



# A Continuum-to-Atomistic Bridging Domain Method for Composite Lattices

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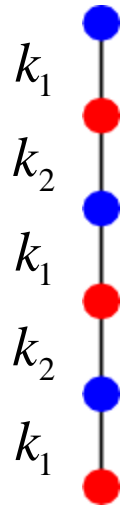
- Motivation
  - Composite lattices
  - Problem with the standard BDM
- Relaxed bridging domain method
- Numerical examples
  - Diatomic chain
  - Graphene lattice
- Conclusions

# Motivation

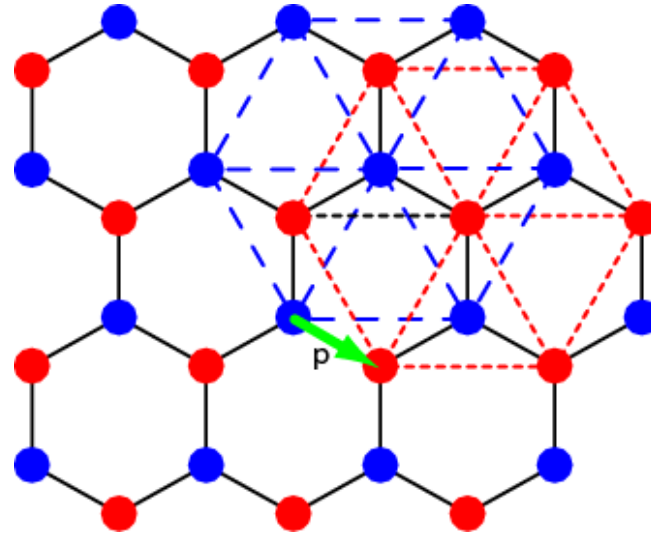


- primary atom
- secondary atom

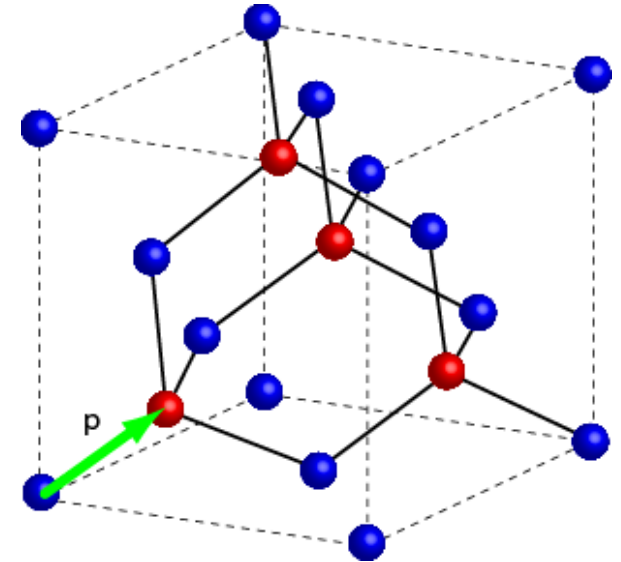
- Composite Lattices



Diatomic chain



Graphene



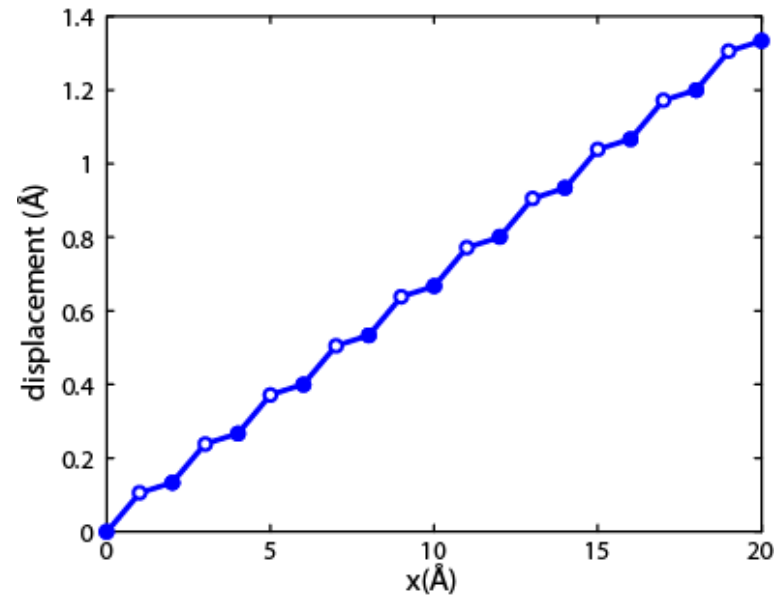
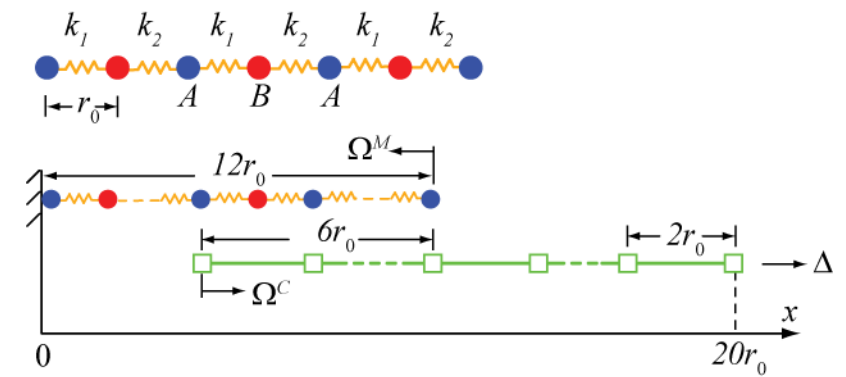
Diamond

Under homogeneous deformation, each sub-lattice undergoes a homogeneous deformation, but the two sub-lattices can move relative to each other. The **relative motions** are usually called the **internal modes**.

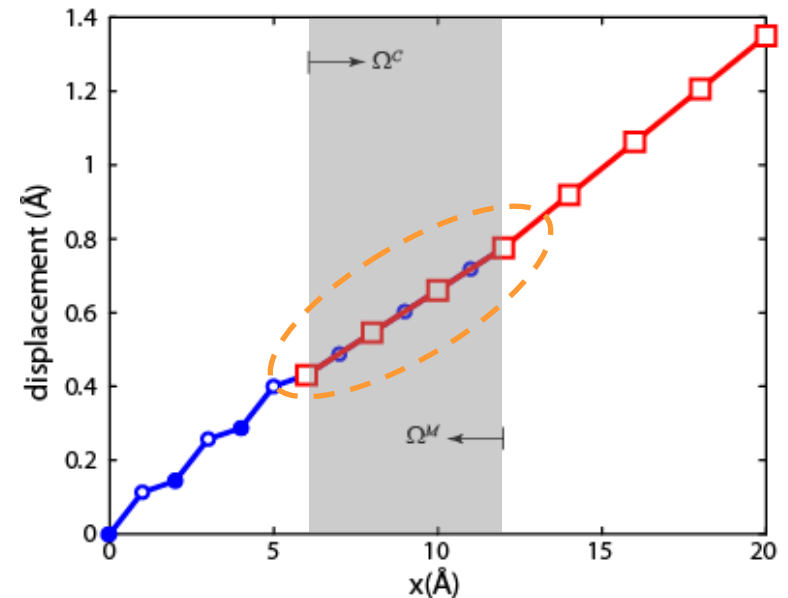
# Motivation



- The standard bridging domain method does not allow internal modes relaxation in the coupling domain



Results with fully MM simulation



Results with the standard BDM

# Relaxed Bridging Domain Method



- Formulation

$$W = W^C + W^M - W^{\text{ext}} + G$$

$$W^C = \int_{\Omega_0^C} (1 - \alpha(\mathbf{X})) \beta w^C d\Omega$$

↑ Continuum strain energy

$$W^M = \frac{1}{2} \sum_{I, J \in \mathcal{M}} \alpha_{IJ} w_{IJ}^M(\mathbf{X}_I, \mathbf{X}_J)$$

↑ Atomistic potential energy

$$W^{\text{ext}} = \sum_{i=1}^{ND} \left( \int_{\Omega_0^C} u_i b_i d\Omega + \int_{\Gamma_i^C} u_i \bar{t}_i d\Gamma + \sum_{I \in \mathcal{M}} d_{iI} f_{iI}^{\text{ext}} \right)$$

↑ External work

$$G = \sum_{i=1}^{ND} \sum_{I \in \mathcal{M}^{cp}} \lambda_i(\mathbf{X}_I) (u_i(\mathbf{X}_I) - d_{iI})$$

↑ Constraints ( $L^2$  coupling)

$\mathcal{M}^c$  → standard BDM

- ◆ Energy decomposition with complementary weight functions  $\alpha$

$\beta$  : Energy scaling factor

$\alpha_{IJ}$  : weight of bond  $I$ - $J$

$w^C$  : strain energy density

$w_{IJ}^M$  : atomistic energy density

$\mathbf{b}$  : body force      $\bar{\mathbf{t}}$  : traction BC

$\mathbf{u}$  : continuum displacement field

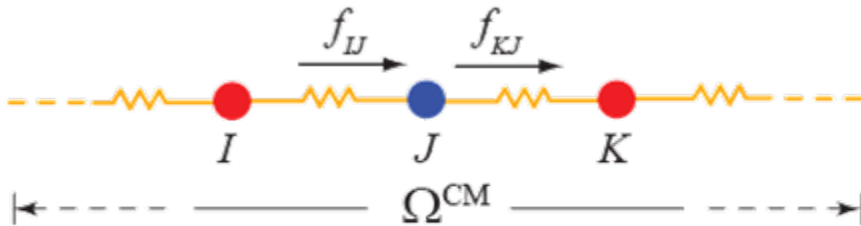
$\mathbf{d}$  : atom displacement

- ◆ Group the atoms into primary and secondary atoms and **only constrain the displacements of the primary atoms** that are in the overlapping domain

# Relaxed Bridging Domain Method



- Bond weights



● primary atom    ● secondary atom

Bond weight is determined by the weight of the secondary atom of the bond

Only applicable on the bonds connecting the primary and secondary atoms. For non-nearest neighbor interactions, a difference weighting scheme is required.

Standard BDM  $\alpha_{IJ} = \frac{\alpha(X_I) + \alpha(X_J)}{2}$

Equilibrium of  $J$

$$\alpha_{JK} f_{KJ} + \alpha_{IJ} f_{IJ} = \frac{\alpha(X_K) - \alpha(X_I)}{2} f_{IJ} \neq 0$$

does not satisfy equilibrium

Relaxed BDM

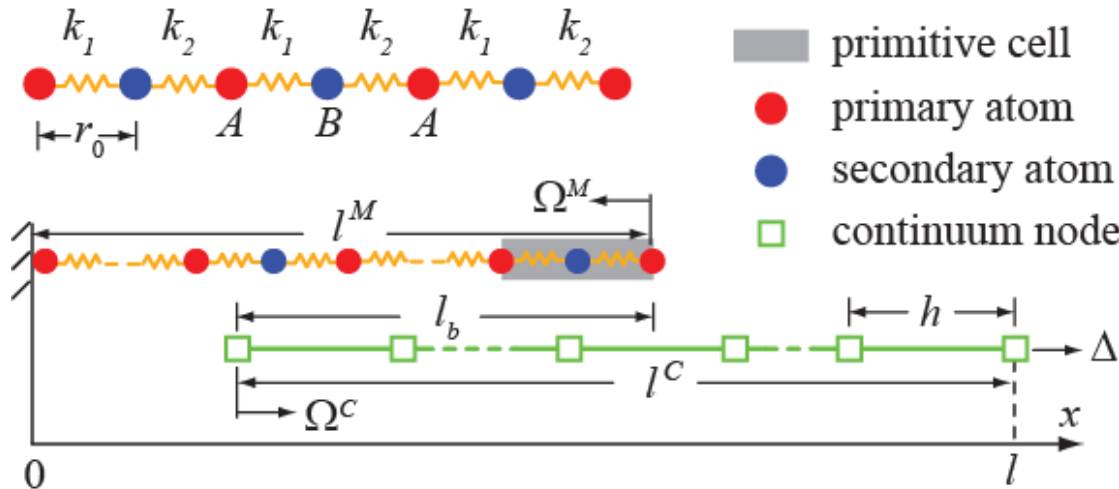
$$\alpha_{IJ} = \begin{cases} \alpha_I & \text{if } I \in \mathcal{M}^s \\ \alpha_J & \text{if } J \in \mathcal{M}^s \end{cases}$$

Equilibrium of  $J$

$$\alpha_{JK} f_{KJ} + \alpha_{IJ} f_{IJ} = \frac{\alpha(X_J) - \alpha(X_J)}{2} f_{IJ} = 0$$

satisfy equilibrium

# Numerical Examples – 1D



$r_0$ : lattice constant

$l^M$ : length of atomistic model

$l_b$ : bridging domain length

$h$ : element size

$l^C$ : length of continuum model

$l$ : length of the entire model

Harmonic potential with nearest neighbor interaction

Exact solution 
$$u^{\text{ex}}(X_I) = \begin{cases} \Delta X_I / l & I \in \mathcal{M}^s \\ [k_2 u(X_{I+1}) - k_1 u(X_I)] / (k_1 + k_2) & \text{otherwise} \end{cases}$$

Error in displacements

Displacement error norm

Error in energy

$$e_u(X_I) = \frac{u(X_I) - u^{\text{ex}}(X_I)}{u^{\text{ex}}(X_I)}$$

$$e_{L^2} = \frac{\sqrt{\sum_{I \in \mathcal{M}} (u_I - u_I^{\text{ex}})^2}}{\sqrt{\sum_{I \in \mathcal{M}} (u_I^{\text{ex}})^2}}$$

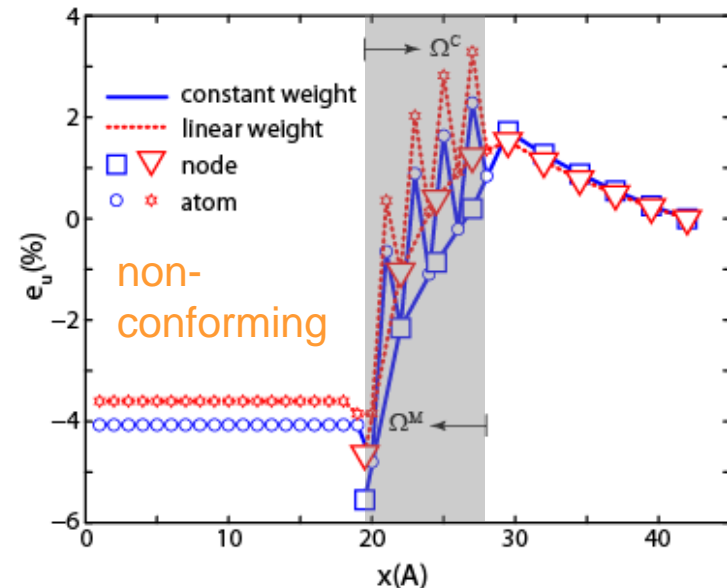
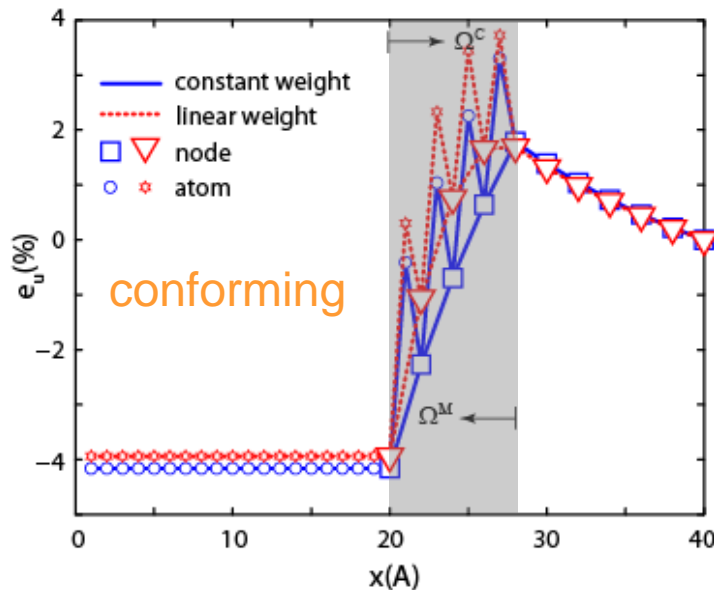
$$e_w = \frac{|\Delta W - \Delta W^{\text{ex}}|}{|\Delta W^{\text{ex}}|}$$

# Numerical Examples – 1D



**Conforming model** – nodes coincide with primary atoms and the element size is an integer multiple of the size of the primitive cell

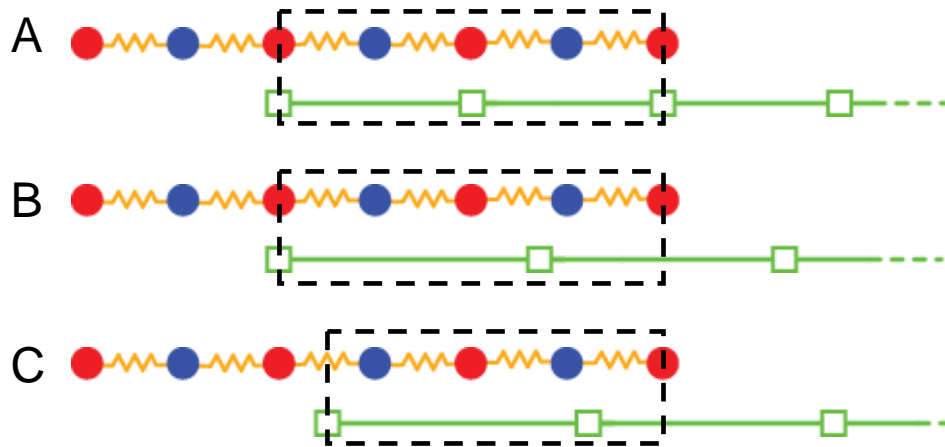
**Non-conforming model** – nodes do not coincide with primary atoms



Results with the standard bridging domain method

The constraints in standard BDM enforce a homogeneous displacement field within each element, which suppresses the internal modes of the lattice.

# Numerical Examples – 1D



Conforming model

Non-conforming model (an element is partially in  $\Omega^{CM}$ )

Non-conforming model (arbitrary)

Model	Constant weight		Linear weight	
	$e_{L^2}$ (%)	$e_W$ (%)	$e_{L^2}$ (%)	$e_W$ (%)
A	3.81 (S)	5.25 (S)	3.96 (S)	3.95 (S)
	$9.40 \times 10^{-14}$ (R)	$2.05 \times 10^{-13}$ (R)	$3.64 \times 10^{-13}$ (R)	$2.46 \times 10^{-13}$ (R)
B	3.35 (S)	3.86 (S)	3.98 (S)	3.00 (S)
	$1.93 \times 10^{-13}$ (R)	$4.97 \times 10^{-13}$ (R)	0.19 (R)	$7.84 \times 10^{-3}$ (R)
C	3.51 (S)	6.11 (S)	3.66 (S)	5.35 (S)
	0.47 (R)	0.16 (R)	0.19 (R)	0.11 (R)

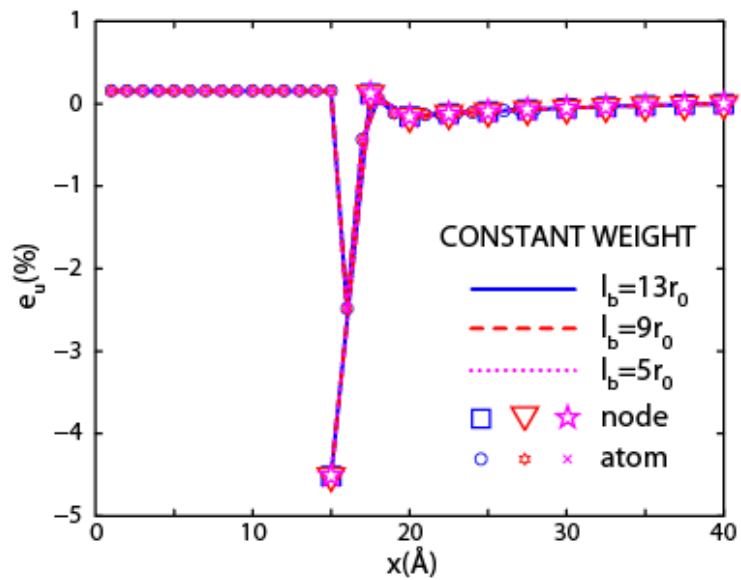
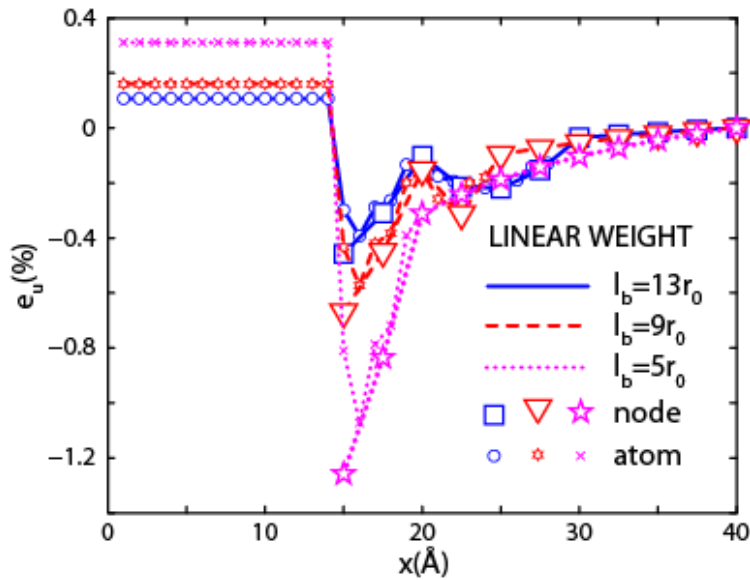
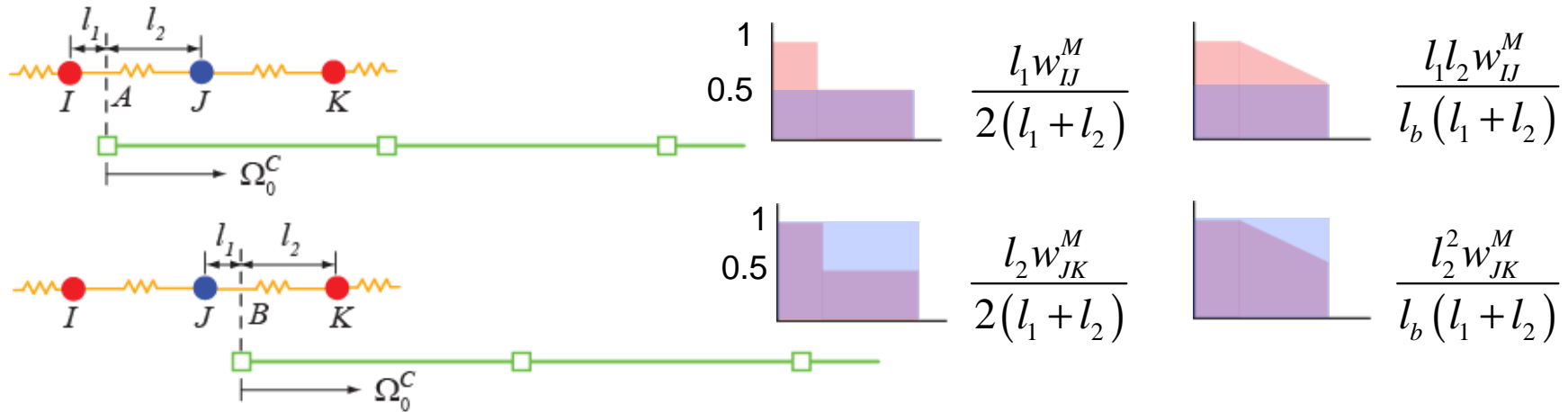
Results with the relaxed bridging domain method

The relaxed constraints allow the **internal modes relaxation**.

# Numerical Examples – 1D



- Weight function



$e_{L^2}$  0.31%  $\rightarrow$  0.16%  $\rightarrow$  0.11%  
 $5r_0$   $9r_0$   $13r_0$

0.16%

# Numerical Examples – 1D



- Lagrange multipliers  $\lambda_i(\mathbf{X}_I) = \sum_{J \in \mathcal{S}^\lambda} N_J^\lambda(\mathbf{X}_I) \lambda_{iJ}$

Diagonal Lagrange multiplier method



$$\frac{\partial W}{\partial \lambda_{iI}} = \sum_{J \in \mathcal{S}} \delta_{IK} N_J(X_K) u_{iJ} - \delta_{IK} d_{iK}$$

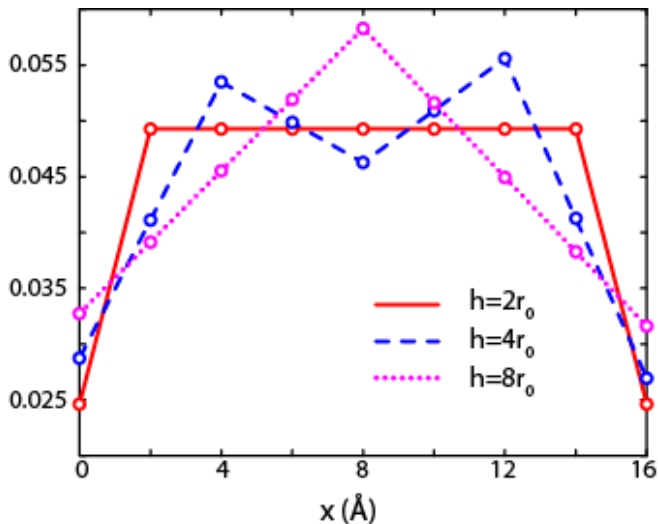
diagonal matrix

Non-diagonal Lagrange multiplier method



$$\frac{\partial W}{\partial \lambda_{iI}} = \sum_{J \in \mathcal{S}, K \in \mathcal{M}^{cp}} N_I^\lambda(X_K) N_J(X_K) u_{iJ} - \sum_{K \in \mathcal{M}^{cp}} N_I^\lambda(X_K) d_{iK}$$

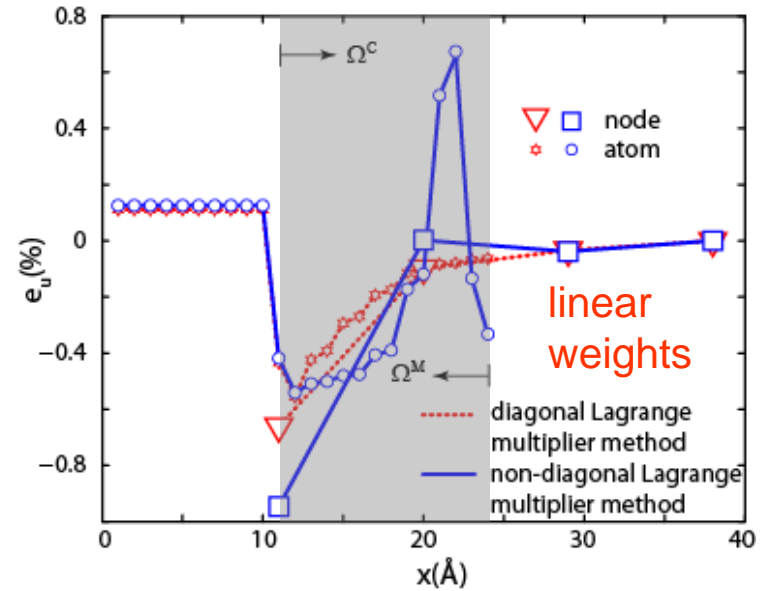
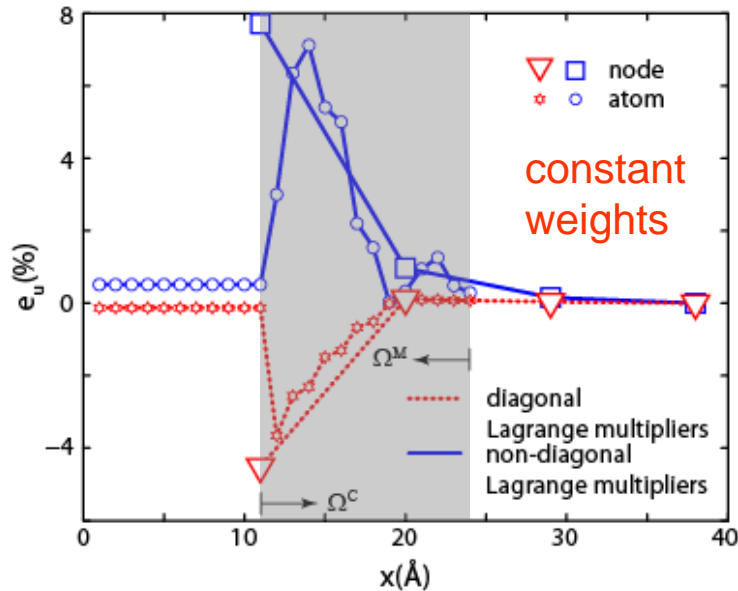
non-diagonal matrix



	Constant Weights		Linear Weights	
	$e_{L^2}$ (%)	$e_W$ (%)	$e_{L^2}$ (%)	$e_W$ (%)
$2r_0$	$1.77 \times 10^{-13}$	$7.68 \times 10^{-14}$	$1.38 \times 10^{-13}$	$5.38 \times 10^{-13}$
$4r_0$	0.76	0.29	0.25	0.01
$8r_0$	2.49	0.99	0.79	0.04

Results of three conforming models with the relaxed BDM

# Numerical Examples – 1D



Results of a non-conforming coupling model

Diagonal Lagrange multiplier method is more accurate

For non-diagonal multiplier method, the error decreases with the element size

# Numerical Examples – 2D



- Graphene sheet coupled with linear triangular finite elements
- Modified Tersoff-Brenner potential is used for interatomic potential

Error in energy of the standard BDM

$$e_w^S = \frac{|\Delta W^S - \Delta W|}{|\Delta W|}$$

Error in energy of the relaxed BDM

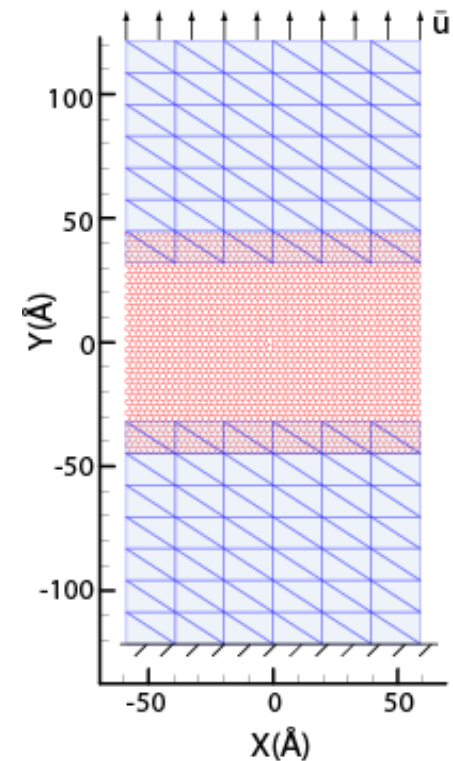
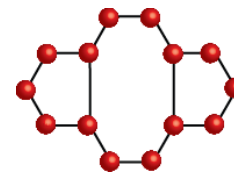
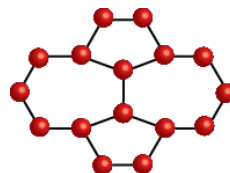
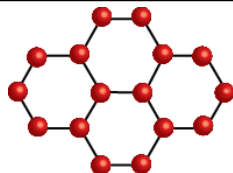
$$e_w^R = \frac{|\Delta W^R - \Delta W|}{|\Delta W|}$$

Model A :  
one-layer  
overlap

	Perfect Lattice	with Stone-Wales defect	with Double-vacancy defect
$e_w^S$	$6.50 \times 10^{-3}$	$6.58 \times 10^{-3}$	$6.67 \times 10^{-3}$
$e_w^R$	$2.77 \times 10^{-4}$	$3.78 \times 10^{-4}$	$4.19 \times 10^{-4}$

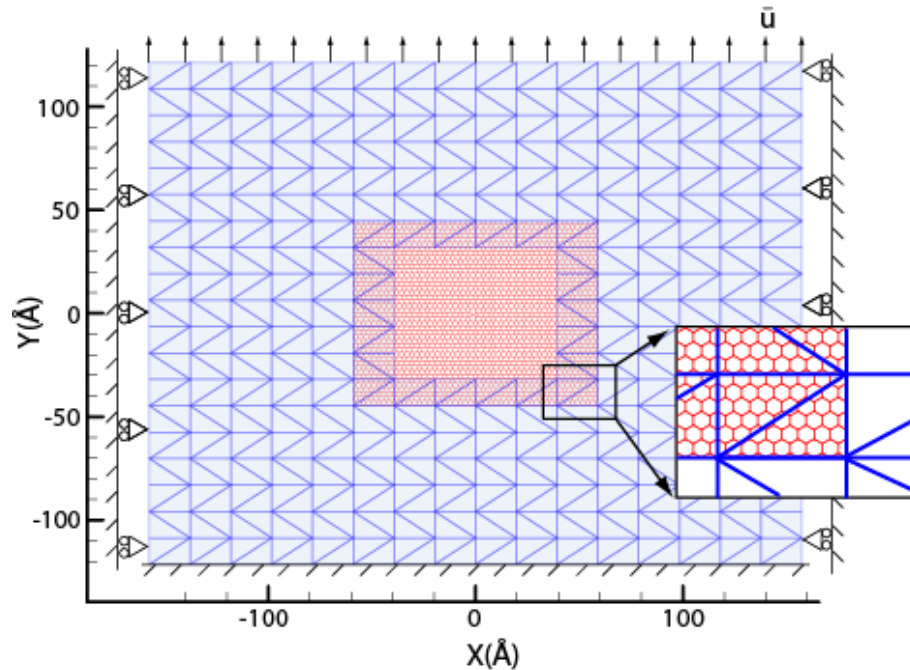
Model B :  
two-layer  
overlap

	Perfect Lattice	with Stone-Wales defect	with Double-vacancy defect
$e_w^S$	$4.41 \times 10^{-3}$	$4.29 \times 10^{-3}$	$1.55 \times 10^{-2}$
$e_w^R$	$8.84 \times 10^{-4}$	$7.29 \times 10^{-4}$	$1.29 \times 10^{-3}$



2D serial bridging domain model

# Numerical Examples – 2D



2D parallel bridging domain model

Energy scaling factor is used to match the atomistic and continuum energy. The factor is parameter dependent. In the two-dimensional examples  $\beta=0.05$  gives the best results.

For serial model, increasing overlapping domain size doesn't increase the accuracy of the results

The accuracy of the relaxed BDM is often an order of magnitude more accurate than the standard BDM

	Perfect Lattice	with Stone-Wales defect	with Double-vacancy defect
$e_W^S$	$8.70 \times 10^{-4}$	$4.68 \times 10^{-3}$	$7.53 \times 10^{-4}$
$e_W^R$	$2.09 \times 10^{-4}$	$1.14 \times 10^{-4}$	$5.47 \times 10^{-4}$

# Conclusions

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- The relaxed bridging domain method is an extended version of the standard bridging domain method
  - Only primary atoms in the overlapping domain are constrained by the Lagrange multiplier
  - Bond weights are determined by the weights of the secondary atoms of the bonds
- The relaxed bridging domain method allows the internal modes relaxation
  - The improvement is obvious; the energy error is an order of magnitude smaller in one-dimensional examples
  - The energy error is almost an order of magnitude smaller than the results from the standard BDM
- We recommend the diagonal Lagrange multiplier method be used with linear weight functions for one- and two-dimensional studies.