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The eXtended Bridging Scale Method (XBSM)

Pattabhi Ramaiah

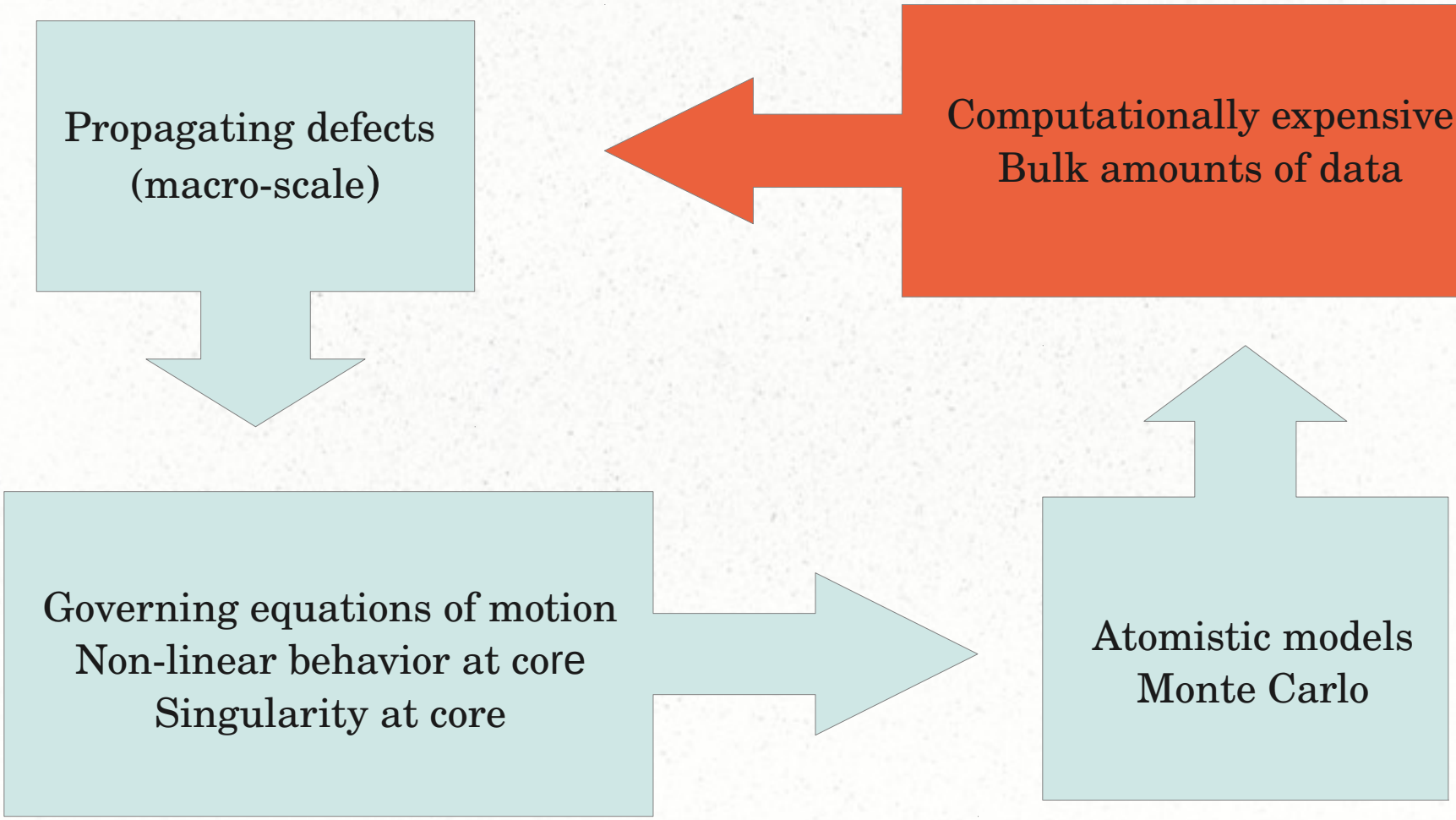
Institute of Structural Mechanics
Bauhaus University of Weimar

Bauhaus-Universität Weimar
Fakultät Bauingenieurwesen
Institut für Strukturmechanik

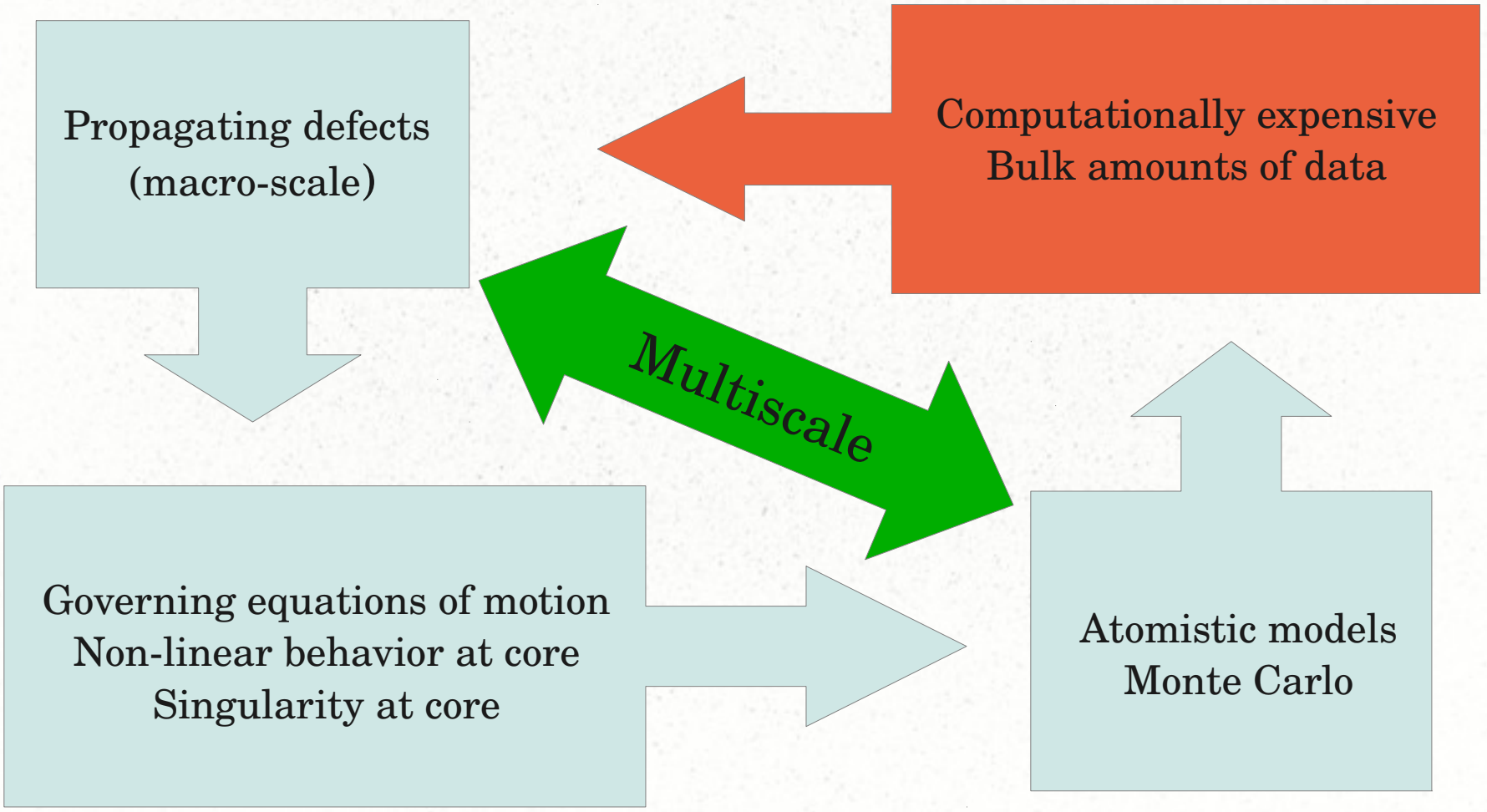
Outline

- **Motivation**
- The eXtended BSM for fracture
- Adaptivity
- Numerical Examples
- Conclusions

Motivation


Propagating defects
(macro-scale)
Computationally expensive
Bulk amounts of data
Governing equations of motion
Non-linear behavior at core
Singularity at core
Atomistic models
Monte Carlo

Motivation


Propagating defects
(macro-scale)
Computationally expensive
Bulk amounts of data
Multiscale
Governing equations of motion
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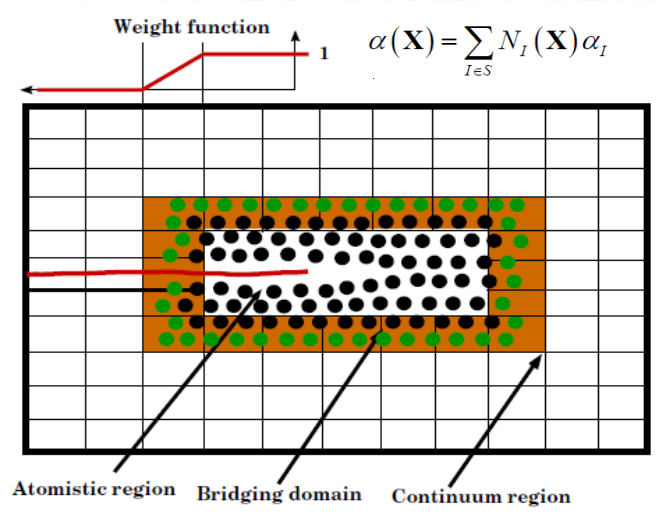
Overview of MM

- Propagating defects
- Must track the defect path
- Adaptivity required

- BDM - Belytschko & Xiao (2003, 2004)
- Adaptive XBDM - Gracie & Belytscko, 2011
- BSM – Liu *et al.*, (2003-2007)
- VAC+BSM – Qian (2003, 2004)
- Phantom node method - Timon, Song (2006, 2008)
- Adaptive XBSM – Current work

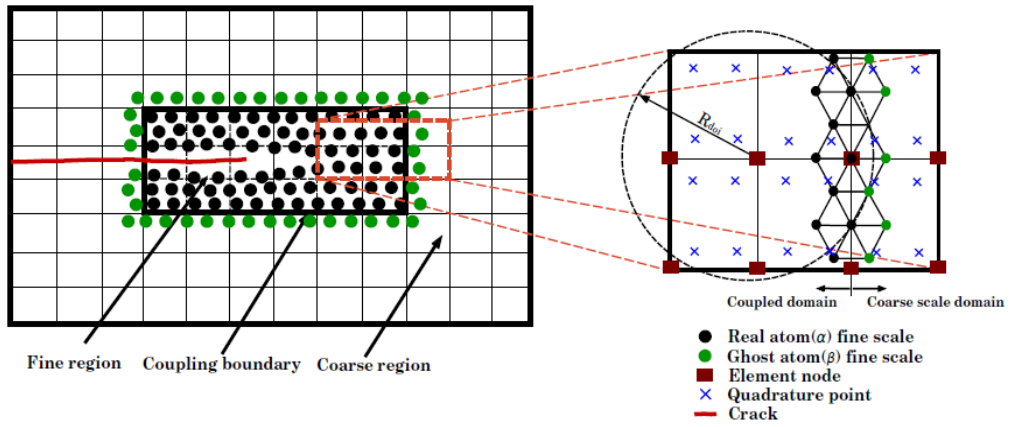
XBDM and XBSM

XBDM



- Overlapping domain decomposition scheme

XBSM



- No coupling domain
- Coupling realized by displacement bc's.

- Motivation
- **The eXtended BSM for fracture**
- Adaptivity
- Numerical Examples
- Conclusions

Why XBSM?

XBSM

Coarse scale

- Everywhere
- Solve independently

Coupling

- Displacement bc's on ghost atoms

XBDM

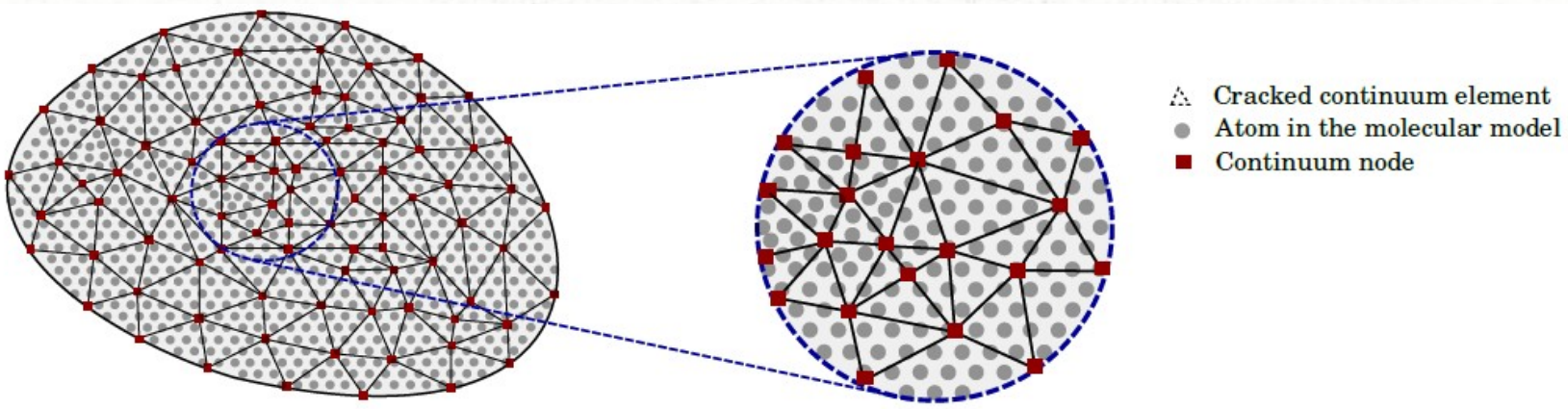
Coarse scale

- Doesn't exist – fine region
- Adaptivity - complicated

Coupling

- Linear energy weighting,
- Compatibility enforced by Lagrange multipliers

Bridging Scale Method

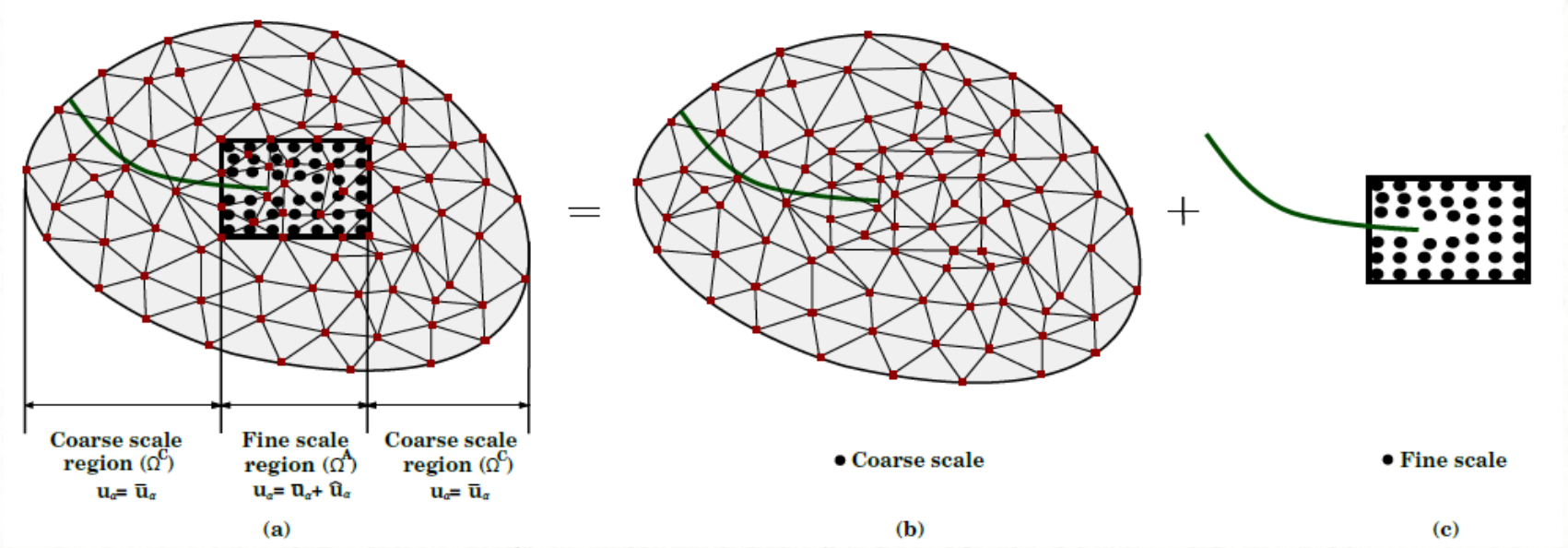


Total displacement $\mathbf{u} = \bar{\mathbf{u}} + \tilde{\mathbf{u}}$

Fine scale displacements exists in the region of interest

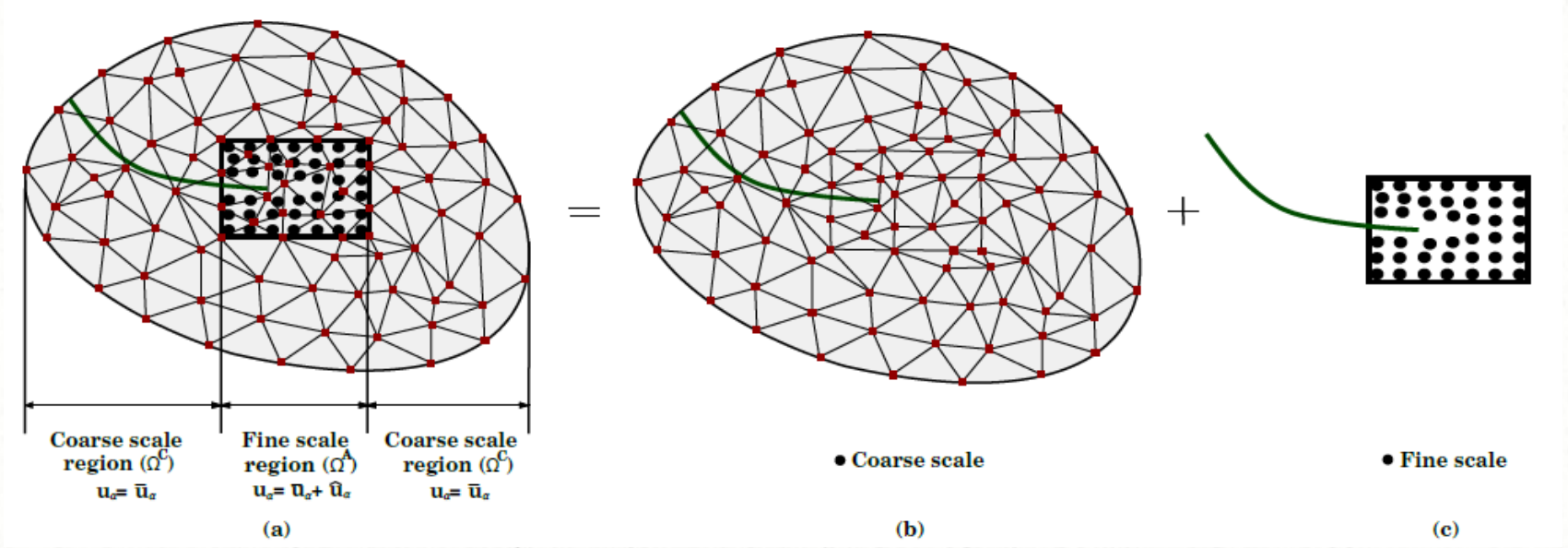
Coarse scale solution $$\bar{\mathbf{u}}_\alpha = \sum_{I=1}^{n^C} N_I(\mathbf{X}_\alpha)\mathbf{d}_I^C$$

XBSM Overview



- Fine scale lattice - (111) atoms of FCC crystal
- Coarse scale – VAC model with phantom node
- Coupling – Displacement bc's.
- Adaptivity implemented

XBSM Overview



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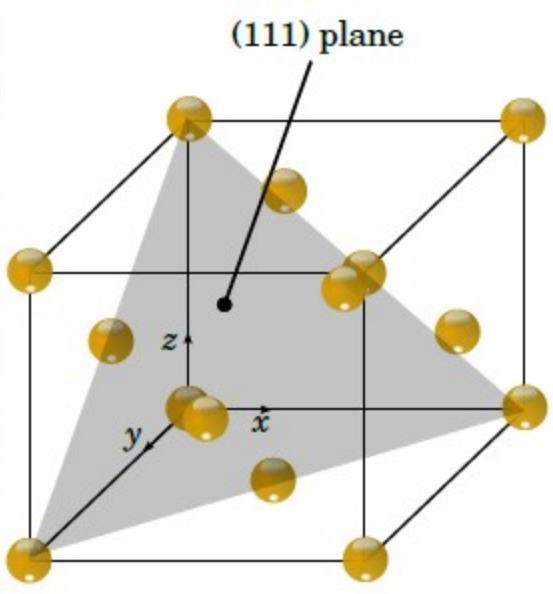
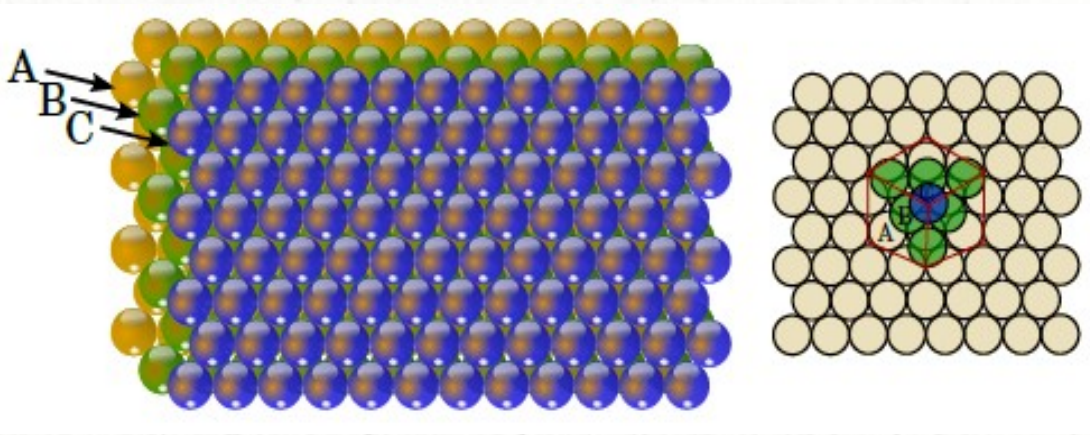
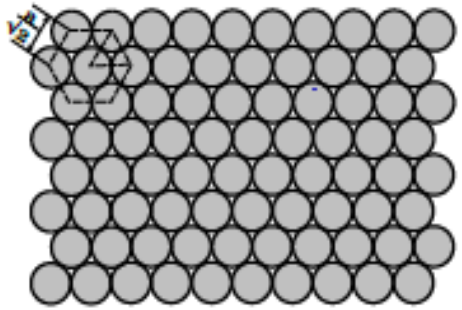
Fine scale model : Lattice

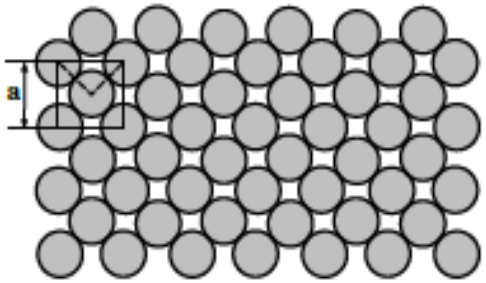


FCC unit lattice



(111) plane atoms





Lattice parameters

LJ potential – to model atom-atom interactions

Fine scale model: Molecular Statics

Total system potential energy

$$\Pi = W^{int} - W^{ext} \quad \text{where} \quad W^{int} = \frac{1}{2}\sum_{\alpha=1}^{n^A}\sum_{\beta\neq\alpha}^{n^A} V(r_{\alpha\beta})$$

Minimization of PE

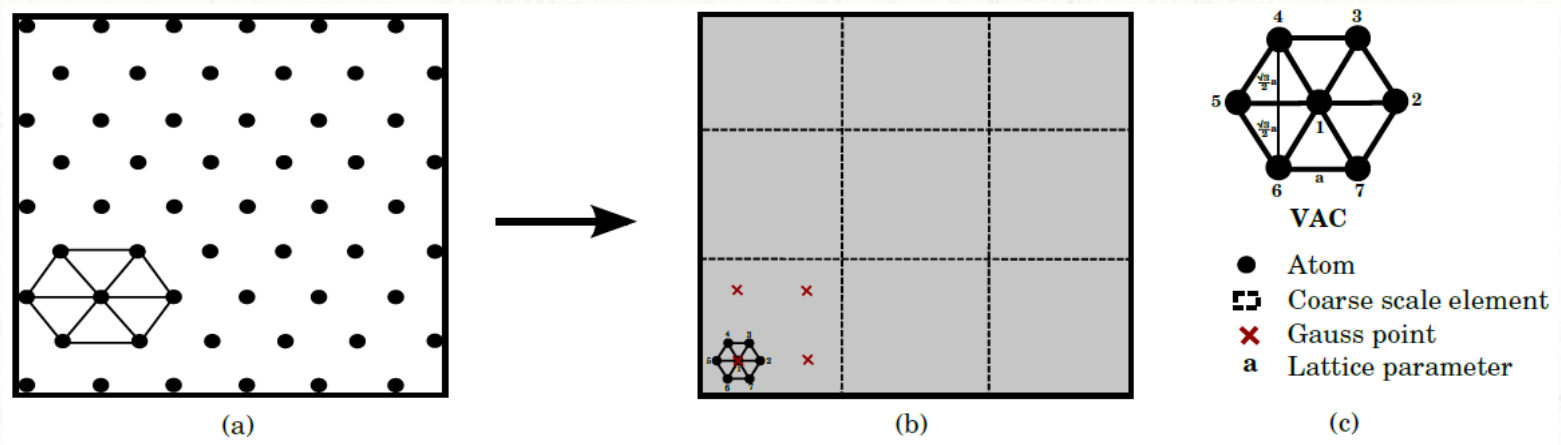
$$\mathbf{F}_\alpha^{int} = \sum_{\beta\neq\alpha}^{n^A} \frac{\partial V(r_{\alpha\beta})}{\partial r}\left(\frac{\mathbf{r}_\alpha - \mathbf{r}_\beta}{r}\right) \quad \text{and} \quad \mathbf{F}_\lambda^{ext} = \frac{\partial W^{ext}}{\partial \mathbf{r}_\lambda}$$

Residual forces

$$\mathbf{R} = \mathbf{F}^{int} - \mathbf{F}^{ext}$$

- Energy minimization – CG method
- Linearization of residual – not required
- Stiffness matrix – not required

Virtual Atom Cluster model



- Each atom has the same environment
- Possess 6 nearest neighbors
- Replace the original structure with VAC
- Energy density parameter

$$W^{int} = \sum_{\alpha=1}^{n^A} \phi_\alpha = \int_{\Omega_0} \phi_\rho d\Omega_0 \approx \sum_G w_G \phi_\rho^G$$

VAC : features

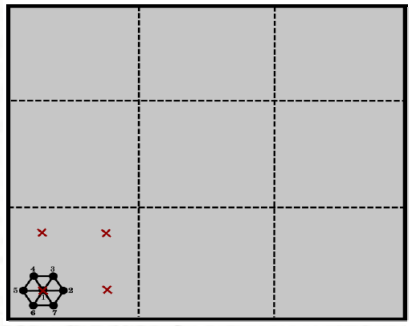
- Not the locations in the original lattice
- Same lattice parameters & inter-atomic potential
- When VAC confirms underlying lattice – Full scale atomistic models
- No continuum measure – no stress update
- Energy density parameter
- Improved computational efficiency

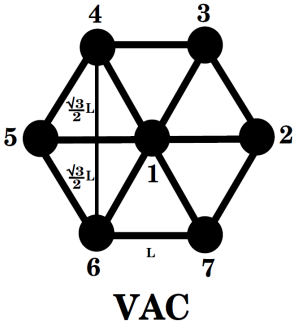
Coarse scale model

Internal energy

$$W^{int} = \sum_{\alpha=1}^{n^A} \phi_\alpha = \int_{\Omega_0} \phi_\rho d\Omega_0 \approx \sum_G w_G \phi_\rho^G$$

$$\frac{\partial W^{int}}{\partial \mathbf{d}_I^c} = \int_{\Omega_0} \frac{\partial \phi_\rho}{\partial \mathbf{d}_I^c} d\Omega_0 = \int_{\Omega_0} \sum_{\alpha=1}^{7} \frac{\partial \phi_\rho}{\partial \bar{\mathbf{u}}_\alpha} \frac{\partial \bar{\mathbf{u}}_\alpha}{\partial \mathbf{d}_I^c} d\Omega_0$$





$$\mathbf{F}_I^{int} = \int_{\Omega_0} \sum_{\alpha=1}^{7} \frac{\partial \phi_\rho}{\partial \bar{\mathbf{u}}_\alpha} N_I(\mathbf{X}_\alpha) d\Omega_0 \approx \frac{1}{\Omega_0} \sum_{G=1}^{n^G} w_G \sum_{\alpha=1}^{7} \frac{\partial \phi_\rho(\bar{\mathbf{u}}_\alpha)}{\partial \bar{\mathbf{u}}_\alpha} N_I(\mathbf{X}_\alpha)$$

$$\phi_\rho = \phi_{12}(r_{12}) + \phi_{13}(r_{13}) + \phi_{14}(r_{14}) + \phi_{15}(r_{15}) + \phi_{16}(r_{16}) + \phi_{17}(r_{17})$$

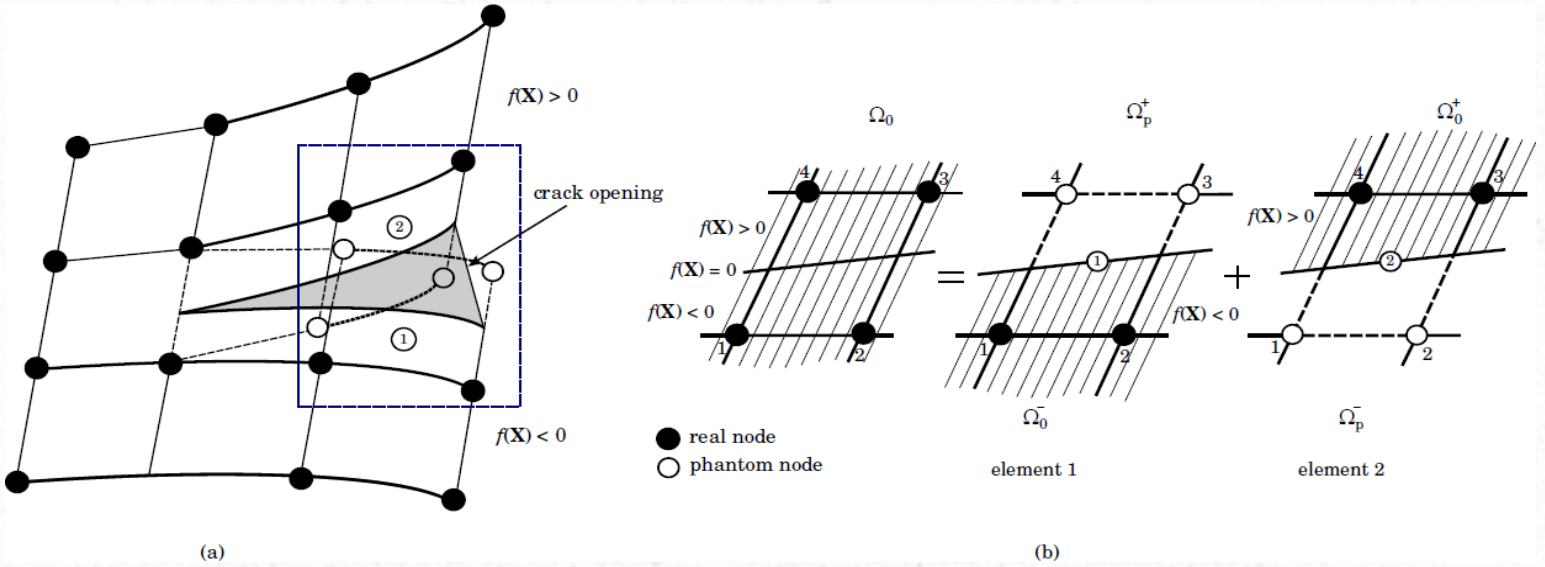
$\alpha = 1$

$$\frac{\partial \phi_\rho}{\partial \bar{u}_{1i}} = \frac{\partial \phi_{12}}{\partial r_{12}} \frac{r_{12i}}{r_{12}} + \frac{\partial \phi_{13}}{\partial r_{13}} \frac{r_{13i}}{r_{13}} + \frac{\partial \phi_{14}}{\partial r_{14}} \frac{r_{14i}}{r_{14}} + \frac{\partial \phi_{15}}{\partial r_{15}} \frac{r_{15i}}{r_{15}} + \frac{\partial \phi_{16}}{\partial r_{16}} \frac{r_{16i}}{r_{16}} + \frac{\partial \phi_{17}}{\partial r_{17}} \frac{r_{17i}}{r_{17}}$$

$\alpha = 2$

$$\frac{\partial \phi_\rho}{\partial \bar{u}_{2i}} = \frac{\partial \phi_{21}}{\partial r_{21}} \frac{r_{21i}}{r_{21}} + \frac{\partial \phi_{23}}{\partial r_{23}} \frac{r_{23i}}{r_{23}} + \frac{\partial \phi_{27}}{\partial r_{27}} \frac{r_{27i}}{r_{27}}$$

The phantom node method



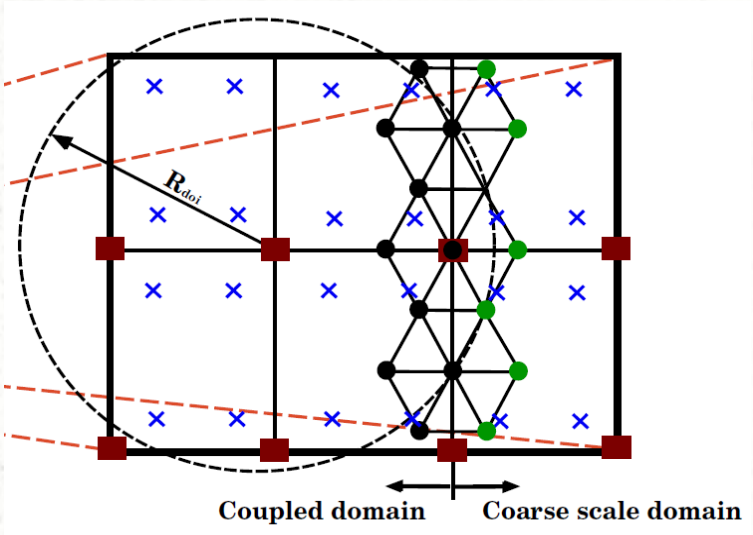
- Cracked element = two overlapping elements
- Theory - Hansbo & Hansbo (2004)
- The phantom node method - Song, Timon(2006,2008)

The total displacement

$$\mathbf{u}(\mathbf{X},t) = \sum_{I\in\{W_0^+,W_p^-\}} \mathbf{u}_I(t)N_I(\mathbf{X})H(f(\mathbf{X})) + \sum_{J\in\{W_0^-,W_p^+\}} \mathbf{u}_J(t)N_J(\mathbf{X})H(-f(\mathbf{X}))$$

Coupled model : solution

- Coarse scale model: Energy & internal forces
  Coupled region – 2 atom sets
  else where – 1 atom set
- Place the phantom nodes
- Apply bc's
- Solve for coarse scale solution
- Ghost atom positions as bc's to fine scale model
- Solve for fine scale solution
- Propagate the crack – based on the crack-tip position



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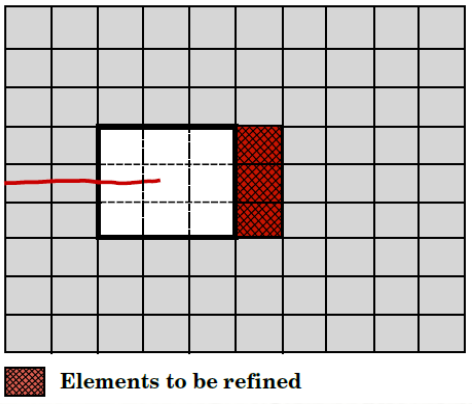
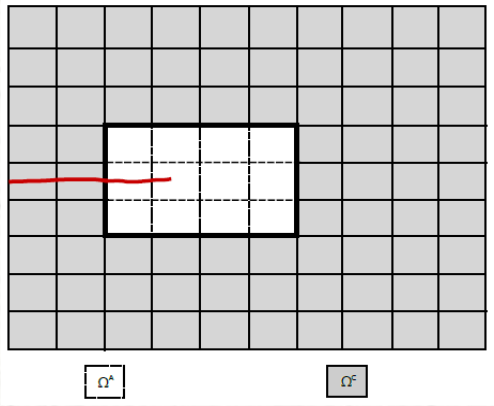
- The eXtended BSM for fracture
- **Adaptivity**
- Numerical Examples
- Conclusions

Adaptivity

1. Adaptive refining – convert the coarse scale region into fine scale region





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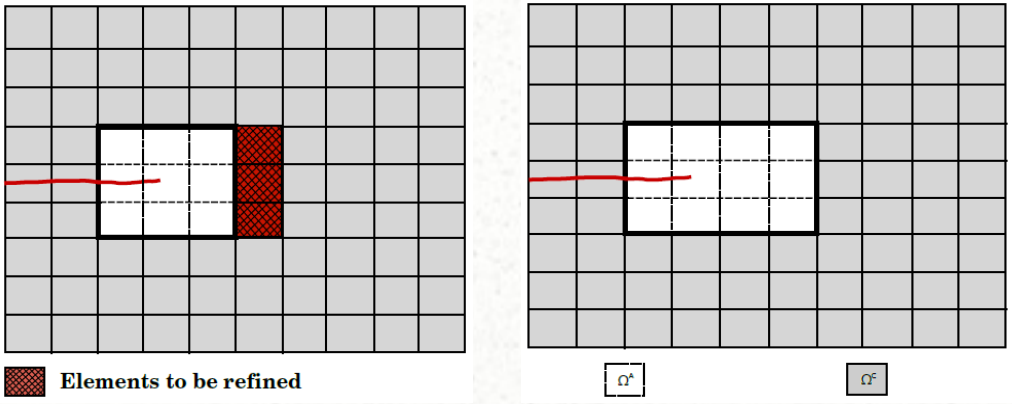
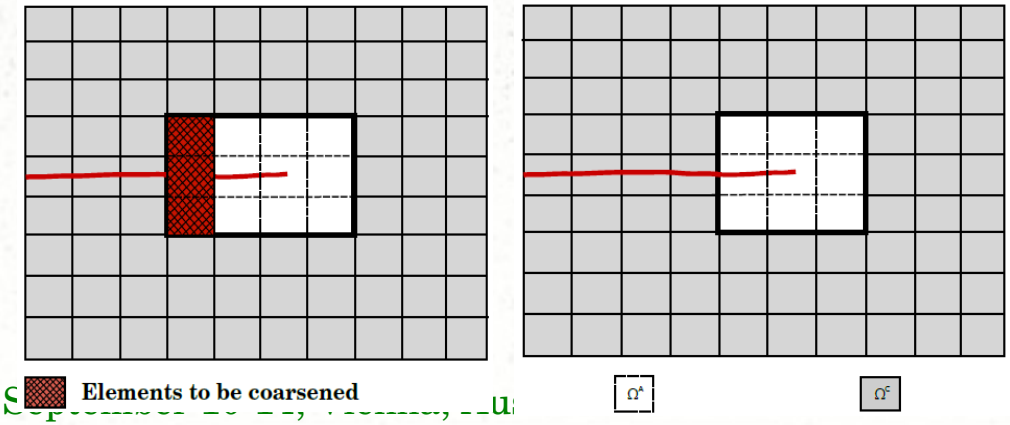


2. Adaptive coarsening – convert the fine scale region into coarse scale region



Adaptivity : steps

- High energy elements

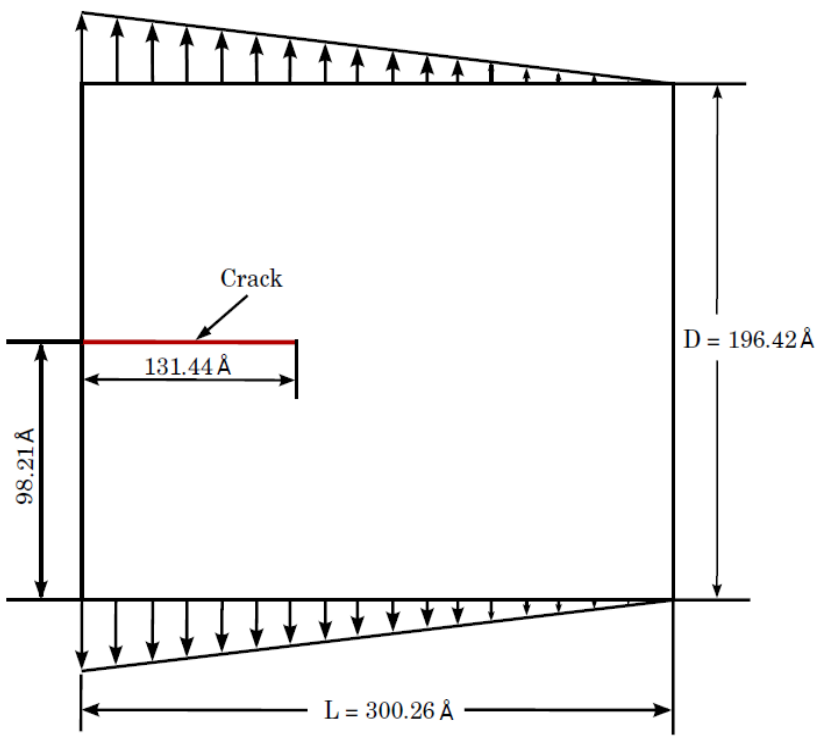
$$\mathcal{E}_n^{HE} = \{e \in \mathcal{E}_n^A \mid energy\ of\ an\ atom\ in\ e > tol^E\}$$

- tol^E – 15-30% higher than the $E_{eqilibrium}$
- Locate the cracktip
- Identify the elements to be refined
- Create and initialize the atoms
- Identify newly cracked elements – phantom nodes
- Propagate the crack
- If coarsening – delete the atoms
- Update the fine scale atoms

- Motivation
- The eXtended BSM for fracture
- Adaptivity
- **Numerical Examples**
- Conclusions

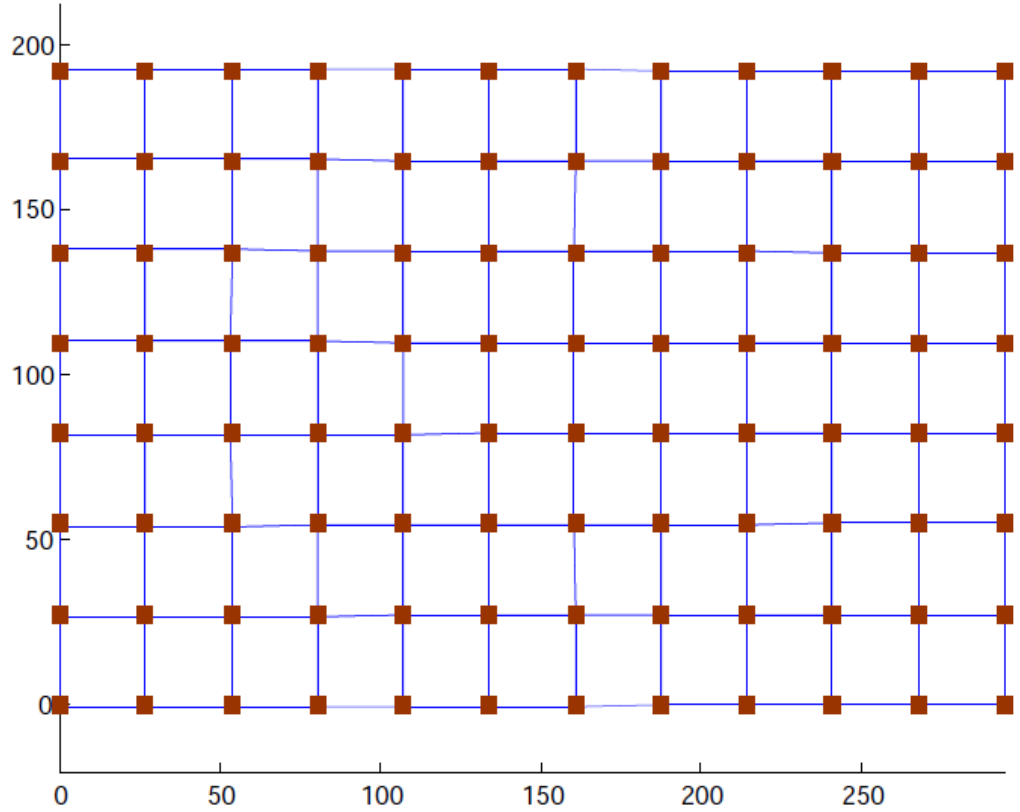
Example 1

- LJ potential
- (111) plane atoms of fcc
- Nearest neighbors only
- Brittle fracture
- Neighbor list not updated
- Displacement load – 5.892 Ang
- Adaptively propagate the crack



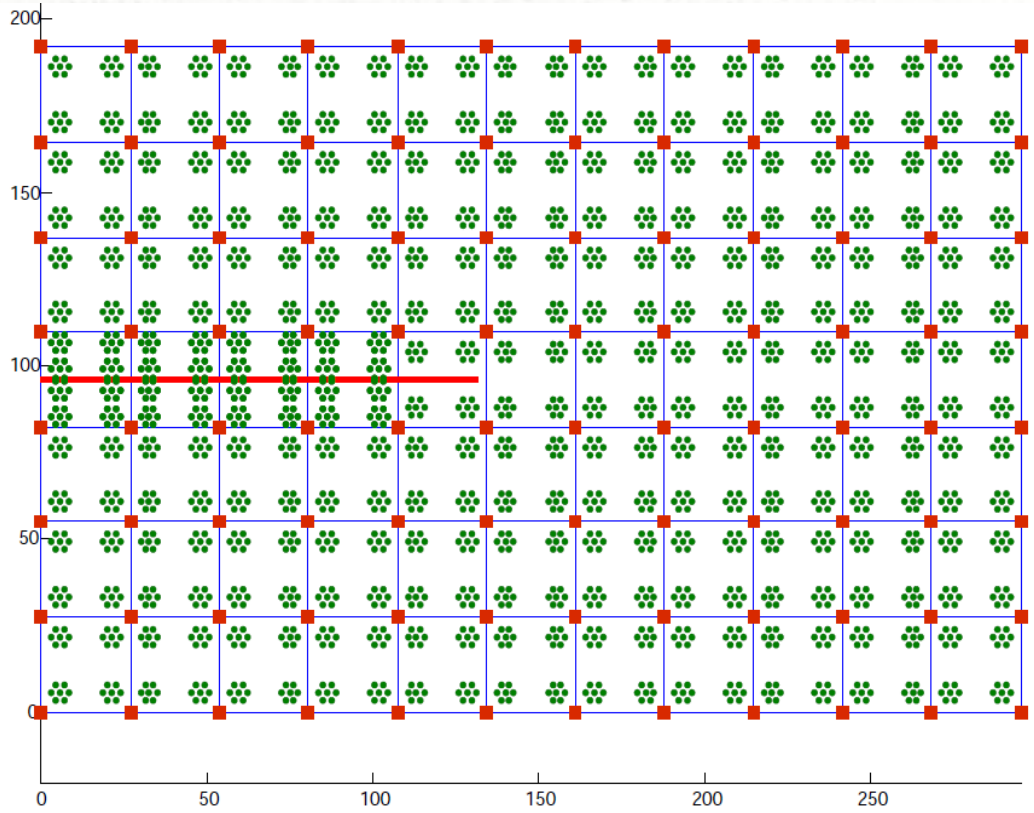
Example 1 : steps

- Coarse scale mesh



Example 1 : steps

- Coarse scale mesh
- Create VAC



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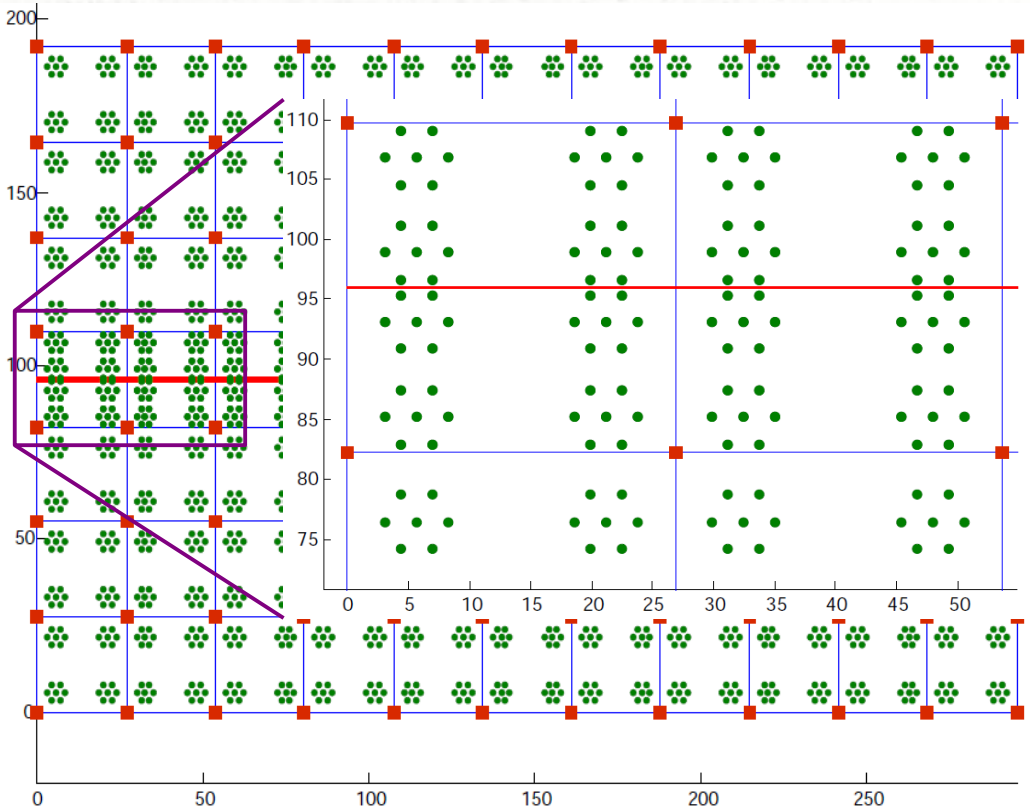
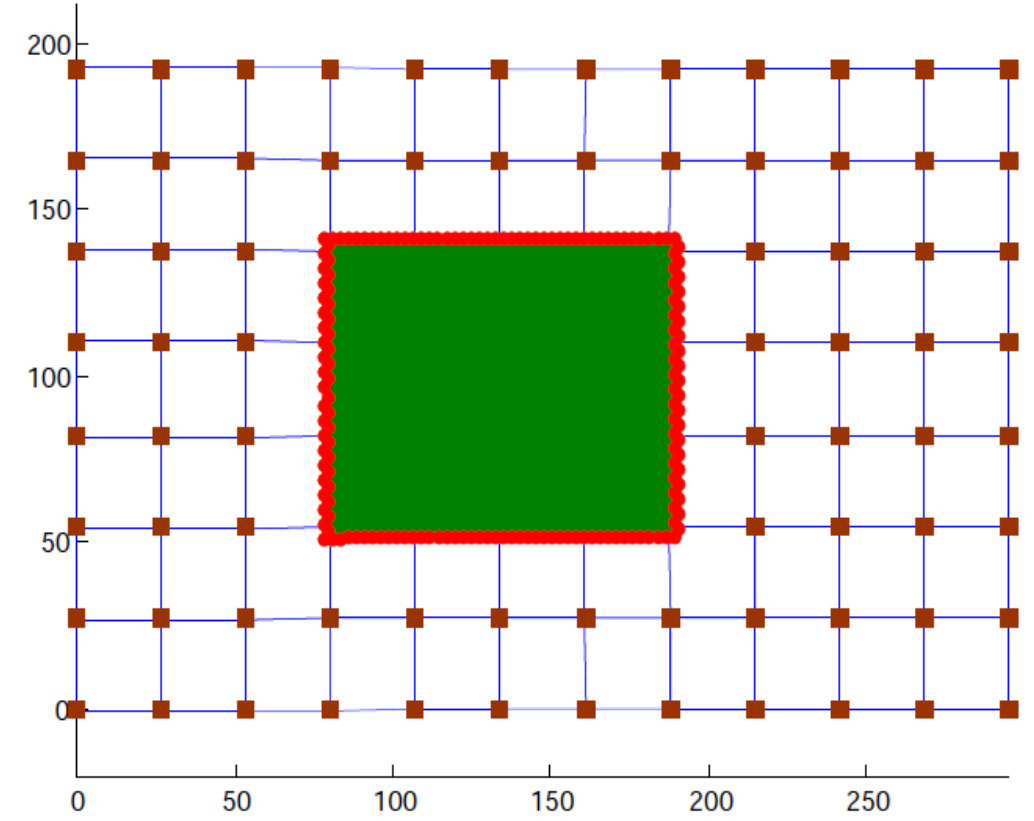


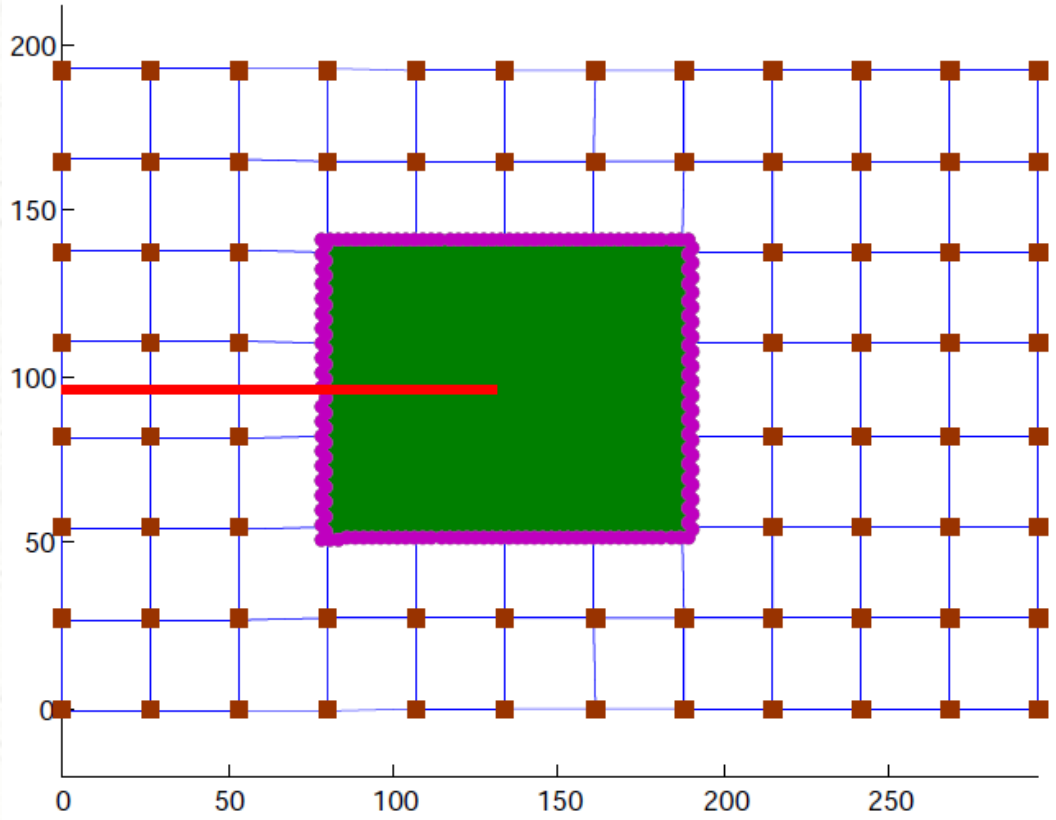
Example 1 : steps

- Coarse scale mesh
- Create VAC
- Fine scale lattice



Example 1 : steps

- Coarse scale mesh
- Create VAC
- Fine scale lattice
- Insert the crack

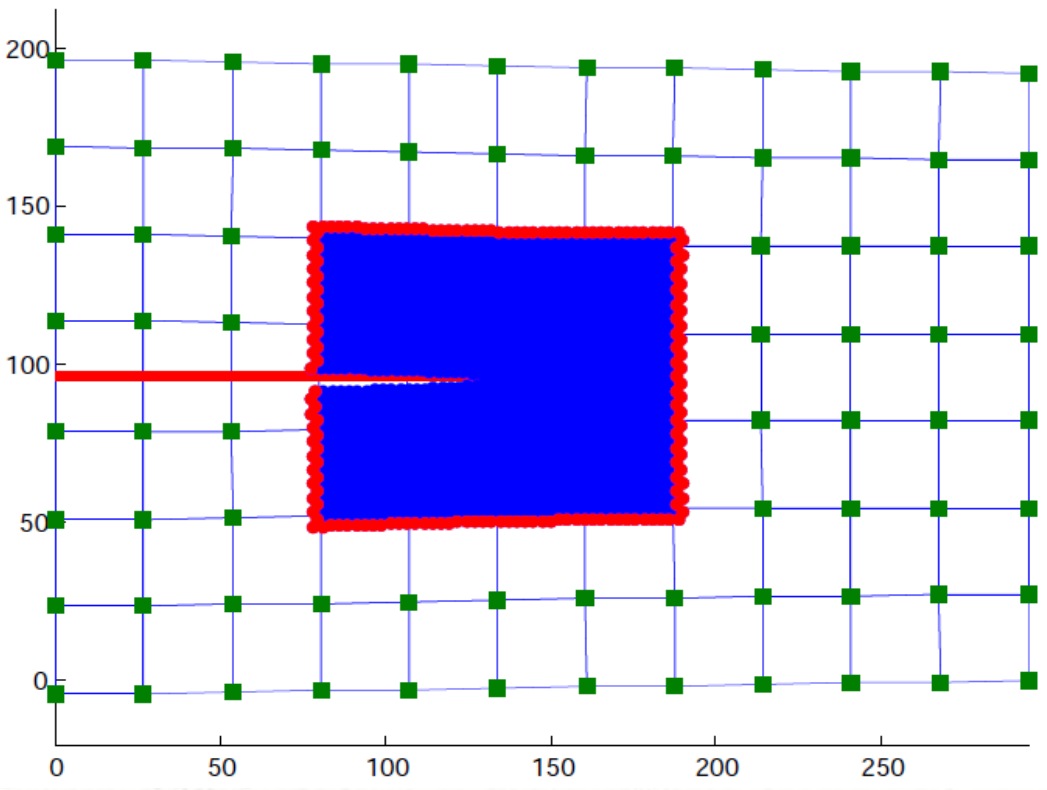


Example 1 : steps

- Coarse scale mesh
- Create VAC
- Fine scale lattice
- Insert the crack
- Apply BC's

  Solve coarse scale

  Solve fine scale

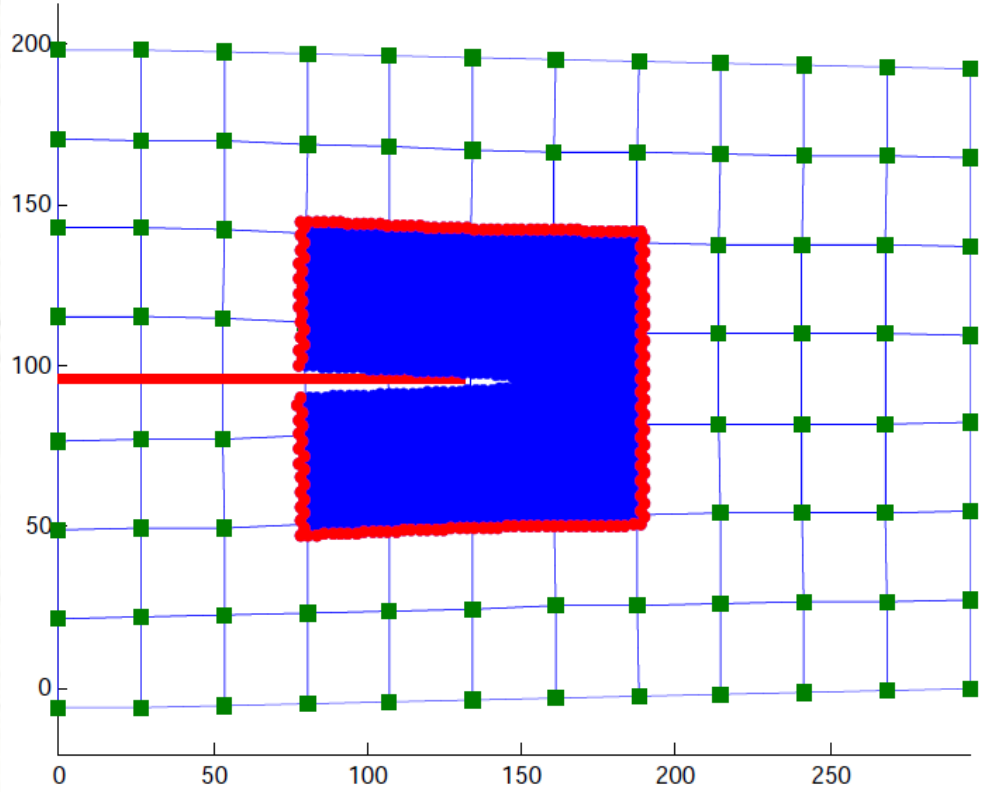


Example 1 : steps

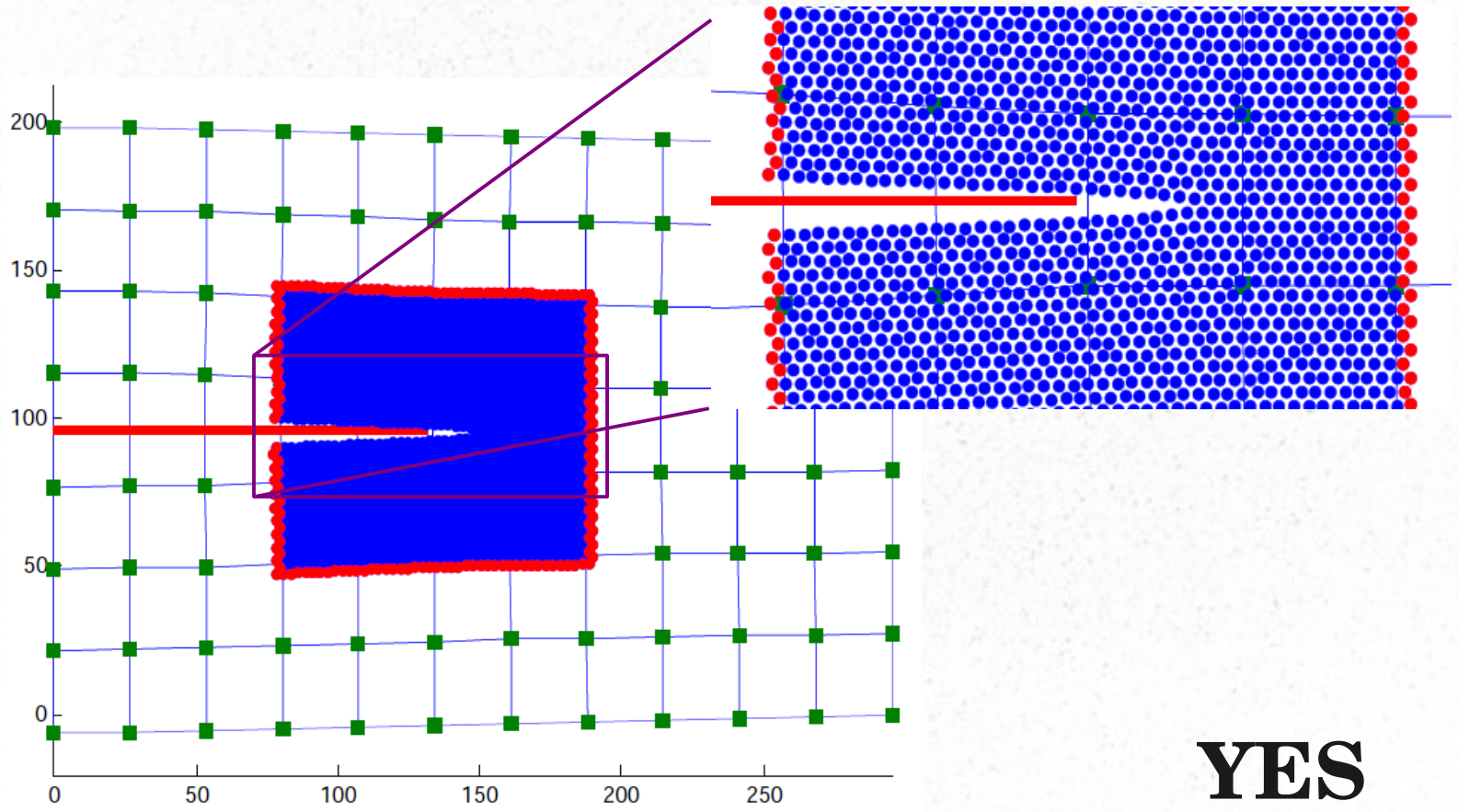
- Coarse scale mesh
- Create VAC
- Fine scale lattice
- Insert the crack
- Apply BC's

  Solve coarse scale

  Solve fine scale
- Adaptivity required?

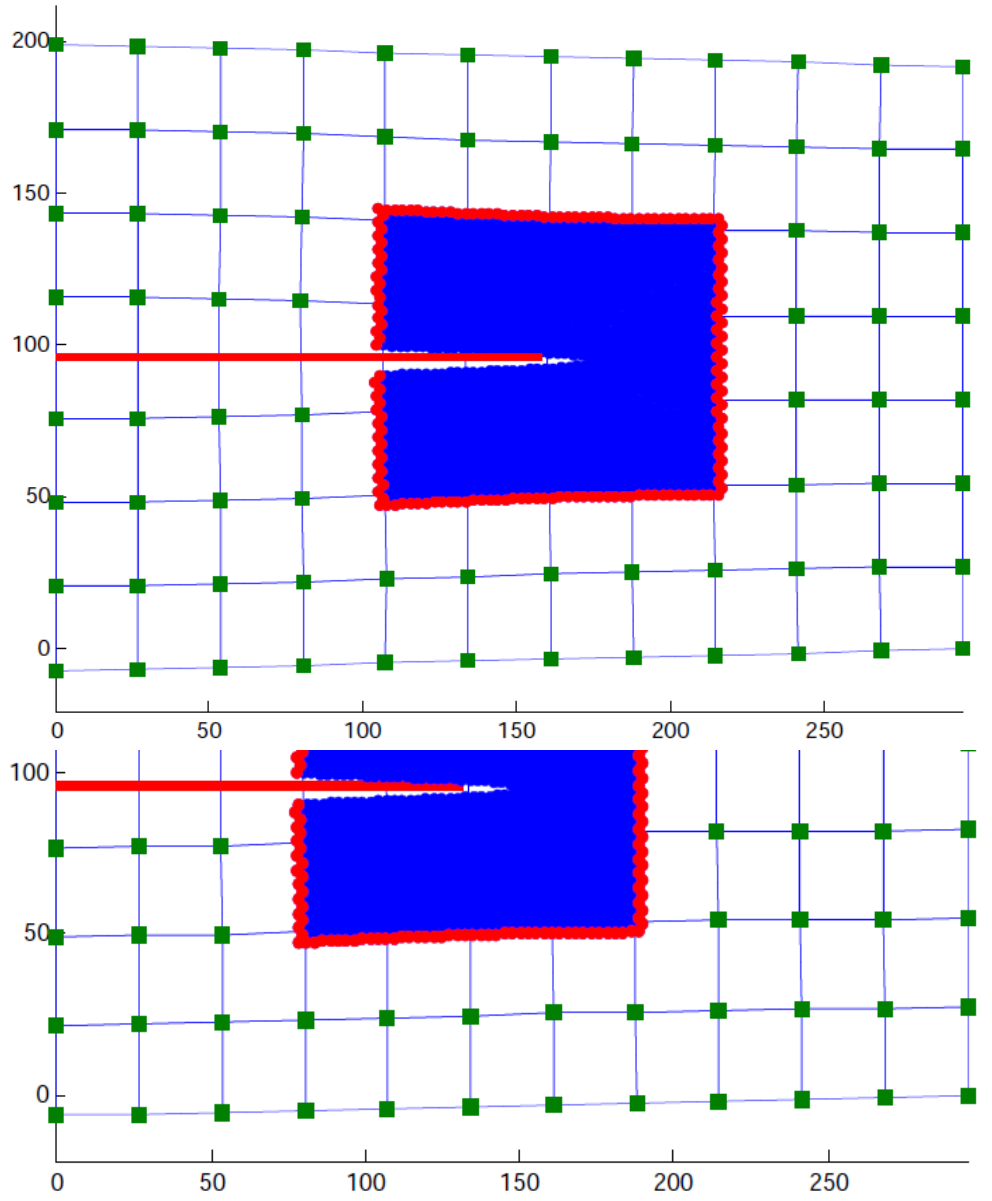


Example 1 : steps



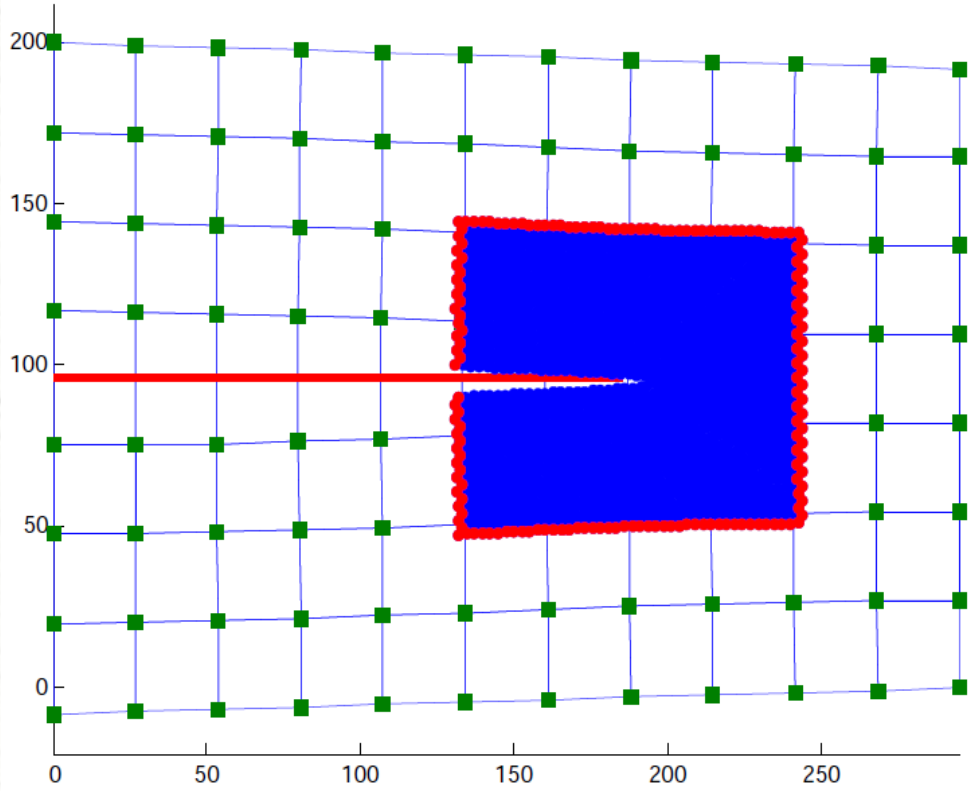
YES

- Coarse scale mesh
- Create VAC
- Fine scale lattice
- Insert the crack
- Apply BC's
  Solve coarse scale
  solve fine scale
- Adaptivity required?
- Refine, coarse-grain



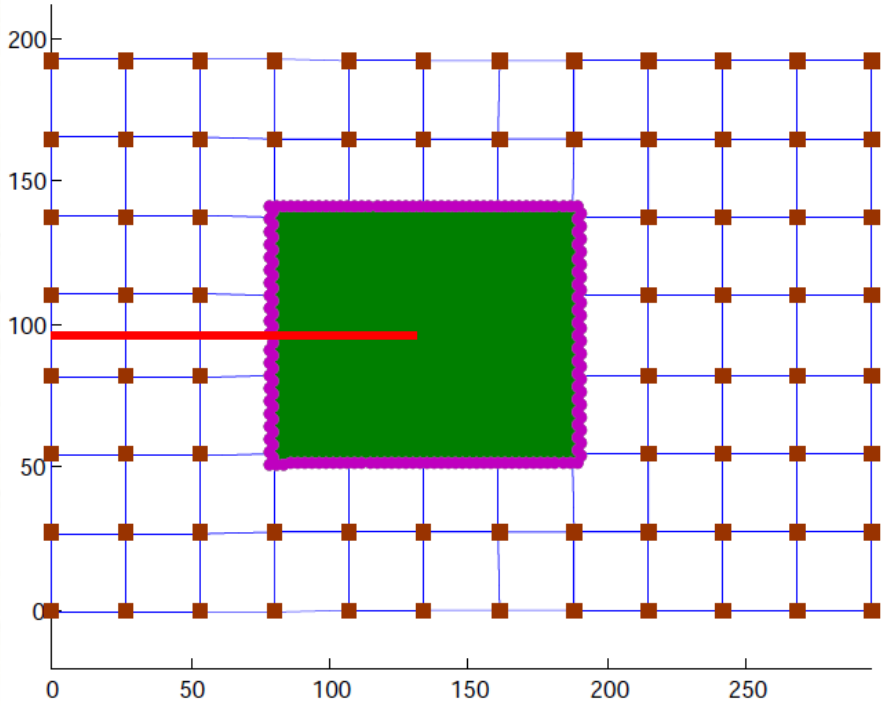
Example 1 : steps

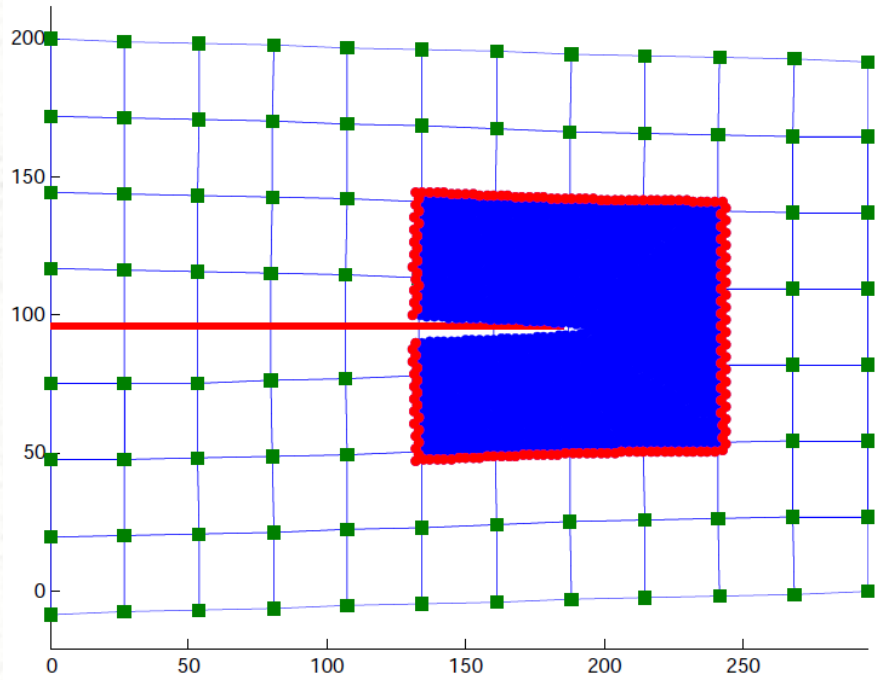
- Coarse scale mesh
- Create VAC
- Fine scale lattice
- Insert the crack
- Apply BC's
  Solve coarse scale
  solve fine scale
- Adaptivity required?
- Refine, coarse-grain
- Propagate the crack



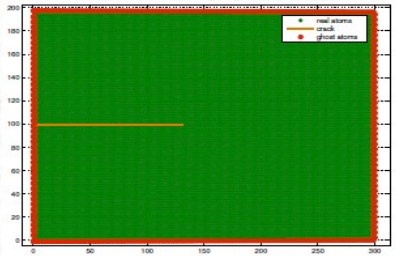
Example 1 : summary

Step 1 to n

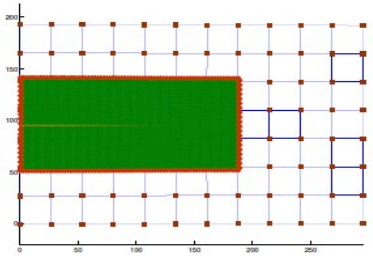




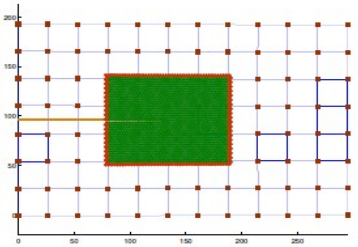
Example 1 : comparison



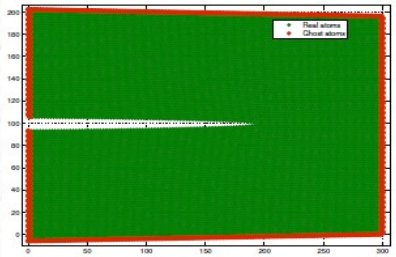
(a) MS model after the first LS



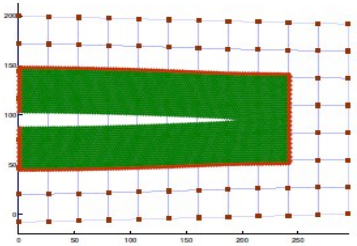
(b) BSM model after the first LS



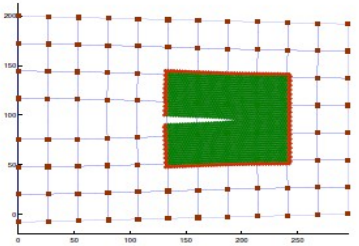
(c) XBSM model after the first LS



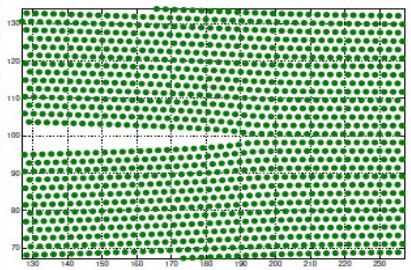
(d) MS model after the final LS



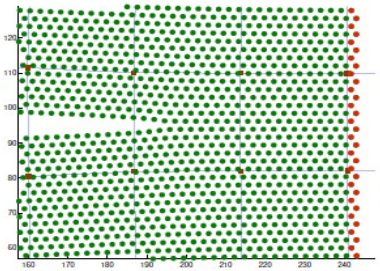
(e) BSM model after the final LS



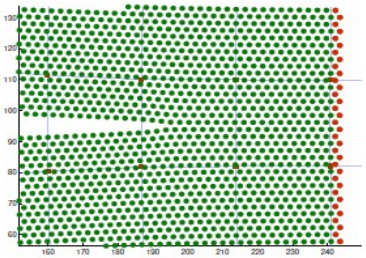
(f) XBSM model after the final LS



(g) zoom of MS model after the final LS

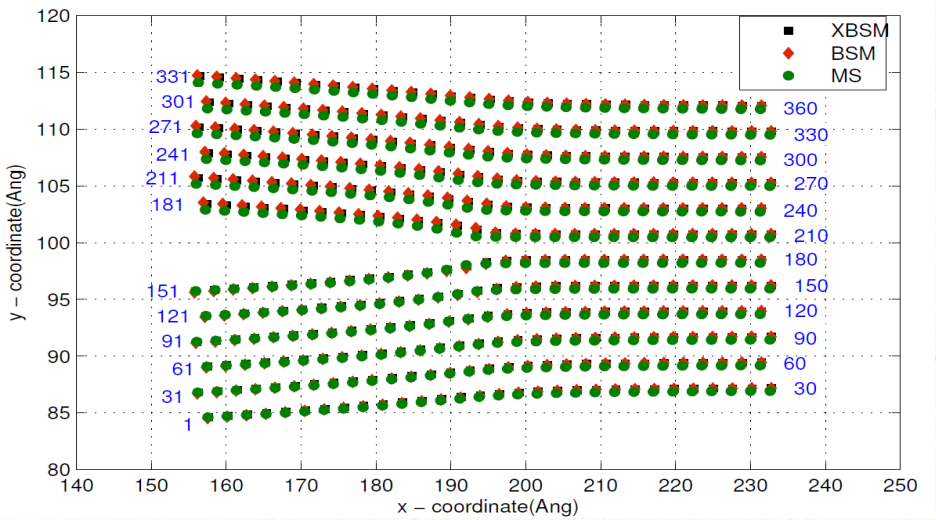


(h) zoom of BSM model after the final LS

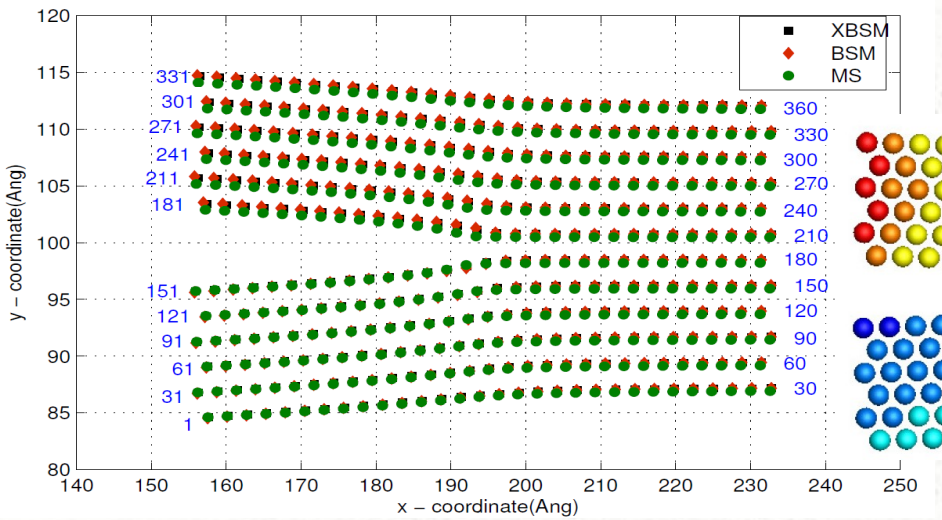


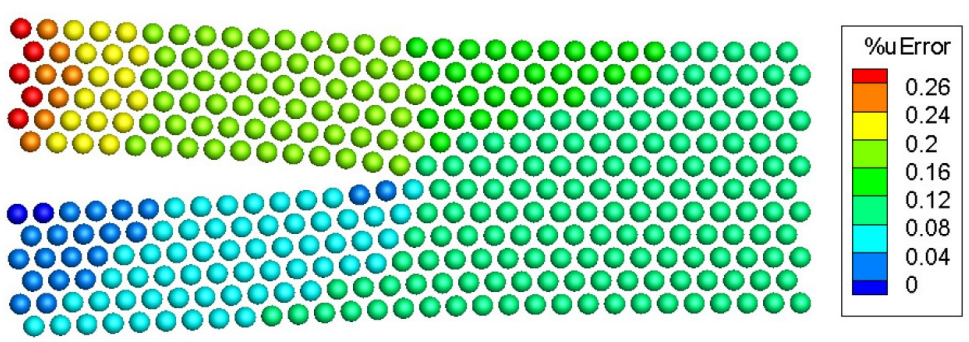
(i) zoom of XBSM model after the final LS

Example 1 : comparison

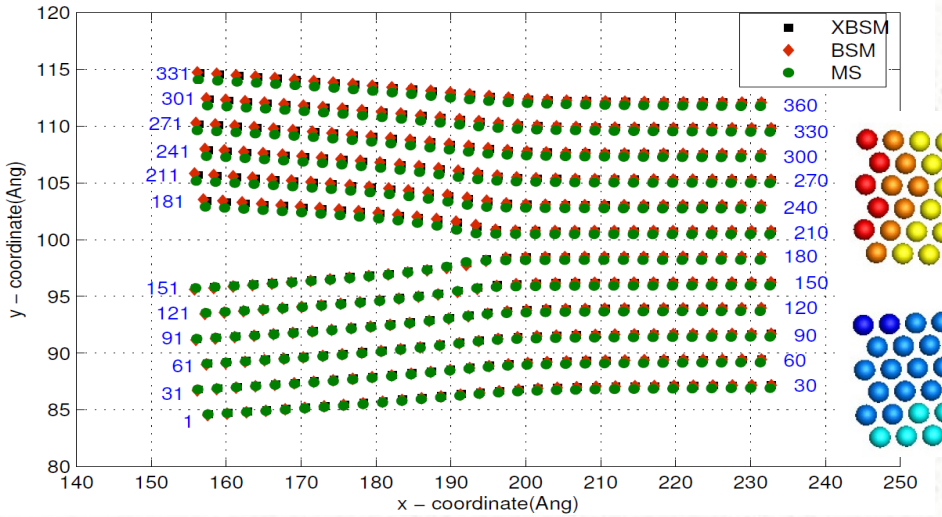


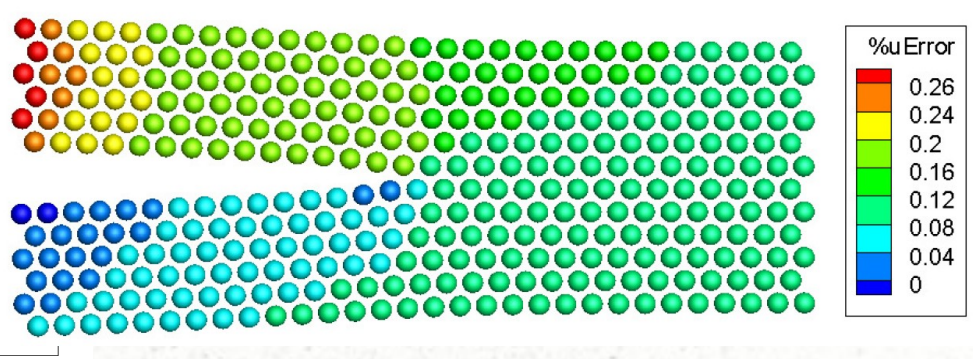
Example 1 : comparison

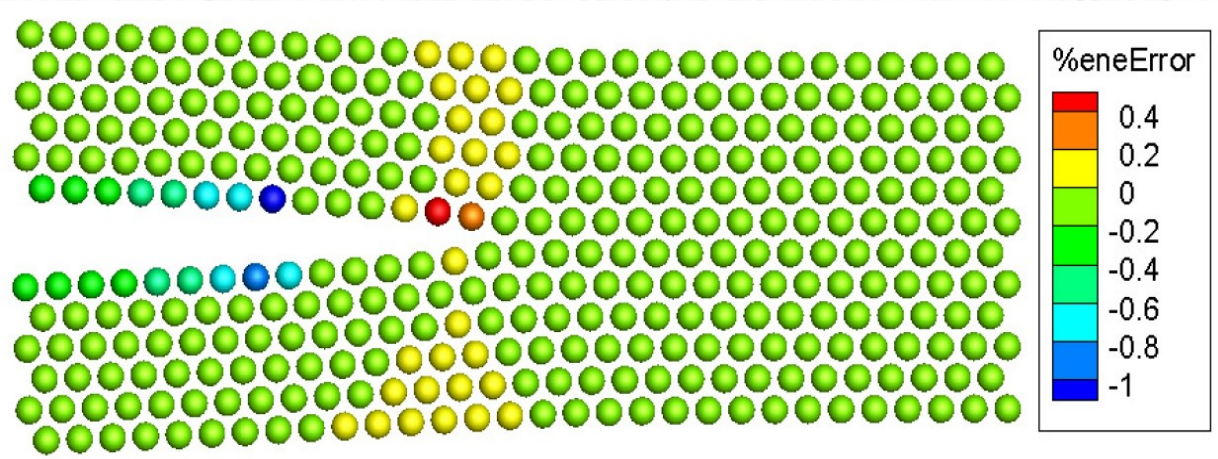




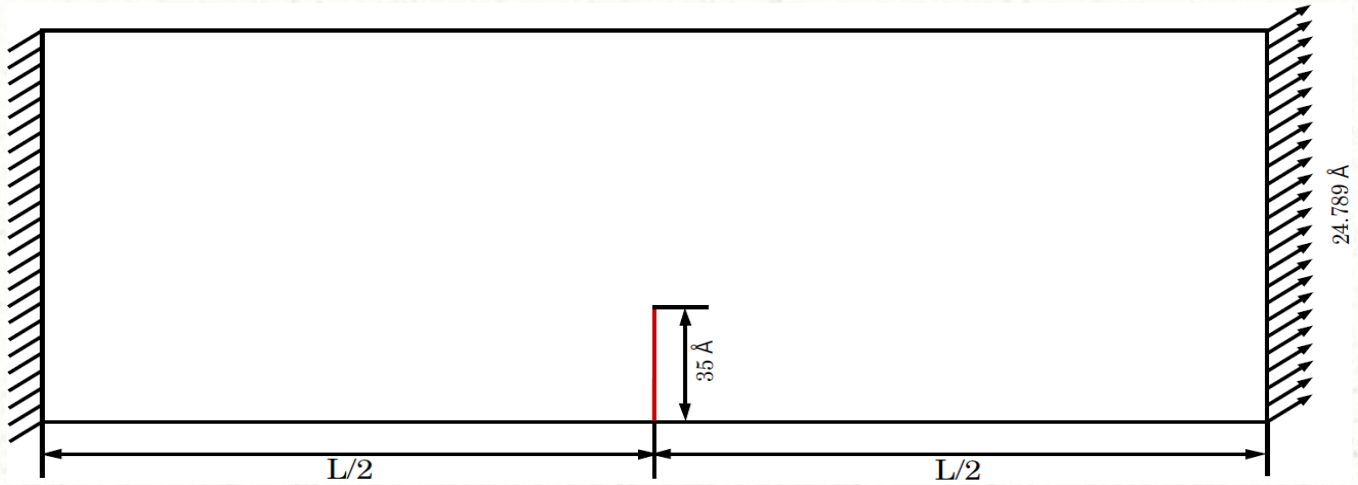
Example 1 : comparison





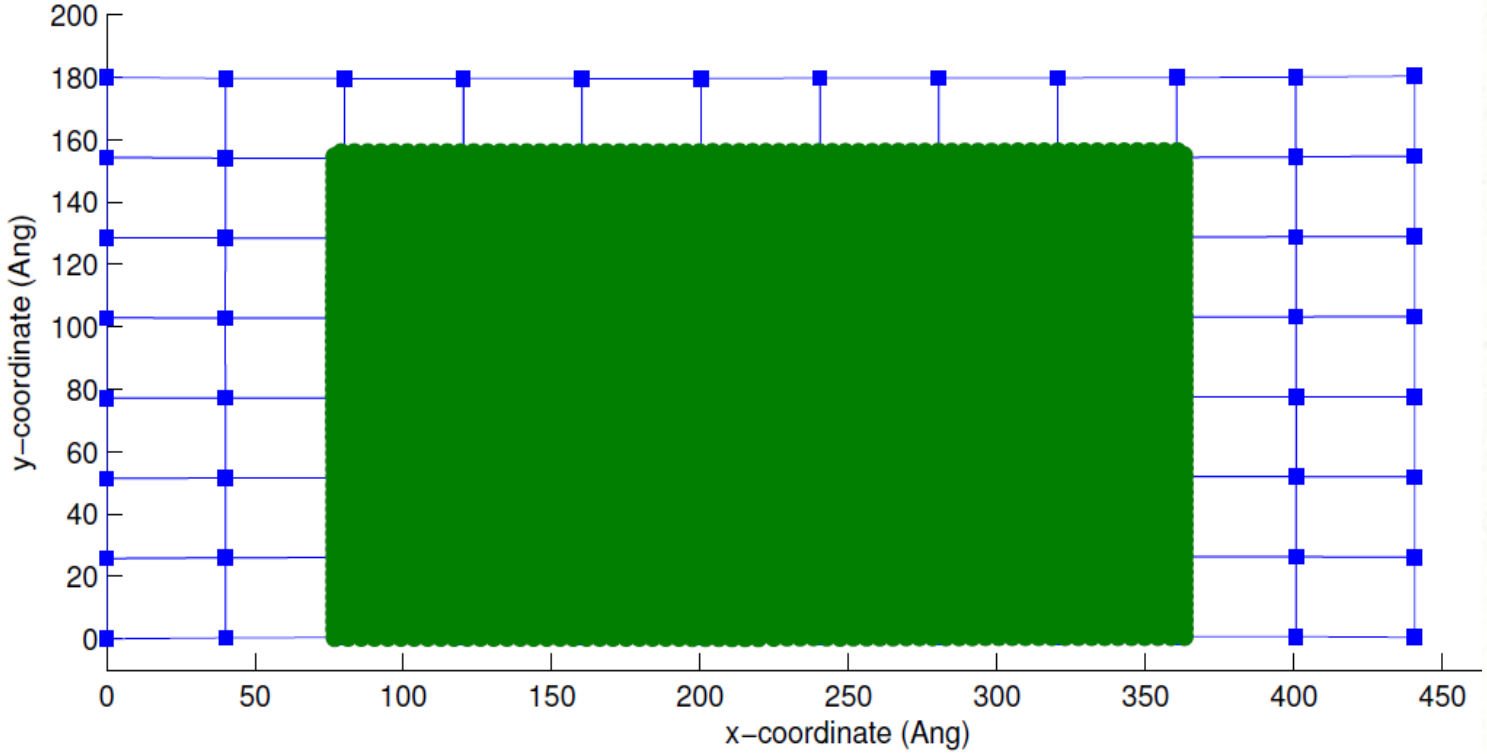


Example 2 : kink crack propagation

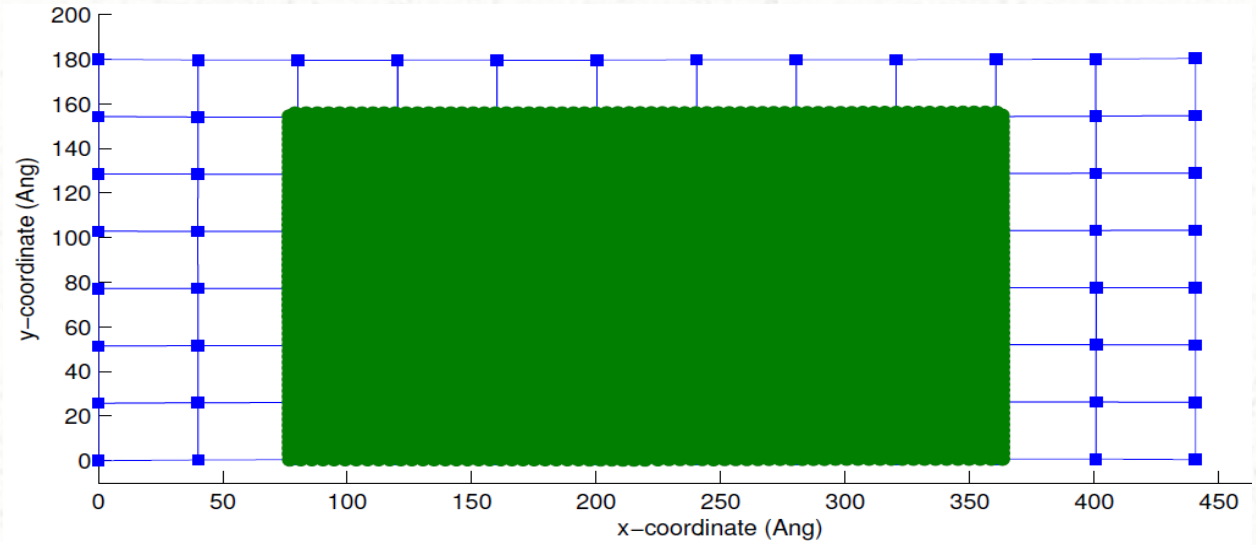


- LJ potential – 440 Ang x 180 Ang
- (111) plane atoms of fcc
- Nearest neighbors only
- Brittle fracture
- Displacement load – 24.798 Ang at 60^0
- Crack not propagated in the coarse scale

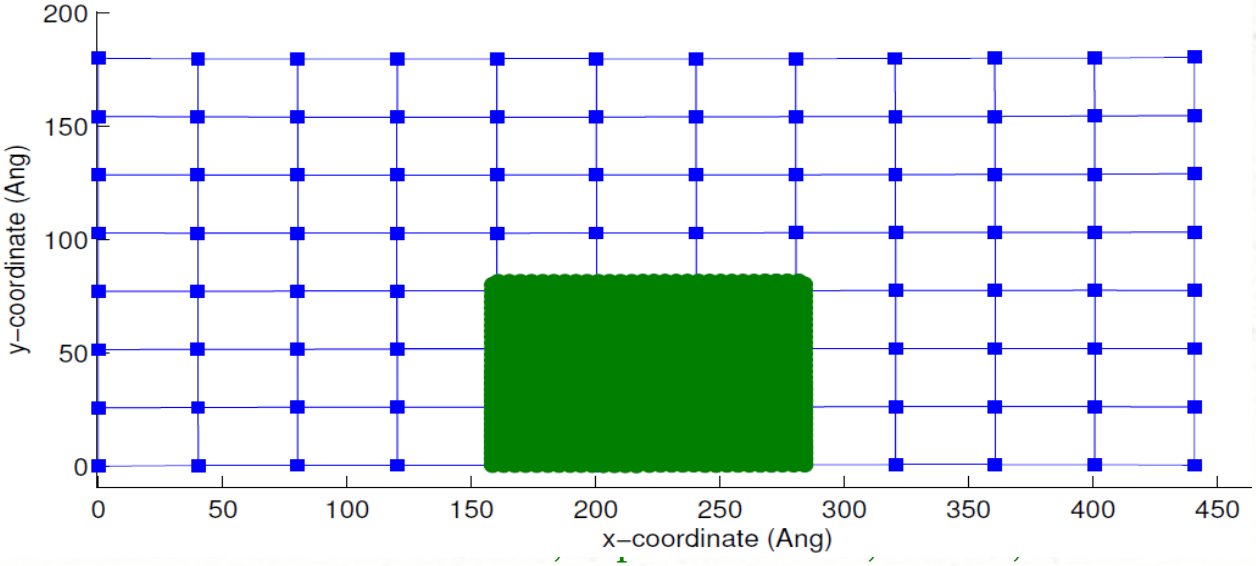
Example 2 : BSM



Example 2 : initial BSM and XBSM

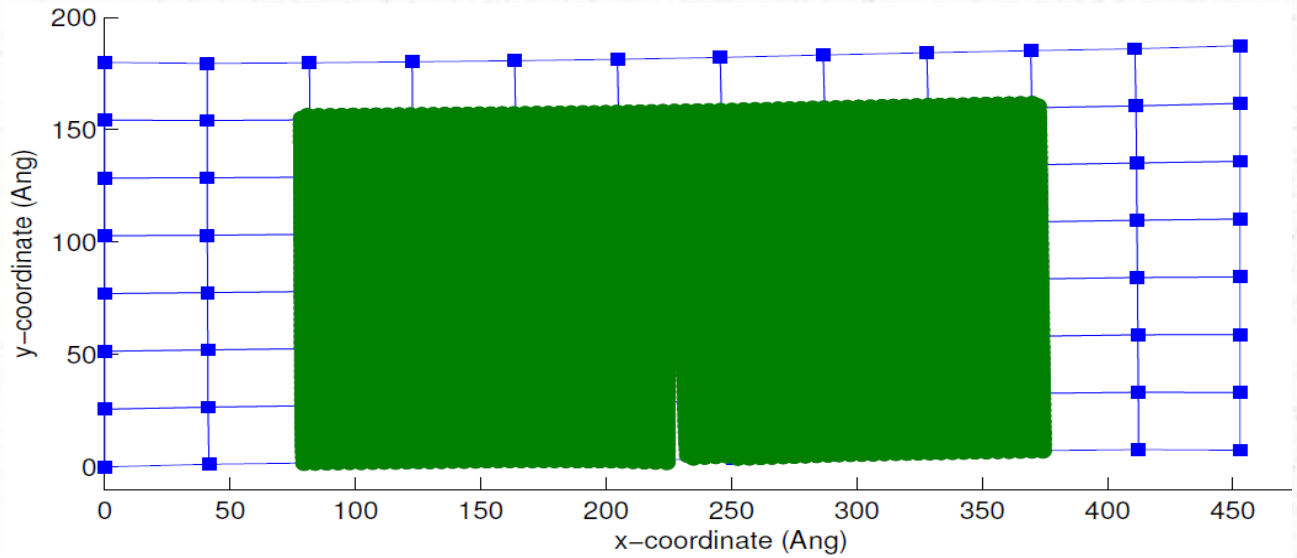


BSM

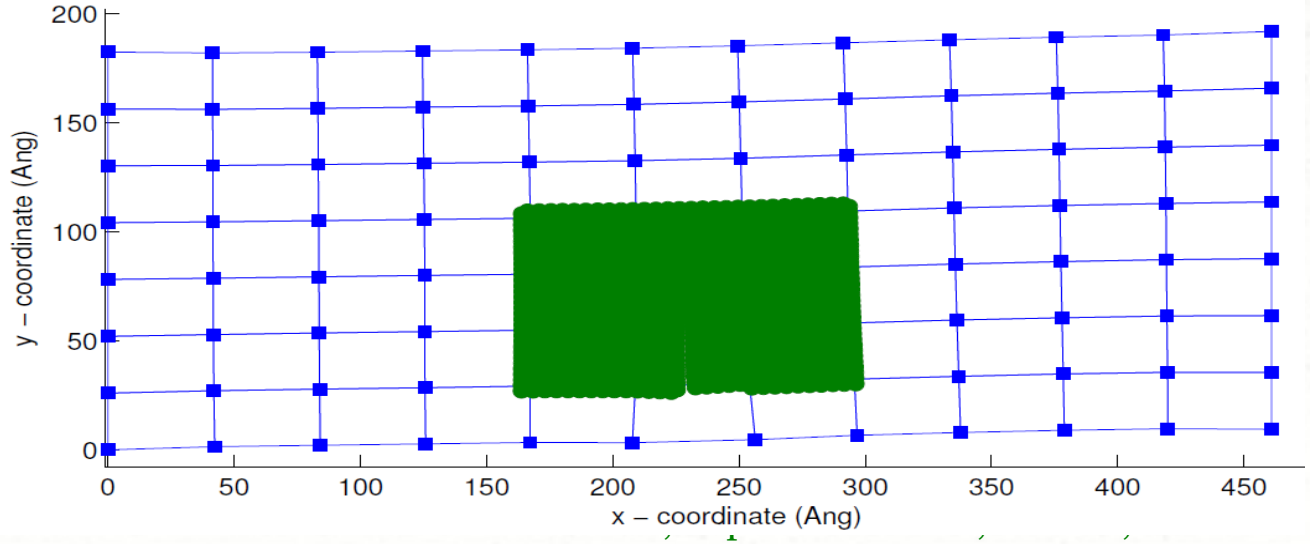


XBSM

Example 2 : BSM and XBSM – 18th LS

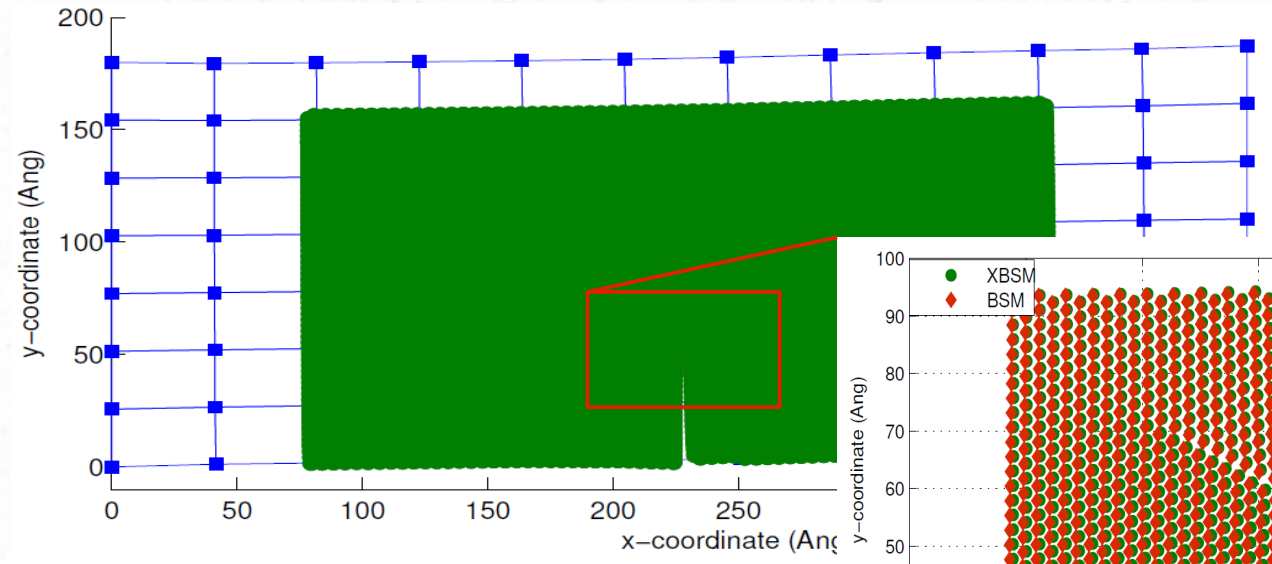


BSM

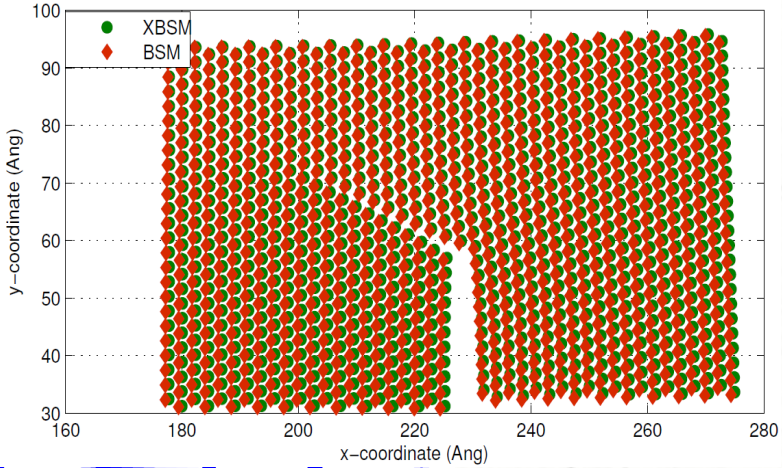


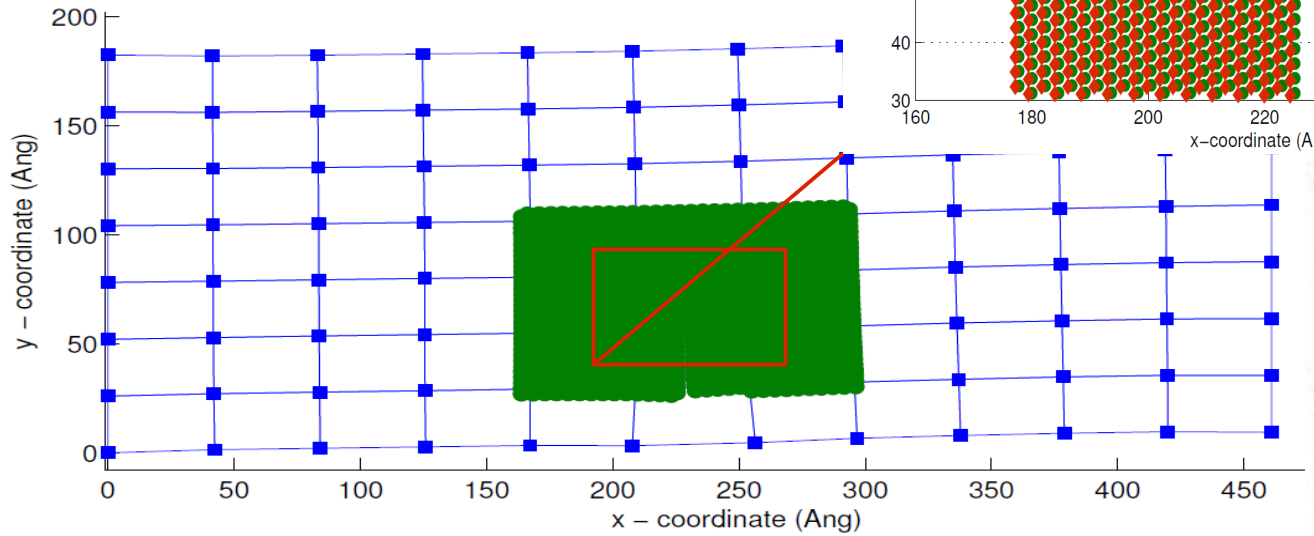
XBSM

Example 2 : BSM and XBSM – 18th LS



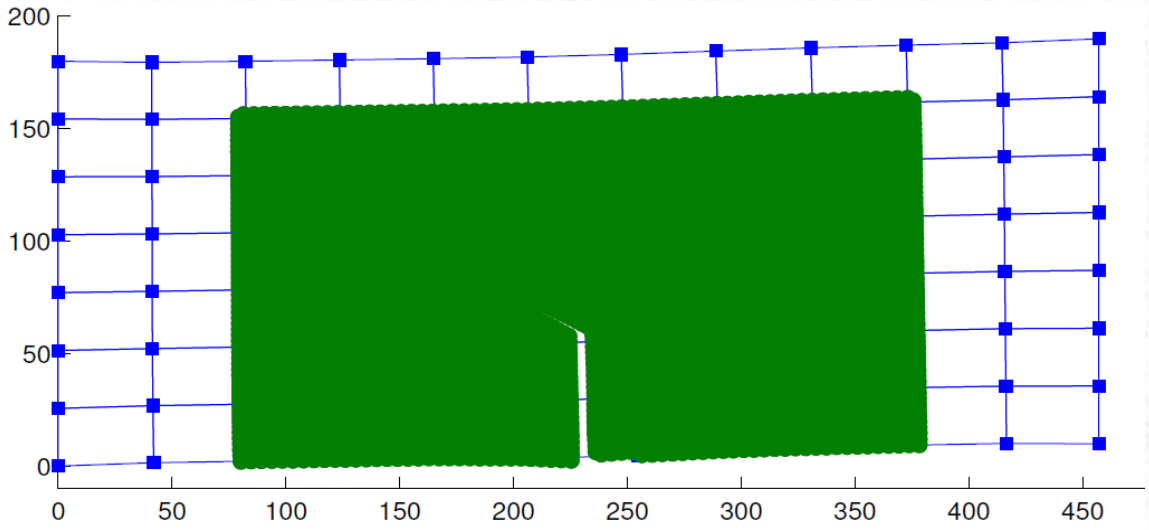
BSM



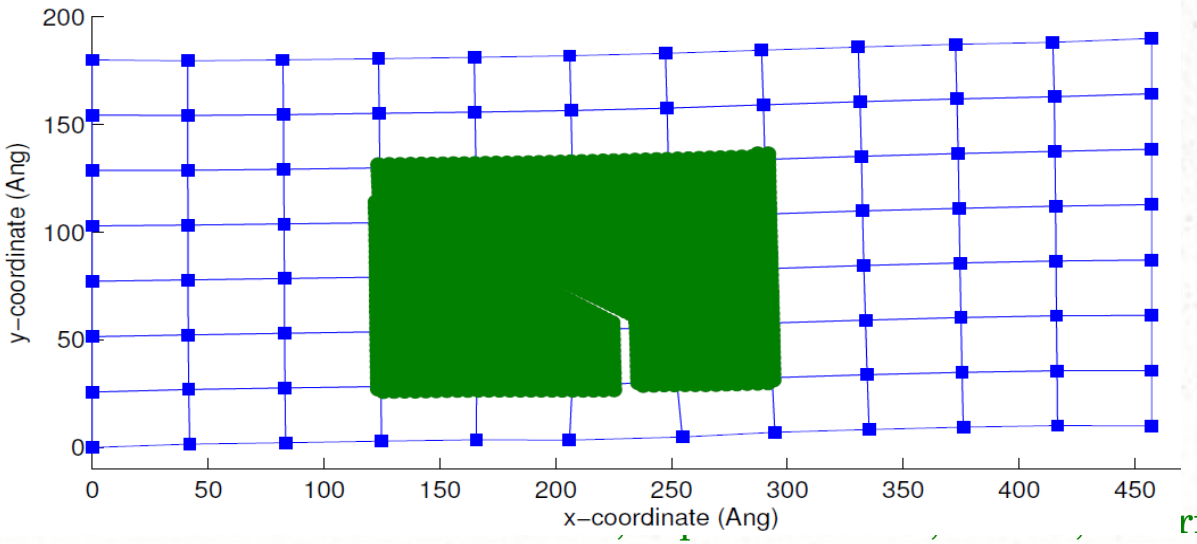


XBSM

Example 2 : BSM and XBSM – 24th LS



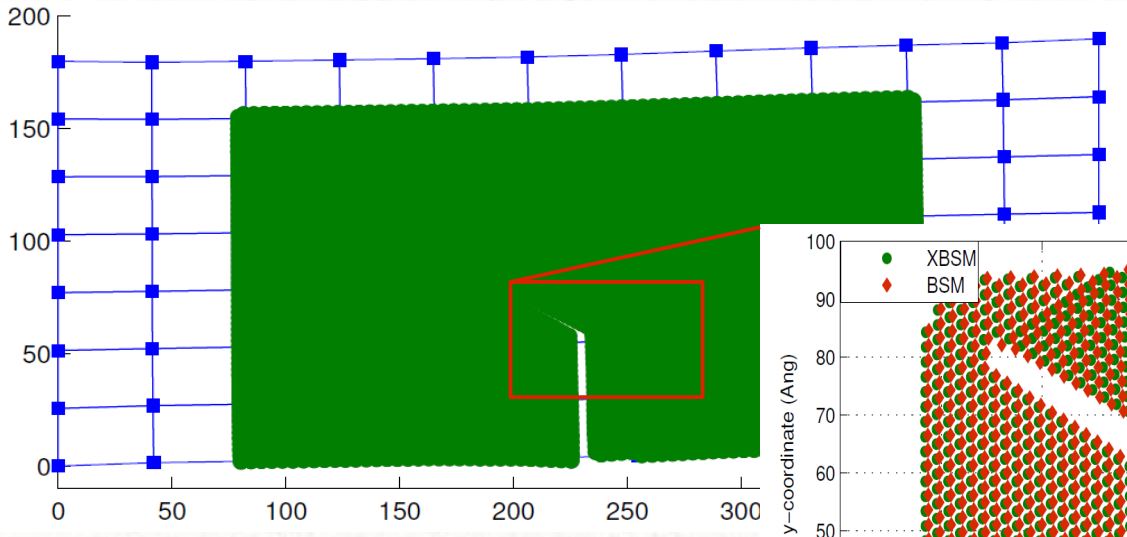
BSM



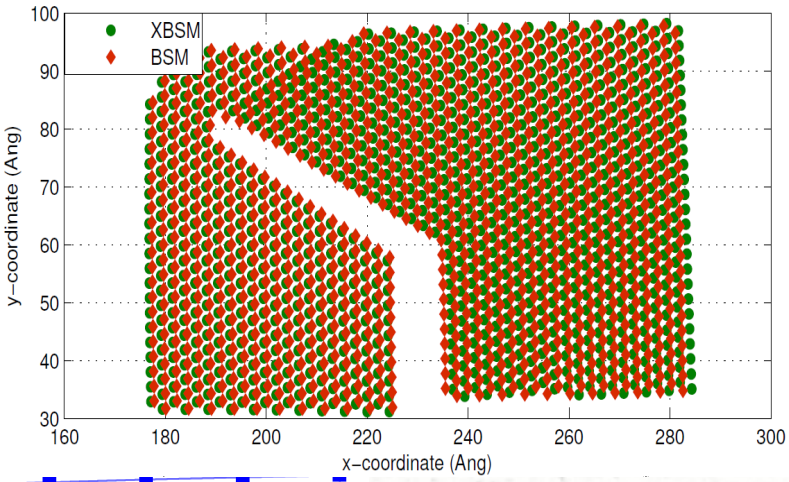
XBSM

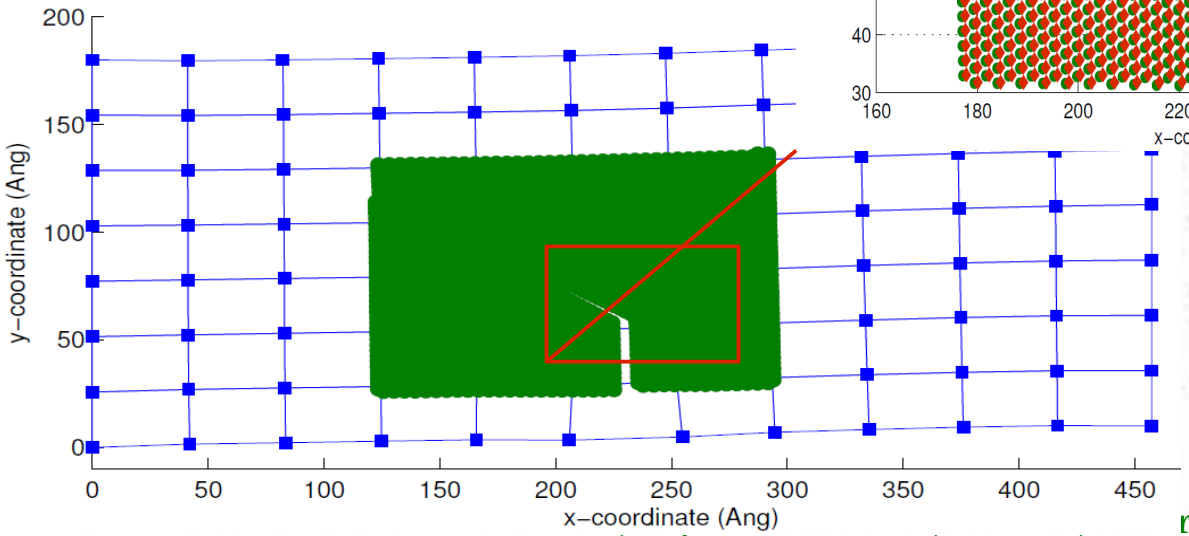
ria

Example 2 : BSM and XBSM – 24th LS



BSM

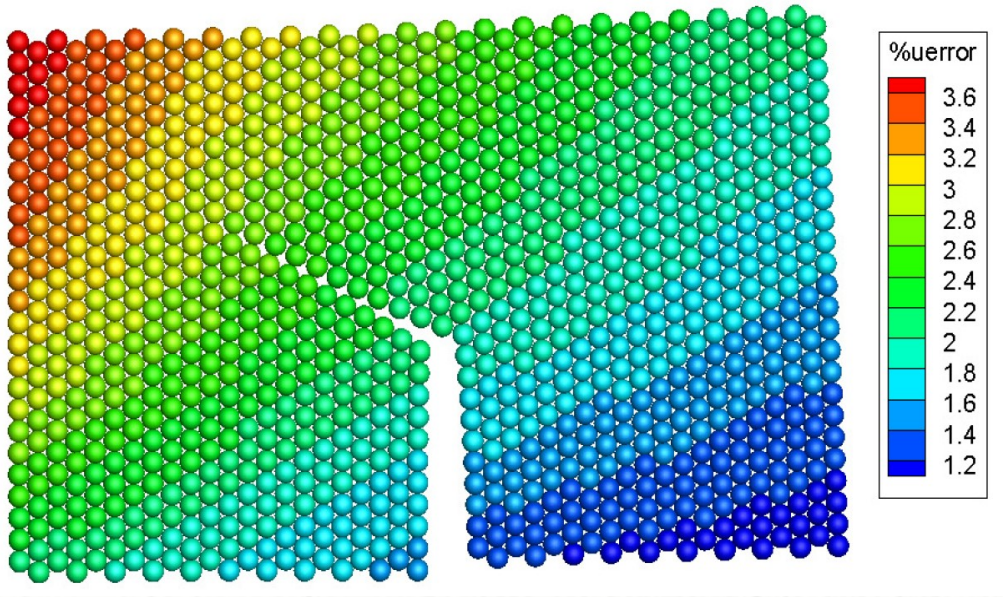




XBSM

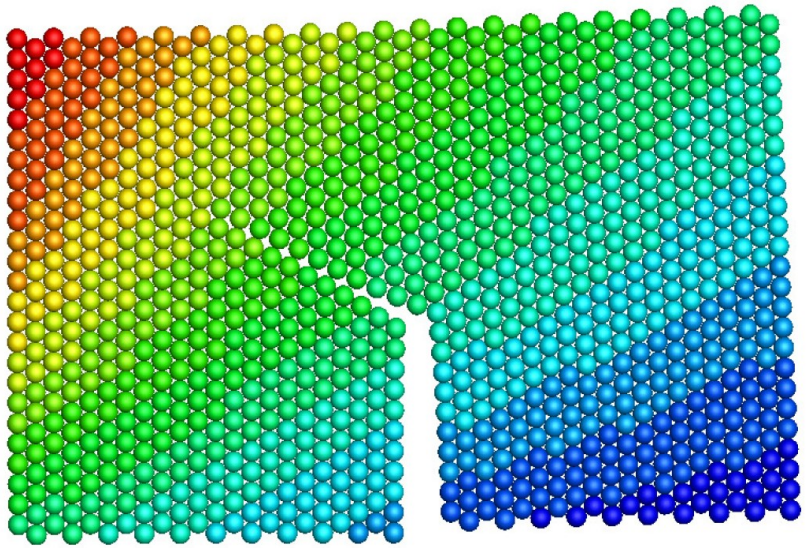
ria

Example 2 : Comparison – 18th & 24th LS

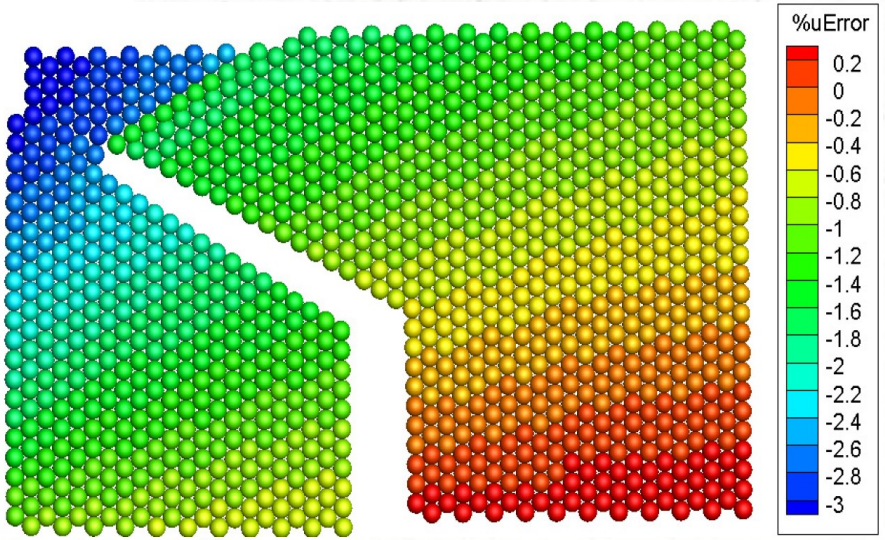


18th LS

Example 2 : Comparison – 18th & 24th LS



18th LS



24th LS

Conclusions and future work

- MS model with crack propagation
- VAC based coarse scale model
- Coupled XBSM model
- Validated through two examples

- Apply XBSM for coupled field problems
- Piezo-electric materials
- Three dimensional models

Collaboration

- Timon Rabczuk
- Robert Gracie
- Stephane Bordas

Thank you for your attention