Boundary conditions for molecular dynamics

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joint work with

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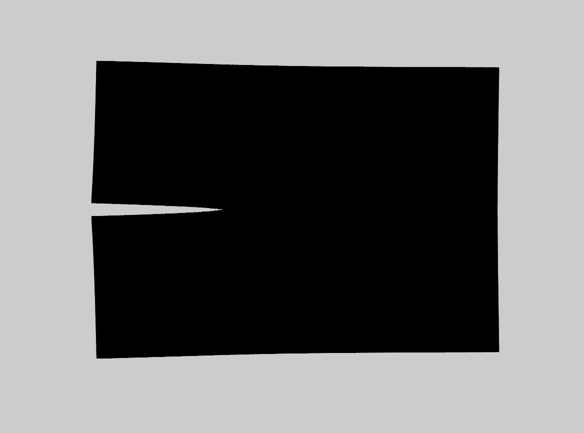
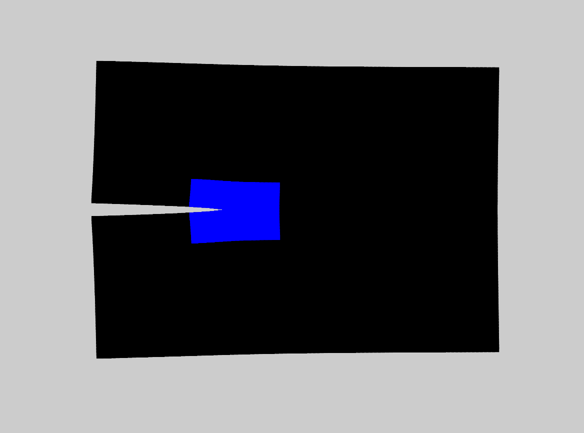
Motivation



Dynamics of cracks

Motivation



Dynamics of cracks

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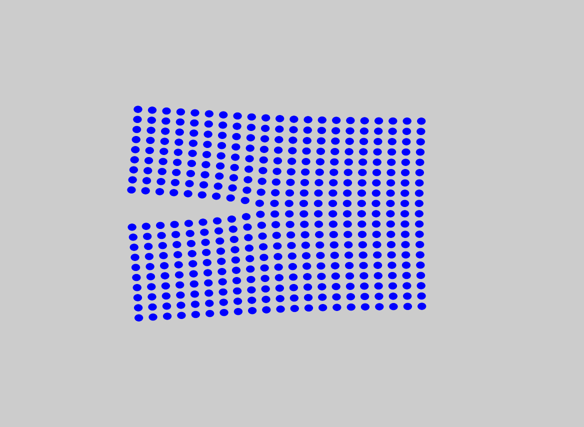
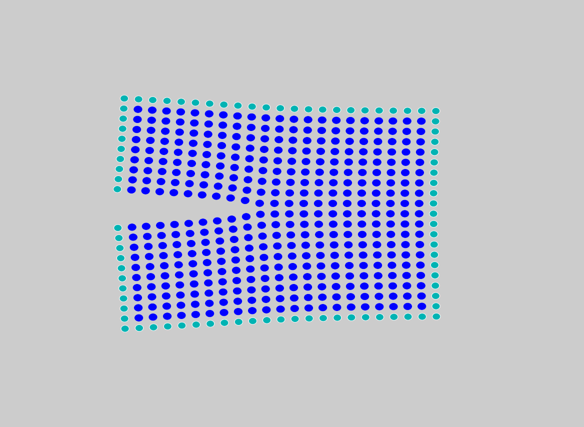


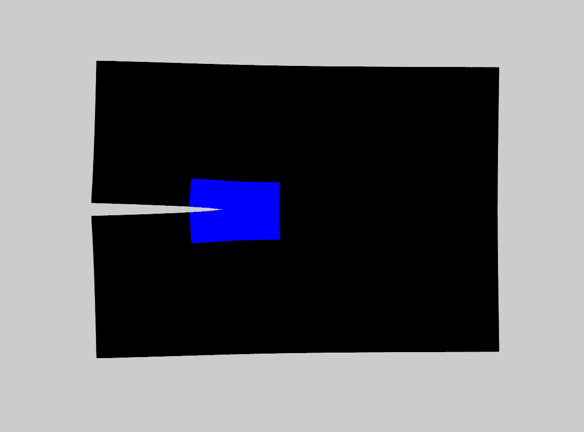
Atomistic study $m\ddot{x}_j = -\frac{\partial V}{\partial x_j}$

Motivation



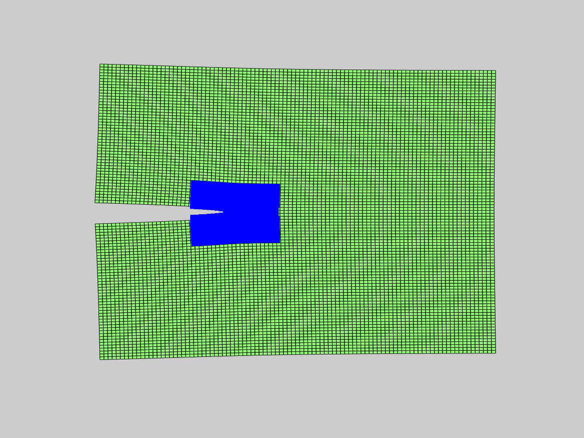
Boundary condition

Motivation



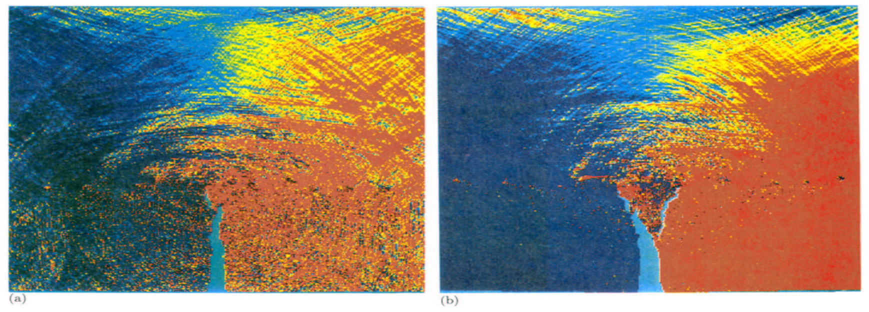
Hybrid model

Motivation



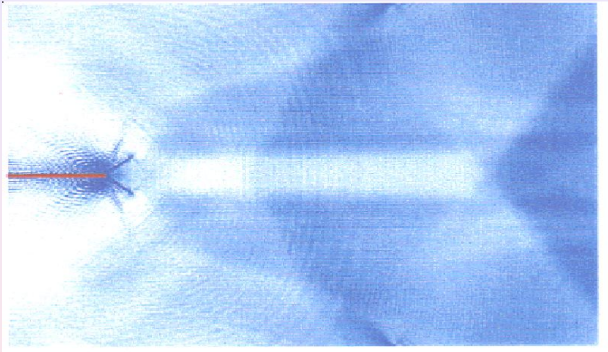
Hybrid model

Boundary effects



Fracture simulation in triangular lattice (Holian et. al. 1996)

Boundary effects



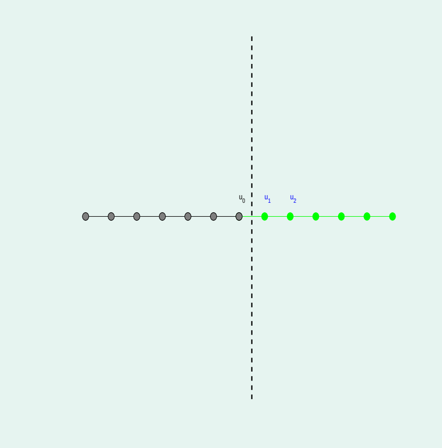
Fracture simulation in BCC iron (Machova and Ackland 1998)

Outline

- Exact boundary conditions
- Phonon reflection
- Variational formulation
- Examples
- Applications to fracture simulation
- Further issues

Exact BC: a 1D example

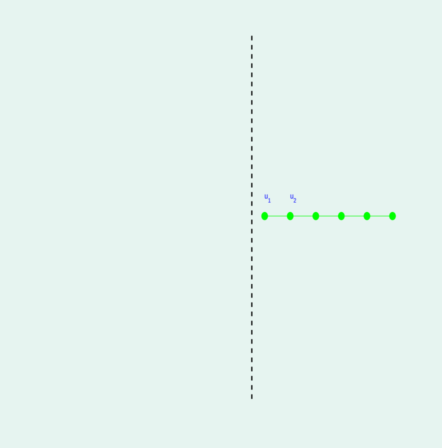
$$\ddot{u}_j = u_{j+1} - 2u_j + u_{j-1}.$$



Boundary condition

Exact BC: a 1D example

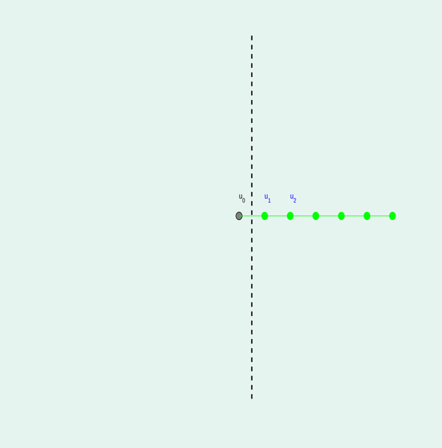
$$\ddot{u}_j = u_{j+1} - 2u_j + u_{j-1}, j > 0.$$



Boundary condition

Exact BC: a 1D example

$$\ddot{u}_j = u_{j+1} - 2u_j + u_{j-1}, j > 0$$
$$u_0(t) \text{ given.}$$



Boundary condition

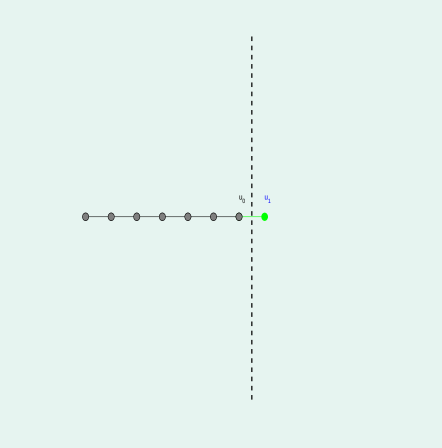
Exact BC: a 1D example

$$\begin{cases} \ddot{u}_j = u_{j+1} - 2u_j + u_{j-1}, & j \le 0 \\ u_j(0) = 0, \quad v_j(0) = 0, & j \le 0 \\ u_1(t) \text{ given.} & \end{cases}$$

Exact B.C. (Adelman and Doll, JChP 1974) :

$$u_j(t) = \int_0^t \beta_j(t-s) u_1(s) ds, j \le 0$$

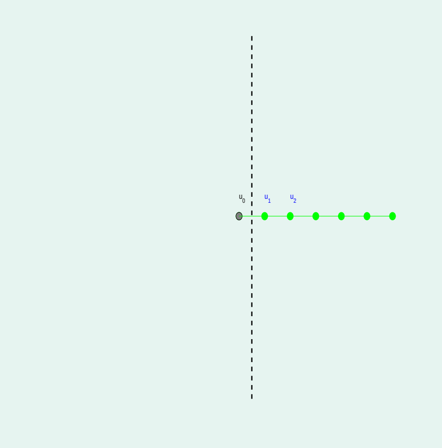
$$\beta_0 = \frac{J_2(2t)}{t}$$



Boundary condition

Exact BC: a 1D example

$$\begin{cases} \ddot{u}_j = u_{j+1} - 2u_j + u_{j-1}, & j > 0 \\ u_0(t) = \int_0^t \beta_0(s) u_1(t-s) ds. \end{cases}$$



Boundary condition

Exact B.C.: 3D lattice

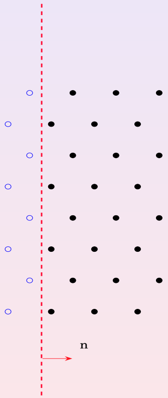
General exact boundary conditions:

$$\mathbf{u}_{0,j,k}(t) = \sum_m \sum_n \int_0^t \boldsymbol{\theta}_{l,j-m,k-n}(t-\tau)\mathbf{u}_{l,m,n}(\tau)d\tau.$$

Numerical approximations:

1. Laplace/Fourier transform:
   (Wagner, Karpov, Liu, Park et al 2004, 2005)
2. test simulations (Cai, de Koning, Bulatov and Yip 2000)

Exact B.C.: 3D lattice



boundary condition for molecular dynamics

Exact B.C.: a 1D example

Exact B.C. :

$$u_0(t) = \int_0^t \theta_j(t-s)u_j(s)ds, j \leq 0$$

$$\tilde{\theta}_j = \tilde{\theta}_1^j = \tilde{\theta}^j.$$

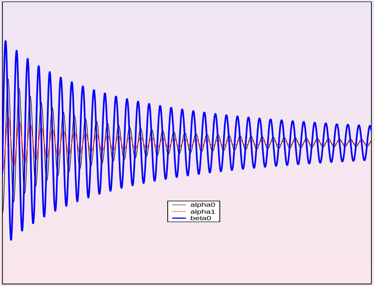
$$\theta_1(t) = \beta_0(t) = \frac{J_2(2t)}{t}.$$

$\theta_j(t)$ delays like $t^{-3/2}$,

Exact B.C.: enhance the decay rate

$$u_0 = \sum_{j=1}^{J} \int_0^t \alpha_j(t-s) u_j(s) ds$$

$$\alpha(t) \sim \frac{C}{t^{J+1/2}}, t \to +\infty.$$



J=2

Exact B.C.: enhance the decay rate

$$u_0 = \sum_{j=1}^{J} \int_0^t \alpha_j(t-s) u_j(s) ds$$

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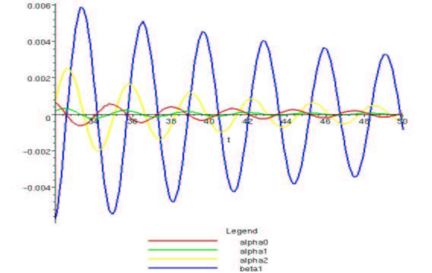

J=3

Implementation issue

Problem with exact boundary conditions:

- difficult to obtain
- **nonlocal** in both space and time
- not practical in MD simulations
- premature truncation leads to large reflection
- not feasible in a multiscale method

Objectives

- **local** boundary conditions
- given stencil, find the BC with minimal phonon reflection
- external loading

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Analogy with absorbing B.C. for wave equations

Local boundary condition for wave equations:
(Engquist and Majda 1977 and 1979)

Local boundary condition for molecular dynamics:
(E and Huang 2001 and 2002)

Phonon spectrum

Harmonic approximation:

$$m_i \ddot{\mathbf{u}}_i = -\sum_j D_{i-j} \mathbf{u}_j.$$

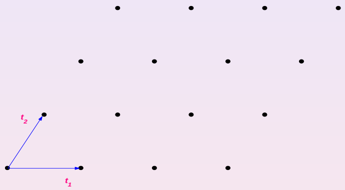
Dynamic matrix

$$\mathcal{D}(\mathbf{k}) = \sum_j D_j e^{-i\mathbf{r}_j \cdot \mathbf{k}},$$

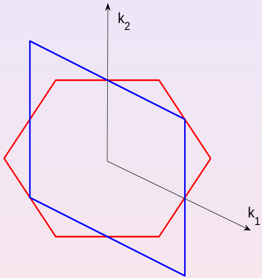
Phonon spectrum

$$\mathcal{D}(\mathbf{k})\varepsilon(\mathbf{k}) = \lambda_s \varepsilon(\mathbf{k}), \omega_s^2 = \lambda_s.$$

Lattice and Brillouin Zone (BZ)

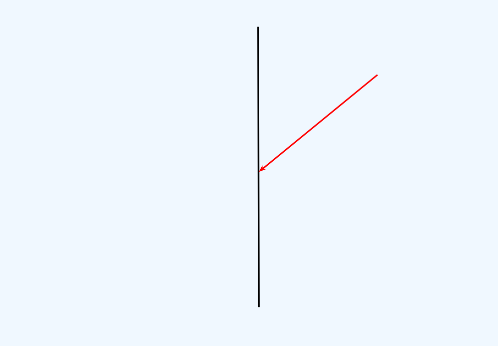


triangular lattice



the first Brillouin zone

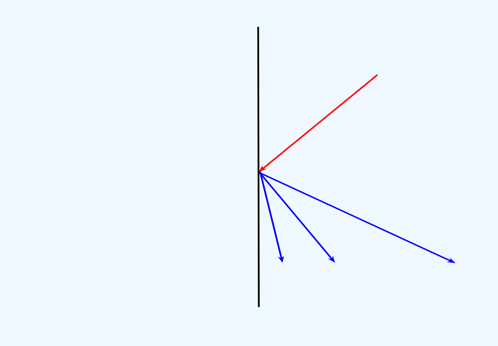
Phonon reflection



$$\mathbf{u}_j = e^{i(\mathbf{r}_j \cdot \mathbf{k}^I - \omega_s t)} \varepsilon_s(\mathbf{k}^I)$$

Reflection of phonon

Phonon reflection

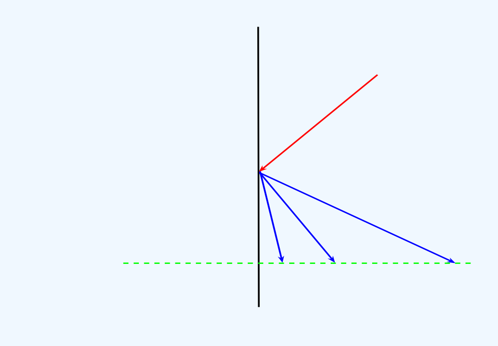


$$\mathbf{u}_j = e^{i(\mathbf{r}_j\cdot\mathbf{k}^I - \omega_s t)}\varepsilon_s(\mathbf{k}^I)$$

$$+e^{i(\mathbf{r}_j\cdot\mathbf{k}^R - \omega_s'(\mathbf{k}^R)t)}\varepsilon_s'(\mathbf{k}^R)$$

Reflection of phonon

Phonon reflection



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$$+e^{i(\mathbf{r}_j\cdot\mathbf{k}^R - \omega_s'(\mathbf{k}^R)t)}\varepsilon_s'(\mathbf{k}^R)$$

Reflection of phonon

Phonon reflection

$$\begin{array}{rcl} \mathbf{k}^I - (\mathbf{k}^I \cdot \mathbf{n})\,\mathbf{n} & = & k^R - (\mathbf{k}^R \cdot \mathbf{n})\,\mathbf{n} \\ \omega_s(\mathbf{k}^I) & = & \omega_{s'}(\mathbf{k}^R). \end{array}$$

Let $\lambda = e^{-i(\mathbf{k}^R \cdot \mathbf{n})a_n}$

$$\det\Big(\mathcal{D}(\mathbf{k}^R) - \omega(\mathbf{k}^I)^2 I\Big) = 0,$$

Wave mode of the reflected phonons:

$$\{\mathbf{k}^R_{ss'_l}, l = 1, 2, \cdots, S \times N_e\}.$$

Phonon reflection: *reflection coefficients*

Boundary condition:

$$\mathbf{u_0}(t) = \sum_{j \in J} \int_0^{t_0} \alpha_j(\tau)\mathbf{u}_j(t-\tau)d\tau.$$

Phonon reflection: *reflection coefficients*

Boundary condition:

$$\mathbf{u_0}(t) = \sum_{j \in J} \int_0^{t_0} \alpha_j(\tau)\mathbf{u}_j(t-\tau)d\tau.$$

Incident and reflected waves:

$$\mathbf{u}_j(t) = c_s^I e^{i(\mathbf{r}_j \cdot \mathbf{k} - \omega_s t)} \varepsilon_s(\mathbf{k})$$

Phonon reflection: *reflection coefficients*

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$$\mathbf{u_0}(t) = \sum_{j \in J} \int_0^{t_0} \alpha_j(\tau) \mathbf{u}_j(t-\tau) d\tau.$$

Incident and reflected waves:

$$\begin{aligned} \mathbf{u}_j(t) &= c_s^I e^{i(\mathbf{r}_j \cdot \mathbf{k} - \omega_s t)} \varepsilon_s(\mathbf{k}) \\ &+ \sum_l c_{ss_l'}^R e^{i(\mathbf{r}_j \cdot \mathbf{k}_{ss_l'}^R - \omega_{s'} t)} \varepsilon_{s_l'}(\mathbf{k}_{ss_l'}^R), \quad \mathbf{c}^R = R\mathbf{c}^I \end{aligned}$$

Phonon reflection: *reflection coefficients*

Boundary condition:

$$\mathbf{u_0}(t) = \sum_{j\in J} \int_0^{t_0} \boldsymbol{\alpha}_j(\tau)\mathbf{u}_j(t-\tau)d\tau.$$

Incident and reflected waves:

$$\mathbf{u}_j(t) = c_s^I e^{i(\mathbf{r}_j\cdot\mathbf{k}-\omega_s t)}\varepsilon_s(\mathbf{k})$$

$$+ \sum_l c^R_{ss'_l} e^{i(\mathbf{r}_j\cdot\mathbf{k}^R_{ss'_l}-\omega_{s'} t)}\varepsilon_{s'_l}(\mathbf{k}^R_{ss'_l}), \quad \mathbf{c}^R = R\mathbf{c}^I$$

$$\mathcal{A}(\mathbf{k}) = \sum_{j\in J} e^{i\mathbf{r}_j\cdot\mathbf{k}} \int_0^{t_0} e^{i\omega\tau}\boldsymbol{\alpha}_j(\tau)d\tau,$$

Linear system:

$$(I-\mathcal{A}(\mathbf{k}))\varepsilon_s(\mathbf{k}) + \sum_l R_{ss'_l}(I-\mathcal{A}(\mathbf{k}^R_{ss'_l}))\varepsilon_{s'_l} = 0.$$

Variational formulation: energy flux

Energy flux at the atomic scale (Irving & Kirkwood 1950):

$$J = \frac{1}{2}\sum(\dot{\mathbf{u}}_i + \dot{\mathbf{u}}_j)D_{i-j}(\mathbf{u}_i - \mathbf{u}_j)\mathbf{r}_{ij}.$$

Convert to Fourier space:

$$J = J^I + J^R.$$

$$\begin{aligned} J^R &= \frac{1}{2}\sum_l \int |c^R_{ss'_l}|^2 \omega_s \nabla\lambda_s(\mathbf{k}^R_{ss'_l}) d\mathbf{k}^R_{ss'_l}, \\ &= \sum_s \int_{\mathbf{k}\in BZ,\ \mathbf{k}\cdot\mathbf{n}\leq 0} |\sum_l c^I_s R_{ss'_l}|^2 \omega_s^2\ (\nabla\omega_s\cdot\mathbf{n}) d\mathbf{k}. \end{aligned}$$

This is the thermal flux due to the applied boundary condition.

Variational formulation: objective function

Seek boundary condition:

$$\mathbf{u}_0(t) = \sum_{j\in J} \int_0^{t_0} \boldsymbol{\alpha}_j(s)\mathbf{u}_j(t-\tau)d\tau,$$

Variational formulation:

$$\min_{\{\alpha_j\}} I[\{\alpha_j\};\mathbf{n}] \triangleq \sum_s \int_{\mathbf{k}\in BZ,\ \mathbf{k}\cdot\mathbf{n}\le 0} \sum_l |R_{ss'_l}|^2 \,(\nabla\omega_s\cdot\mathbf{n})d\mathbf{k}$$

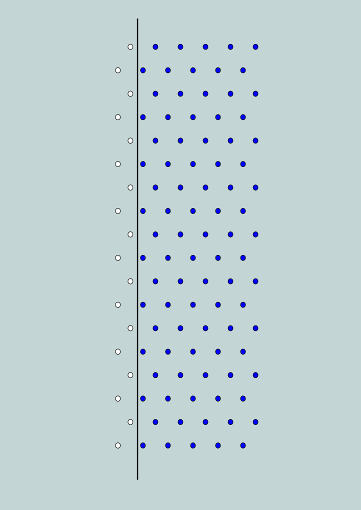
subject to certain constraints.

Variational formulation: constraints

$$R(0) = 0 \Rightarrow \sum_j \int_0^{t_0} \boldsymbol{\alpha}_j(\tau) d\tau = I.$$

$$\sum_j \int_0^{t_0} \boldsymbol{\alpha}_j(\tau) \tau d\tau \; \partial_{\boldsymbol{\xi}} \omega_s(0) \boldsymbol{\varepsilon}_s + \sum_j \int_0^{t_0} \boldsymbol{\alpha}_j(\tau) d\tau \mathbf{r}_j \cdot \boldsymbol{\xi} \boldsymbol{\varepsilon}_s = 0.$$

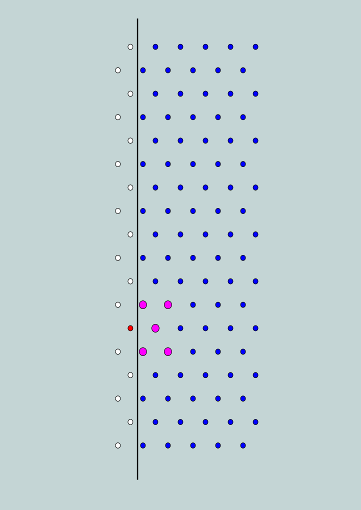
Choosing the stencil



Discrete boundary conditions:

$$\mathbf{u}_i^n = \sum_{\mathbf{r}_j - \mathbf{r}_i \in J} \sum_{m=1}^{M} \alpha_j^m \mathbf{u}_j^{n-m}.$$

Choosing the stencil



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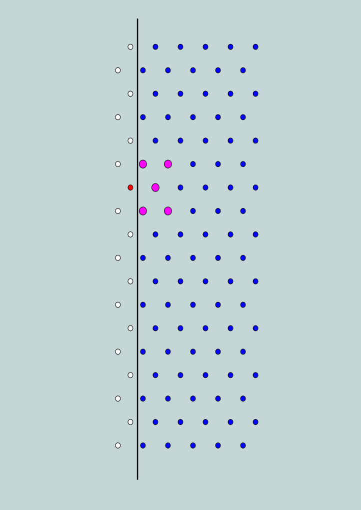

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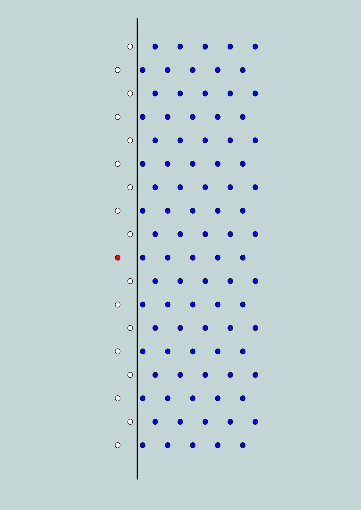

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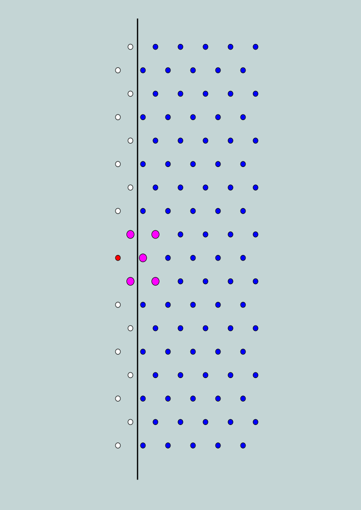

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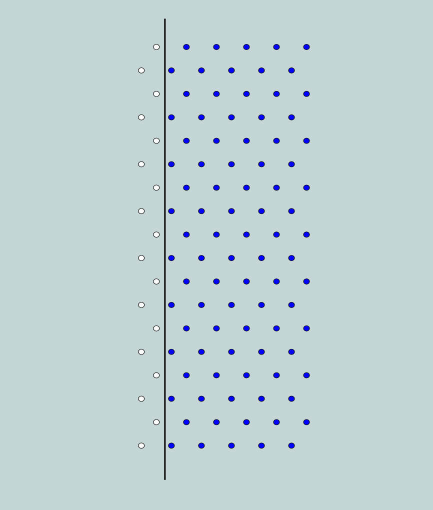
Symmetry properties

$$\tilde{\alpha}_{j'} = P\alpha_j P^T,$$

$$I[\tilde{\alpha}, \mathbf{n}'] = I[\alpha, \mathbf{n}].$$



equivalent planes

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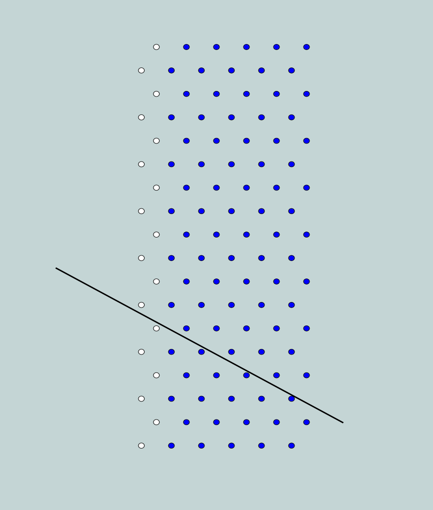


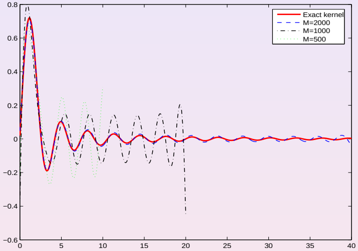
equivalent planes

Numerical procedure

1. Compute the dispersion relation and the polarization vectors,
2. For each $\mathbf{k}$, such that $\mathbf{k} \cdot \mathbf{n} \leq 0$, find all the possible wavenumbers for the reflected phonon,
3. Select the stencil: the set J and the number of time steps M,
4. Initialize the time history kernels $\{\alpha_j^m\}$,
5. Compute the reflection coefficients $R_{ss_l'}$ and the objective function
6. Use a optimization subroutines to obtain new values for the time history kernels.
7. Go to step 5 unless certain convergence criterion is met.

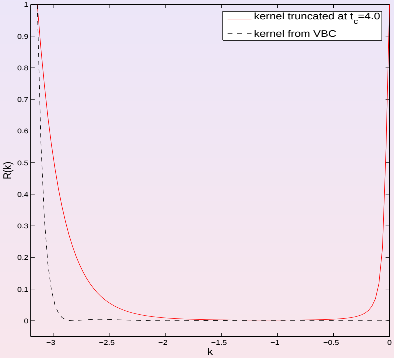
Example I: 1D chain

$$R(k) = \frac{1 - \sum_j e^{ijk} \int_0^{t_0} \alpha_j(\tau) e^{i\omega\tau} d\tau}{1 - \sum_j e^{-ijk} \int_0^{t_0} \alpha_j(\tau) e^{i\omega\tau} d\tau}.$$



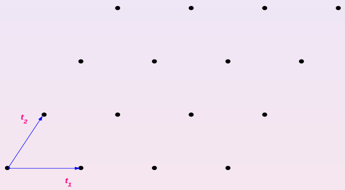
time history kernels

Example I: 1D chain

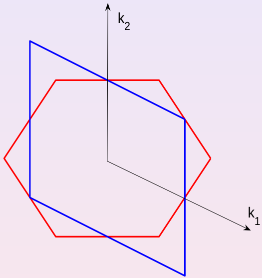


phonon reflection

Example II: 2D triangular lattice

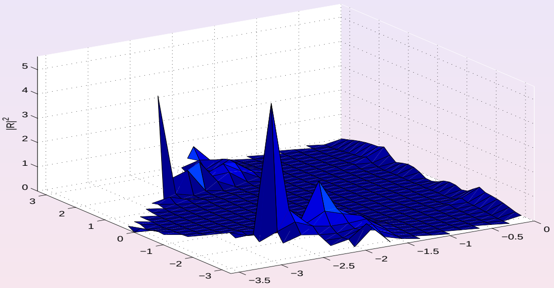


triangular lattice



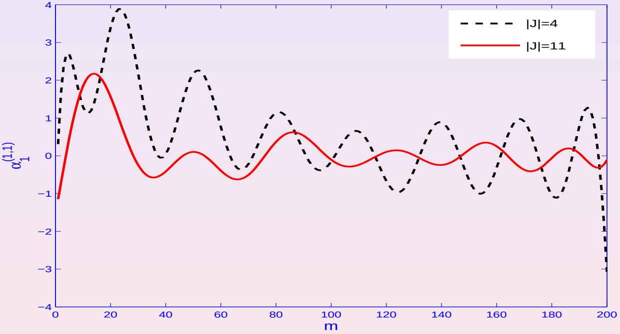
the first Brillouin zone

Example II: reflection coefficients



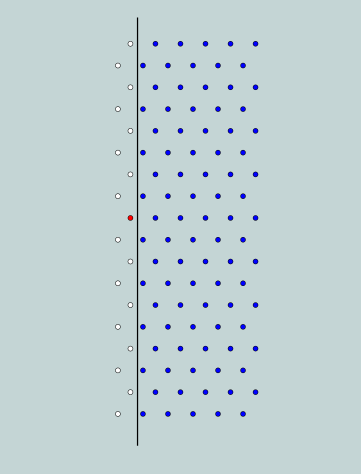
the total reflection

Example II: time history kernels



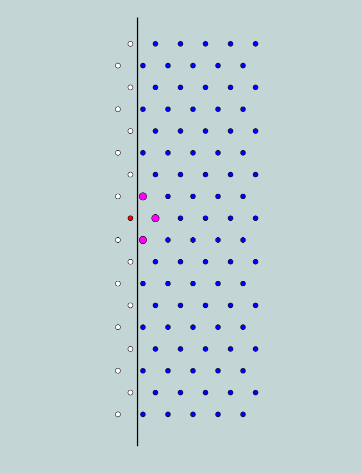
the memory kernels

Example II: comparing different stencils



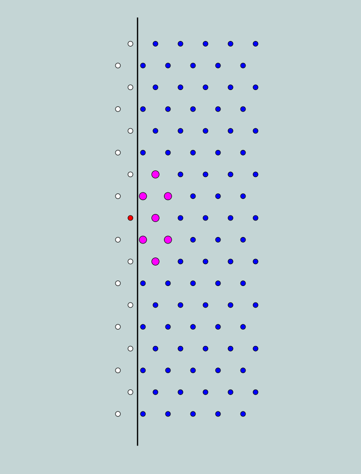
Selection of the stencil

Example II: comparing different stencils



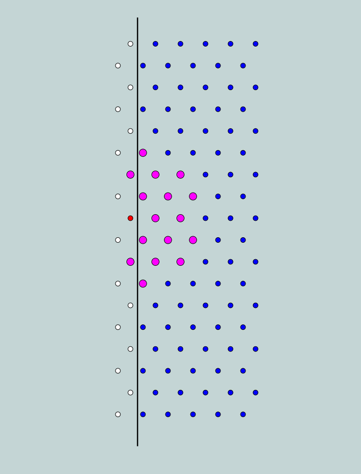
$|J| = 4$

Example II: comparing different stencils



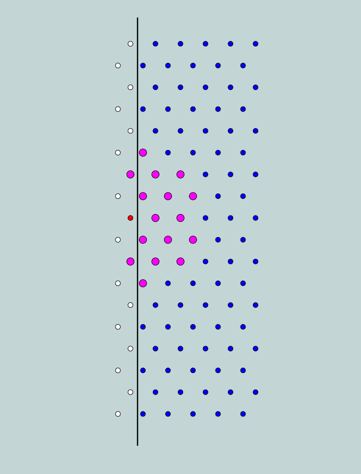
$$|J| = 8$$

Example II: comparing different stencils

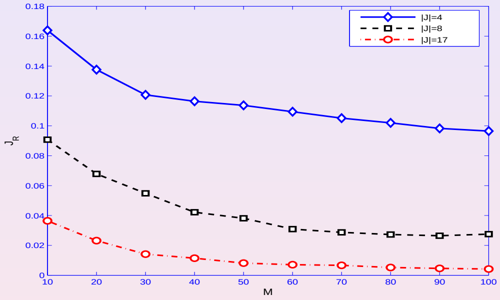


$|J| = 17$

Example II: comparing different stencils

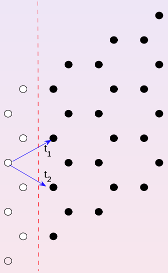


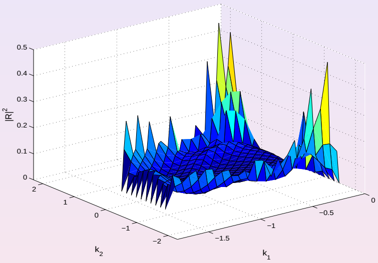
$|J| = 17$



Total reflection on various stencil

Example III: graphene sheet





Graphene lattice structure

Total reflection

Application: fracture simulation in BCC Iron

fixed boundary condition

variational boundary condition

Implementations

1. **minimization**
   `BFGS routines e.g. Zhu et al 1997`
2. **integration over the Brillouin zone**
   `K-point method`
3. **boundary conditions for the corners**
   `create new planes`
4. **external loading**
   `specify displacement, apply traction`

Work in progress

1. standardization
2. stability analysis
3. comparison with damping method
4. extension to finite temperature

Summary

1. exact boundary condition
2. analysis of phonon reflection
3. variational formulation to minimize phonon reflection
4. **local** boundary condition
5. implementation issues
6. applications to fracture simulations

Reference: X. Li and W. E, Variational boundary conditions for molecular dynamics simulations of solids at low temperature, comm. comp. phys. **1** (2006), 136--176.