Boundary conditions for molecular dynamics

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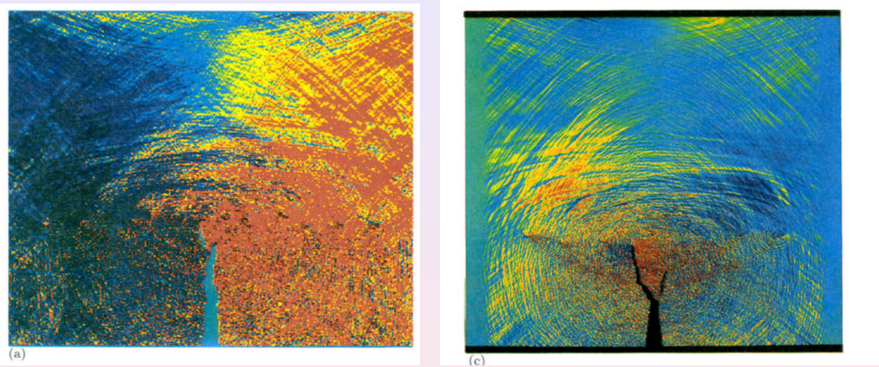
Motivation

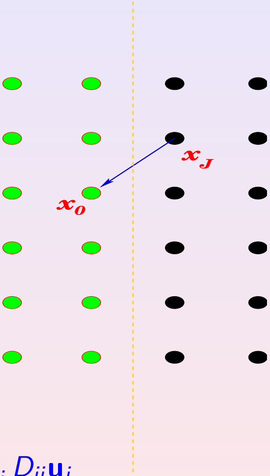


Holian and Ravelo PRB 1994

Outline

- Exact boundary conditions
- Phonon reflection
- Variational formulation
- Examples
- Application to fracture simulation

Problem setup

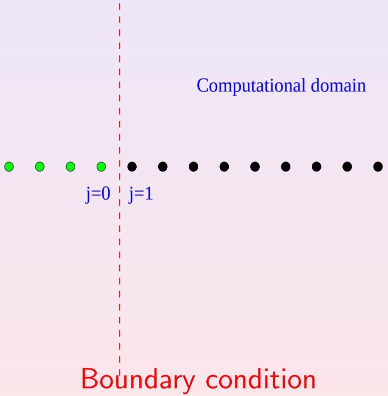


$$m\ddot{\mathbf{u}}_i = -\sum_j D_{ij}\mathbf{u}_j \qquad\qquad m\ddot{\mathbf{u}}_i = -\frac{\partial V}{\partial \mathbf{x}_i}.$$

MD boundary condition: a 1D example

Exact boundary condition can be obtained by solving the **half space problem:**

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



1D example: exact boundary condition

Exact boundary condition (`Adelman et. al. 1974, 1976`):

$$u_0(t) = \int_0^t \beta(t-s)u_1(s)ds, j \leq 0$$

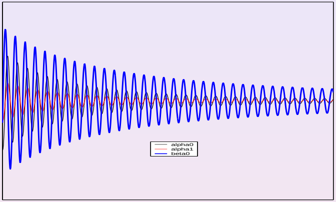
$$\beta(t) = \frac{J_2(2t)}{t}.$$

Faster decay by using more atoms

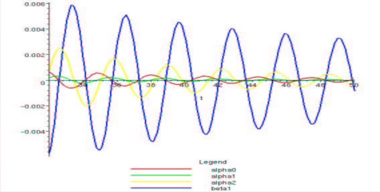
$$u_0 = \sum_{j=1}^{J} \int_0^t \alpha_j(t-s) u_j(s) ds$$

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

J=2



J=3



General lattice

Linearized equation of motion,

$$M\ddot{\mathbf{u}}_{i,j,k} = \sum_{l,m,n} D_{i-l,j-m,k-n}\mathbf{u}_{l,m,n},$$

Fourier transform in the j and k direction,

$$M\ddot{\mathbf{U}}_i(\eta,\zeta) = \sum_l \mathcal{D}_{i-l}(\eta,\zeta)\mathbf{U}_l(\eta,\zeta).$$

$$\mathbf{U} = \mathcal{F}_{j\to\eta,k\to\zeta}[\mathbf{u}],\ \mathcal{D} = \mathcal{F}_{j\to\eta,k\to\zeta}[D].$$

Exact boundary condition:

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

Existing work

- W. Cai, M. de Koning, V. V. Bulatov and S. Yip 2000,
- G.J. Wagner, G.K. Eduard and W.K. Liu 2004,
- H.S. Park, E.G.Karpov, W.K. Liu and P.A. Klein 2004.

Practical issue

Exact boundary conditions:

- **nonlocal** in both space and time
- 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
- take into account of external loading

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An analogy: boundary condition for the wave equation: ABC (`Engquist and Majda 1979`), and many other methods.

Phonon spectrum

Harmonic approximation:

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

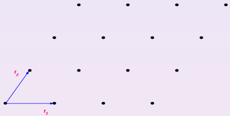
Dynamic matrix:

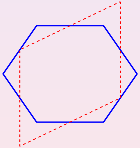
$$M\mathcal{D}(\mathbf{k}) = \sum_j D_j e^{-i\mathbf{r}_j \cdot \mathbf{k}},$$

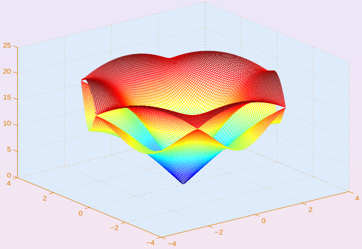
Phonon spectrum

$$\mathcal{D}(\mathbf{k})\varepsilon_s(\mathbf{k}) = \lambda_s \varepsilon_s(\mathbf{k}).$$

Brillouin zone: triangular lattice



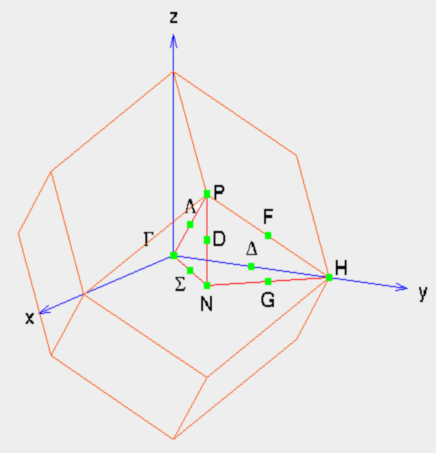




the first Brillouin zone

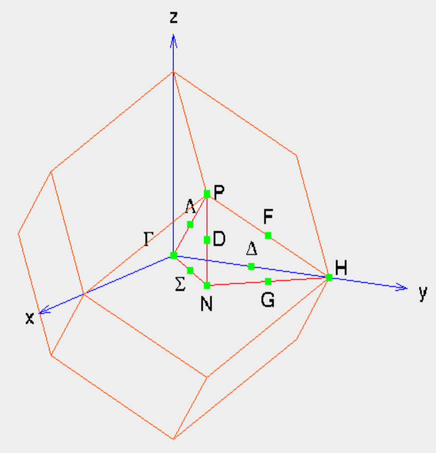
Phonon spectrum

Brillouin zone



BZ for BCC lattice

Brillouin zone

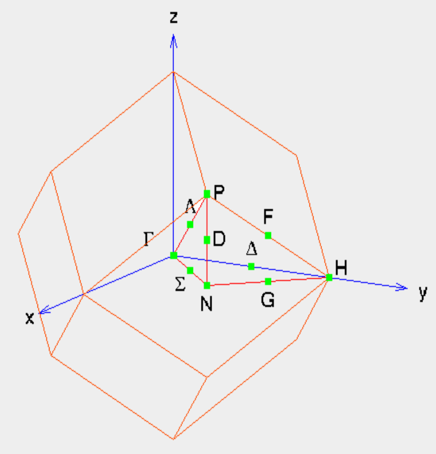


BZ for BCC lattice

Symmetry of the spectrum:

$$\omega(\mathbf{k}) = \omega(P\mathbf{k}), \quad \varepsilon(P\mathbf{k}) = P\varepsilon(\mathbf{k}).$$

Brillouin zone



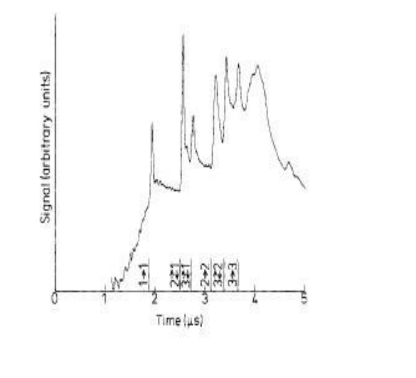
BZ for BCC lattice

Integration over the BZ: K point method (Monkhorst and Pack 1976).

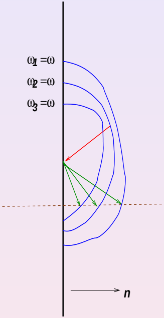
$$
\begin{aligned}
u_i &= (2i - nq - 1)/(2nq) \\
\mathbf{k}_{ijl} &= u_i \mathbf{b}_i + u_j \mathbf{b}_j + u_l \mathbf{b}_l .
\end{aligned}
$$

The symmetry of the grid points substantially reduces the computation.

Phonon reflection



Taborek and Goodstein 1979



Incident and reflected waves

Phonon reflection:

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

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

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

leads to a polynomial for λ. The roots of the polynomial come in pairs $(\lambda, 1/\lambda^*)$. The degree of the polynomial: $Nd \times Ne \times Na$. The wavenumber:

$$
\mathbf{k}^R_{s,s'} \cdot \mathbf{n} = k_r + i k_i.
$$

Phonon reflection: *reflection coefficients*

Boundary condition:

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

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Incident and reflected waves:

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

Phonon reflection: *reflection coefficients*

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Incident and reflected waves:

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

Phonon reflection: *reflection coefficients*

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$$\mathbf{c}^R = R\mathbf{c}^I,$$

Linear system:

$$(I-\mathcal{A}(\mathbf{k}))\varepsilon_s(\mathbf{k}) + \sum_{s'} R_{ss'}(I-\mathcal{A}(\mathbf{k}_{ss'}^R))\varepsilon_{s'}(\mathbf{k}).$$

Thermal flux

Energy flux at the atomic scale:

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

Convert to Fourier space:

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

$$\begin{aligned} J^R &= \int |c^R_{ss'}|^2 \omega_{s'} \nabla\lambda_{s'}(\mathbf{k})d\mathbf{k}, \\ J^R_n &= 2\sum_s \int_{\mathbf{k}\in BZ,\ \mathbf{k}\cdot\mathbf{n}\le 0} |\sum_{s'} c^I_{s'} R_{ss'}|^2 \omega_s^2\ (\nabla\omega_s \cdot \mathbf{n})d\mathbf{k}. \end{aligned}$$

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

Variational boundary conditions

Discrete boundary condition:

$$\mathbf{u}_0^{n+1} = \sum_{j=1}^{J} \sum_{m=1}^{M} \alpha_j^m \mathbf{u}_j^{n-m} \Delta t,$$

Variational formulation:

$$\min_{\{\alpha_j^m\}} \sum_s \int_{\mathbf{k}\in BZ,\ \mathbf{k}\cdot\mathbf{n}\le 0} \sum_{s'} |R_{ss'}|^2 \, |(\nabla\omega_s \cdot \mathbf{n})| d\mathbf{k}$$

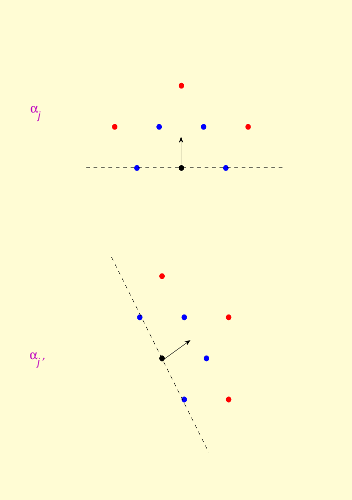
subject to certain constraints.

Symmetry properties

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

Reflection matrices:

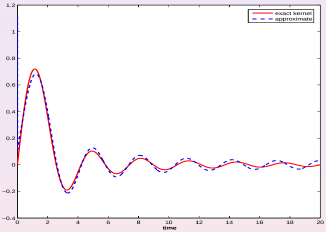
$$R\big(\mathbf{k}; \{\alpha_{j'}\}\big) = R\big(P^T \mathbf{k}; \{\alpha_j\}\big).$$



Example: 1D chain

Reflection (E and Huang 2001, 2002)

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



exact kernel

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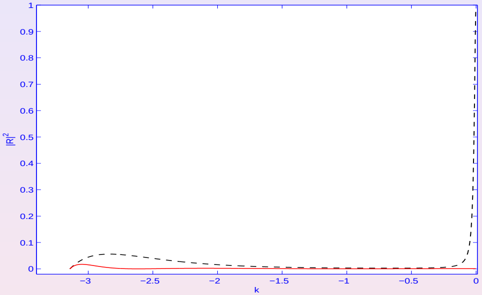
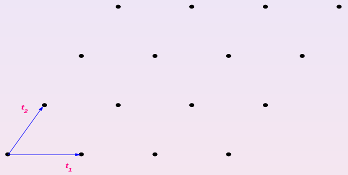
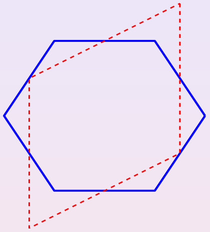


Premature truncation vs variational BC

Example: 2D triangular lattice



the triangular lattice



the first Brillouin zone

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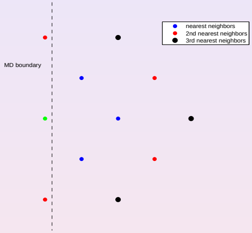
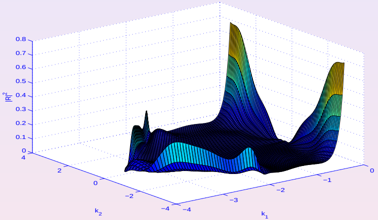
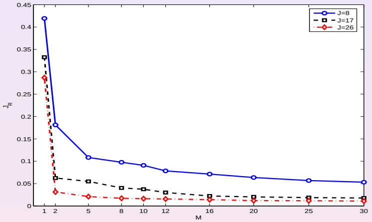


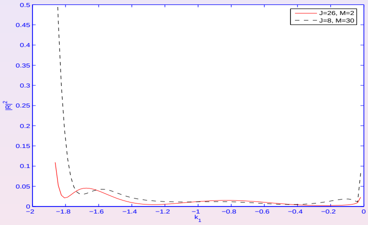


neighbor atoms

phonon reflection for $J = 26, M = 2$

Example: 2D triangular lattice

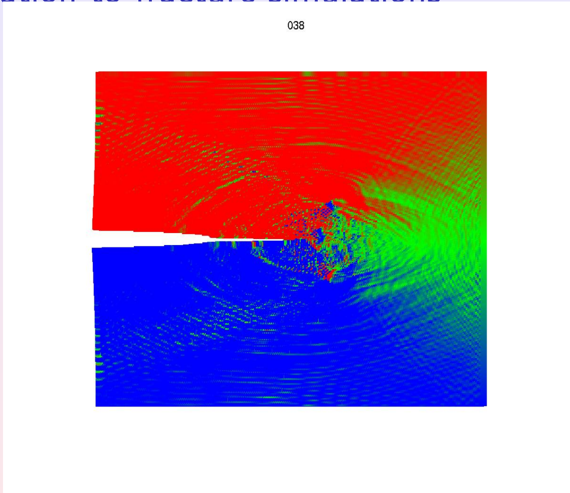




size of the stencil

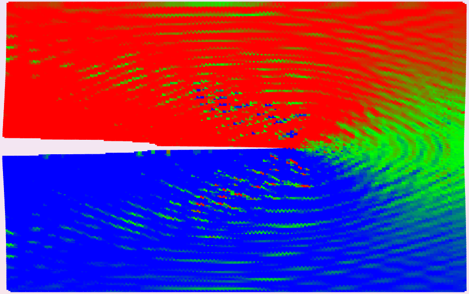
phonon reflection along $\theta = 2\pi/3$

Application to fracture simulations



Fixed BC

Application to fracture simulations



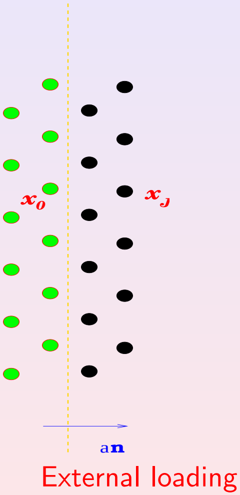
Local BC

More practical issues: external loading

stress free?

The reflection coefficient $|R(k)| \equiv 1$!

More practical issues: external loading



Applied deformation:

$$\mathbf{W} = \mathbf{F}\mathbf{n} - \mathbf{n} = \frac{\partial \mathbf{u}}{\partial \mathbf{n}},$$

Boundary condition:

$$\mathbf{w}_0 = \sum_j \int_0^{t_0} \alpha_j(s)\mathbf{w}_j(t-s)ds.$$

In Fourier space:

$$\hat{w}(k) = \hat{u}(k)(1 - e^{ia\mathbf{k}\cdot\mathbf{n}}).$$

Summary

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