Controlled time integration with discrete exterior calculus

Applications in electro-magnetism, acoustics and more

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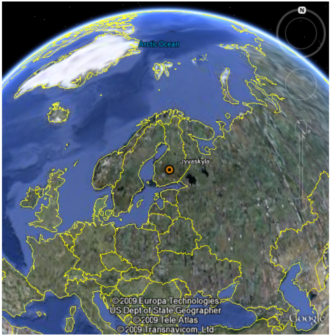
About us

Research group: Computational Field Theory

Members

- Tuomo Rossi
- Lauri Kettunen
- Sanna Mönkölä
- Tytti Saksa
- Mikael Myyrä
- Sampsa Kiiskinen
- Markus Kivioja



Formers members: Jukka Räbinä, Jonni Lohi, Joona Räty

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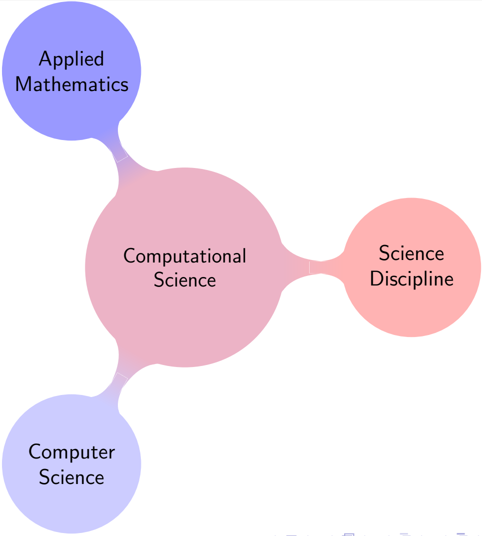
Computational Field Theory - Group's activities

- Algorithm / Method development
- Computational tools / Software development
- Applications in physics: wave propagation



Computational Field Theory - Group's activities

- "Systematization" of boundary value problems (BVPs) (Rossi et al. 2021)
    - Motivated by aim to solve several problems with a single software system
- Computational wave propagation: Application to wave problems in electromagnetism, acoustics, elastodynamics, quantum mechanics
- We look at the BVPs from the application and software point of view

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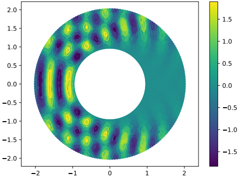
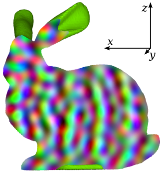
Computational wave propagation

- Time evolution of wave problems in acoustics, electro-magnetism, elasticity, quantum mechanics
- Discretization via discrete exterior calculus (DEC)
- Solving time-harmonic problems in time domain (not in frequency domain)
  - more suitable for some application areas, or for problems with a high wave number
  - Controlled time integration (controllability algorithm introduced by Roland Glowinski)





Acoustic wave propagation

For scalar v (0-form) and vector $\mathbf{p}$ (1-form), in $\Omega \times (0, T)$

$$\frac{\partial v}{\partial t} - c^2 \mathrm{div}\ \mathbf{p} = 0\ ,$$
$$\frac{\partial \mathbf{p}}{\partial t} - \mathrm{grad}\ v = 0\ .$$

$$\partial_t v - c^2 \star \mathrm{d} \star \mathbf{p} = 0\ ,$$
$$(-1)^n \star \partial_t \star \mathbf{p} - \mathrm{d}\ v = 0\ .$$

and boundary conditions and initial conditions
Notice, that if we select $v = \frac{\partial w}{\partial t}$, $\mathbf{p} = \mathrm{grad}\ w$, we obtain a more classical formulation of wave problem with variable w.

Electromagnetic wave propagation

For vector fields **b** (1-form) and **e** (2-form), in $\Omega \times (0, T)$

$$\frac{\partial \mathbf{b}}{\partial t} + \text{curl } \mathbf{e} = 0 \, ,$$
$$-\mu_0 \epsilon \frac{\partial \mathbf{e}}{\partial t} + \text{curl } \mathbf{b} = \mu_0 \mathbf{j} \, ,$$

$$\partial_t \mathbf{b} + \mathrm{d}\mathbf{e} = 0 \, ,$$
$$- \star \partial_t \star_\epsilon \mathbf{e} + \star \mathrm{d} \star_\mu \mathbf{b} = \star \mathbf{j} \, .$$

and boundary conditions and initial conditions

$\mathbf{b} = \mu_0 \mathbf{h}$, $\mathbf{d} = \epsilon \mathbf{e}$ $\qquad$ $\mathbf{b} = \star_\mu \mathbf{h}$, $\mathbf{d} = \star_\epsilon \mathbf{e}$

Generalized wave propagation, step 1

Observation (Räbinä, Kettunen, et al. 2018): A class of wave propagation problems (electromagnetism, sound propagation, elastic waves, quantum mechanics, etc.) can be characterized by a system of partial differential equations

$$\partial_t(\mathrm{M}\mathbf{u}) + \mathrm{D}\mathbf{u} = \mathbf{f} + \mathrm{F}\mathbf{u} \, ,$$

where

$$\mathrm{D} = \begin{bmatrix} & \mathrm{div} & & \\ \mathrm{grad} & & -\mathrm{curl} & \\ & \mathrm{curl} & & -\mathrm{grad} \\ & & -\mathrm{div} & \end{bmatrix} .$$

This framework coincides with Rainer Picard's "Mother PDE" suggesting a setting from which a large class of linear partial differential equations can be inherited. (Picard and McGhee 2011)

Generalized wave propagation, step 2: spacetime

Let symbols F and G denote formal sums of general differential forms. By the action principle, the conservation law is defined for such a general field. On a four dimensional differentiable manifold Ω with Minkowski metric, signature $(-,+,+,+)$, for $F = f^0 + \ldots + f^4$ and $G = g^0 + \ldots + g^4$, we obtain a system (Rossi et al. 2021):

$$\begin{bmatrix} \partial_t & & & & & \star\mathrm{d}\star & & \\ & \partial_t & & & -\mathrm{d} & & \star\mathrm{d}\star & \\ & & \partial_t & & & -\mathrm{d} & & \star\mathrm{d}\star \\ & & & \partial_t & & & -\mathrm{d} & \\ & \star\mathrm{d}\star & & & -\star\partial_t\star & & & \\ \mathrm{d} & & \star\mathrm{d}\star & & & \star\partial_t\star & & \\ & \mathrm{d} & & \star\mathrm{d}\star & & & -\star\partial_t\star & \\ & & \mathrm{d} & & & & & \star\partial_t\star \end{bmatrix} \begin{bmatrix} f^0 \\ f^1 \\ f^2 \\ f^3 \\ f_s^0 \\ f_s^1 \\ f_s^2 \\ f_s^3 \end{bmatrix} = \begin{bmatrix} g_s^0 \\ g_s^1 \\ g_s^2 \\ g_s^3 \\ g^0 \\ g^1 \\ g^2 \\ g^3 \end{bmatrix}.$$

where $\star\mathrm{d}\star f_s^1 = \operatorname{div} f_s^1$, $\star\mathrm{d}\star f_s^2 = \operatorname{curl} f_s^2$, $\star\mathrm{d}\star f_s^3 = \operatorname{grad} f_s^3$ and $\mathrm{d}f_s^0 = \operatorname{grad} f_s^0$, $\mathrm{d}f_s^1 = \operatorname{curl} f_s^1$, $\mathrm{d}f_s^2 = \operatorname{div} f_s^2$
($\star\star = (-1)^{p(n-p)+1}$ where p is the degree of the differential form and n is the dimension of our Minkowski manifold)

From general system of equations back to BVPs

- For Maxwell's equations in space and time, we choose $F = b + e \wedge dt = b + dt \wedge (-e)$ and $G = \star j - dt \wedge \star q$. This corresponds to setting $f_s^1 = -e$, $f^2 = b$, $g^1 = \star j$, and $g_s^0 = - \star q$, and by substituting these to the system of equation (to obtain the Maxwell's equations).
- Similarly, by appropriate choices, one may derive equations for e.g. acoustics, and non-relativistic Scrödinger equation.
- Small-strain elasticity can be modelled by extending the system to E-valued forms (corresponding to tensors).

Generalized model in spacetime

- DEC is a natural discretization tool,
- covers relativistic hyperbolic boundary value problems by nature,
- parabolic and elliptic problems are simplifications,
- space and time-stepping can be separated

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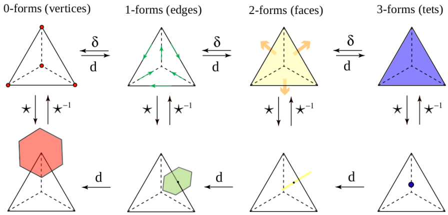
Discrete exterior calculus, DEC

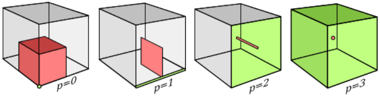
- DEC is based on the works by A. N. Hirani (2003), Desbrun, A. Hirani, and Marsden (2003) (generalization of the FDTD)
- In DEC, discrete forms are discretized as cochains.
- Discrete exterior derivative is defined with the help of a coboundary operator.
- The Stokes theorem holds exactly.



M. Desbrun, E. Kanso, Y. Tong. Discrete differential forms for computational modeling. In: ACM SIGGRAPH 2006 Courses. SIGGRAPH '06. Boston, Massachusetts: Association for Computing Machinery, pp. 39–54, 2006.

Discretization/approximation of Hodge star

- The Hodge star operator $\star$ maps a differential p-form to a differential $(n-p)$-form.
- The "discrete Hodge star" operator is a matrix mapping between the primal and dual mesh.
- For the dual grid, a circumcentric subdivision (producing an orthogonal dual)], one can straightforwardly choose a diagonal matrix as an approximation for the Hodge star (Delaunay-Voronoi duality)



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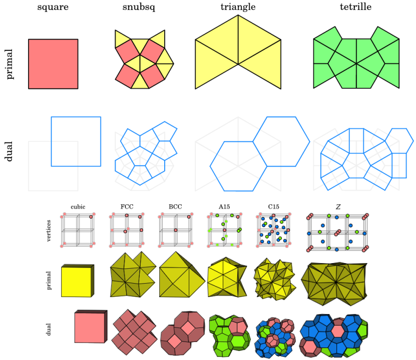
On choosing a mesh

For the quality of meshes in the case of DEC, one desires well-centered (or self-centered) simplices (or triangles), i.e. each circumcenter lies inside its associated simplex.



For a general geometry, there exist so-called Hodge optimized triangulations (HOT-meshes) (Mullen et al. 2011).

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Time integration

- Time stepping is done in a leapfrog manner.
- Leapfrog time stepping is conditionally stable: subject to the Courant-Friedrichs-Lewy (CFL) condition ($\Delta t < c\Delta x$).
- If we get a diagonal approximation for Hodge star ("a mass matrix"), leapfrog time stepping is fast (time integration is performed by a matrix multiplication at every time step)
- Utilizing preknown properties of the time-harmonic solution (depending on the wave number), we may derive a better approximation for the discrete Hodge star for time-harmonic waves. Such a "harmonic Hodge" can be presented as a diagonal matrix as well, and it seems to improve remarkably the accuracy of time-harmonic solutions

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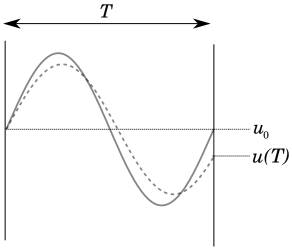
Controlled time integration

- In the controlled time integration, we do not solve the time-dependent problem directly but instead we accelerate the convergence of solution by minimizing the difference between an initial solution and the corresponding solution after one time period.
- The advantage of the mixed formulation is, that the related controllability problem takes place in $L^2(\Omega)^{n+1}$



Controlled time integration, some history

- Controllability methods by Glowinski et al. were first formulated basing on variational methods. (Bristeau, Glowinski, and Periaux 1993, 1998)
- For a scalar wave equation in a mixed formulation, controllability algorithm was proposed by Glowinski and Rossi 2006 (variational formulation).
- Theoretical framework on the controllability techniques has further been discussed by Pauly and Rossi 2011, generalizing the theory for a generalized Maxwell's equation in the context of differential forms.
- Chaumont-Frelet et al. (2022) combined discontinuous Galerkin method with the exact controllability in the context of Maxwell's equations.

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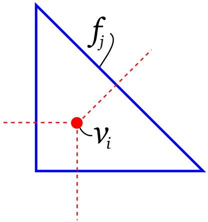
and boundary conditions and initial conditions



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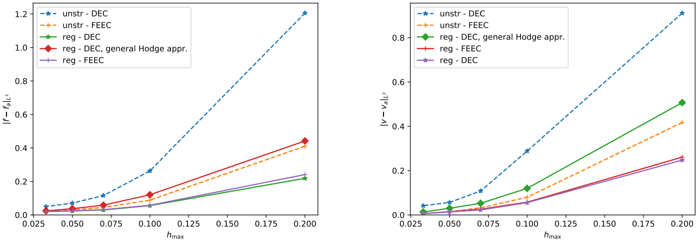
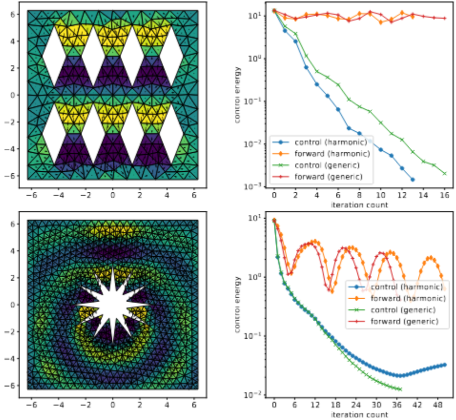
Acoustics, scattering from circular scatterer

Computational errors of solutions by the DEC and the FEEC (finite element exterior calculus) methods were very close to each other, when the diagonal approximation of Hodge was corrected with the "harmonic" multiplier. However, DEC's sensitivity to mesh quality is very visible (but time integration fast!).



Results published in (Saksa 2025). In numerical computations, the PyDEC software (Bell and A. N. Hirani 2012) was used for building the simplicial complexes and the matrices. For 3D case, see also (Rossi et al. 2021).

Acoustics, scattering from non-convex scatterer



Results published in (Myyrä 2026). In numerical computations, the PyDEC software (Bell and A. N. Hirani 2012) was used for building the simplicial complexes and the matrices.

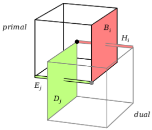
Electromagnetic wave propagation

For vector fields **b** (1-form) and **e** (2-form), in $\Omega \times (0, T)$

$$\frac{\partial \mathbf{b}}{\partial t} + \text{curl } \mathbf{e} = 0 \,,$$
$$-\mu_0 \epsilon \frac{\partial \mathbf{e}}{\partial t} + \text{curl } \mathbf{b} = \mu_0 \mathbf{j} \,,$$

$$\partial_t \mathbf{b} + \mathrm{d}\mathbf{e} = 0 \,,$$
$$-\star \partial_t \star \mathbf{e} + \star \mathrm{d} \star \mathbf{b} = \star \mathbf{j} \,.$$

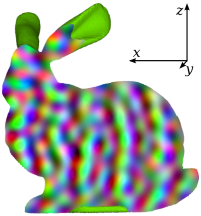
and boundary conditions and initial conditions

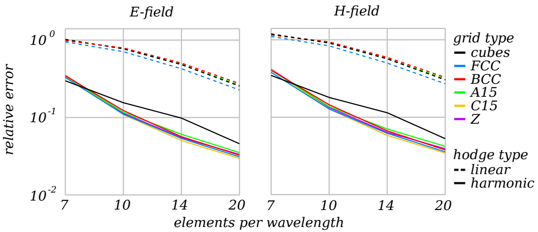


ϵ and μ_0 are embedded into the Hodge operators. (In general, material laws can be embedded into the Hodge operator.)

Electromagnetism, scattering of a plane wave from a non-convex obstacle

As an incident wave, we used a circularly polarized plane wave propagating in the direction of the positive x_1-axis. The outermost layer was implemented as a PML.





(Mönkölä, Räbinä, and Rossi 2023)

More

- Controlled time integration for meteor radar reflections in 3D (CPU parallelization)(Räbinä, Mönkölä, et al. 2016)
- A coupled problem of linear elasticity and acoustics (Räbinä, Kettunen, et al. 2018)
- Spacetime simulations (wave propagation in e.g. shrinking and rotating cavities) (Rossi et al. 2021) https://sites.google.com/jyu.fi/gfd/meshing/space-time-meshing
- Atomic Bose–Einstein condensates at ultra low temperature (GPU parallelization) (Räbinä, Kuopanportti, et al. 2018)
- Higher-order discretizations (Lohi 2022)

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Concluding remarks

- Discrete exterior calculus provides us with a diagonal mass matrix for fast time integration.
- Discrete exterior calculus is particularly sensitive to the quality of the mesh to achieve a desired solution accuracy.
- The controlled time integration has shown its potential for complex geometries, e.g. scattering problems with non-convex scatterers.
    - Harmonic Hodge correction increases accuracy.
- The flexibility of discrete exterior calculus from parallelization and its suitability for complex geometries makes it a competitive computing tool for wave applications in physics.

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Computational tools developed in Jyväskylä

- GFD Library By Räbinä (C++)
  https://sites.google.com/jyu.fi/gfd/
- Dexterior Library by Myyrä (Rust)
  https://codeberg.org/molentum/dexterior
- GpuDecGpe by Kivioja
  https://github.com/markus-kivioja/GpuDecGpe

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