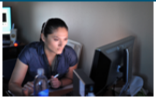
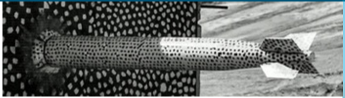
A (vector) bundle-valued discrete exterior calculus in $\mathbb{R}^3$





Chris Eldred (SNL)

Presented by:

Chris Eldred (SNL)

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September 3rd, 2025

Structure-Preserving Models of Continuum Mechanics

Want to build (numerical) models of physical system with same properties as continuous equations:

- Conservation laws: mass, momentum, energy, etc.
- Involution constraints: $\nabla \cdot \mathbf{B} = 0$, etc.
- Entropy behaviour: conserved by reversible dynamics, generated by irreversible dynamics (across shocks)

How can we do this?

- Obtain equations using *geometric mechanics* (GM; variational/Lagrangian, Hamiltonian, metriplectic, etc.) and discretize them using *structure-preserving* (SP) spatial and temporal discretizations, based on *exterior calculus*!

This talk will illustrate this in the context of discrete exterior calculus as a spatial discretization

Intro to "Modern" DEC

Where is DEC used?

- Electrodynamics (Maxwell)
  - FDTD, Yee scheme = spacetime DEC
- Low-Mach Fluids = Velocity-Based Formulations
  - Incompressible Flow, VVP Stokes: MAC scheme
  - GFD: Arakawa C-Grid, TRiSK (Dynamico/WAVETRISK, MPAS-O, ICON-IAP, PAM)
- Also: port-Hamiltonian, Cell method (Tonti)
- Key here is all quantities are *scalar-valued differential forms*

What about high-Mach fluids = momentum-based formulations?

This requires the use of *(vector) bundle-valued differential forms*, main subject of this talk!

Structure-Preserving Spatial Discretizations

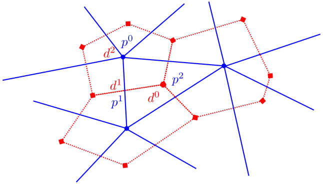
Structure preserving (ie. mimetic, compatible) = discrete version of (scalar-valued) exterior calculus

- Discrete analogues of key (exterior) calculus identities such as:
  - Annihilation/Exact Sequence: $\mathrm{d}\,\mathrm{d} = 0$
    - ex. $\nabla \cdot \nabla \times = 0$, $\nabla \times \nabla = 0$
  - Integration by Parts: $\langle \alpha, \mathrm{d}\,\beta \rangle - \langle \delta\,\alpha, \beta \rangle = \langle \alpha, \beta \rangle_{d\Omega}$
    - ex. $\int_\Omega a \nabla \cdot \mathbf{b} + \int_\Omega \nabla a \cdot \mathbf{b} = \int_{\partial\Omega} a\mathbf{b} \cdot \hat{\mathbf{n}}$
  - Hodge decomposition/deRham cohomology: $\alpha = \mathrm{d}\,\psi + \delta\,\phi + h$, with $\mathrm{d}\,h = \delta\,h = 0$
    - ex. $\mathbf{a} = \nabla\psi + \nabla \times \phi + \mathbf{h}$ with $\nabla \cdot \mathbf{h} = \nabla \times \mathbf{h} = 0$
    - Spaces ψ, ϕ and h have the correct dimension (depending on topology of manifold)

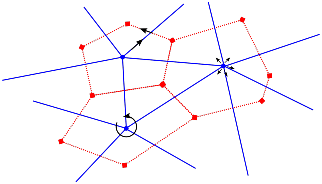
How does DEC achieve these?

Key ideas of DEC

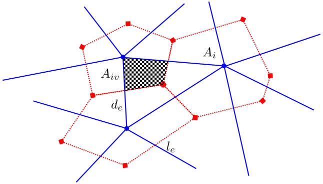
- Two grids in duality (straight and twisted , 1-1 relationship between k and $(n-k)$ cells on opposite grids
- Discrete differential forms are **integrated values** over **geometric entities**, 1-1 relationship between k-form and $(n-k)$-forms on opposite grids (**Hodge star**)
- Operators are either **topological** (exterior derivative, wedge product) or **metric** (Hodge star, inner product), discretize accordingly + separately



Staggering



Topological



Metric

Why use discrete exterior calculus (DEC)?

Useful Features of DEC (compared to FEEC)

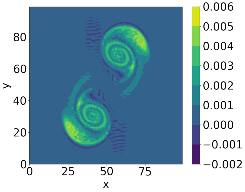
- Distinguishes between straight and twisted forms (especially important for electrodynamics and electromagnetic fluids)
- Pointwise limiting is easier (strong connections with existing staggered finite-volume methods)
- Explicit (no linear systems unless physical system needs them)

New-ish Developments in DEC at SNL

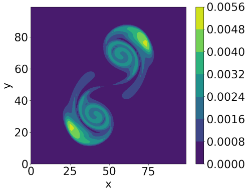
- Consistent treatment of boundaries + arbitrary boundary conditions
  - Inflow/outflow, slip and no-slip, etc.
- High-order Hodge stars on structured, uniform grids
- Structure-presering, high-resolution, oscillation-limiting, property-preserving (SPHROL-PP) Lie derivatives for arbitrary SVDFs

SPHROL-PP Transport Operators

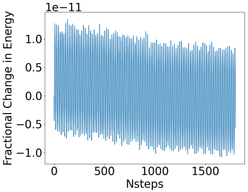
- **Structure-preserving**: Lie derivative $\mathscr{L}$ and diamond $\diamond$ are *discrete adjoints*
- **High-resolution**: *resolve sharp gradients* or *discontinuities* using as few grid points as possible
- **Oscillation-limiting**: reduce or eliminate *unphysical numerical oscillations*, especially in regions of sharp gradients or discontinuities
- **Property-preserving**: preserve solution properties ex. solution bounds (invariant domain) such as positivity of densities



Usual



SPHROL-PP



Energy

SPHROL-PP eliminates spurious oscillations, reduces overshoots/undershoots, still conserves

How exactly does a SPHROL-PP transport operator work?

- Split $\mathscr{L}_{\mathbf{u}}\alpha$ and $\alpha \diamond \beta$ into exterior derivative d and interior product i using Cartan's magic formula:

$$\mathscr{L}_{\mathbf{u}}\alpha = \mathrm{d}\, i_{\mathbf{u}}\alpha + i_{\mathbf{u}}\mathrm{d}\,\alpha \qquad \alpha \diamond \beta = \mathrm{d}\,\alpha \triangle \beta + \alpha \triangle \mathrm{d}\,\beta \tag{1}$$

- SP = discrete d using discrete exterior derivatives, obtain discrete $\triangle$ as discrete adjoint of i
- HROL = discretize i using *flowed-out definition* and (WENO-based) reconstructions
- PP = limit reconstructions using flux-corrected transport

Volume form version looks like "convential" schemes, k-form version is new
Has been done for arbitrary k-forms on unstructured grids
Have a similar operator for velocity self-advection term ($\frac{\nabla \times \mathbf{v}}{D} \times \mathbf{F}$)

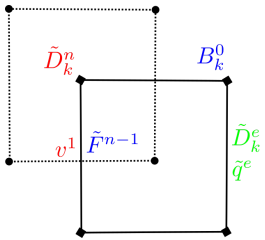
A DEC scheme for (low-Mach) neutral fluids

Advected densities model: n densities D_k ($k = 1, \dots, n$; ex. component masses ρ_i, entropic variable density $S = \rho\eta$) and velocity $\mathbf{v}$

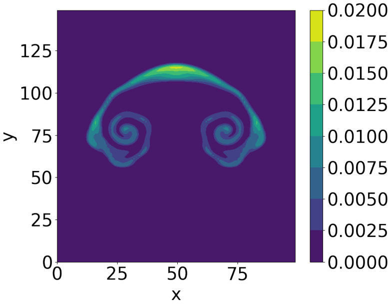
$$\begin{matrix} \frac{\partial \mathbf{v}}{\partial t} + \frac{\nabla\times\mathbf{v}}{D} \times \mathbf{F} + \sum_k \frac{D_k}{D} \nabla B_k = 0 \\ \frac{\partial D_k}{\partial t} + \nabla\cdot\left(\frac{D_k}{D}\mathbf{F}\right) = 0 \end{matrix} \quad \rightarrow \quad \begin{matrix} \frac{\partial \mathbf{v}}{\partial t} + \mathbf{Q}\,\mathbf{F} + \sum_k \tilde{D}_k \mathbf{D}_1 B_k = 0 \\ \frac{\partial D_k}{\partial t} + \tilde{\mathbf{D}}_2 \tilde{D}_k \mathbf{F} = 0 \end{matrix} \tag{2}$$

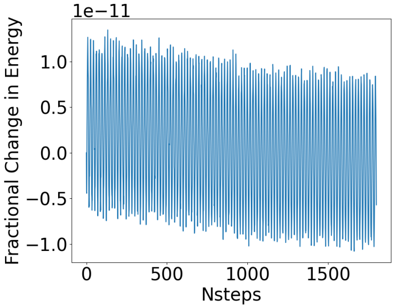
$$\mathbf{F} = \frac{\delta \mathscr{H}}{\delta \mathbf{v}} \qquad B_k = \frac{\delta \mathscr{H}}{\delta D_k} \qquad \mathbf{Q} = \frac{1}{2}\left[q^e\,\mathbf{W} + \mathbf{W}\,q^e\right] \tag{3}$$

- Choice of D_k and $\mathscr{H}[\mathbf{v}, D_k]$ closes the model: can get (thermal) shallow water, (moist) compressible Euler, (moist) anelastic, etc.
- Discrete $\mathscr{H}[\mathbf{v}, D_k]$ has Hodge stars/inner products (and wedge products), independent of topological properties



Quick example from atmospheric modelling





Conservation to **machine-precision** with spatial and temporal discretization (discrete gradients), including SPHROL-PP transport*

*- energy-conserving time integrator is not property-preserving yet

DEC for (tensor)-valued differential forms

BVDF DEC in $\mathbb{R}^n$

Focus on tensor-valued forms (key for continuum mechanics)

- In $\mathbb{R}^n$, tensor bundles become vector spaces instead of vector bundles
  - *Connection* is trivial, *global basis* for bundles
- Represent a tensor-valued k-form as r (size of tensor in components) scalars attached to a k-cell
  - SVDFs are just special case with $r = 1$
- BVDF DEC is essentially just *component-wise* version of SVDF DEC
  - Discrete exterior derivatives and Hodges stars both act on components independently
- Can formulate Lie derivatives and diamond operators exactly as in the SVDF case
- On general manifolds $\mathbb{M}$, much more complicated construction is needed

Let's see an application of this for compressible flow

Lie-Poisson Hamiltonian Formulation for Neutral Fluids

Lie-Poisson Hamiltonian formulation for momentum **m**, advected densities D_k

$$\frac{\partial \mathbf{m}}{\partial t} + \mathscr{L}_{\frac{\delta H}{\delta \mathbf{m}}} \mathbf{m} + \sum_k D_k \nabla \frac{\delta H}{\delta D_k} = 0 \quad (4)$$

$$\frac{\partial D_k}{\partial t} + \nabla \cdot \left(D_k \frac{\delta H}{\delta \mathbf{m}}\right) = 0 \quad (5)$$

System is closed by specifying D_k and $H[\mathbf{m}, D_k]$: different choices yield (thermal) shallow water, compressible Euler, etc.

To discretize, need a way to represent m and D_k, along with Lie derivatives $\mathscr{L}_{\frac{\delta H}{\delta \mathbf{m}}} \mathbf{m}$, $\nabla \cdot (D_k \frac{\delta H}{\delta \mathbf{m}})$ and diamond operator $D_k \nabla \frac{\delta H}{\delta D_k}$

Note: can extend to arbitrary advected quantities α noting that $\nabla \cdot (D_k \frac{\delta H}{\delta \mathbf{m}}) = \mathscr{L}_{\frac{\delta H}{\delta \mathbf{m}}} \alpha$ and $D_k \nabla \frac{\delta H}{\delta D_k} = \alpha \diamond \frac{\delta H}{\delta \alpha}$

DEC Spatial Discretization of LP Formulation

- D_k is a twisted volume form, **m** is a covector-valued twisted volume form
  - Both live at dual grid cell centers = unstaggered scheme
- Discretize Lie derivatives (and diamong operators) using structure-preserving, high-resolution, oscillation-limiting, property-preserving (SPHROL-PP) transport operators

Conserves total energy (locally) and (some) Casimirs

LP DEC scheme works well for *smooth solutions* ex. thermal shallow water; fails for *discontinuous solutions* ie high-mach compressible Euler. Why?

Why does LP DEC scheme fail for discontinuous solutions?

- The model is wrong: entropy is generated across shocks!
- Fix with a *thermodyamically compatible viscous regularization*
  - Closely related to ideas from Guermond, Brenner, Svard

$$\frac{\partial \mathbf{m}}{\partial t} + \cdots + \nabla \cdot (\varepsilon_{\mathbf{m}} \nabla \mathbf{m}) = 0 \tag{6}$$

$$\frac{\partial \rho}{\partial t} + \ldots \nabla \cdot (\varepsilon_{\rho} \nabla \rho) = 0 \tag{7}$$

$$\frac{\partial S}{\partial t} + \ldots \nabla \cdot (\varepsilon_{S} \nabla S) = \Pi \geq 0 \tag{8}$$

with $T\Pi = \varepsilon_{\mathbf{m}} \nabla \mathbf{m} \cdot \nabla \mathbf{u} + \varepsilon_{\rho} \nabla \rho \cdot \nabla \frac{\delta \mathscr{H}}{\delta \rho} + \varepsilon_{S} \nabla S \cdot \nabla \frac{\delta \mathscr{H}}{\delta S} \geq 0$ recalling $T = \frac{\delta \mathscr{H}}{\delta S}$. Relies on positive definiteness of Hessian $\frac{\delta^2 \mathscr{H}}{\delta^2 \mathbf{x}}$ and ε's.

Connections with entropy-stable schemes

Most (all?) entropy-stable schemes solve:

$$\frac{\partial \mathbf{m}}{\partial t} + \nabla \cdot (\mathbf{u}\,\mathbf{m}) + \nabla p = 0 \quad (9)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\,\mathbf{u}) = 0 \quad (10)$$

$$\frac{\partial h}{\partial t} + \nabla \cdot ((h+p)\,\mathbf{u}) = 0 \quad (11)$$

with a numerical fluxes that can be decomposed into *inviscid* and *regularization/viscous* parts ex. for ρ they are:

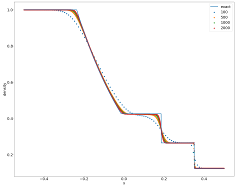
$$\nabla \cdot (\rho\,\mathbf{u}) \approx \nabla \cdot (\rho\,\mathbf{u}) + \nabla \cdot (\varepsilon \nabla \rho) \quad (12)$$

for a *flow and grid size dependent* ε, and further imply an equation of the form

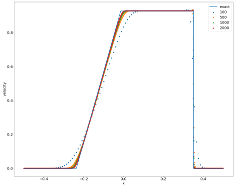
$$\frac{\partial S}{\partial t} + \nabla \cdot (S\,\mathbf{u}) + \nabla \cdot (\varepsilon \nabla S) = \Pi \geq 0 \quad (13)$$

The LP scheme with regularization just makes this process explicit!

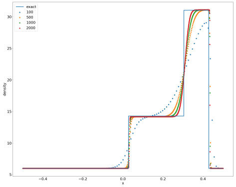
LP DEC Scheme Results- Sod Shock Tube and Toro Problem 5



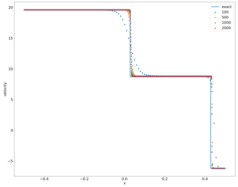
Density ρ



Velocity $\mathbf{u}$



Density ρ

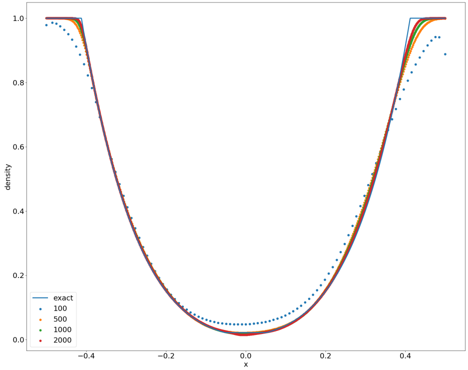


Velocity $\mathbf{u}$

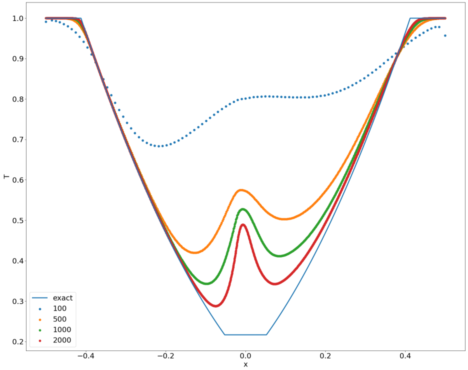
Regularized LP DEC scheme correctly captures shock location and magnitude, no unphysical oscillations

- Rusanov viscosity $\varepsilon = \frac{1}{2}|\Delta x| s_{max}$ with minbee limiter
- 7th order WENO reconstructions
- 2nd order Hodge stars
- SPPRK3 time stepping

LP DEC Scheme Results- Enfield123



Density ρ



Temperature T

Density is good, but there is a temperature anomaly
Regularization is generating uphysical entropy!

Ongoing/Future Work and Conclusions

Electromagnetic Fluids I- Continuous

Single component electromagnetic fluid with (elementary) charge q

$$\frac{\partial \mathbf{m}}{\partial t} + \mathscr{L}_{\frac{\delta \mathrm{H}}{\delta \mathbf{m}}} \mathbf{m} + \rho \nabla \frac{\delta \mathrm{H}}{\delta \rho} + S \nabla \frac{\delta \mathrm{H}}{\delta S} + q\rho \frac{\delta \mathrm{H}}{\delta \mathbf{D}} + q\rho \frac{\delta \mathrm{H}}{\delta \mathbf{m}} \times \mathbf{B} = 0 \tag{14}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \frac{\delta \mathrm{H}}{\delta \mathbf{m}}) = 0 \tag{15}$$

$$\frac{\partial S}{\partial t} + \nabla \cdot (S \frac{\delta \mathrm{H}}{\delta \mathbf{m}}) = 0 \tag{16}$$

$$\frac{\partial \mathbf{D}}{\partial t} - \nabla \times \frac{\delta \mathrm{H}}{\delta \mathbf{B}} - q\rho \frac{\delta \mathrm{H}}{\delta \mathbf{m}} = 0 \tag{17}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \frac{\delta \mathrm{H}}{\delta \mathbf{D}} = 0 \tag{18}$$

Involution constraints $\nabla \cdot \mathbf{B} = 0$, $\nabla \cdot \mathbf{D} = q\rho$, connects ρ and $\mathbf{D}$ equations

$\mathbf{B}$ is straight 2-form, $\mathbf{D}$ is twisted 2-form

Electromagnetic Fluids II- Discretization

Discretization (essentially) just combines neutral fluids scheme with Yee scheme!

$q\rho \frac{\delta H}{\delta \mathbf{m}}$, $q\rho \frac{\delta H}{\delta \mathbf{m}} \times \mathbf{B}$ and $q\rho \frac{\delta H}{\delta \mathbf{D}}$ are interior product terms that can be treated using SPHROL-PP ideas

Key features of proposed scheme:

- For **any** choice of Hodge stars (Hamiltonian), reconstruction and property-preserving limiting
  - Conserves energy (locally) and some Casimirs
  - Gets involution constraints
- Both **B** and **D** equations are strong form
- Likely requires same (fluid) regularization as neutral fluids scheme

Conclusions

- GM-EC formulations + SP discretizations are a powerful tool for building (numerical) models of physical systems with key properties: conservation laws, involution constraints, entropy behaviour, etc.
- Key examples for SVDFs using DEC:
  - FDTD/Yee scheme (electrodynamics)
  - MAC scheme (velocity-based incompressible fluids)
  - TRiSK scheme (velocity-based low-Mach fluids)
- BVDF DEC developed, used for discretization of Lie-Poisson (momentum-based) formulations
  - Works for smooth flows and (some) discontinuous flows

Future Work

- Implement and test LP DEC scheme for electromagnetic fluid models
- Better (flow-adaptive) viscous regularization, alternative reconstructions: active only at shocks? entropy-based viscosity? how to handle contact discontinuities?
- DEC Improvements
  - HO Hodge stars on unstructured and hierachical/AMR meshes
  - Hierarchical/AMR DEC
  - Extend BVDF DEC to manifolds
  - SPRHOL-PP transport for BVDFs
- SciML DEC: learn Hodge stars (ie Hamiltonians) and reconstructions, use in both full order and surrogate models
- Extend ideas to solid mechanics and/or shock hydrodynamics

Thanks for listening! Questions?

Very incomplete list of (biased) references (contact me for many more!):

Eldred2022 C. Eldred, W. Bauer. **Understanding TRiSK from a discrete exterior calculus perspective**, arxiv

Eldred2024a C. Eldred **Extending discrete exterior calculus with boundaries**, in preparation

Eldred2024b C. Eldred, M. Waruszewski, M. Norman, M. Taylor **Structure-preserving, high-resolution, oscillation-limiting, property-preserving (SPHROL-PP) transport operators in discrete exterior calculus**, in preparation

Eldred2024c C. Eldred **A discrete exterior calculus scheme for momentum-based formulations of neutral fluids**, in preparation