Simulating waves with discrete exterior calculus

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In this presentation

Note: our applications are not inverse problems, but if you use FEM or similar in your work, this might be an interesting addition to your toolbox.

Slides available online at https://molentum.me/id2025dec.pdf

A brief introduction to DEC

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A geometric approach to discretizing differential equations.

Discrete operations that mimic continuous theory (i.e. preserve certain properties, e.g. Stokes theorem, Leibniz rule)

Advantages:

- geometric flexibility
- efficient time-stepping schemes
- composable implementation
- generalizes to higher dimensions and curved spaces

Exterior calculus

Starting point: differential equation expressed in terms of **differential forms**

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1-forms are **covectors** (row vectors), $\overset{1}{\boldsymbol{\alpha}} = \boldsymbol{a}\,\mathbf{d}\boldsymbol{x} + \boldsymbol{b}\,\mathbf{d}\boldsymbol{y}$

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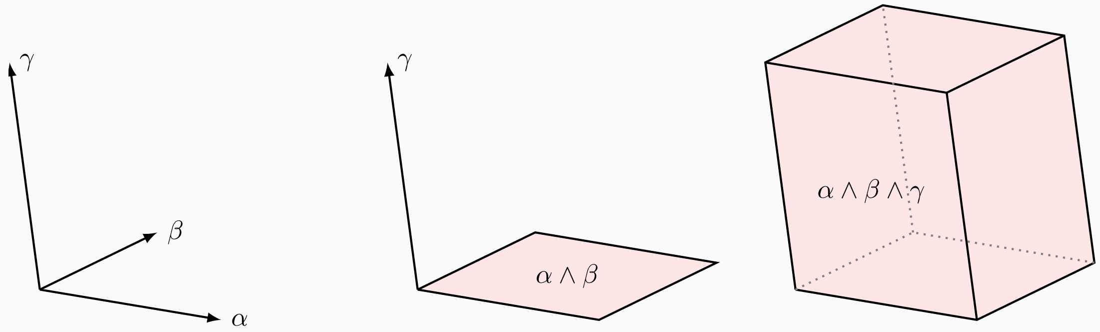
Higher-dimensional forms measure oriented parallelograms, parallelepipeds, ...

2-form $\overset{2}{\omega} = \overset{1}{\alpha} \wedge \overset{1}{\beta} = (x_1, x_2) \mapsto \alpha(x_1)\beta(x_2) - \alpha(x_2)\beta(x_1)$



Exterior calculus

Computing with forms is done with **exterior calculus** operators:

- exterior derivative $\boldsymbol{d}$
- Hodge star $\star$
- wedge product $\wedge$
- interior product $\imath_X$
- Lie derivative $\mathscr{L}_X$
- musical isomorphisms $\flat$ and $\sharp$

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Exterior calculus

$\boldsymbol{d}$ generalizes the **differential** of a function. Takes a $\boldsymbol{k}$-form and produces a $(\boldsymbol{k}+1)$-form.

Correspondence with classical vector calculus (in $\mathbb{R}^3$):

- $\boldsymbol{d}\overset{0}{\boldsymbol{f}} \sim \nabla \boldsymbol{f}$ (a 0-form is a scalar function)
- $\boldsymbol{d}\overset{1}{\boldsymbol{v}} \sim \nabla \times \boldsymbol{v}$
- $\boldsymbol{d}\overset{2}{\boldsymbol{w}} \sim \nabla \cdot \boldsymbol{w}$

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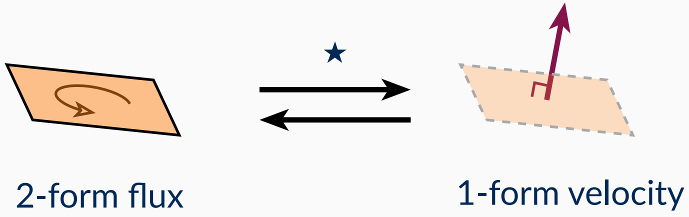
Hodge star $\star$ represents the "orthogonal complement": Transforms a $\boldsymbol{k}$-form to the perpendicular $(\boldsymbol{n}-\boldsymbol{k})$-form



Discretization

Main idea of DEC: discretize the **operators** (and operands), try to preserve key properties

Discretization becomes a drop-in replacement!

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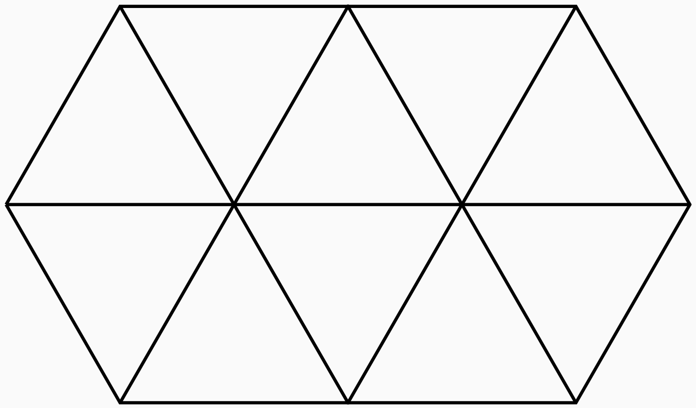
Domain discretized as a polyhedral (usually simplicial) mesh



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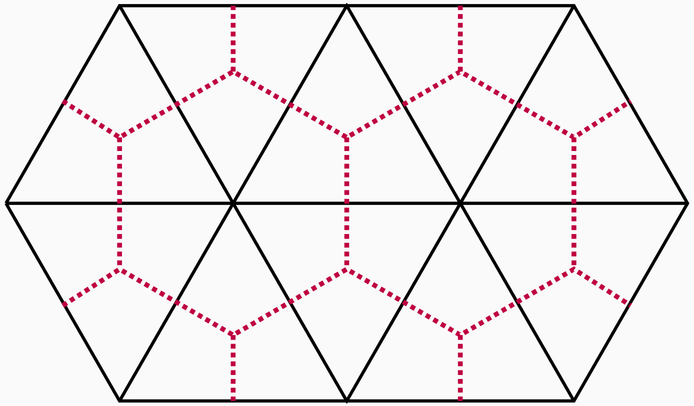
Domain discretized as a polyhedral (usually simplicial) mesh

...and its (Voronoi-Delaunay) **dual**

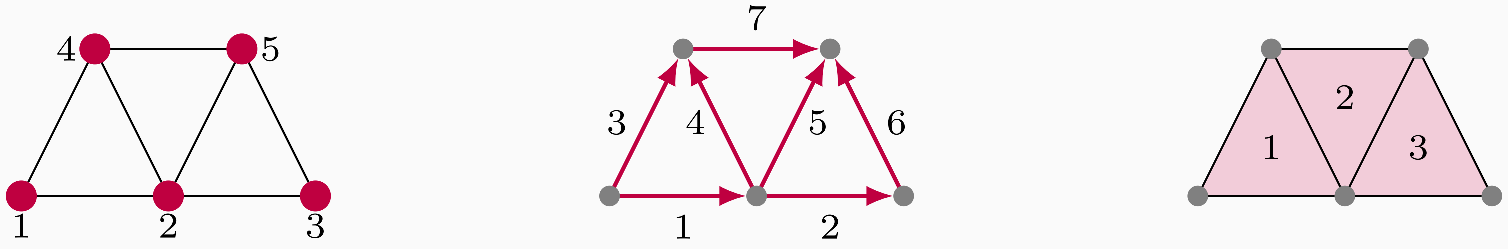


Discretization

Differential forms discretized as cochains: vectors of values associated with mesh elements

Discretizing a continuous $\boldsymbol{k}$-form $\boldsymbol{x}$:

$$X_i = \int_{\sigma_i} x$$



Discretization

Operators discretized as **matrices**

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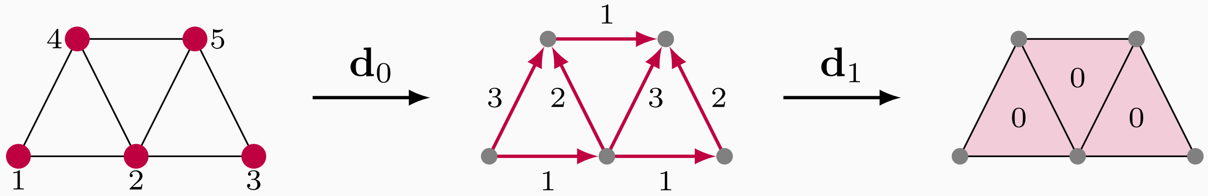
Operators discretized as **matrices**

Discrete $\boldsymbol{d}$ is the *coboundary operator*, takes a $\boldsymbol{k}$-cochain to a $\boldsymbol{(k+1)}$-cochain using Stokes theorem $\int_\sigma d\omega = \int_{\partial\sigma} \omega$



$$\mathbf{d}_0 = \begin{bmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ -1 & & & 1 & \\ & -1 & & 1 & \\ & -1 & & & 1 \\ & & -1 & & 1 \\ & & & -1 & 1 \end{bmatrix}, \quad \mathbf{d}_1 = \begin{bmatrix} 1 & & -1 & 1 & & & \\ & & & -1 & 1 & & -1 \\ & 1 & & & -1 & 1 & \end{bmatrix}$$

Stokes theorem is satisfied **exactly**, using only topological information!

Discretization

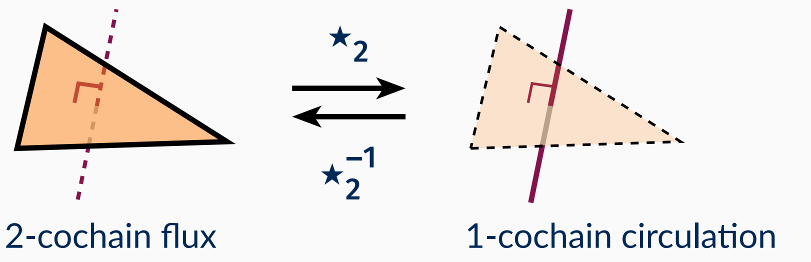
Discrete $\star$ takes a k-cochain to a $(n-k)$-cochain on the other (primal/dual) mesh

An approximation of the **metric** geometry

Many possible definitions. The standard $\star$ is a diagonal matrix of primal-dual volume ratios

$$\star_{ii} = \frac{|\sigma_i^*|}{|\sigma_i|}$$

Diagonality of $\star$ is the key to DEC's efficiency.



Implementation

DEC primitives are simple matrices and vectors ⇒ generic and composable!

Rust library: `dexterior` (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 visualization (2D only for now)

Summary

In summary, DEC represents

- geometry as a primal-dual pair of meshes
- differential forms as values on mesh elements (cochains)
- operators as matrices describing geometric relationships

Drawbacks:

- need for the dual mesh; sensitivity to mesh quality
- higher-order schemes are challenging to formulate and lose the diagonality of the Hodge star

Recommended reading

- **Desbrun, Kanso & Tong (2006)**. Discrete Differential Forms for Computational Modeling [1]
  - Concise but thorough summary of DEC theory, great intermediate resource.
- **Crane, de Goes, Desbrun & Schröder (2013)**. Digital geometry processing with discrete exterior calculus [2]
  - Detailed course materials with great visualizations.
- **Blair Perot & Zusi (2014)**. Differential Forms for Scientists and Engineers. [3]
  - Exterior calculus for beginners.
- **Myyrä (2023)**. Discrete Exterior Calculus and Exact Controllability for Time-Harmonic Acoustic Wave Simulation [4]
  - My own master's thesis, where I tried to give a layman-friendly introduction.
- **Hirani (2003)**. Discrete Exterior Calculus [5]
  - The thesis that coined DEC.

Case study: 2D acoustics

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Scalar wave equation for velocity potential $\boldsymbol{\Phi}$:

$$\frac{\partial^2 \boldsymbol{\Phi}}{\partial t^2} - c^2 \Delta \boldsymbol{\Phi} = 0$$

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expressed in terms of velocity $\boldsymbol{v} = \nabla \Phi$ and pressure $p = \frac{\partial \Phi}{\partial t}$ as a first-order system

$$\begin{cases} \frac{\partial p}{\partial t} - c^2 \nabla \cdot \boldsymbol{v} = 0 \\ \frac{\partial \boldsymbol{v}}{\partial t} - \nabla p = 0 \end{cases}$$

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$$\begin{cases} \frac{\partial p}{\partial t} - c^2 \nabla \cdot v = 0 \\ \frac{\partial v}{\partial t} - \nabla p = 0 \end{cases}$$

Converted to exterior calculus with 0-form $\overset{0}{\mathrm{p}}$ and 1-form $\overset{1}{\mathrm{v}}$:

$$\begin{cases} \frac{\partial \overset{0}{\mathrm{p}}}{\partial t} - c^2 \star d \star \overset{1}{\mathrm{v}} = 0 \\ \frac{\partial \overset{1}{\mathrm{v}}}{\partial t} - d \overset{0}{\mathrm{p}} = 0 \end{cases}$$

DEC spatial discretization

Replace $\overset{0}{\mathbf{p}}$, $\overset{1}{\mathbf{v}}$ with primal 0-cochain $\boldsymbol{P}$, $\boldsymbol{P}_i = \overset{0}{\mathbf{p}}(\boldsymbol{x}_i)$, and primal 1-cochain $\boldsymbol{V}$, $\boldsymbol{V}_i = \int_{e_i} \overset{1}{\mathbf{v}}$.

Replace $\boldsymbol{d}, \star$ with discrete $\mathbf{d}, \star$.

$$\Rightarrow \begin{cases} \frac{\partial P}{\partial t} - c^2 \star_0^{-1} \mathbf{d}_1^T \star_1 V = 0 \\ \frac{\partial V}{\partial t} - \mathbf{d}_0 P = 0 \end{cases}$$

Leapfrog timestepping

Place variables at staggered time instances and use central differences

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

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Multiply by Δt and reorganize, get the explicit timestep formulas

$$P^{n+1} = P^{n} + \Delta t c^2 \star_0^{-1} \mathbf{d}_1^T \star_1 V^{n+\frac{1}{2}}$$

$$V^{n+\frac{3}{2}} = V^{n+\frac{1}{2}} + \Delta t \mathbf{d}_0 P^{n+1}$$

(Conditionally stable with short enough Δt, subject to CFL condition)

Implementation with `dexterior`

Now that we have the timestep formulas

$$P^{n+1} = P^n + \Delta t c^2 \star_0^{-1} \mathbf{d}_1^T \star_1 V^{n+\frac{1}{2}}$$

$$V^{n+\frac{3}{2}} = V^{n+\frac{1}{2}} + \Delta t \mathbf{d}_0 P^{n+1}$$

implementation in code is very simple:

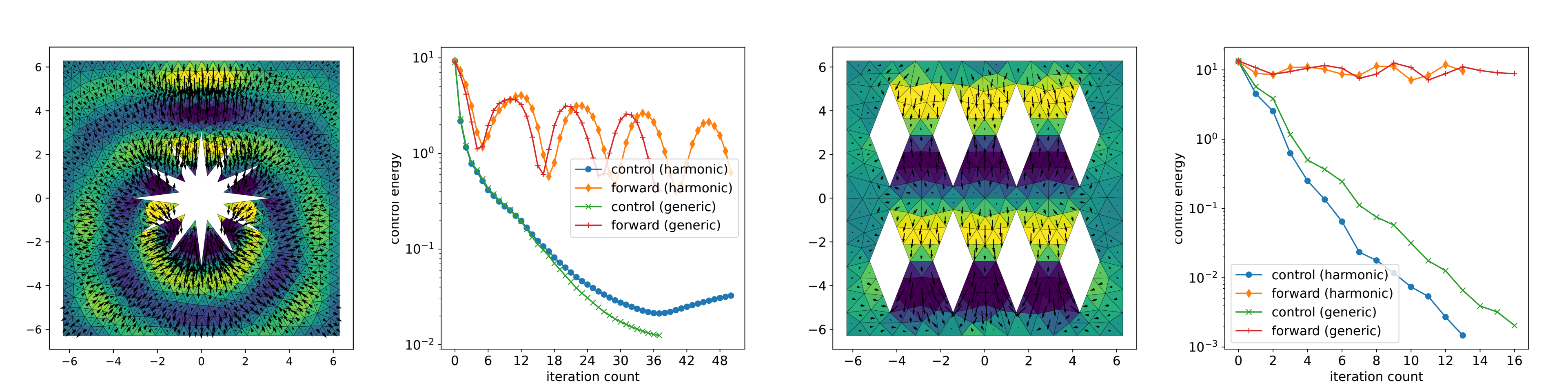
```
use dexterior::*;
let mesh = SimplicialMesh::new(vertices, indices);
let mut p: Cochain<Primal, 0> = mesh.integrate_cochain(...);
let mut v: Cochain<Primal, 1> = mesh.integrate_cochain(...);
loop {
  p += dt * c_sq * mesh.star() * mesh.d() * mesh.star() * &v;
  v += dt * mesh.d() * &p;
}
```

Results

Master's thesis [4], upcoming paper [6]

DEC + controllability-based optimization for time-harmonic acoustic scattering problems
+ alternative Hodge star for spatially harmonic problems

(using PyDEC – `dexterior` didn't exist yet)



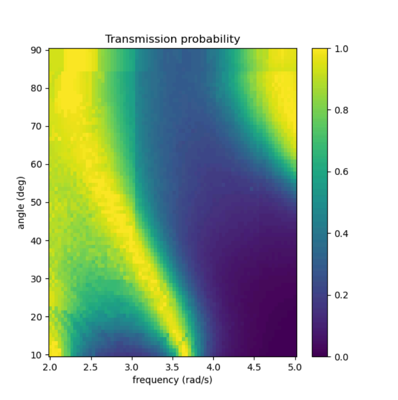
More applications

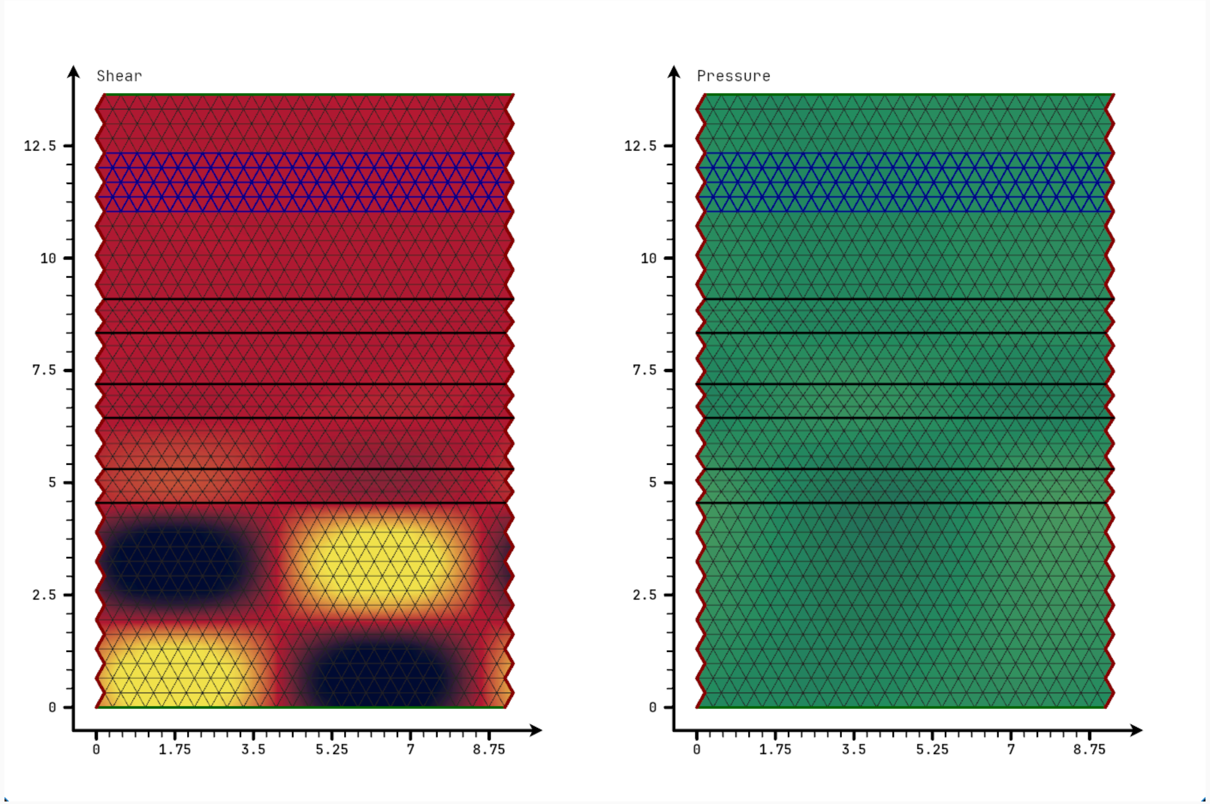
Phonon transmission

Ongoing work: elastic waves in vertically layered, horizontally periodic structures

Applications in nanoscale heat transport (current focus), seismology, etc.

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





Other works from our research group

Electromagnetics and generalized wave propagation problems (Räbinä et al.) [7], [8]

GPU-accelerated quantum mechanics (Kivioja) [9], [10]

Minkowski spacetime meshing (Mönkölä et al.) [11]

Higher-order discretizations (Lohi) [12]

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