Discrete exterior calculus for phonon propagation in layered periodic structures

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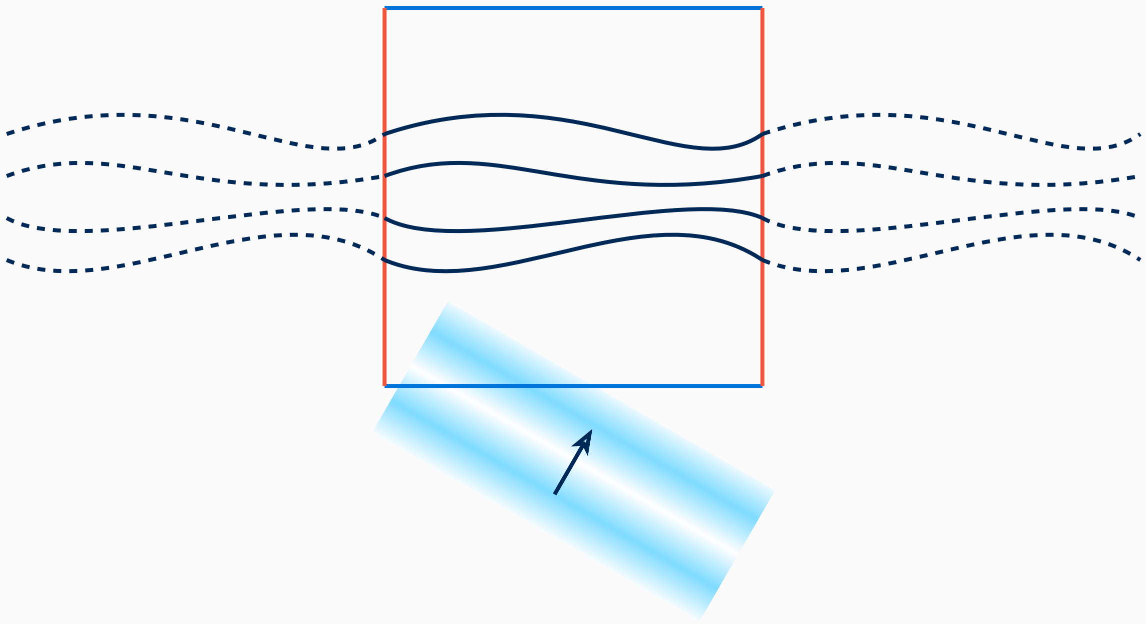
In this presentation

Problem description

Phonon: quasiparticle described by a vibration in an elastic material

Given some material structure, compute transmission and reflection probabilities for different phonon modes



Applications at different wavelength scales: heat (nm), acoustics (m), seismology (km) [1]

Elastic waves

Hooke's law: stress is linearly proportional to strain

$$\boldsymbol{\sigma}_{ij} = \boldsymbol{C}_{ijkl}\boldsymbol{u}_{k;l}$$

Isotropic material and $\boldsymbol{F} = \boldsymbol{ma}$:

$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} = (\lambda + 2\mu)\boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{u}) + \mu\boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \boldsymbol{u}$$

Governing equations

Hooke's law: stress is linearly proportional to strain

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Isotropic material and $\boldsymbol{F} = m\boldsymbol{a}$:

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Helmholtz decomposition of displacement velocity $\boldsymbol{v} = \frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{\nabla}\Phi + \boldsymbol{\nabla} \times \boldsymbol{\Psi}$ leads to system

$$\begin{cases} \frac{\partial p}{\partial t} = (\lambda + 2\mu)\boldsymbol{\nabla} \cdot \boldsymbol{v} \\ \frac{\partial \boldsymbol{w}}{\partial t} = \mu \boldsymbol{\nabla} \times \boldsymbol{v} \\ \rho \frac{\partial \boldsymbol{v}}{\partial t} = \boldsymbol{\nabla} p + \boldsymbol{\nabla} \times \boldsymbol{w} \end{cases}$$

where $p = \rho \frac{\partial \Phi}{\partial t}$, $\boldsymbol{w} = \rho \frac{\partial \boldsymbol{\Psi}}{\partial t}$ represent longitudinal and transverse stress potentials

Differential forms for 2D (P,SV) polarized waves (displacement in (x, y) plane):

$\overset{1}{\mathbf{q}} = \star\overset{1}{\mathbf{v}}$ for displacement flux,
$\overset{0}{\mathbf{p}}$ for pressure,
$\overset{0}{\mathbf{w}}$ for (z-component of) shear potential

$$\begin{cases} \dfrac{\partial \overset{0}{\mathbf{p}}}{\partial t} = (\lambda + 2\mu)\star d\overset{1}{\mathbf{q}} \\ \dfrac{\partial \overset{0}{\mathbf{w}}}{\partial t} = \mu\star d\star\overset{1}{\mathbf{q}} \\ \rho\dfrac{\partial \overset{1}{\mathbf{q}}}{\partial t} = \star d\overset{0}{\mathbf{p}} - d\overset{0}{\mathbf{w}} \end{cases}$$

Discretization

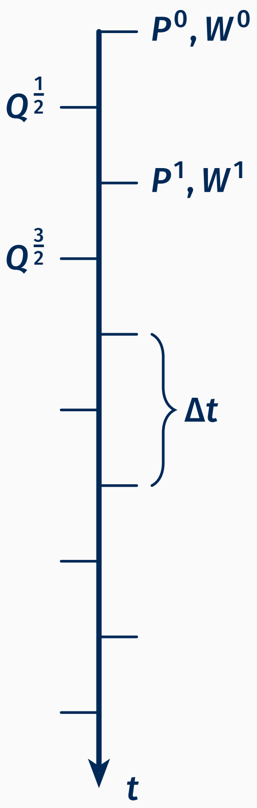
Discretization

DEC space discretization: replace differential forms with cochains, exterior calculus operators with matrices

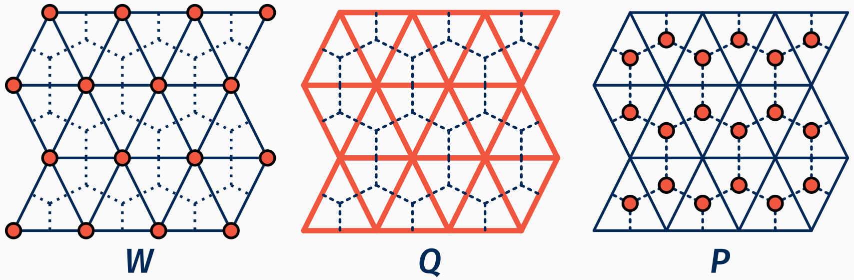
Leapfrog time discretization (central differences in time with staggered variables)

Timestep equations:

$$\begin{cases} P^{n+1} = P^{n} + \Delta t(\lambda + 2\mu) \star \mathbf{d} Q^{n+\frac{1}{2}} \\ W^{n+1} = W^{n} + \Delta t \mu \star \mathbf{d} \star Q^{n+\frac{1}{2}} \\ Q^{n+\frac{3}{2}} = Q^{n+\frac{1}{2}} + \frac{\Delta t}{\rho}(\star \mathbf{d} P^{n+1} - \mathbf{d} W^{n+1}) \end{cases}$$



W (shear) is a primal 0-cochain, ***Q*** (flux) is a primal 1-cochain, ***P*** (pressure) is a dual 0-cochain



Remark: energy conservation

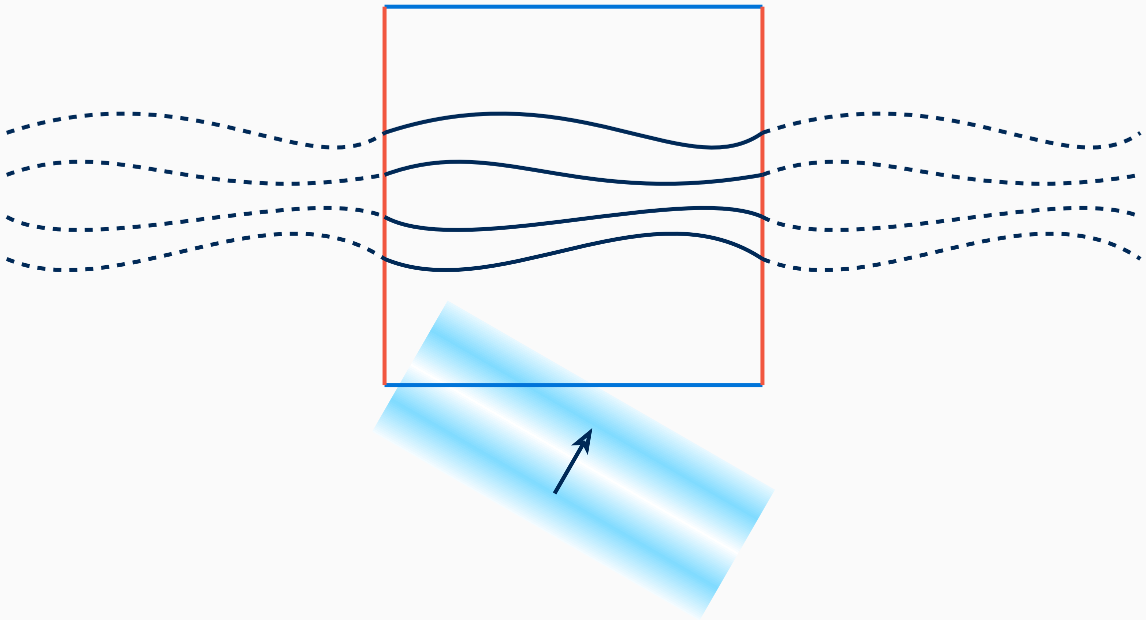
This scheme preserves the discrete energy

$$E^n = \begin{bmatrix} P^n & W^n & Q^n \end{bmatrix} \begin{bmatrix} (\lambda + 2\mu)^{-1} & & \\ & \mu^{-1} & \\ & & \rho \end{bmatrix} \begin{bmatrix} P^n \\ W^n \\ Q^n \end{bmatrix}$$

(shown for a general class of wave propagation problems by Räbinä et al. [2])

Can be verified by a simple numerical experiment: set a reflecting boundary condition and observe energy over time

Domain and boundary conditions



Horizontally periodic, vertically finite structure with piecewise constant materials

Top and bottom: absorbing boundary

Left and right: periodic boundary

Within the domain: material boundaries

Absorbing boundary

First order Engquist-Majda absorbing boundary condition [3]

$$\frac{1}{c}\frac{\partial u}{\partial t} + \hat{n} \cdot \nabla u = 0$$

Applied to each potential $\boldsymbol{P}, \boldsymbol{W}$ by setting fluxes and circulations over boundary edges

Absorbing boundary

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$$\frac{1}{c}\frac{\partial u}{\partial t} + \hat{n} \cdot \nabla u = 0$$

Applied to each potential P, W by setting fluxes and circulations over boundary edges

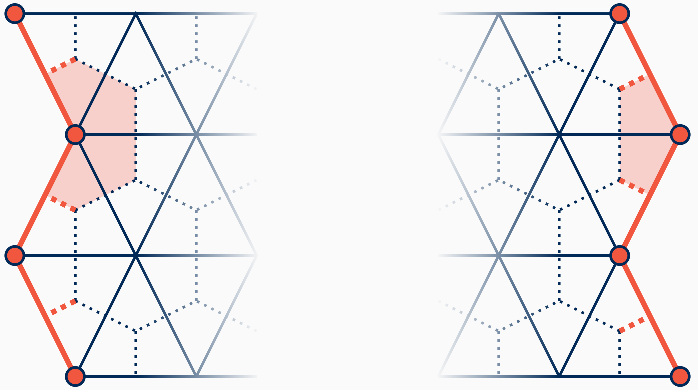
Only absorbs waves at a specific propagating angle completely. Multiply by $\cos\theta$ to optimize the boundary condition for angle θ

For structures with a dominant axis we can compute θ *a priori* using Snell's law

Projection operator on cochains that sums values of opposite edges and vertices:

$$P_{ij} = \begin{cases} 1, & \text{if } i = j \text{ or } \sigma_i \text{ is opposite to } \sigma_j \\ 0, & \text{otherwise} \end{cases}$$

Adjusted Hodge star that sums together opposite dual volumes ($\star_{ii} = \frac{\text{dual vol}}{\text{primal vol}}$)



Material boundaries

Materials in welded contact: continuity of displacement and traction

~~Achieved automatically with appropriate assigning of material parameters as in FDTD~~

Not true: decomposition $\frac{\partial \boldsymbol{v}}{\partial t} = \boldsymbol{\nabla} \boldsymbol{p} + \boldsymbol{\nabla} \times \boldsymbol{w}$ is not valid on material boundary

Haven't solved this yet; investigating alternative formulation using vector-valued differential forms

Numerical experiments

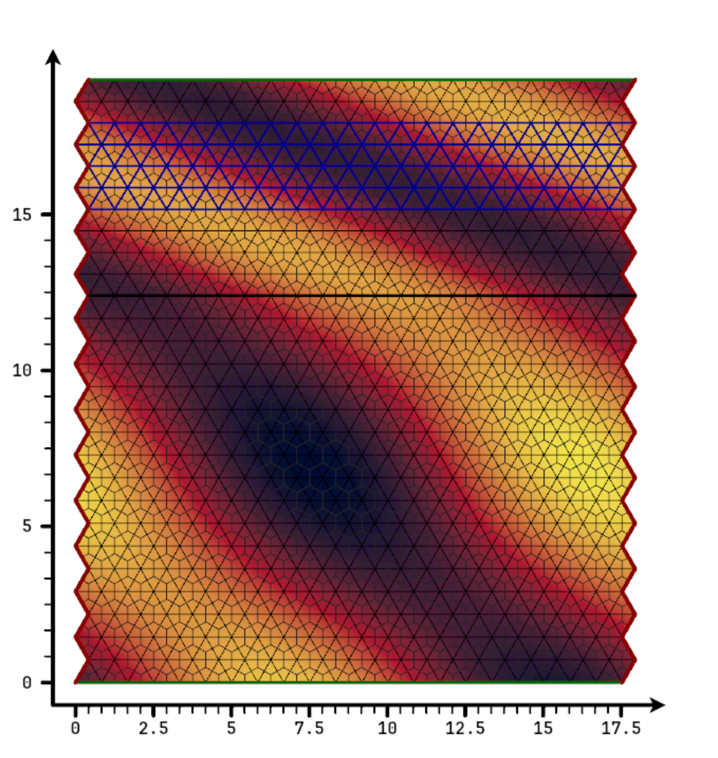
Single planar boundary

Incident plane wave with given polarization (P/SV), frequency and propagation angle

Analytic solutions for reflection and transmission coefficients can be computed from continuity of displacement and stress [4]

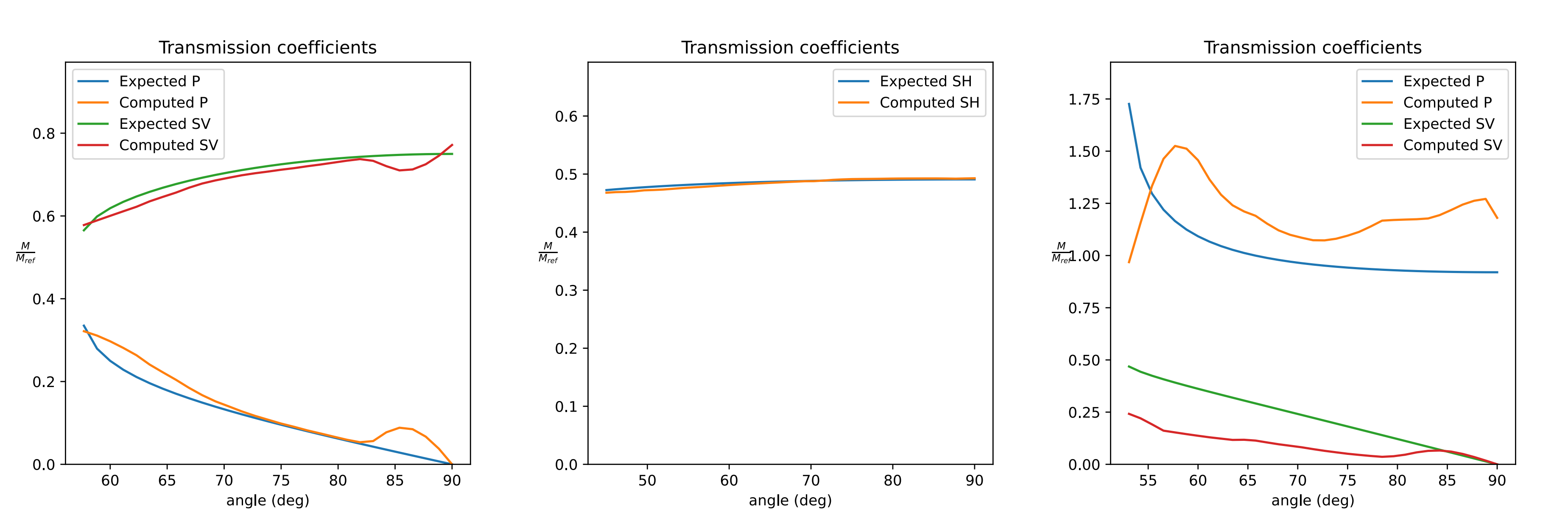
Measurement of energy and velocity amplitudes in a strip of triangles in the top layer

Run the simulation twice: with constant material parameters to obtain free-space reference measurements $\boldsymbol{M}_{\text{ref}}$ and with materials applied to get $\boldsymbol{M}$; compute transmission coefficients as $\frac{\boldsymbol{M}}{\boldsymbol{M}_{\text{ref}}}$; compare against analytic values



Numerical experiments

Initial results with a few random combinations of materials:



Currently works well with some material combinations but fails with others due to incomplete handling of the material interface. Energy is conserved but change of polarization (P ↔ SV) at the interface is not reliably captured

Bragg mirror

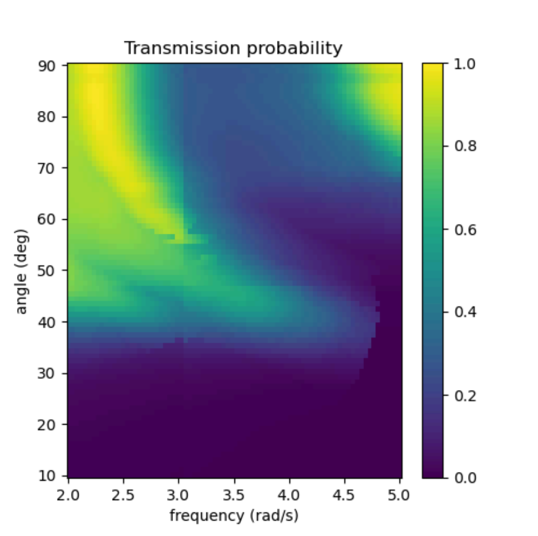
Multiple planar layers of alternating materials with quarter-wavelength thickness (for a specific wavelength we wish to reflect)

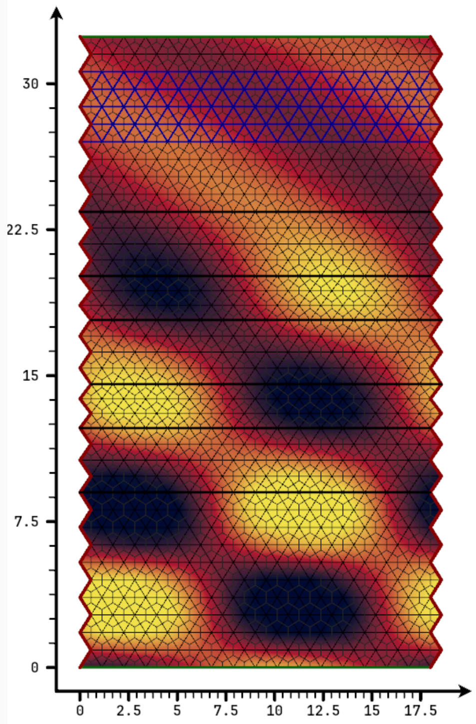
Otherwise exactly the same as the one-interface case

More limited analytic solutions still available

Compute phonon transmission probability (square of transmission coefficient) for a range of frequencies and angles

Useful for estimating heat conductivity





Implementation

Implementation

`dexterior`: general-purpose Rust library, inspired by PyDEC [5],

https://codeberg.org/molentum/dexterior/

Given a simplicial mesh of any dimension, generates $\mathbf{d}$, $\star$ and various utilities
(plus several unfinished experiments: vector-valued forms, interpolation, Lie derivatives...)

Type safe: dimensions of cochains and operators checked at compile time

Real-time visualizer (2D only for now)

Code example: SH wave

```
use dexterior::*;

let mesh = SimplicialMesh::new(vertices, indices);

type Velocity = Cochain<0, Primal>;
type Shear = Cochain<1, Primal>;

let mut v: Velocity = mesh.integrate_cochain(...);
let mut w: Shear = mesh.integrate_cochain(...);

let v_step: Op<Shear, Velocity>
  = (dt / dens) * mesh.star() * mesh.d() * mesh.star();
let w_step: Op<Velocity, Shear> = -dt * mu * mesh.d();

loop {
  w += &w_step * &v;
  v += &v_step * &w;
}
```

$$V^{n+1} = V^n + \frac{\Delta t}{\rho} \star \mathbf{d} \star W^{n+\frac{1}{2}}$$

$$W^{n+\frac{3}{2}} = W^{n+\frac{1}{2}} - \Delta t \mu \mathbf{d} V^{n+1}$$

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Slides available online at https://molentum.me/publications/

and source code at https://codeberg.org/molentum/phononic/

References

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[3] B. Engquist and A. Majda, "Radiation boundary conditions for acoustic and elastic wave calculations," *Communications on Pure and Applied Mathematics*, vol. 32, no. 3, pp. 313–357, May 1979, doi: 10.1002/cpa.3160320303.

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