An Extended Bridging Domain Method for Continuum-Atomistic Simulations of Discontinuities

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Outline

- Motivation
- Extended FEM for Dislocations
- Bridging Domain Method for Discontinuities
- Numerical Examples
- Conclusions and future work

Focus Materials

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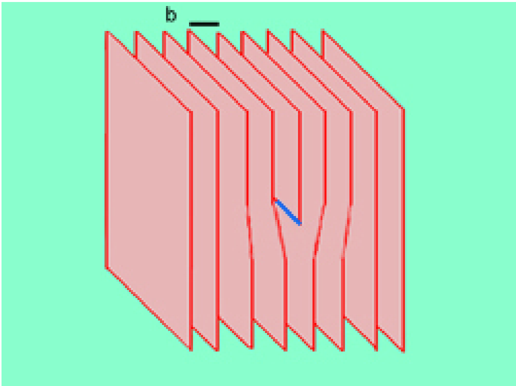
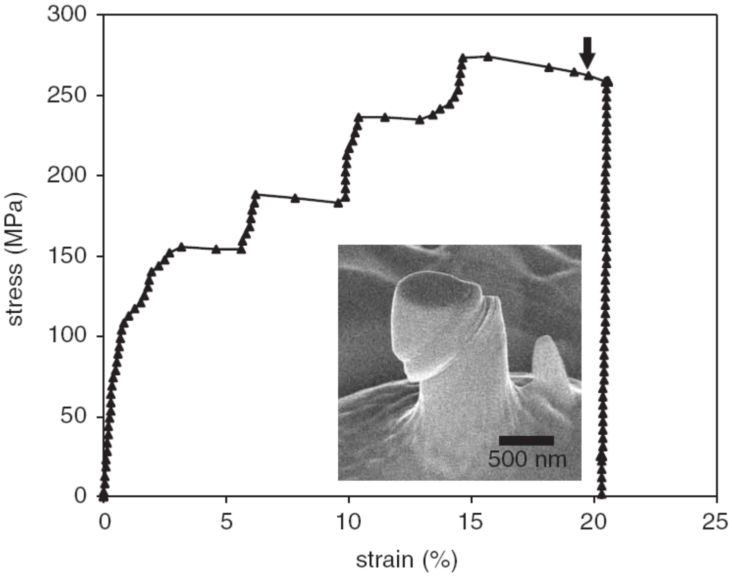
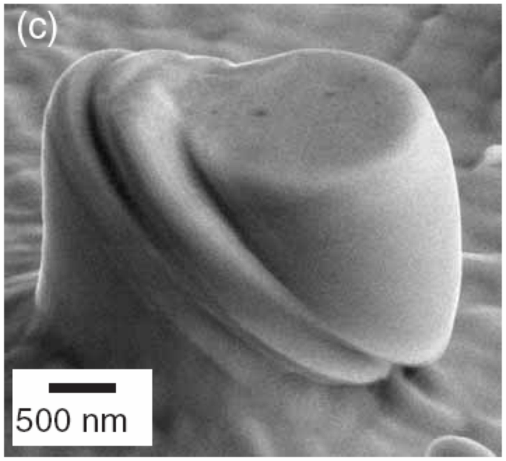
- Crystalline materials. (Metals, Graphene, etc)
- Plastic behaviour is the result of dislocation motion.
- Recent experiments allow for more quantitative comparisons with simulations







Submicron Au Columns Volkert, 2006

Motivation Summary

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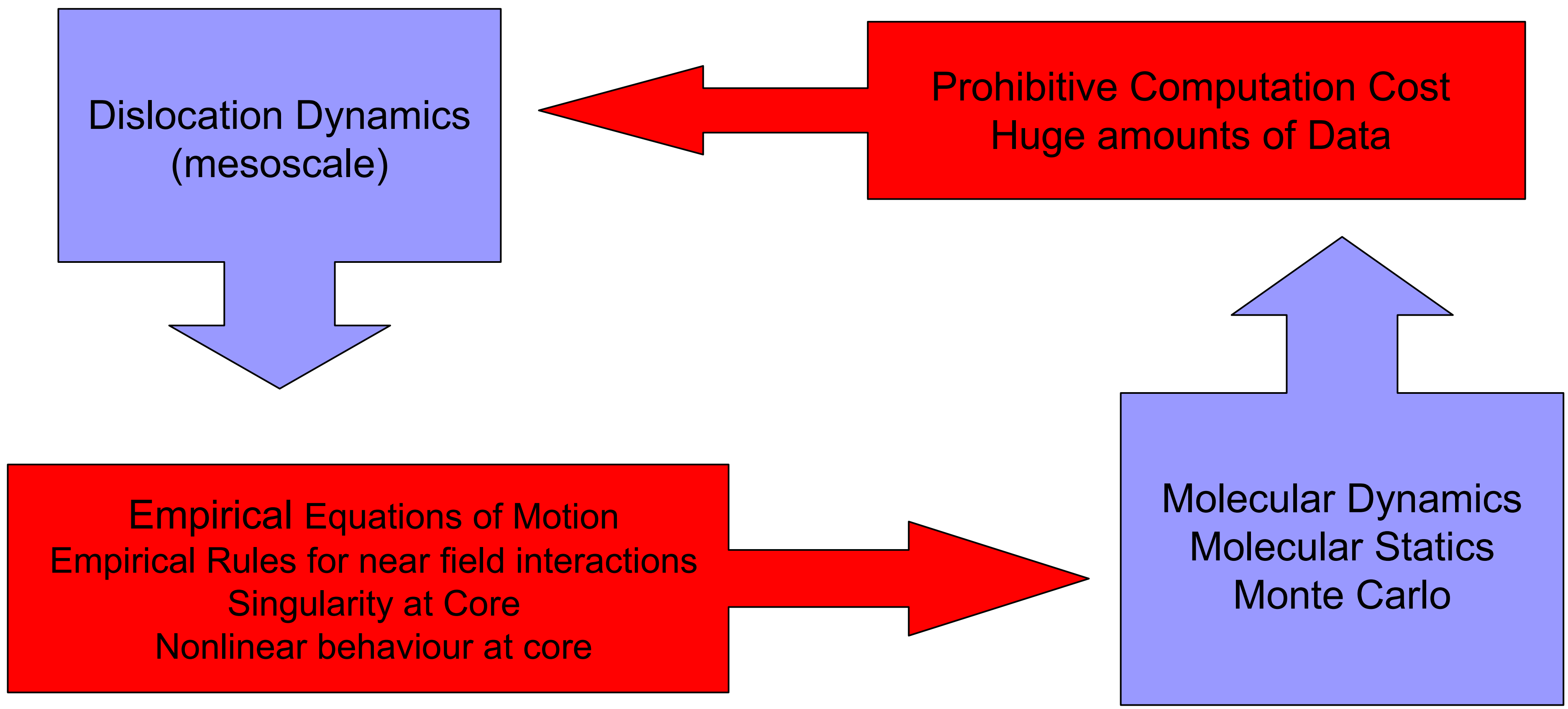

Motivation Summary

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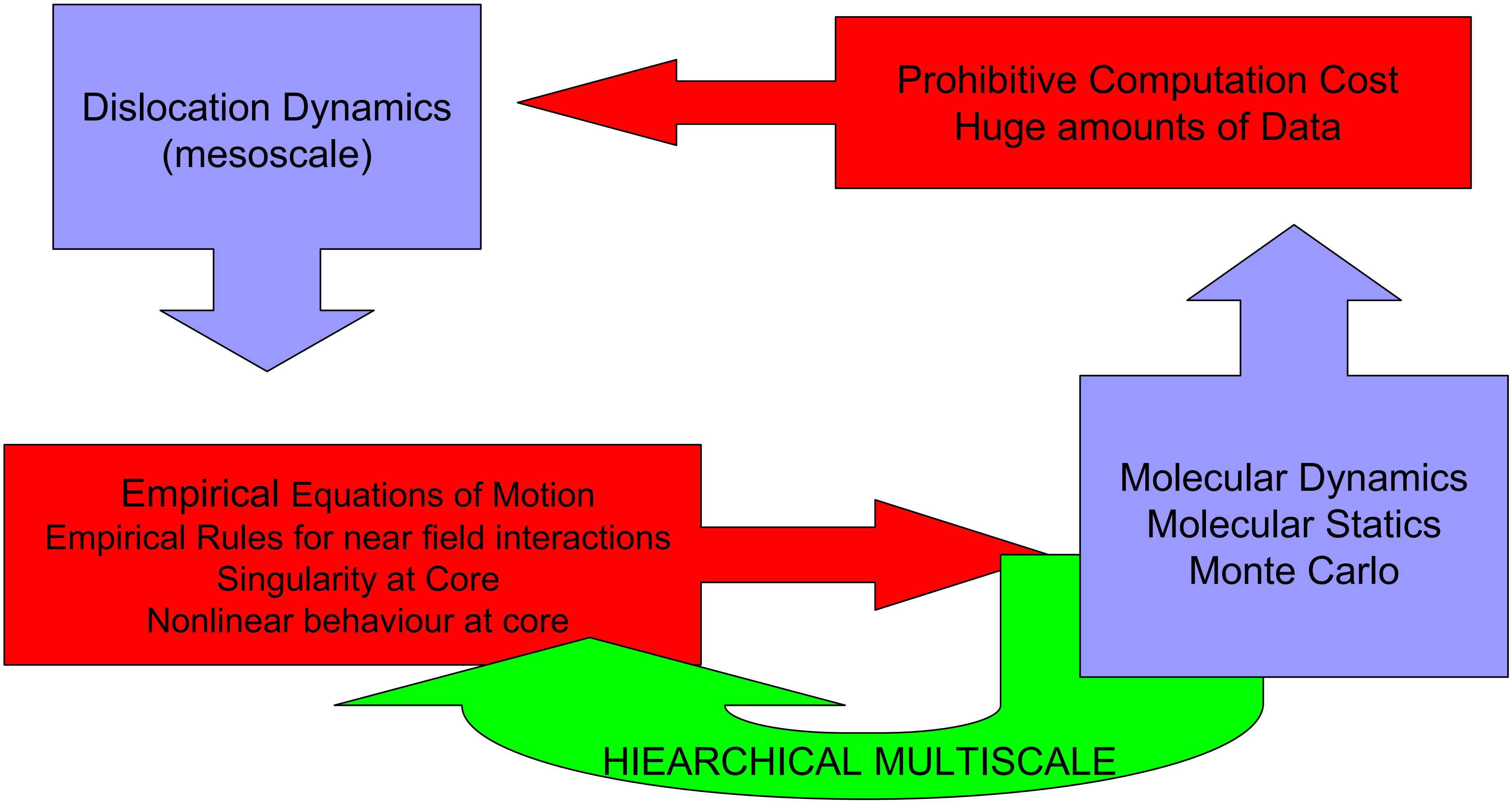

Motivation Summary

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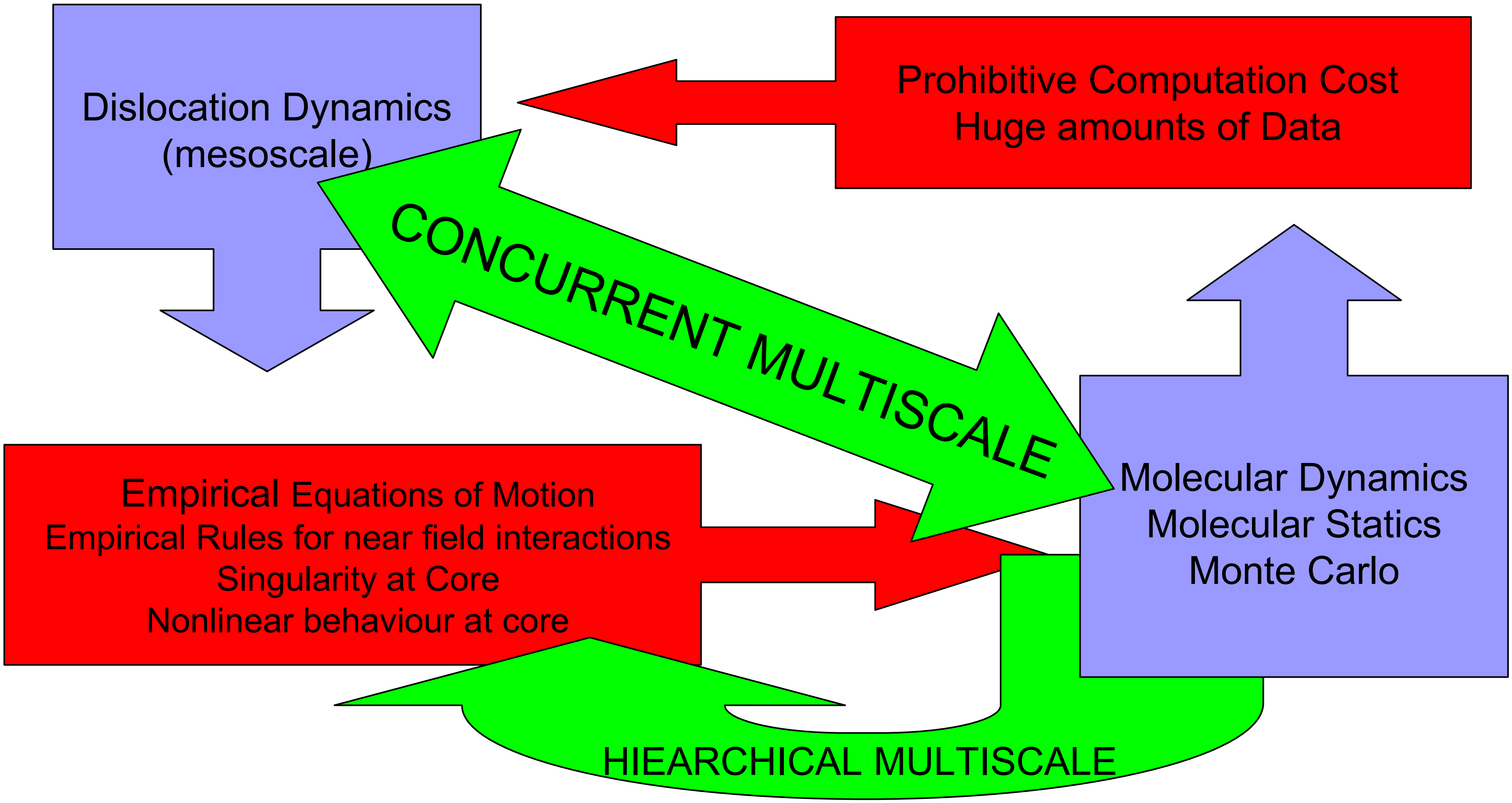

Characteristics of Concurrent Multiscale Models

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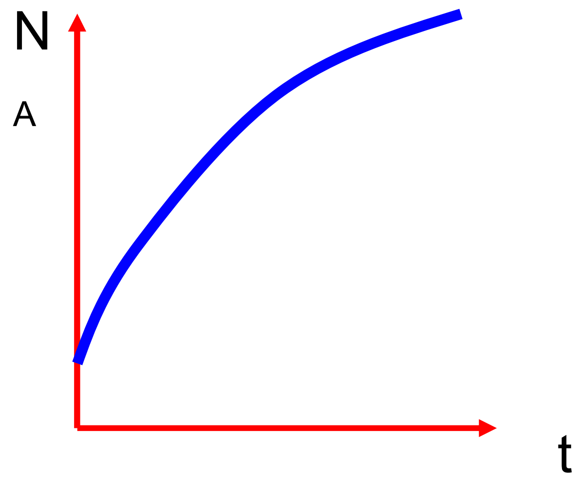
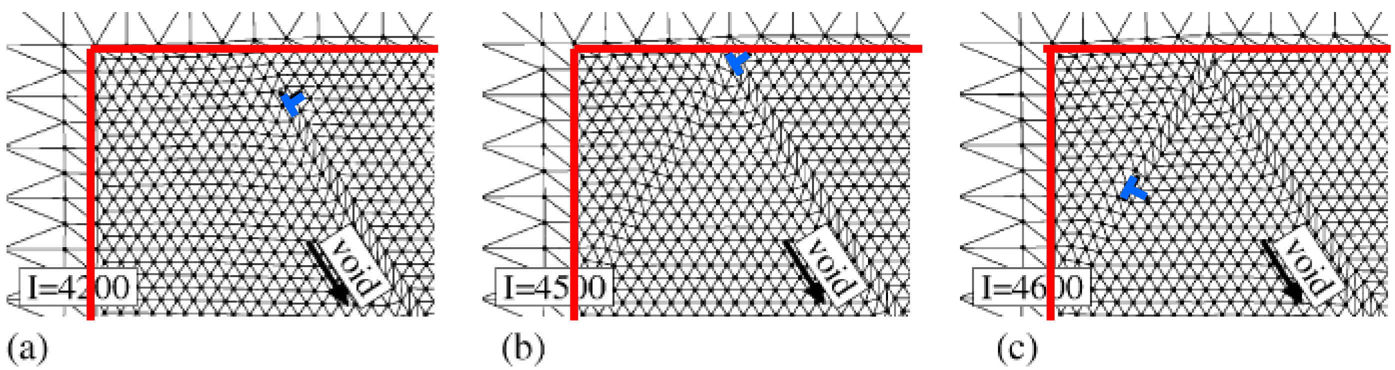
- Dislocations tend to move towards MM/CM interface
- Adaptivity required
- Must follow complete dislocation path
- Total number of atoms becomes very large.





Shilkrot, Miller, Curtin (2004)

CADD: Coupled Atomistic and DD

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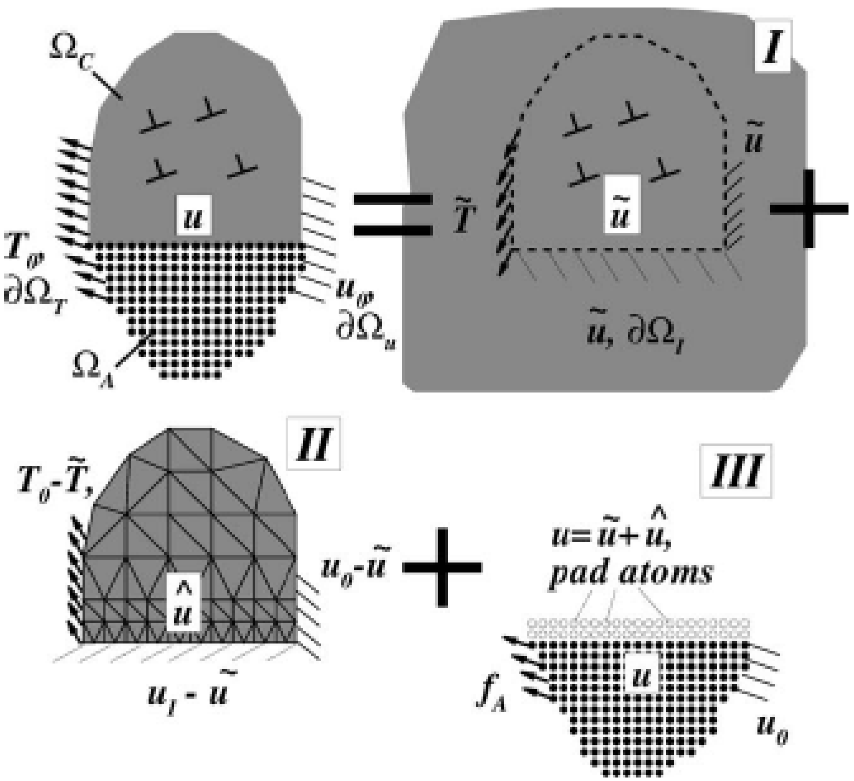
- Shilkrot,Miller,Curtin 2002, 2004
- Quasicontinuum based coupling.
- Superposition based DD.
- Linear Isotropic Continuum.
- Dislocation “JUMP” across MM/CM interface
- Significant reduction of number of atoms
- Difficult to see extension to 3D.
- Empirical DD rules and laws



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- **Bridging Domain Method for Discontinuities**
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XFEM Dislocation Model

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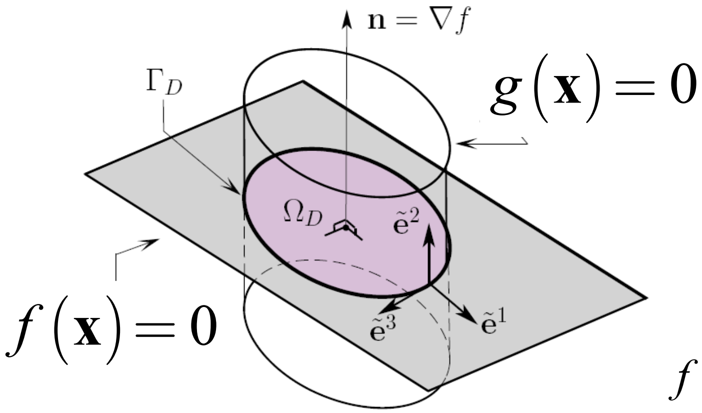
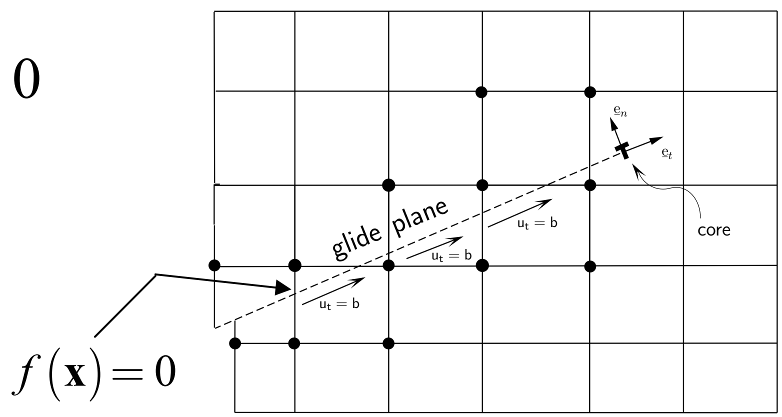
- Introduced by Gracie, Ventura, & Belytschko IJNME 2007
  - Belytschko and Gracie IJP, 2008 & Gracie, et al. JMPS 2008.





$$\mathbf{u}(\mathbf{x}) = \sum_I N_I(\mathbf{x})\mathbf{u}_I + \mathbf{b}H\big(f(\mathbf{x})\big)H\big(-g(\mathbf{x})\big)\sum_{J\in S^D} N_J(\mathbf{x})$$

H( ) is the Heaviside step function

Burgers Vector **b** is a known quantity, so no additional degrees of freedom

Bridging Domain Method

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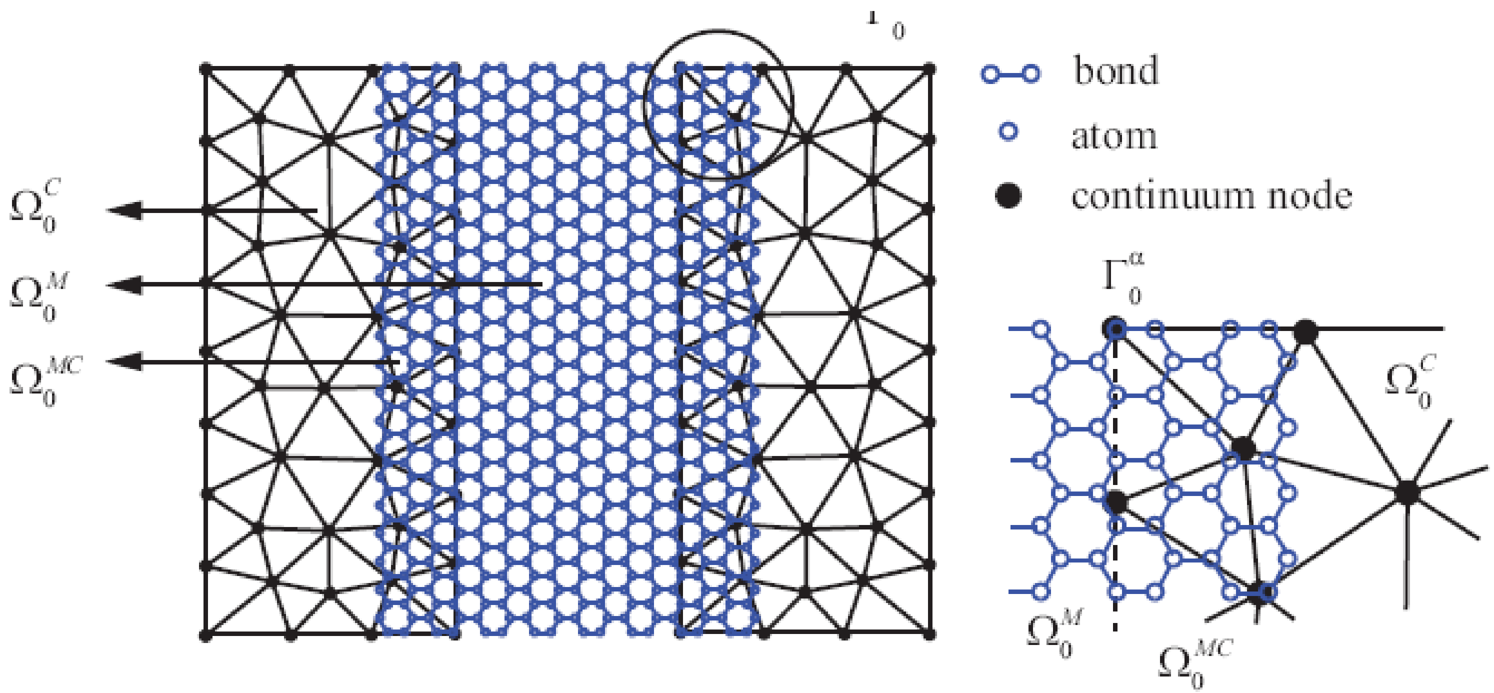
- Belytschko & Xiao (2003,2004)
- Overlapping domain decomposition scheme.
- Compatibility in the handshaking domain is enforced by Lagrange Multipliers.



Bridging Domain Method

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Total Energy Potential:

$$E = E_\alpha^C(\mathbf{u}) + E_\alpha^M(\mathbf{s}) + \boldsymbol{\lambda}^T \bullet \mathbf{g}(\mathbf{u},\mathbf{s})$$

Constraints:

$$g_{iI} = u_i^h(\mathbf{X}_I) - d_{iI}^A, \ \forall I \,|\, \mathbf{X}_I \in \Omega^{MC}$$

Energy of Continuum:

$$E_\alpha^C(\mathbf{u}) = \int_{\Omega^C} (1-\alpha) w^C(\mathbf{F}(\mathbf{u}))\, d\Omega$$

Energy of Atomistics:

$$E_\alpha^M(\mathbf{u}) = \frac{1}{2}\sum_i^{n^A}\sum_{i\neq j}^{n^A}\frac{\alpha_i+\alpha_j}{2}V(r_{ij})$$

Ω^C : Continuum domain

Ω^M : Molecular domain

Ω^{MC} : Coupling domain

$\mathbf{d}_I^A$: disp. of atom I

$\boldsymbol{\lambda}$: Lagrange Multipliers

w^C : Strain energy density

V : Atomic Potential

α : weight

BDM – weight function

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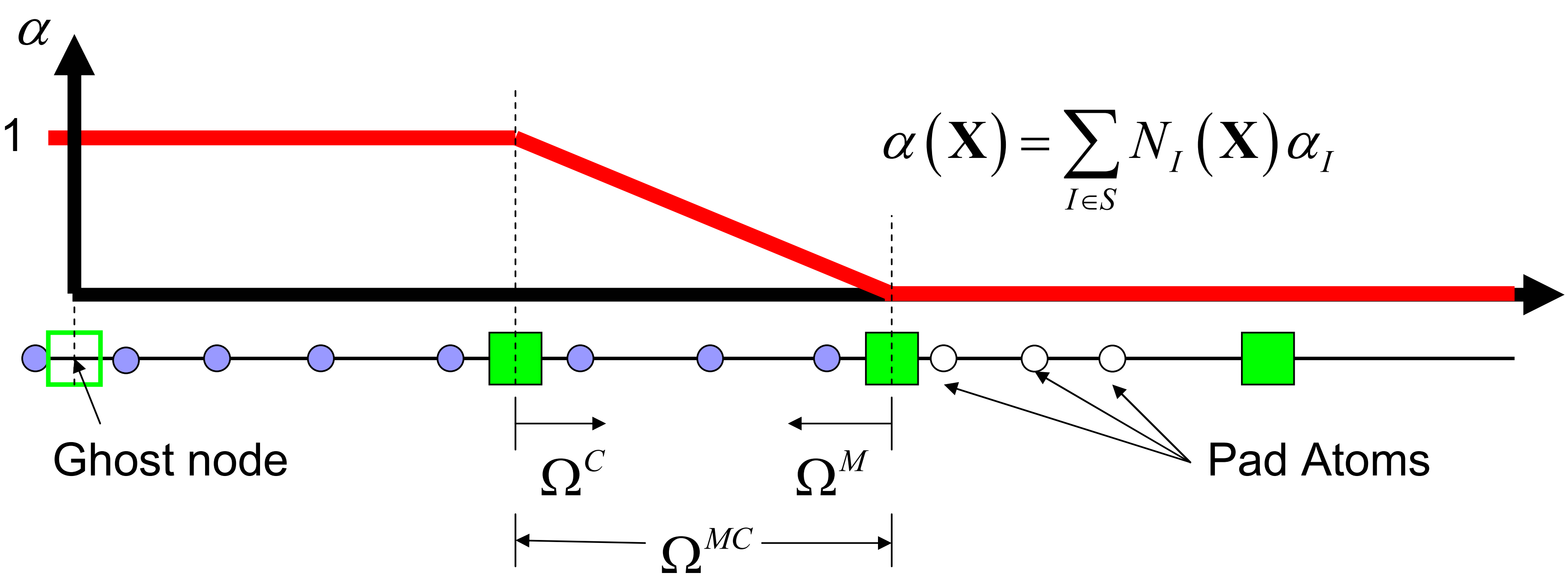

$$\mathbf{u}(\mathbf{X}) = \sum_{I \in S} N_I(\mathbf{X})\mathbf{u}_I, \forall \mathbf{X} \in \Omega^C$$

$$\boldsymbol{\lambda}(\mathbf{X}) = \sum_{I \in S^\lambda} N_I(\mathbf{X})\boldsymbol{\lambda}_I, \forall \mathbf{X} \in \Omega^{MC}, S \cup S^\lambda = \varnothing$$

BDM for dislocations

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- Extended BDM by using dislocation enrichment from XFEM

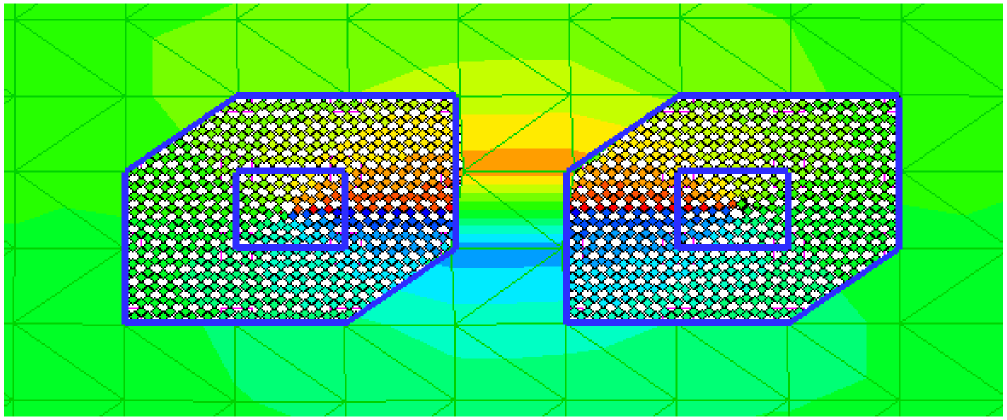
$$\mathbf{u}(\mathbf{X}) = \sum_{I \in S} N_I(\mathbf{X})\mathbf{u}_I + \mathbf{b}H\left(f(x)\right)\sum_{J \in \mathrm{S}^{\mathrm{D}}} N_J(\mathbf{x}), \forall \mathbf{X} \in \Omega^C, S^D \subseteq S$$

- Equilibrium equations found by minimize Energy

$$\frac{\partial E(\mathbf{u},\mathbf{s},\boldsymbol{\lambda})}{\partial \mathbf{u}_I} = 0, \forall I \in S$$

$$\frac{\partial E(\mathbf{u},\mathbf{s},\boldsymbol{\lambda})}{\partial \mathbf{s}_J} = 0, J \in [1, n^A]$$

$$\frac{\partial E(\mathbf{u},\mathbf{s},\boldsymbol{\lambda})}{\partial \boldsymbol{\lambda}_K} = 0, \forall K \in S^\lambda$$



Model Generation

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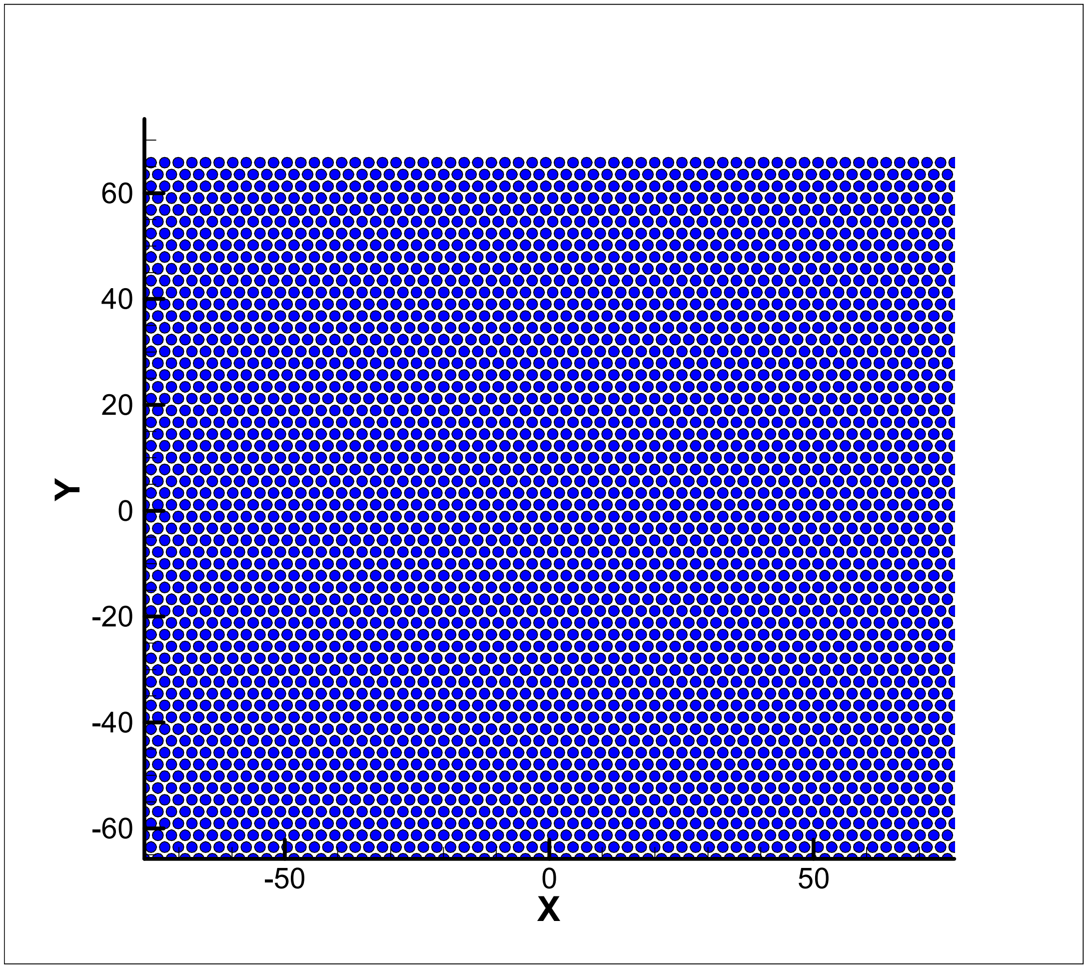
1. Create Lattice



Model Generation

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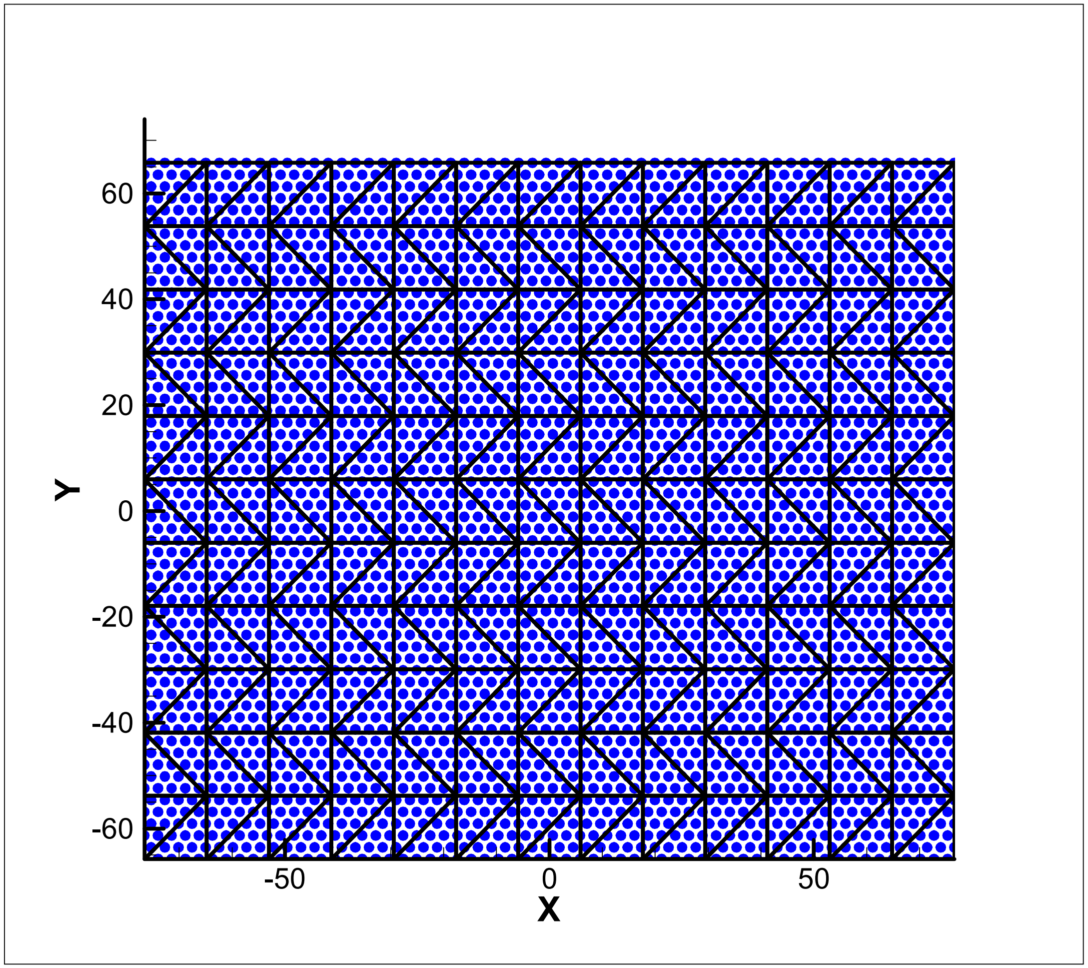
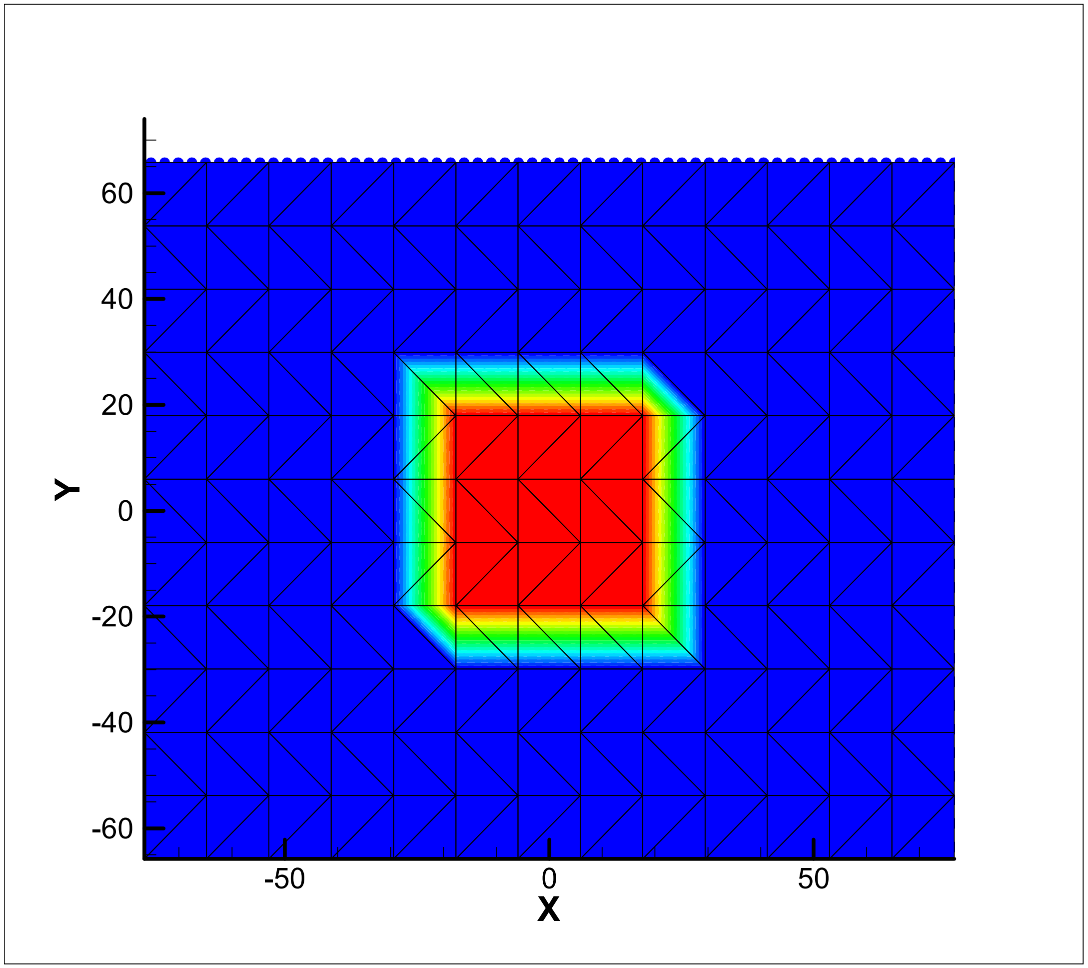
1. Create Lattice
2. Create Mesh



Model Generation

R. Gracie – Northwestern University

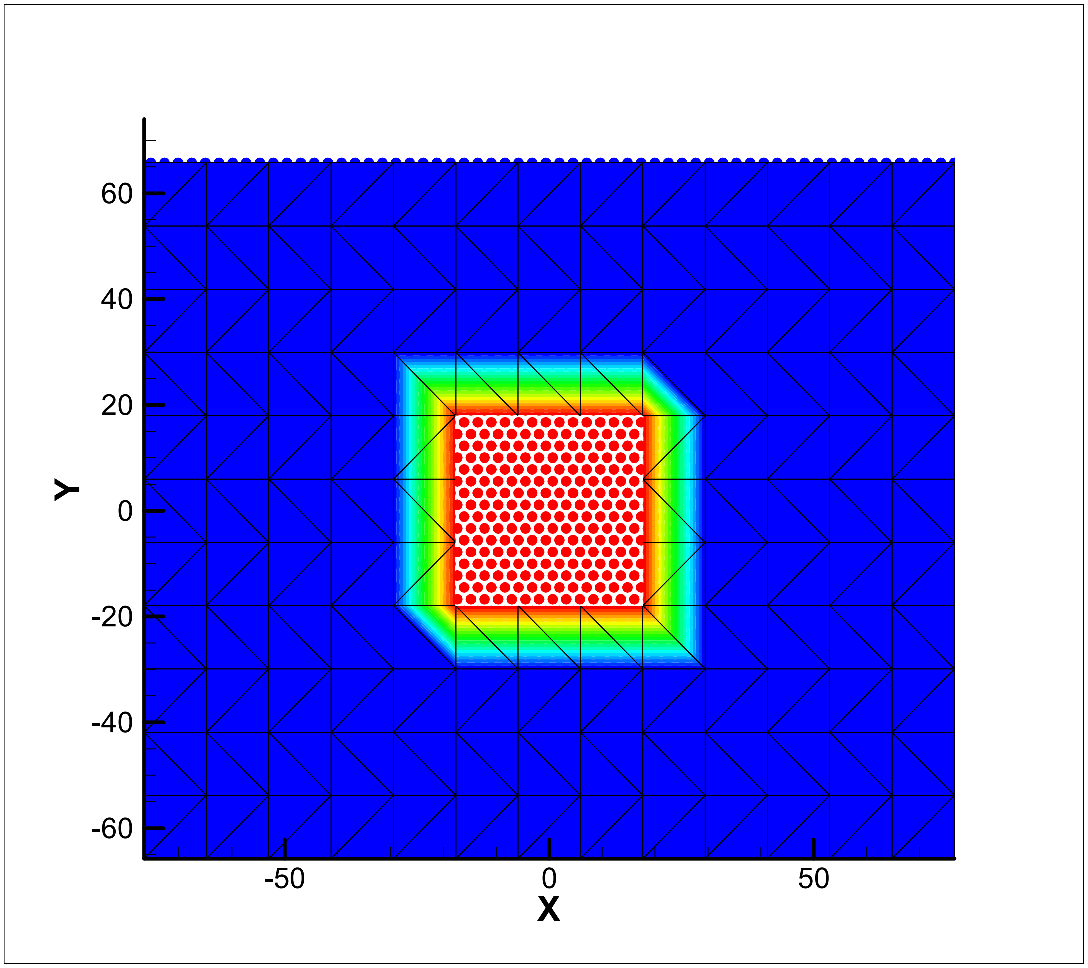
1. Create Lattice
2. Create Mesh
3. Identify MM elements. Set weights at nodes to 1.



Model Generation

R. Gracie – Northwestern University

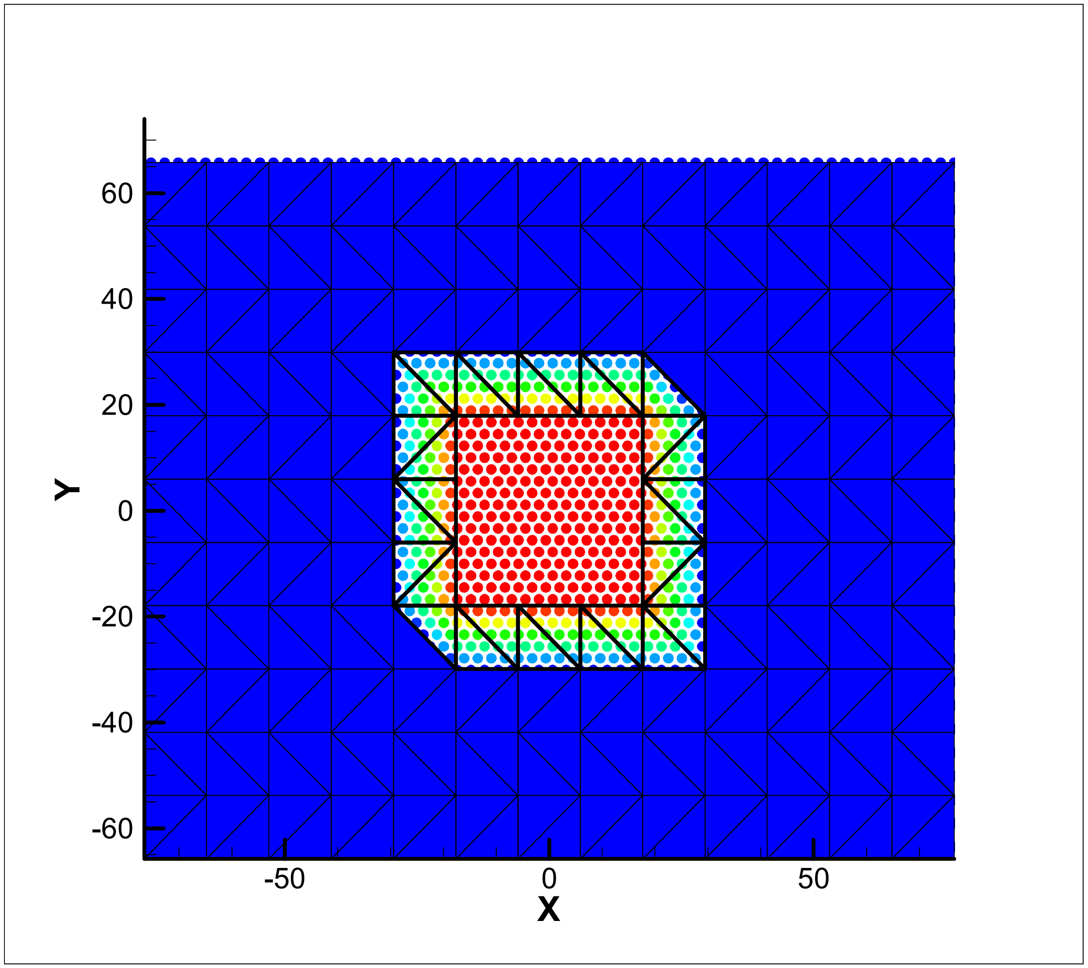
1. Create Lattice
2. Create Mesh
3. Identify MM elements. Set weights at nodes to 1.
4. Remove elements where MM will be performed



Model Generation

R. Gracie – Northwestern University

1. Create Lattice
2. Create Mesh
3. Identify MM elements. Set weights at nodes to 1.
4. Remove elements where MM will be performed
5. Create Lagrange Multiplier Mesh.
6. Solve



Homogenization of Slip

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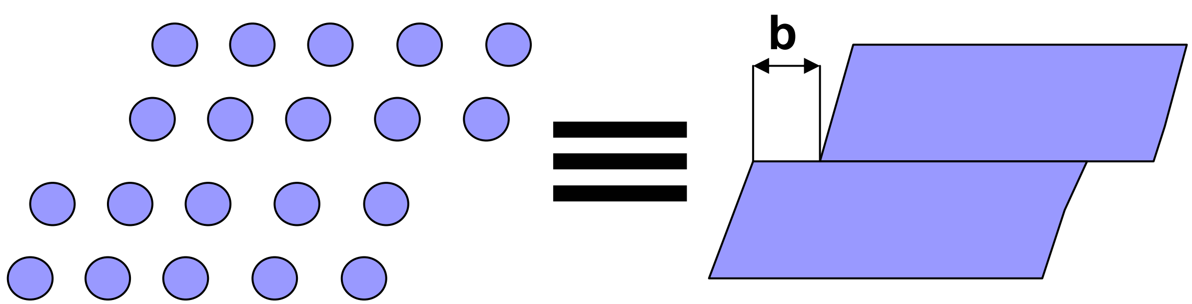
- Homogenization of Atomistic Displacements within an element by minimization of L2 displacement norm.



$$\Pi = \frac{1}{2}\sum_{\beta\in\Omega_e}\left(u_i\left(\mathbf{X}_\beta\right)-d_{i\beta}^A\right)^2$$

$$\Pi = \frac{1}{2}\sum_{\beta\in\Omega_e}\left(\sum_{I\in S_e}N_I\left(\mathbf{X}_\beta\right)u_{iI}+\sum_{\eta=1}^{n_S}\left[b_i^\eta H\left(f^\eta\left(\mathbf{X}_\beta\right)\right)\right]-d_{i\beta}^A\right)^2$$

Homogenization of Slip

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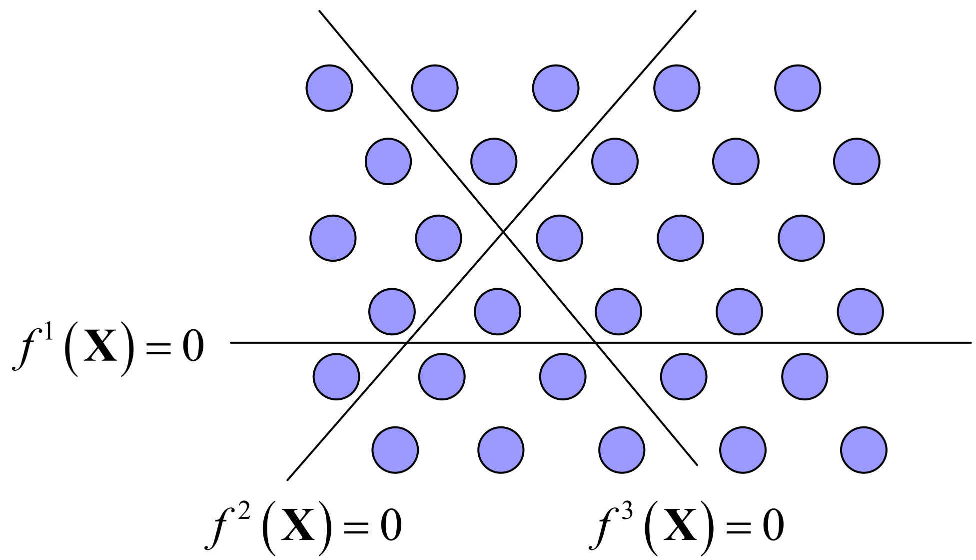
$$\Pi = \frac{1}{2}\sum_{\beta\in\Omega_e}\left(\sum_{I\in S_e} N_I\left(\mathbf{X}_\beta\right)u_{iI} + \sum_{\eta=1}^{n_S}\left[b_i^\eta H\left(f^\eta\left(\mathbf{X}_\beta\right)\right)\right] - d_{i\beta}^A\right)^2$$

- Know location of slip planes for a given lattice structure
- Minimize L2 norm.

$$\frac{\partial\Pi}{\partial u_{iI}} = 0,\ \forall I \in S_e, i\in[1,3]$$

$$\frac{\partial\Pi}{\partial b_i^\eta} = 0,\ \forall \eta \in [1,n_s], i\in[1,3]$$



Graphene Sheet with Defects

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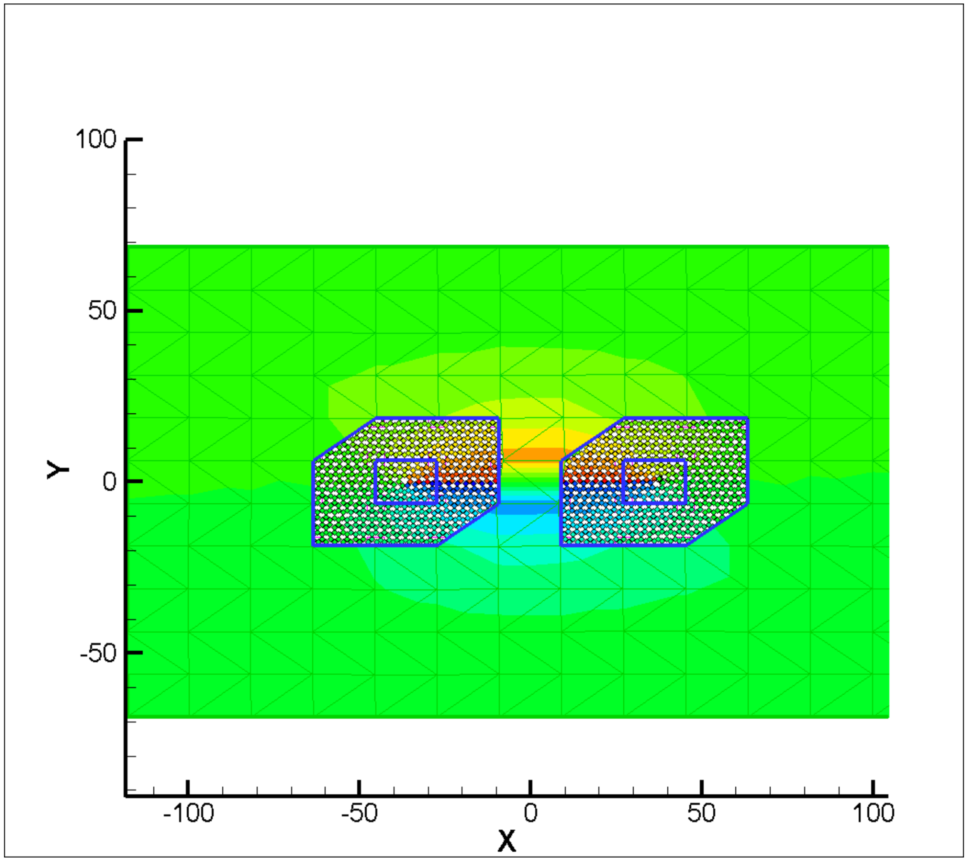

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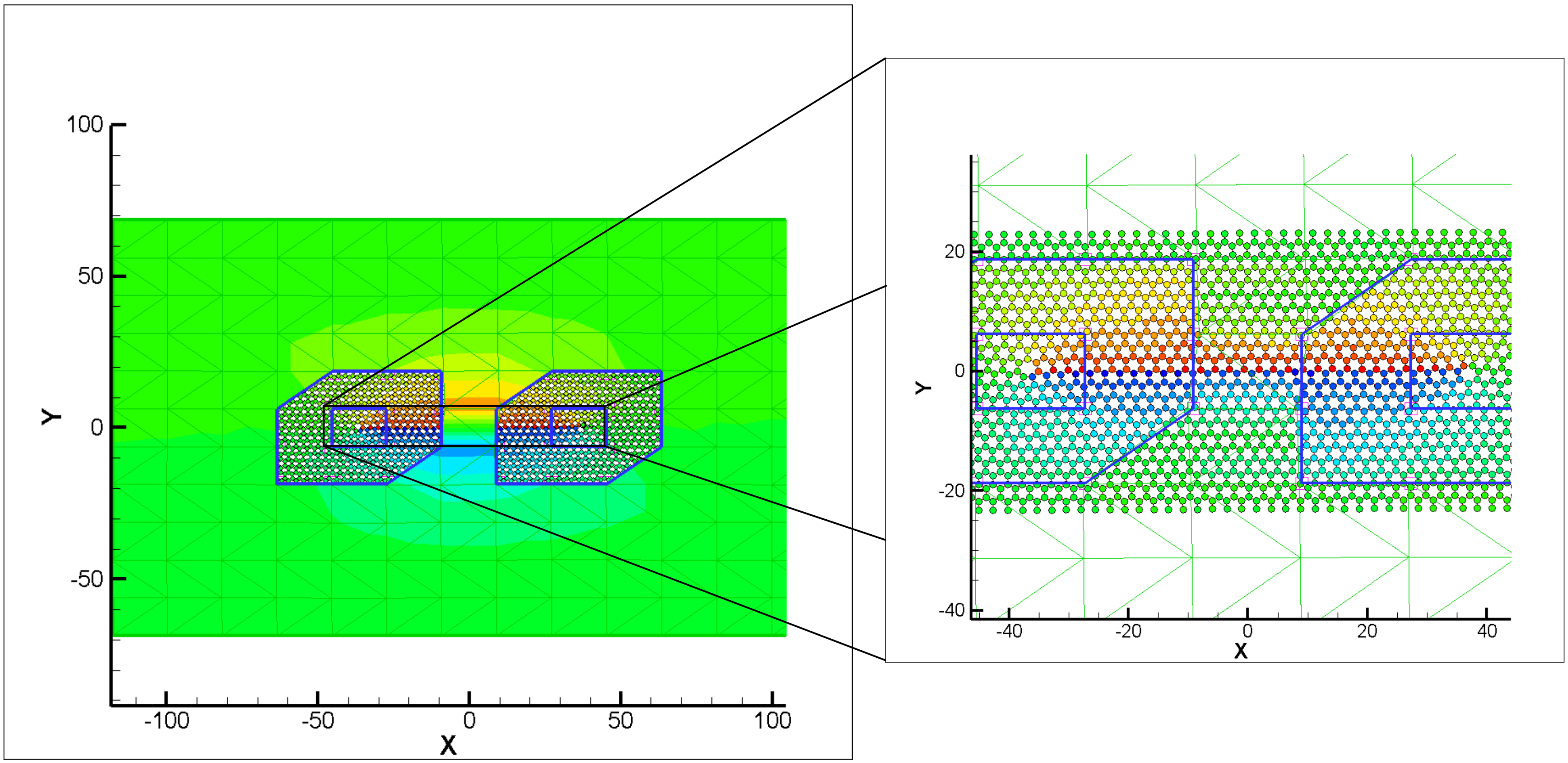

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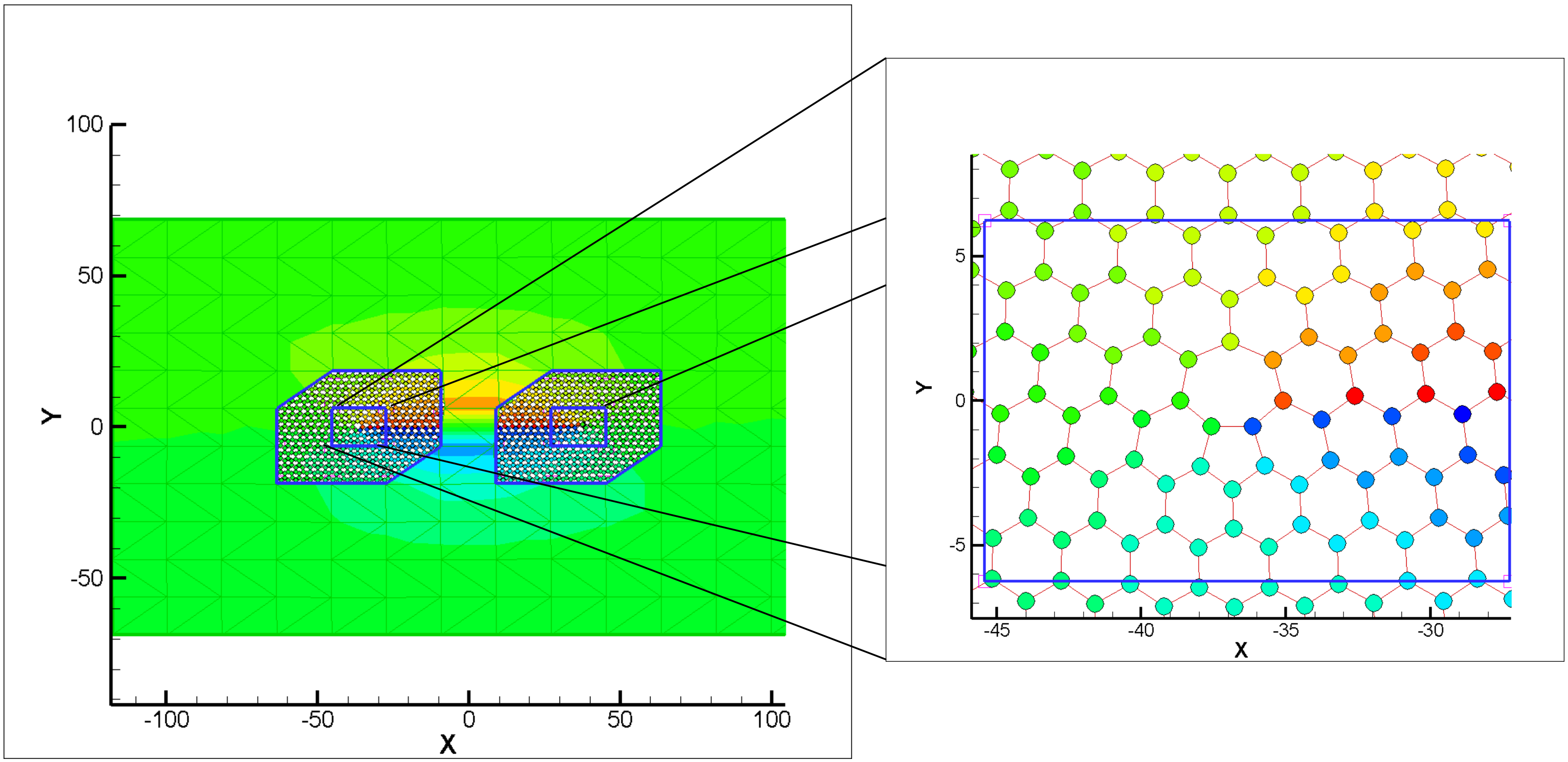

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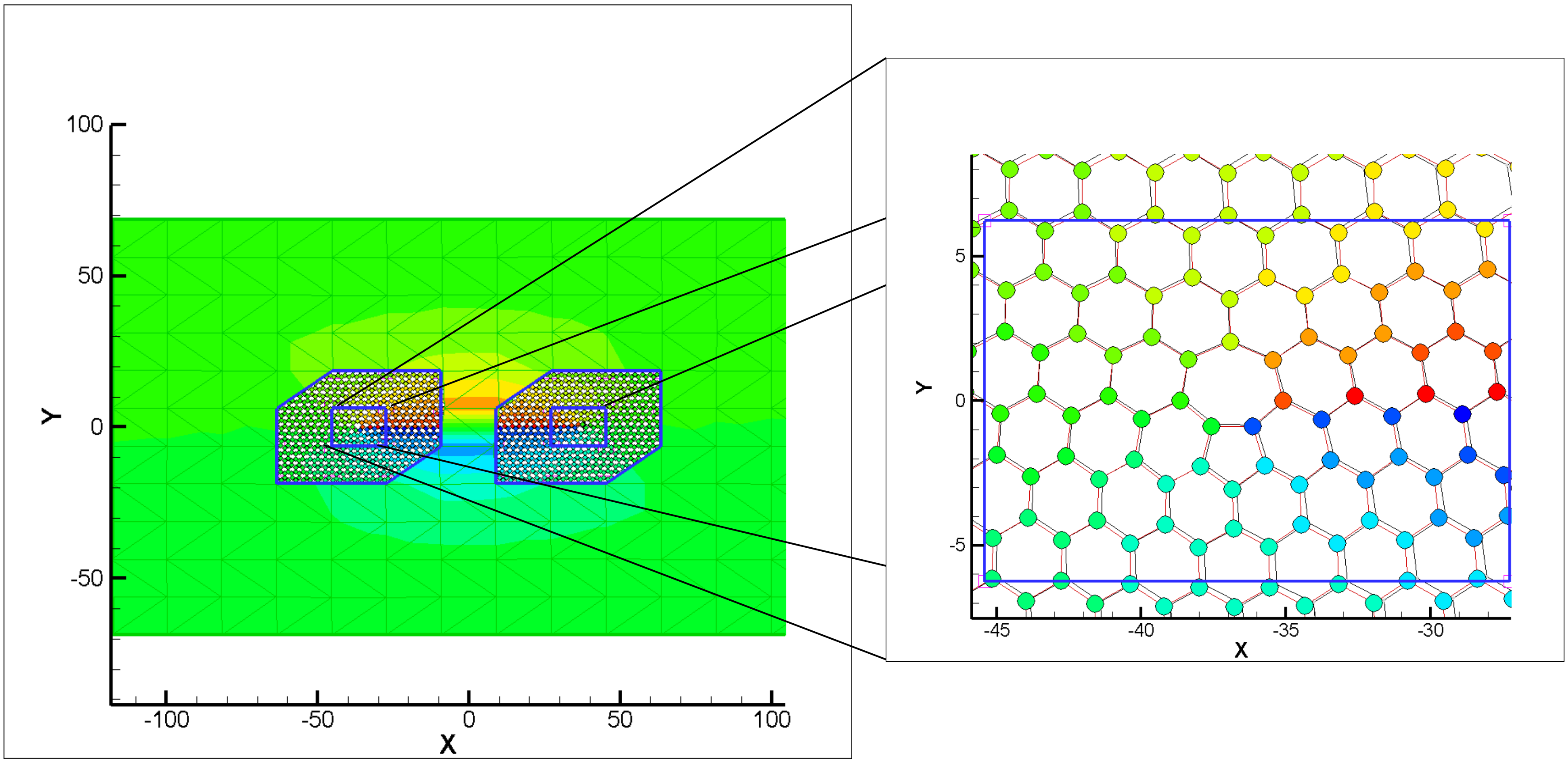

Dislocation Nucleation from a Void

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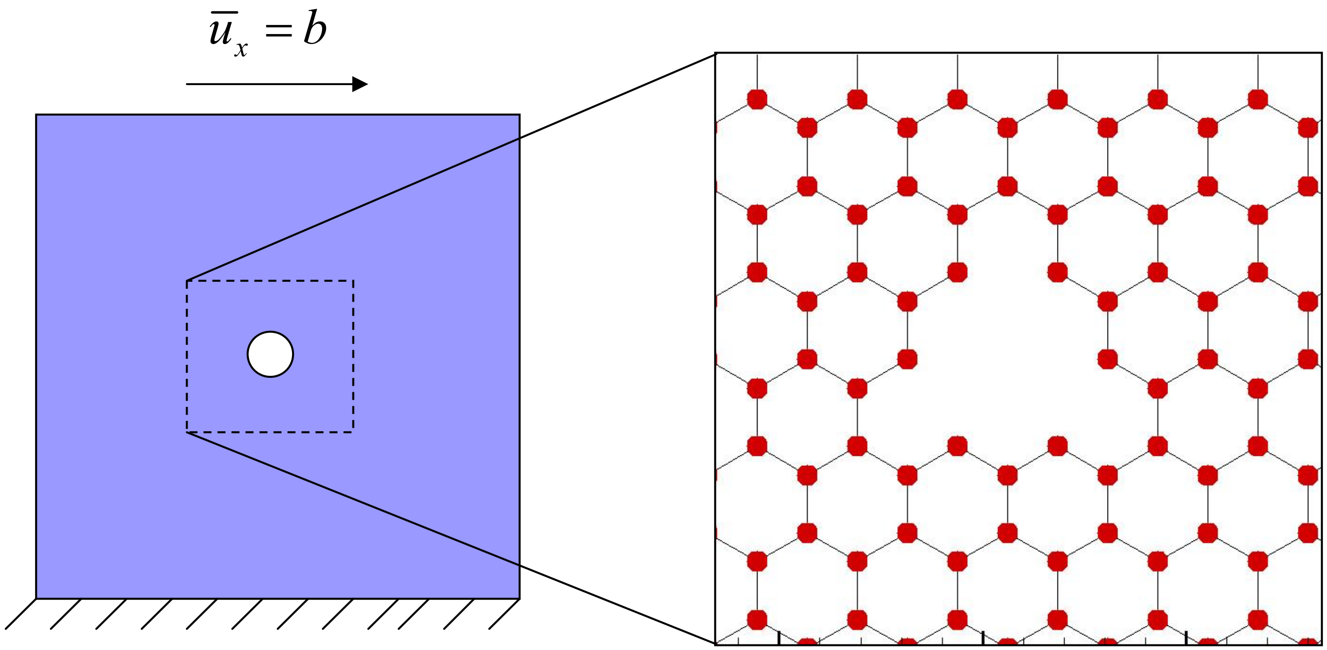
- Tersoff-Brenner Potential
- Linear Elastic Material



Dislocation Nucleation from a Void

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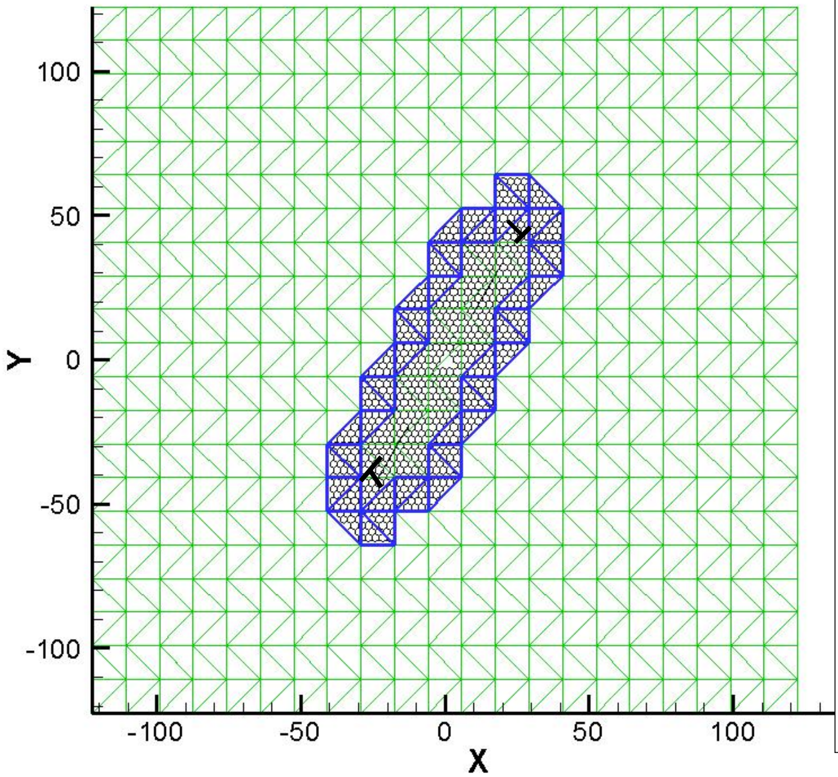
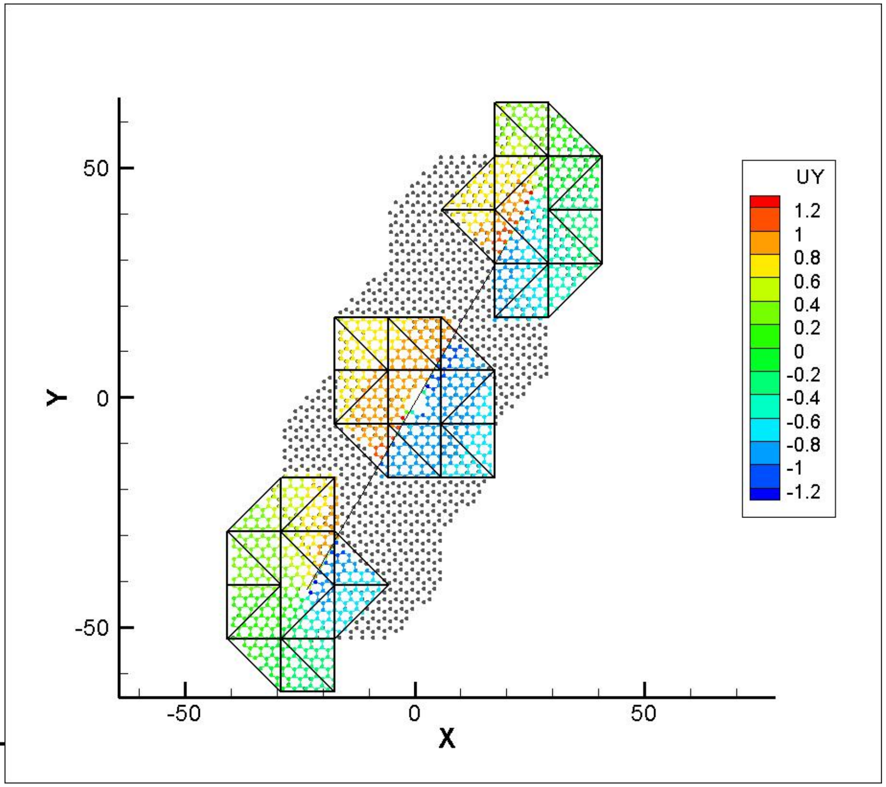
BDM



BDM-XFEM

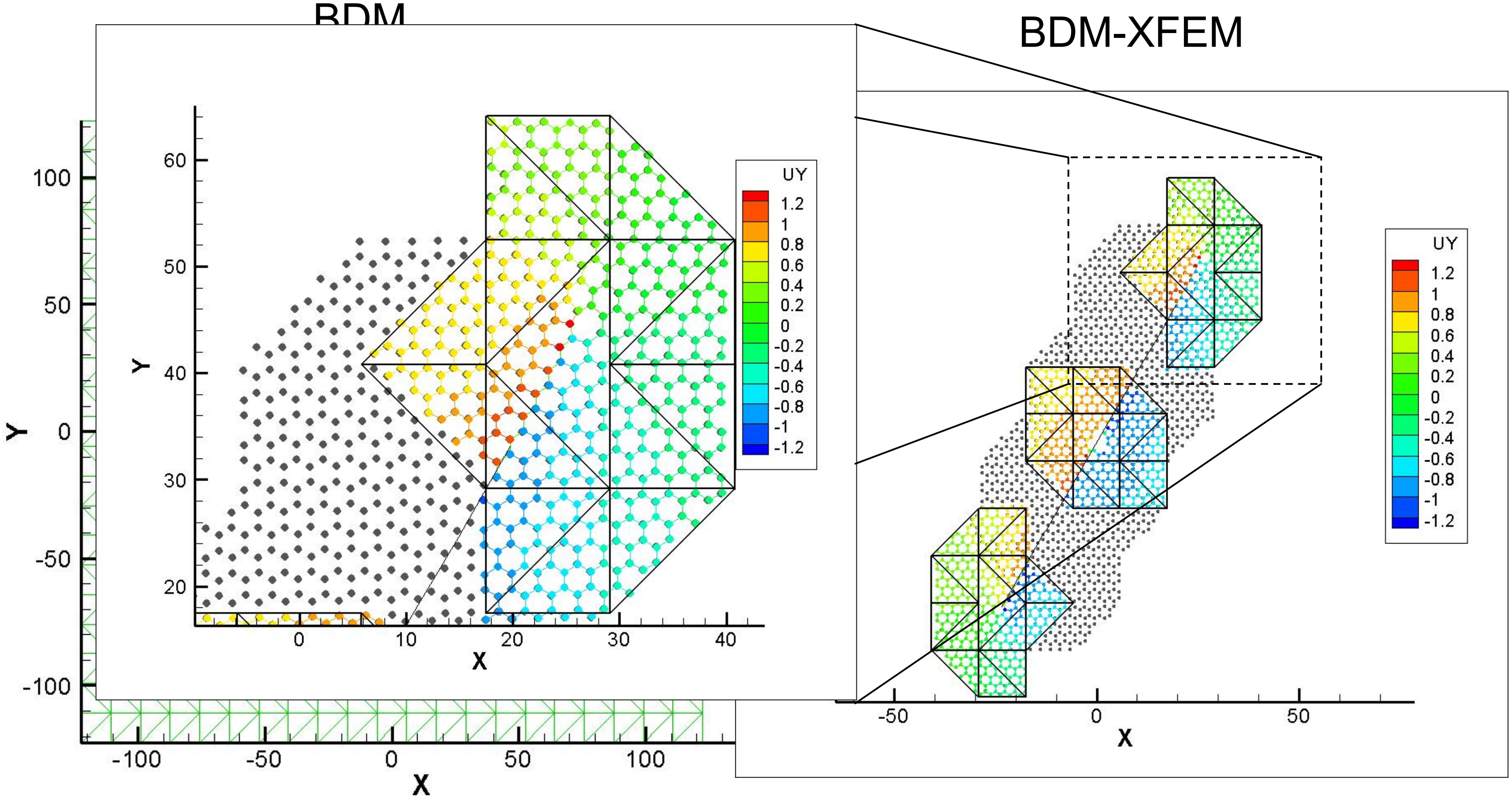


Dislocation Nucleation from a Void

R. Gracie – Northwestern University

BDM

BDM-XFEM



Dislocation Nucleation from a Void

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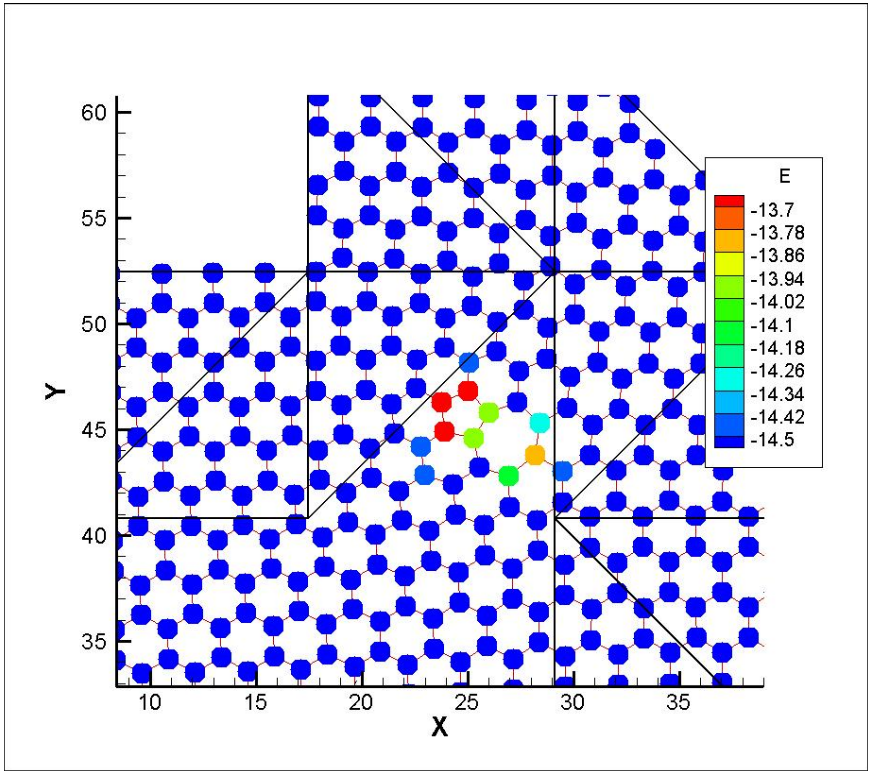
Energy Per Atom

BDM



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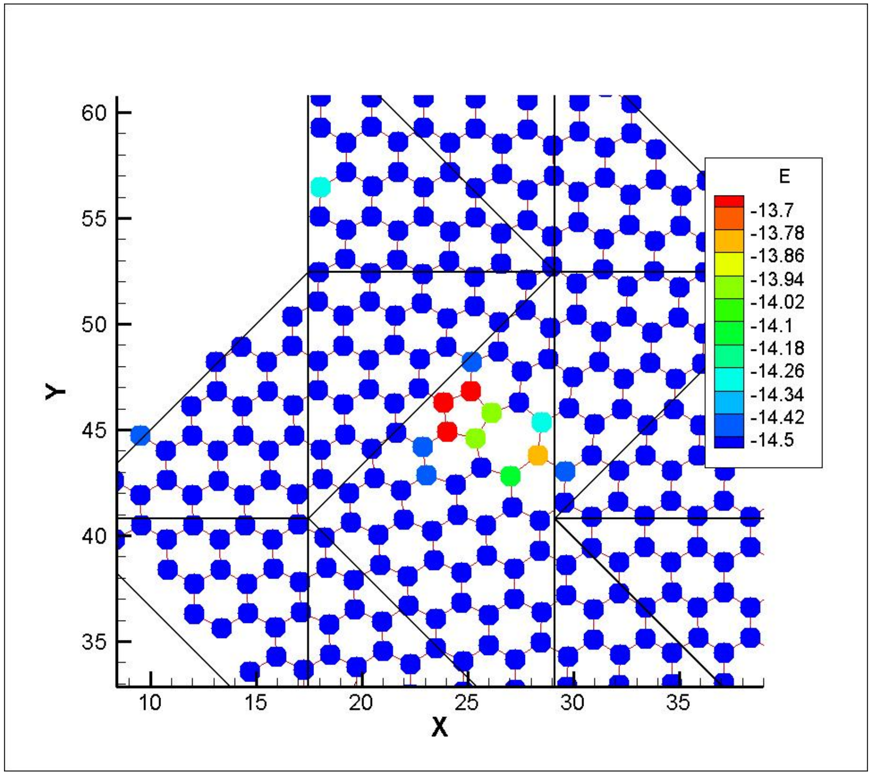

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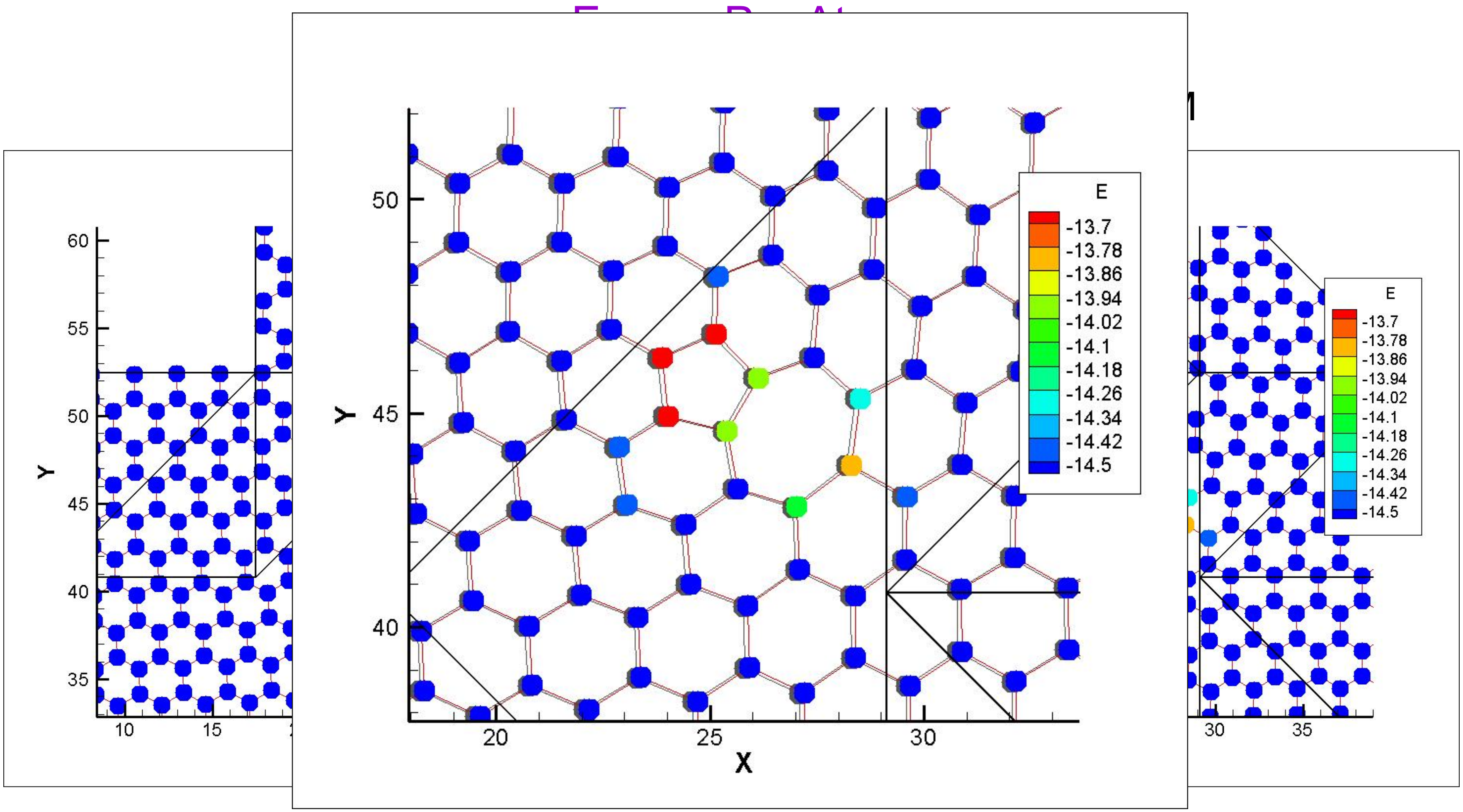

Conclusions

- 0 K continuum-atomistic multiscale framework.
- Homogenization of discontinuities.
- Significant reduction in the number of atoms
- Applicable to complicated lattice structures (ex. graphene)
- Anisotropic/Nonlinear Continuum
- Clearly extendable to 3D
- Extendable to Dislocation Dynamics without phemenological rules or equations of motion
- Further research to improve adaptivity.
- Extension to Finite Temperature