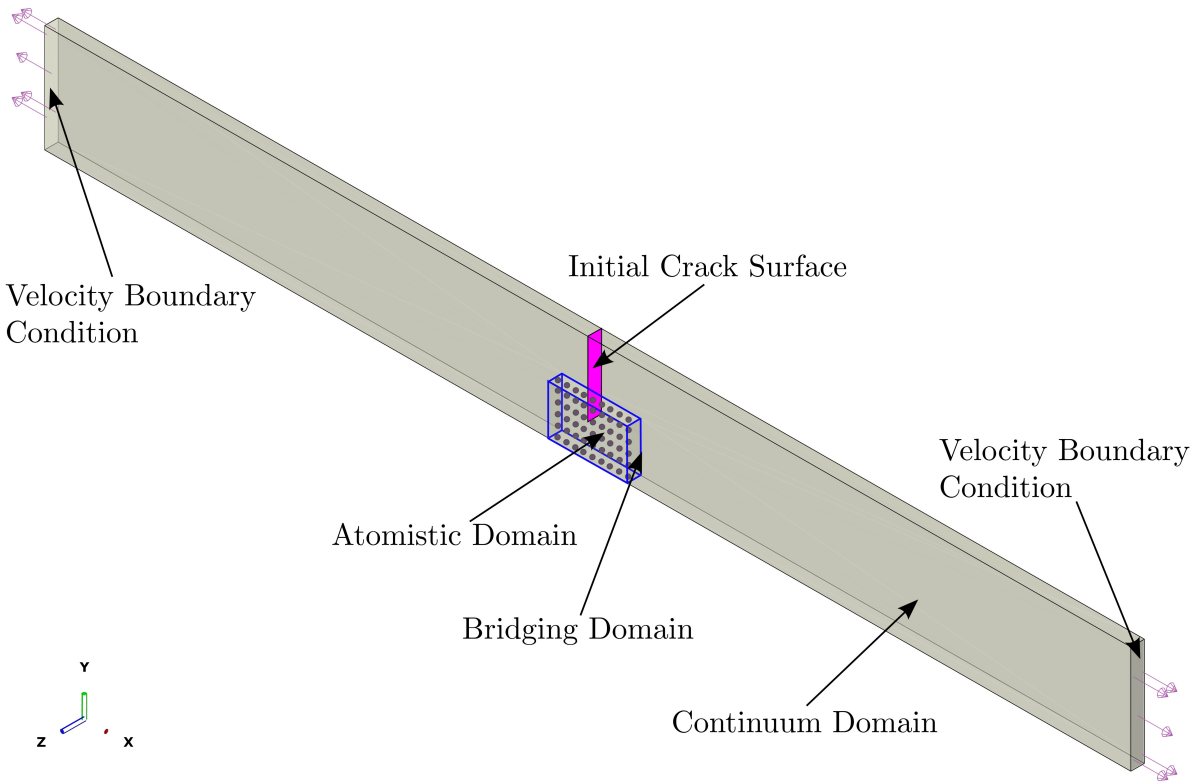
Example 1: FE-XFEM Coupling

Displacement Contour, Movie 2



Example 2: MD-XFEM Coupling

Example 2: Coupled MD-XFEM



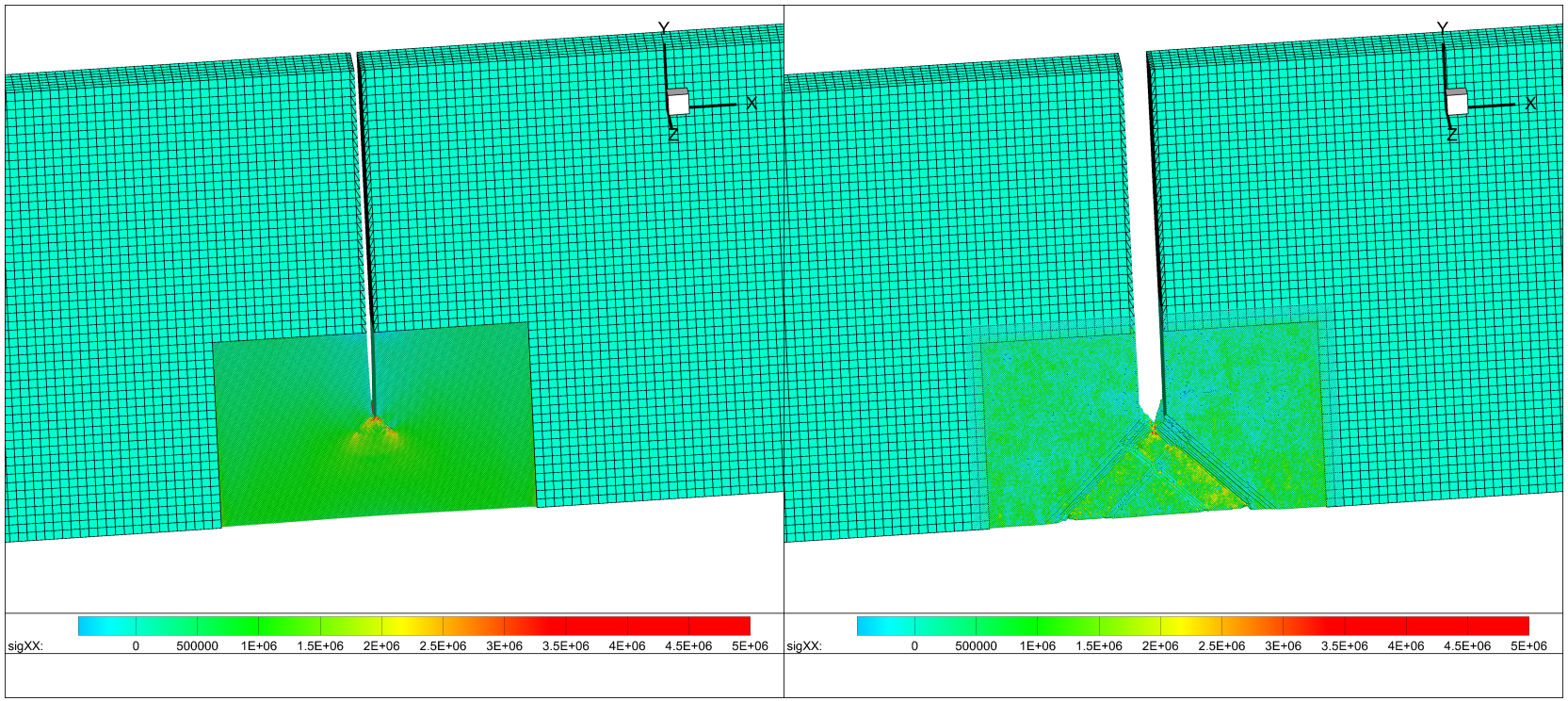
Example 2: MD-XFEM Coupling

Simulation Details

- A 3D rectangular specimen (8000x800x100 ^{3})
- LAMMPS is used for MD part
- Cauchy-Born method for continuum material
- Crack length 620
- 197,743 elements and 692,064 DOFs.
- Atomistic domain is FCC lattice with constant 3.645
- Atomistic region has the size of 540x340x100A3 with 1,626,240 active and 166,815 bridging atoms.
- Lennard-Jones constants are: $\sigma = 2.29$ and $\epsilon = 0.467\ eV$ Velocity of 0.1 A/picoseconds applied to both ends, time step is .003 picoseconds.

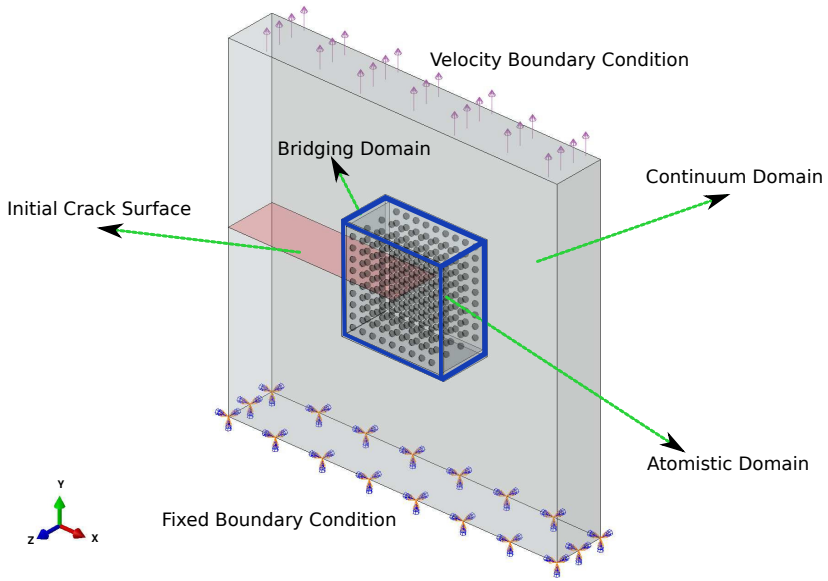
Example 2: MD-XFEM Coupling 1

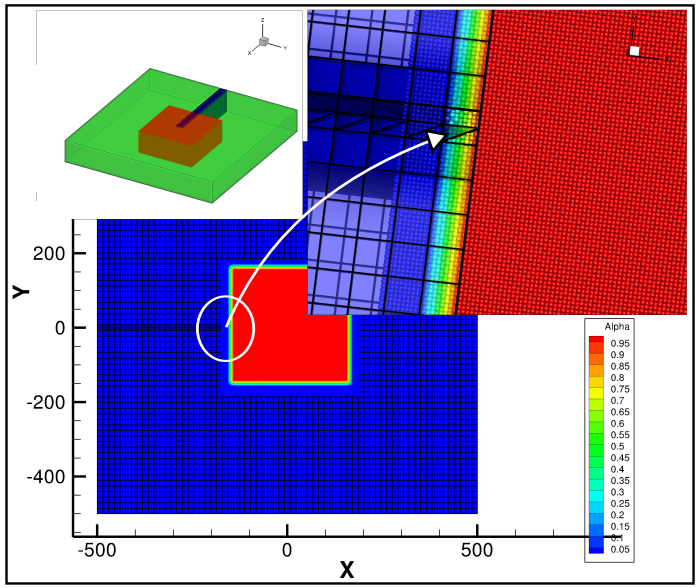
Results at time steps: 32400,63400
Movie 3



Example 3: MD-XFEM Coupling 2

Coupled MD-XFEM using LAMMPS





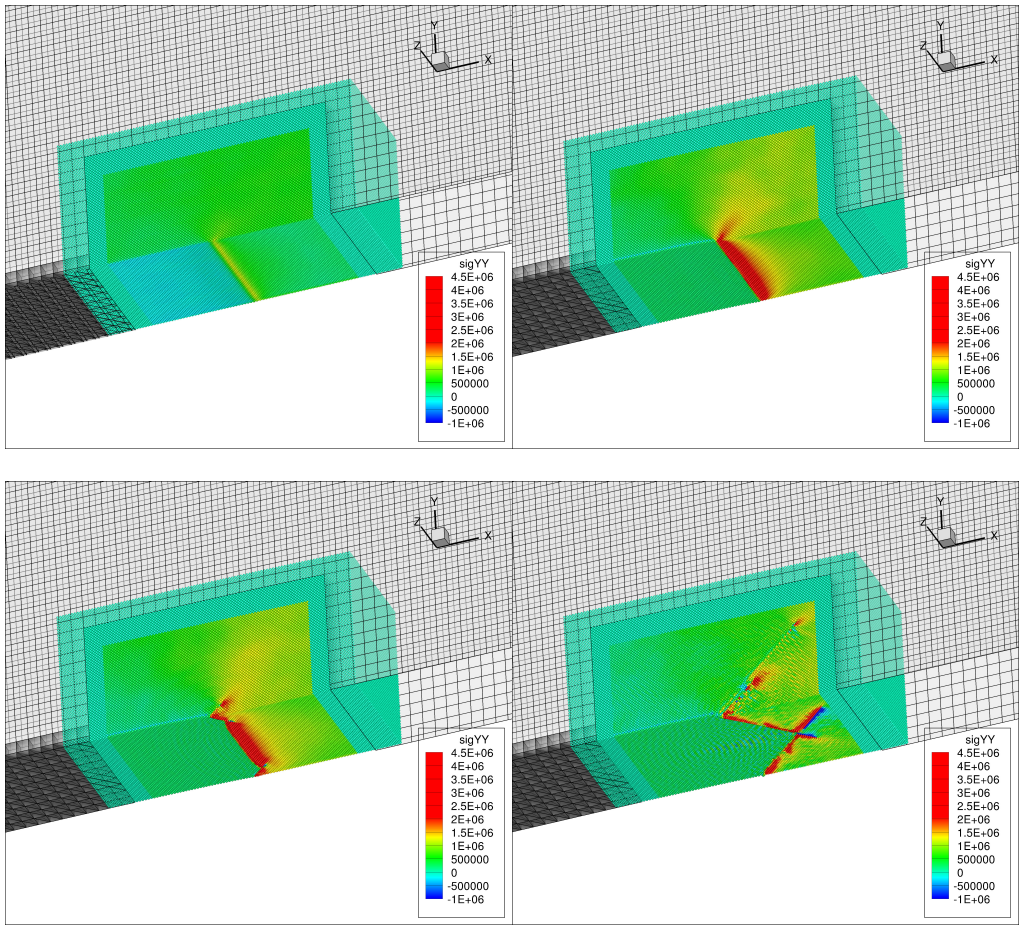
Example 3: MD-XFEM Coupling

Simulation Details

- A 3D rectangular specimen (1000x1000x150A3)
- Cauchy-Born method for continuum material
- Crack length 620A
- 44,890 elements and 152,592 DOFs.
- Element size is 15A
- Atomistic domain is FCC lattice with constant 3.645A
- Atomistic region has the size of 310x310x150A3 with 1,368,575 active atoms
- Velocity B.C. on top nodes

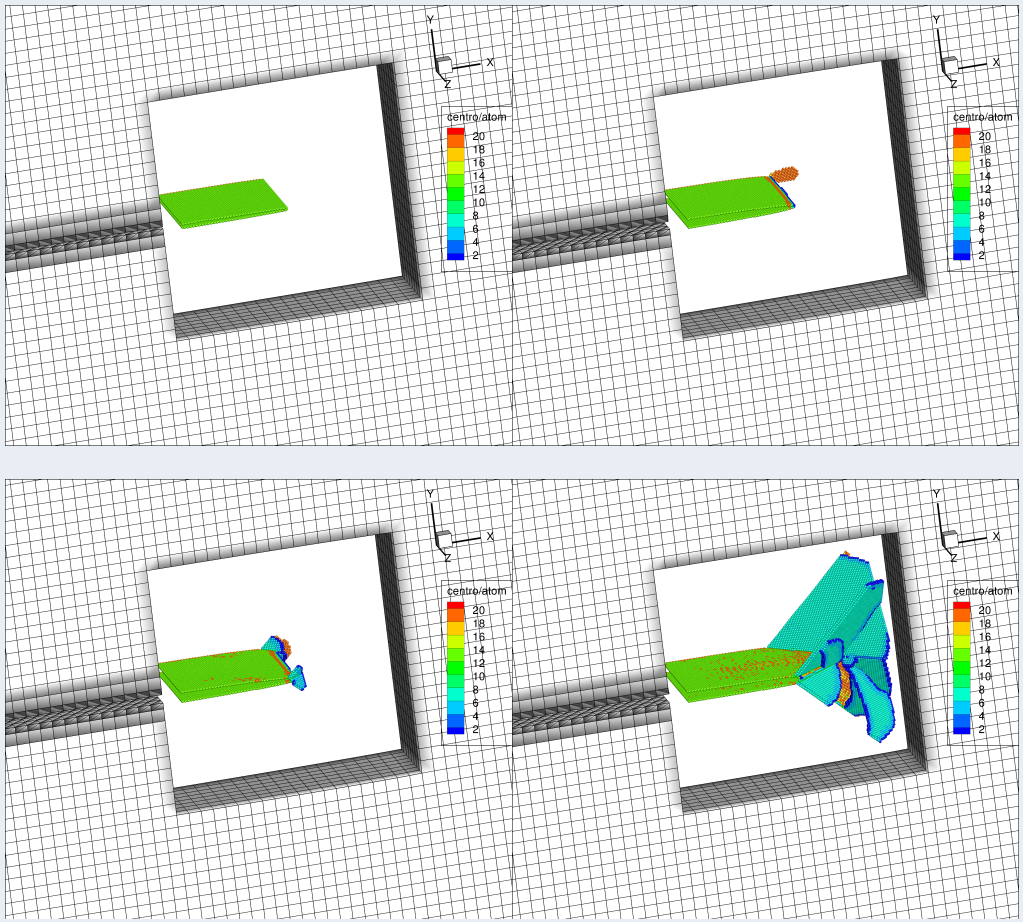
Example 3: MD-XFEM Coupling

Results at time steps: 10000,33000,34000,35800



Example 3: MD-XFEM Coupling Results (Movie 4)

Results at time steps: 10000,33000,34000,35800



Discussion

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- In XFEM-MD coupling, dislocations should be handled when they propagate close to the continuum domain
  I. Adaptive refinement of the atomistic domain
  II. XFEM enrichment for dislocations
  III. CG method of Y. Chen et al.
  (A concurrent scheme for passing dislocations from atomistic to continuum domains, Acta Materiala, 2012)

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  III. CG method of Y. Chen et al.
  (A concurrent scheme for passing dislocations from atomistic to continuum domains, Acta Materiala, 2012)
- Cauchy-Born method is not always valid
  I. Strain range, II. Surface effects, III. Temperature range, IV. Material, V. Efficiency

Discussion

- Modeling higher temperatures
- Isothermal simulations can be done with the current method
- A strain rate, temperature dependent material model should be used at the coarse scale
- Computing the material model can be automated based on a hierarchical multiscale method
- Polymeric materials can be modeled with this method

Conclusions and Future Plans

- An extended bridging domain method was presented.
- A multiscale software framework was introduced.
- The verification examples show that the method is stable in dynamics in both FE-FE coupling and FE-MD coupling.
- A comparison between full MD and coupled FE-MD
- Several examples modeling crack propagation was shown.
- Handling dislocation propagating to the continuum domain was discussed.

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- A comparison between full MD and coupled FE-MD
- Several examples modeling crack propagation was shown.
- Handling dislocation propagating to the continuum domain was discussed.
- Future work includes isothermal multiscale simulations, and extension to other materials.
- Efficient parallelization for distributed memory systems is also another challenge.

Thanks you for your attention.

Collaborators:
Prof. Timon Rabczuk (Bauhaus – Supervisor)
Prof. Stephane Bordas (Cardiff)
M.S. Mohammad Silani (IUT)