Discrete exterior calculus for phonon propagation in layered periodic structures

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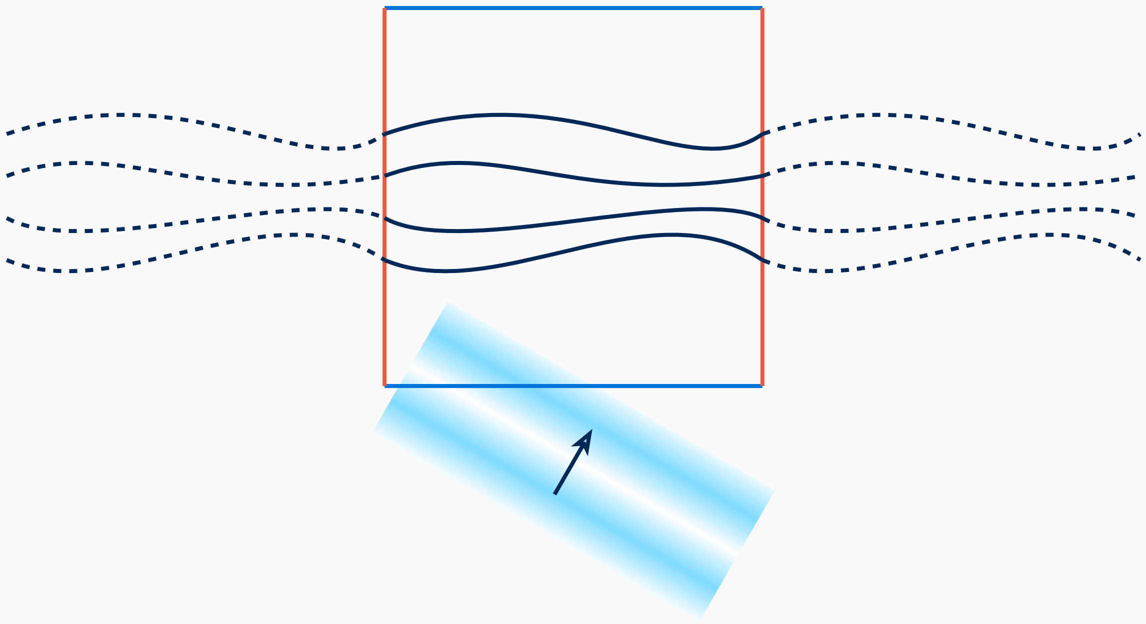
In this presentation

Problem description

Phonon: pseudoparticle 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

Governing equations

Hooke's law: stress is linearly proportional to strain

$$\sigma_{ij} = C_{ijkl} u_{k;l}$$

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

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

..but can't solve directly with first-order DEC

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

Φ and Ψ satisfy independent scalar wave equations

$$\begin{cases} \rho \frac{\partial^2 \Phi}{\partial t^2} = (\lambda + 2\mu)\nabla^2 \Phi \\ \rho \frac{\partial^2 \Psi}{\partial t^2} = \mu \nabla^2 \Psi \end{cases}$$

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

Additionally we have (by definition + smoothness)

$$\frac{\partial \boldsymbol{v}}{\partial t} = \boldsymbol{\nabla}\frac{\partial \Phi}{\partial t} + \boldsymbol{\nabla} \times \frac{\partial \Psi}{\partial t}$$

Introduce $\boldsymbol{p} = \rho\frac{\partial \Phi}{\partial t}$, $\boldsymbol{w} = \rho\frac{\partial \Psi}{\partial t}$ representing longitudinal and transverse stress potentials, get the first-order system

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

Exterior calculus and reduction to 2D

3D elastic waves come in three polarizations: P, SV, SH

P-waves are longitudinal (pressure) waves with displacement velocity $\boldsymbol{v_p} = \boldsymbol{\nabla\Phi}$

SV waves are transverse (shear) waves with $\boldsymbol{v_s} = \boldsymbol{\nabla} \times \boldsymbol{\Psi}$ in the $(\boldsymbol{x}, \boldsymbol{y})$ plane

SH waves are shear waves with $\boldsymbol{v_s}$ along the $\boldsymbol{z}$ axis

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Differential forms for 2D (P,SV) waves:
$\overset{1}{\mathbf{q}} = \star \overset{1}{\mathbf{v}}$ for flux of velocity,
$\overset{0}{\mathbf{p}}$ for pressure,
$\overset{0}{\mathbf{w}}$ for (z-component of) shear potential

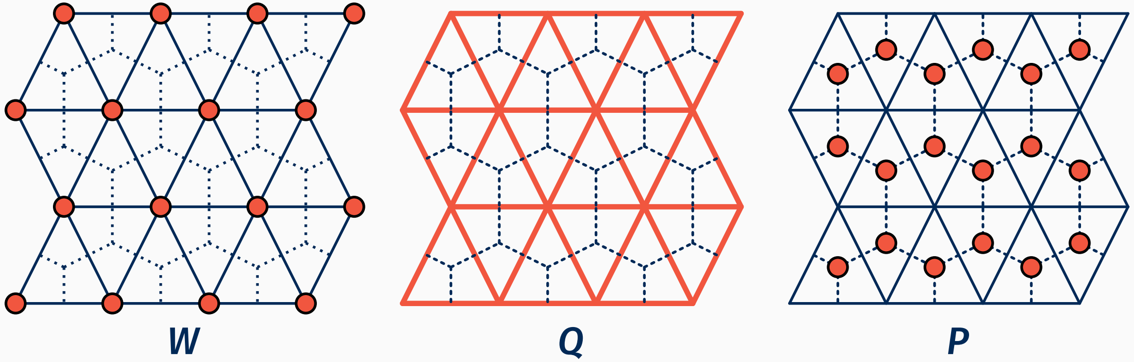
$$\begin{cases} \dfrac{\partial \overset{0}{\mathbf{p}}}{\partial t} = (\lambda + 2\mu) \star d \overset{1}{\mathbf{q}} \\ \dfrac{\partial \overset{0}{\mathbf{w}}}{\partial t} = \mu \star d \star \overset{1}{\mathbf{q}} \\ \rho \dfrac{\partial \overset{1}{\mathbf{q}}}{\partial t} = \star d \overset{0}{\mathbf{p}}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

Discretization

DEC space discretization: replace differential forms with cochains, exterior calculus operators $\boldsymbol{d}, \star$ with matrices $\mathbf{d}_k, \star_k$

$$\begin{cases} \dfrac{\partial \overset{0}{\mathrm{p}}}{\partial t} = (\lambda + 2\mu)\star d\overset{1}{\mathrm{q}} \\ \dfrac{\partial \overset{0}{\mathrm{w}}}{\partial t} = \mu \star d \star \overset{1}{\mathrm{q}} \\ \rho \dfrac{\partial \overset{1}{\mathrm{q}}}{\partial t} = \star d\overset{0}{\mathrm{p}} - d\overset{0}{\mathrm{w}} \end{cases} \Rightarrow \begin{cases} \dfrac{\partial P}{\partial t} = (\lambda + 2\mu)\star_2 \mathbf{d}_1 Q \\ \dfrac{\partial W}{\partial t} = \mu \star_0^{-1} \mathbf{d}_0^T \star_1 Q \\ \rho \dfrac{\partial Q}{\partial t} = \star_1^{-1} \mathbf{d}_1^T P - \mathbf{d}_0 W \end{cases}$$

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

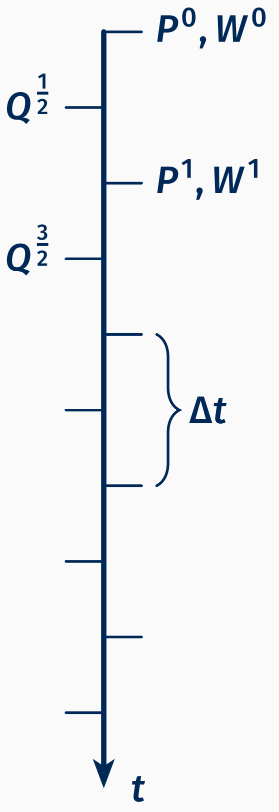


Leapfrog time discretization (central differences in time, $X^n \coloneqq X(n\Delta t)$)

$$\frac{\partial P}{\partial t} \approx \frac{P^{n+1} - P^n}{\Delta t}, \qquad \frac{\partial W}{\partial t} \approx \frac{W^{n+1} - W^n}{\Delta t}, \qquad \frac{\partial Q}{\partial t} \approx \frac{Q^{n+\frac{3}{2}} - Q^{n+\frac{1}{2}}}{\Delta t}$$

Substitute and multiply by Δt, get timestep equations

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



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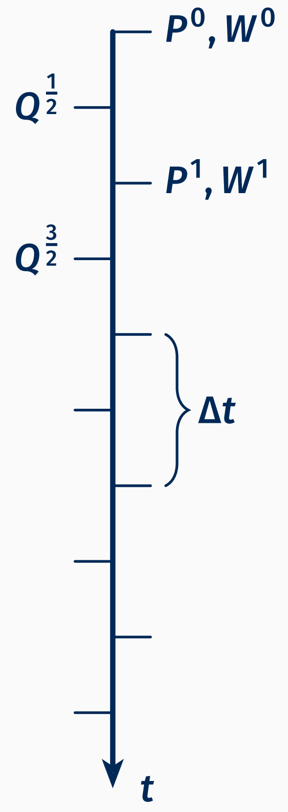

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Explicit ⇒ efficient!

Conditionally stable: $\frac{c_{\max}}{h_{\min}} \Delta t$ must be low enough (CFL condition)

Remark: energy conservation

This scheme preserves the discrete energy

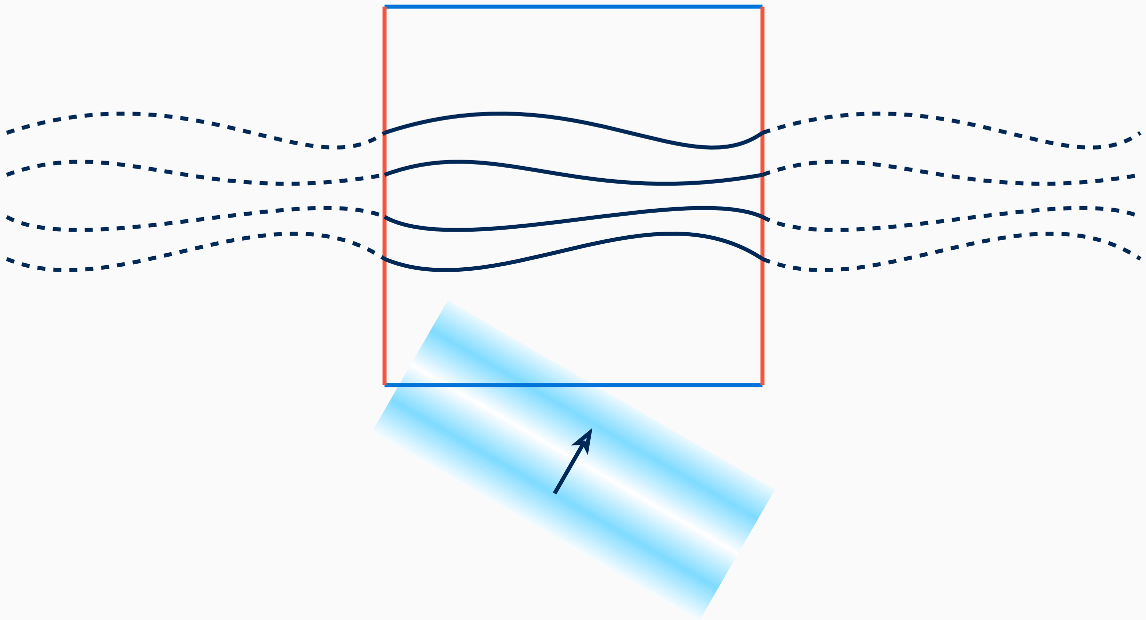
$$E^n = \begin{bmatrix} P^n & W^n & Q^n \end{bmatrix} \begin{bmatrix} (\lambda + 2\mu)^{-1} & & \\ & \mu^{-1} & \\ & & \rho \end{bmatrix} \begin{bmatrix} P^n \\ W^n \\ Q^n \end{bmatrix}$$

(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

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

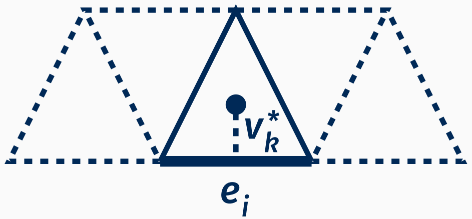
Absorbing boundary

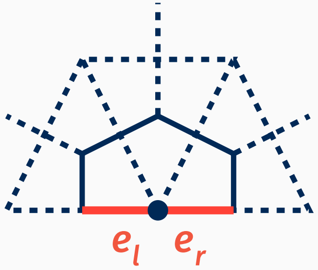
First order Engquist-Majda absorbing boundary condition [3]

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

Applied separately to velocity potentials $\Phi = \frac{p}{\rho}, \Psi = \frac{w}{\rho}$, becomes

$$\frac{1}{\rho c_p} p + \underbrace{\hat{n} \cdot v}_{=q} = 0, \qquad \frac{1}{\rho c_s}(w \times \hat{n}) \times \hat{n} + v \times \hat{n} = 0$$





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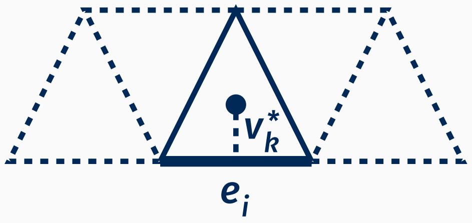

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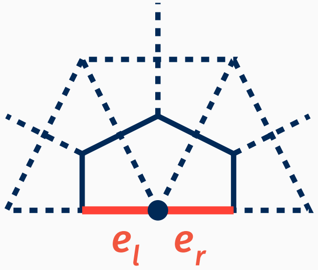

Implemented in the discrete case as

$$Q_i^{n+\frac{1}{2}} = -\frac{1}{\rho c_p}|e_i| P_k^n \text{ (replaces timestep)}, \qquad W_i^n = W_i^n - \frac{1}{2}(|e_l| + |e_r|) c_s W_i^n \text{ (extra term prior to timestep)}$$

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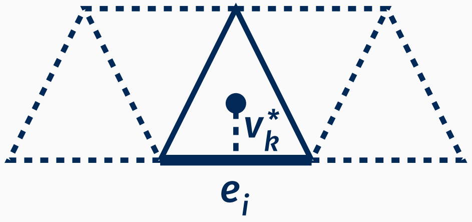

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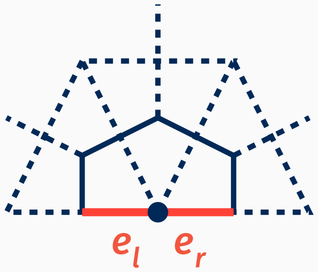

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Only absorbs waves at a specific propagating angle completely. Multiply by $\cos\theta$ to optimize the boundary condition for angle θ

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

Velocity decomposition

Problem: cannot satisfy both P and SV absorbing boundaries simultaneously

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Solution: split velocity into two components: $\boldsymbol{Q} = \boldsymbol{Q}_p + \boldsymbol{Q}_s$ where $\boldsymbol{\nabla} \times \boldsymbol{Q}_p = \boldsymbol{\nabla} \cdot \boldsymbol{Q}_s = \boldsymbol{0}$ everywhere except at material boundaries

Now we can apply absorbing boundaries separately to $\boldsymbol{Q}_p$ and $\boldsymbol{Q}_s$ and still capture the interaction between P and SV waves at material boundaries

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Timestep equations are now

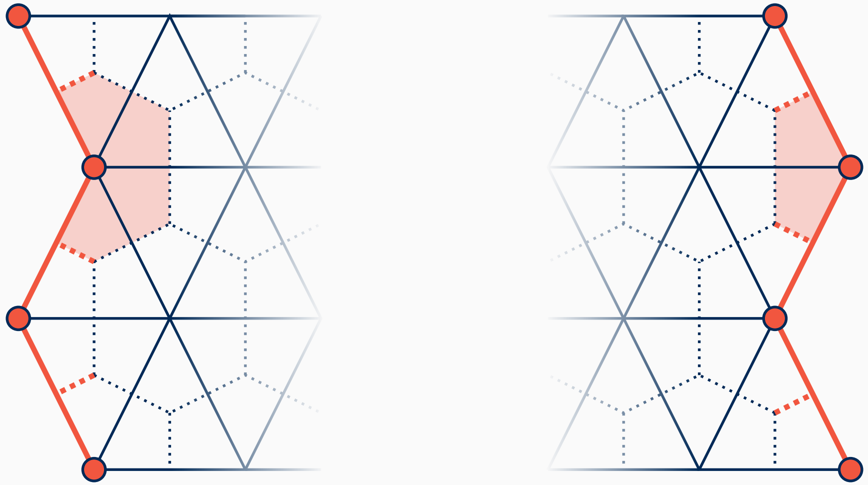
$$
\begin{cases}
P^{n+1} = P^n + \Delta t(\lambda + 2\mu) \star \mathbf{d}\left(Q_p^{n+\frac{1}{2}} + Q_s^{n+\frac{1}{2}}\right) \\
W^{n+1} = W^n + \Delta t \mu \star \mathbf{d} \star \left(Q_s^{n+\frac{1}{2}} + Q_p^{n+\frac{1}{2}}\right) \\
Q_p^{n+\frac{3}{2}} = Q_p^{n+\frac{1}{2}} + \frac{\Delta t}{\rho}(\star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

Periodic boundary

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

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

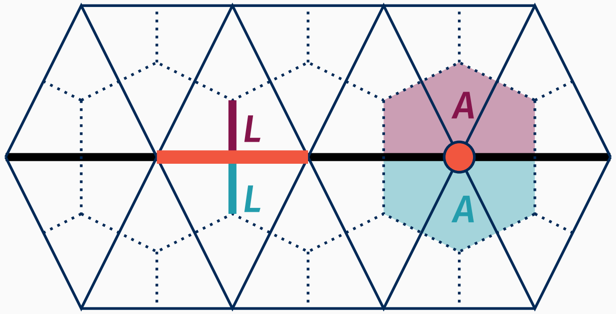
Adjusted Hodge star that sums together opposite dual volumes ($\star_{ii} = \frac{\text{dual vol}}{\text{primal vol}}$)



Materials in welded contact: continuity of displacement and stress

Achieved automatically: single value of velocity and stress (potentials) per mesh element

Material parameters assigned as averages weighted by dual volume as in FDTD [4]



$$\mu_{\bullet} = \frac{A + A}{\frac{A}{\mu} + \frac{A}{\mu}}$$ (harmonic average)

$$\rho_{-} = \frac{L\rho + L\rho}{L + L}$$ (arithmetic average)

Source terms

Plane wave with values $\boldsymbol{w}_{\text{in}}, \boldsymbol{q}_{\text{in}}, \boldsymbol{p}_{\text{in}}$ incident from below at angle $\boldsymbol{\theta}_{\text{in}}$

Applied by adding source values to cochains $\boldsymbol{W}, \boldsymbol{Q}, \boldsymbol{P}$ at the bottom boundary

Eased in and out by multiplying with $f(t) = \left(2 - \sin\left(\frac{t}{t_{\text{tr}}}\frac{\pi}{2}\right)\right)\sin\left(\frac{t}{t_{\text{tr}}}\frac{\pi}{2}\right)$ [5]

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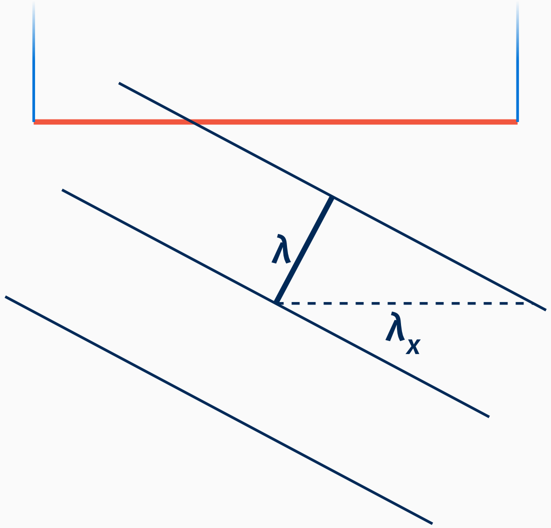
Problem: plane wave has angle-dependent horizontal wavelength $\boldsymbol{\lambda}_x = \frac{\lambda}{\cos\theta_{\text{in}}}$

If domain width isn't a multiple of $\boldsymbol{\lambda}_x$, incident wave is discontinuous at the periodic boundary



Plane wave with values $\boldsymbol{w}_{\text{in}}, \boldsymbol{q}_{\text{in}}, \boldsymbol{p}_{\text{in}}$ incident from below at angle θ_{in}

Applied by adding source values to cochains $\boldsymbol{W}, \boldsymbol{Q}, \boldsymbol{P}$ at the bottom boundary

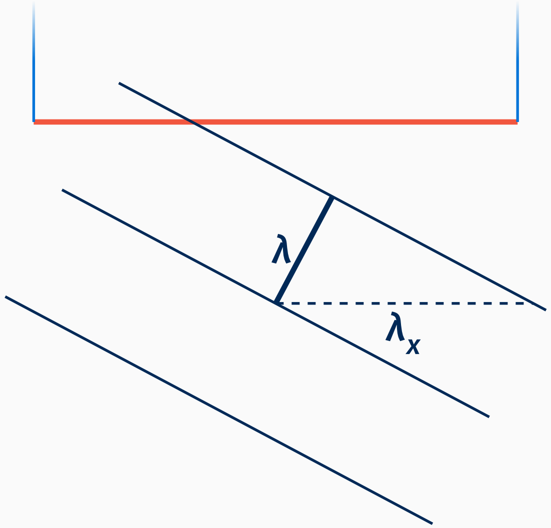
Eased in and out by multiplying with $f(t) = \left(2 - \sin\left(\frac{t}{t_{\text{tr}}}\frac{\pi}{2}\right)\right)\sin\left(\frac{t}{t_{\text{tr}}}\frac{\pi}{2}\right)$ [5]

Problem: plane wave has angle-dependent horizontal wavelength $\lambda_x = \frac{\lambda}{\cos\theta_{\text{in}}}$

If domain width isn't a multiple of λ_x, incident wave is discontinuous at the periodic boundary

If all material boundaries are planar, we can choose width of the domain ⇒ no problem!

Otherwise, phase-shifting periodic boundary needed (not implemented yet)



Numerical experiments

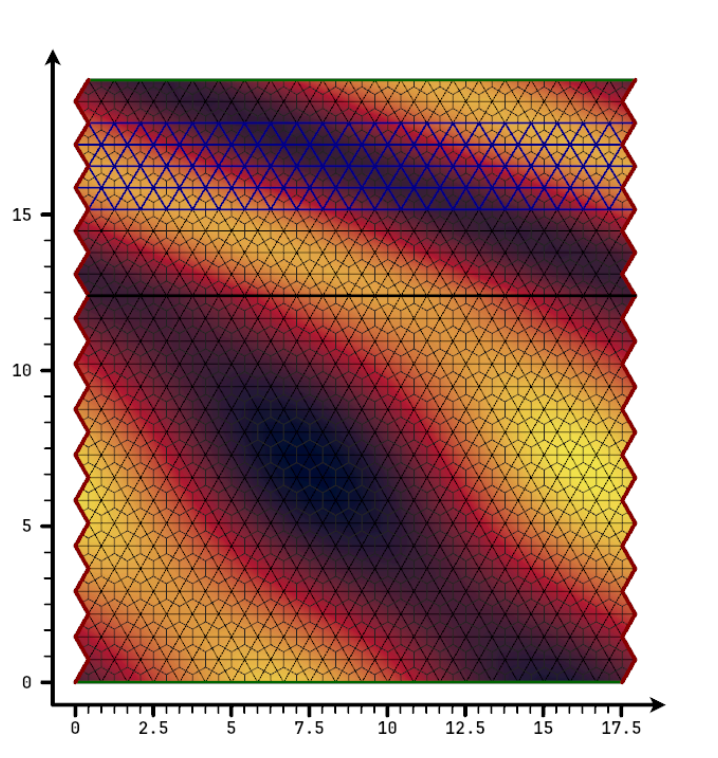
Single planar boundary

Analytic solutions for reflection and transmission coefficients can be computed from continuity of displacement and stress [6]

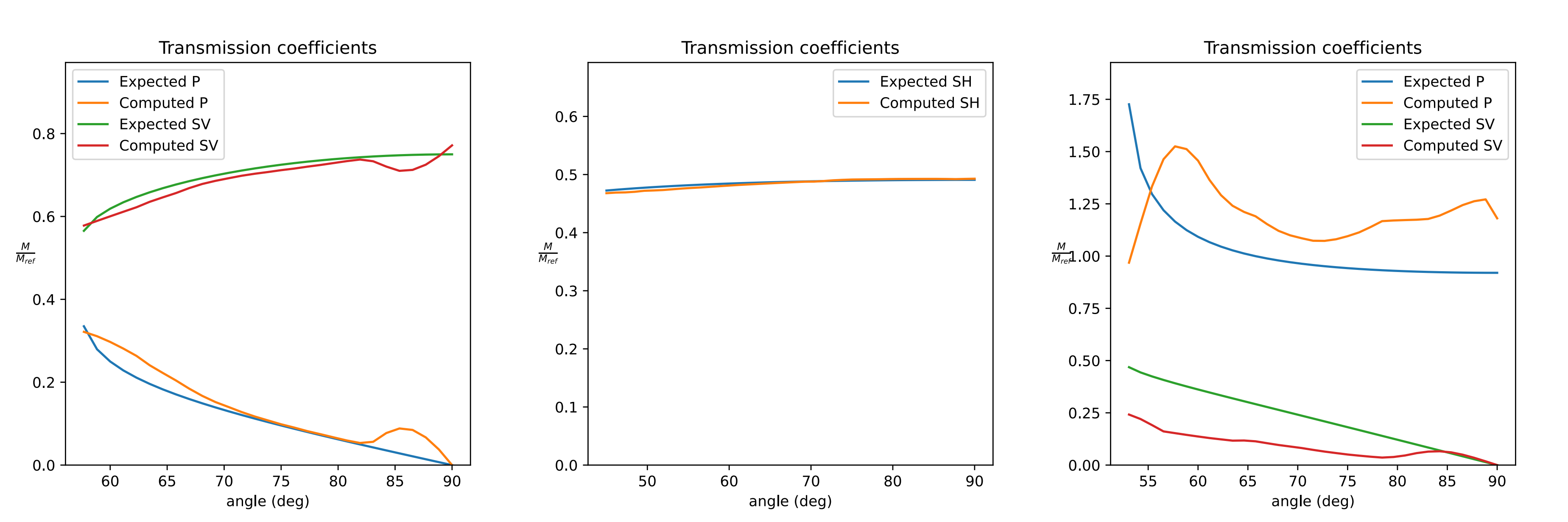
Structured mesh of (approximately) equilateral triangles generated on the fly to match width with λ_x

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

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



Initial results with a few random combinations of materials:



Works well with most material combinations but sometimes fails (as in rightmost figure); investigation underway

Bragg mirror

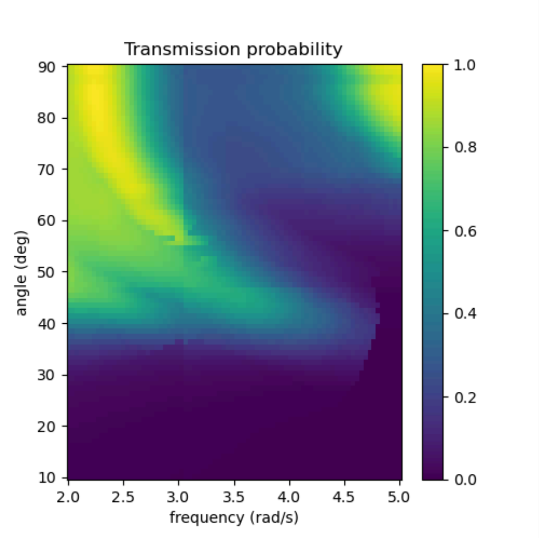
Multiple planar layers of alternating materials with quarter-wavelength thickness (for a specific wavelength we wish to reflect)

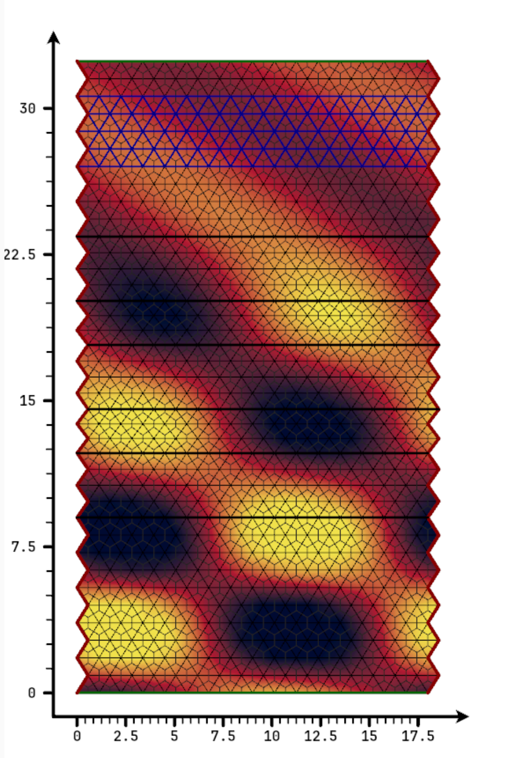
Otherwise exactly the same as the one-interface case

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





Future plans

More complicated 2D geometry

- requires phase-shifting periodic boundary and a different mesh generating strategy (FEM mesh generators like `gmsh` are ok but not optimal)

3D proof of concept

- mesh generation is an issue again, but DEC scheme generalizes easily

Implementation

Implementation

`dexterior`: general-purpose Rust library, inspired by PyDEC [7]

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

Given a simplicial mesh of any dimension, generates $\mathbf{d}$, $\star$ and various utilities

Type inference and compile-time checks to ensure dimensions match

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;
}
```

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

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

Acknowledgments

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Thanks also to Felix Mende for discussions on physics and applications

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

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

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