Structure-preserving, high-order and oscillation-limited transport operators

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(I) What is a transport operator?

- Many quantities of interest in geophysical fluid dynamics are *advected* (*transported*) quantities: they obey an equation of the form

$$\frac{\partial a}{\partial t} + \mathscr{L}_{\mathbf{u}} a = 0$$

where $\mathscr{L}_{\mathbf{u}} a$ is the *Lie derivative*. This is the most general form of a *transport operator*.

- Examples: entropy, potential temperature, mass, moisture/salt/trace species, potential vorticity, etc.
- In this work we focus on densities (scalar-valued volume or n-forms), for which the Lie derivative is:

$$\frac{\partial a}{\partial t} + \nabla\cdot(a\mathbf{u}) = 0$$

(II) Transport operators and structure-preservation

- The equations of motion for a general fluid in $\mathbb{R}^2$ with K advected densities* D_k ($k = 1,\dots,K$), total mass $\rho = \sum_k c_k D_k$ and absolute velocity $\mathbf{v}$ can be written in *symplectic form* using a *Hamiltonian* $\mathscr{H}[\mathbf{v}, D_k]$ as

$$\frac{\partial \mathbf{v}}{\partial t} + q\mathbf{F}^T + \sum_k \frac{D_k}{\rho}\nabla B_k = 0$$

$$\frac{\partial D_k}{\partial t} + \nabla\cdot\left(\frac{D_k}{\rho}\mathbf{F}\right) = 0$$

with potential vorticity $q = \frac{\nabla^T\cdot\mathbf{v}}{\rho}$, where $\mathbf{F} = \frac{\delta\mathscr{H}}{\delta\mathbf{v}}$ and $B_k = \frac{\delta\mathscr{H}}{\delta D_k}$ are *functional derivatives* of $\mathscr{H}$. Examples: (thermal) shallow water, (moist) compressible Euler in Cartesian coordinates**

- Using predicted variables $\mathbf{x} = (\mathbf{v}, D_k)$ and symplectic operator $\mathbb{J}[\mathbf{x}]$ this is

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbb{J}\frac{\delta\mathscr{H}}{\delta\mathbf{x}}$$

where

$$\mathbb{J} = -\begin{pmatrix} q\square^T & \frac{D_k}{\rho}\nabla\square \\ \nabla\cdot(\frac{D_k}{\rho}\square) & 0 \end{pmatrix} \qquad \frac{\delta\mathscr{H}}{\delta\mathbf{x}} = \begin{pmatrix}\mathbf{F} \\ B_k\end{pmatrix}$$

- **Key point**: each D_k leads to a corresponding term (the $\diamond$ operator) in the $\mathbf{v}$ equation. In other words, $\mathbb{J}$ is anti-symmetric under the appropriate inner product. **This is the structure that should be emulated in a numerical method.**
- Note: can write transport equations for D_k in terms of *transport velocity* $\mathbf{U} = \frac{\mathbf{F}}{\rho}$ as

$$\frac{\partial D_k}{\partial t} + \nabla\cdot(D_k\mathbf{U}) = 0$$

* When quantities such as temperature T that are not (purely) advected are predicted, this type of formulation is still useful because part of their dynamics is described by transport operators with corresponding diamond operator terms in the $\mathbf{v}$ equation.

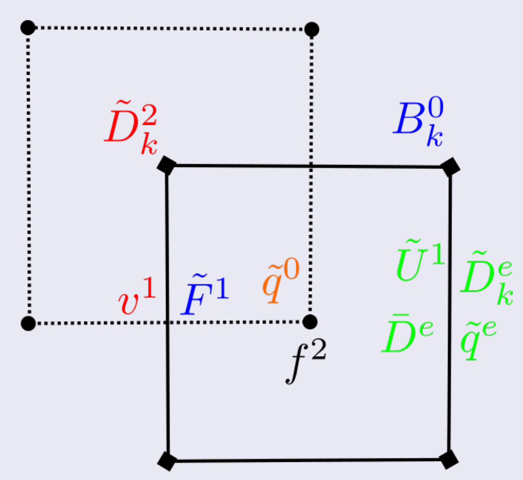
** Similar related formulations apply in $\mathbb{R}^3$ (or for arbitrary 2D/3D manifolds, in fact), in other coordinate systems (such as Lagrangian, height or mass-based terrain-following vertical coordinates) and with other types of advected quantities; and for various dynamical (hydrostatic, semi-compressible, etc.) and metric (shallow, traditional, etc.) approximations.

(III) Structure-preserving numerical transport operators

- We use a *discrete exterior calculus* (DEC) based approach, essentially an extension of the *TRiSK scheme*:

$$\frac{\partial v^1}{\partial t} + \mathbf{Q}\tilde{F}^{n-1} + \sum_k \frac{\tilde{D}_k^e}{\tilde{\rho}^e}\mathbf{D}_1 B^0 = 0$$

$$\frac{\partial \tilde{D}_k^n}{\partial t} + \tilde{\mathbf{D}}_n\left(\frac{\tilde{D}_k^e}{\tilde{\rho}^e}\tilde{F}^{n-1}\right) = 0$$



where $\tilde{F}^{n-1} = \frac{\delta\mathscr{H}}{\delta v^1}$ and $B^0 = \frac{\delta\mathscr{H}}{\delta\tilde{D}_k^n}$ for discrete Hamiltonian $\mathscr{H}[v^1, \tilde{D}_k^n]$.

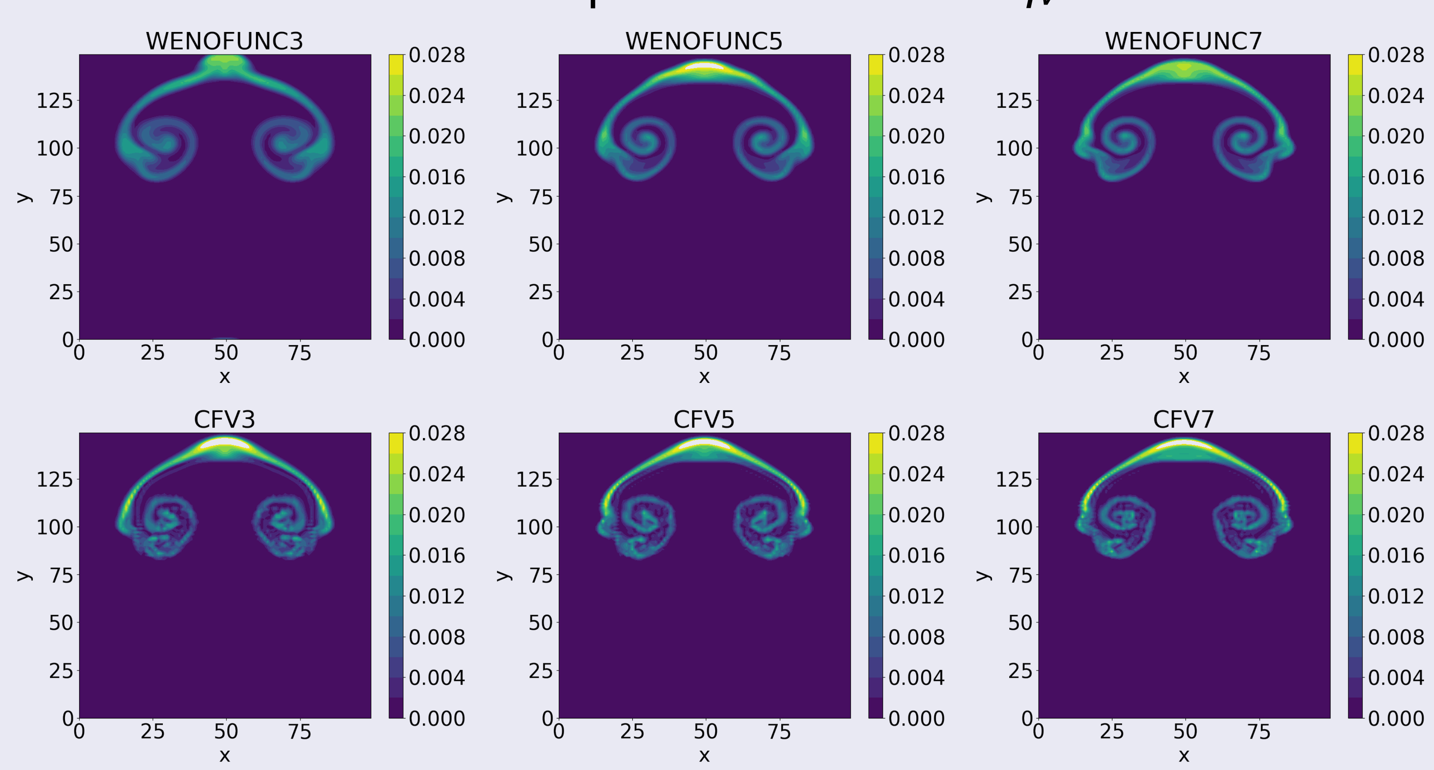
- Can write transport equation for $\tilde{D}_k^n$ in terms of transport velocity $\tilde{U}^{n-1}$ (defined through $\tilde{F}^{n-1} = \tilde{\rho}^e\tilde{U}^{n-1}$) as

$$\frac{\partial \tilde{D}_k^n}{\partial t} + \tilde{\mathbf{D}}_2(\tilde{D}_k^e\tilde{U}^{n-1}) = 0$$

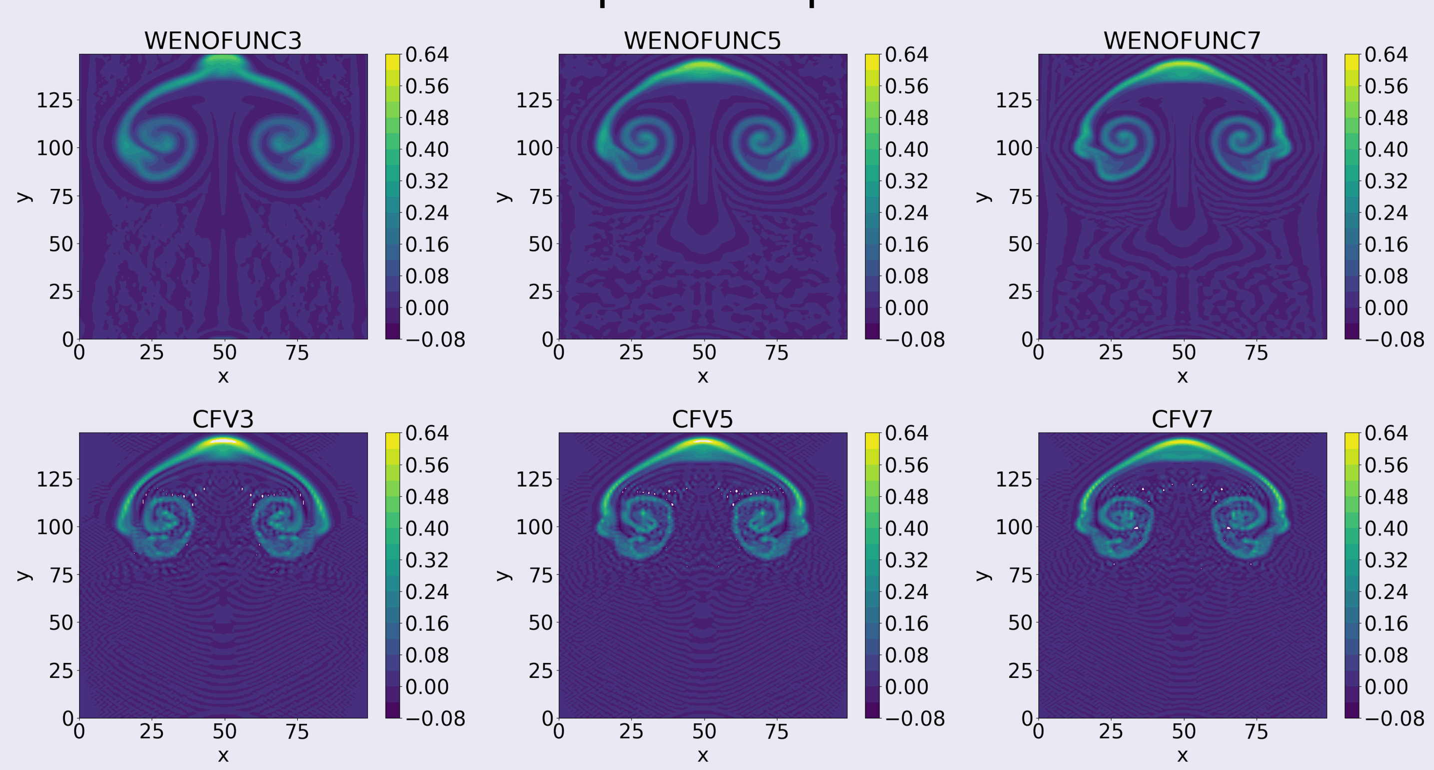
Key: This is a standard staggered FV transport scheme, and $\tilde{D}_k^e$ are arbitrary (high-order) *centered finite volume* (CFV) or *weighted essentially non-oscillatory* (WENO) reconstructions.

(IV) Results

Water vapor concentration q_v

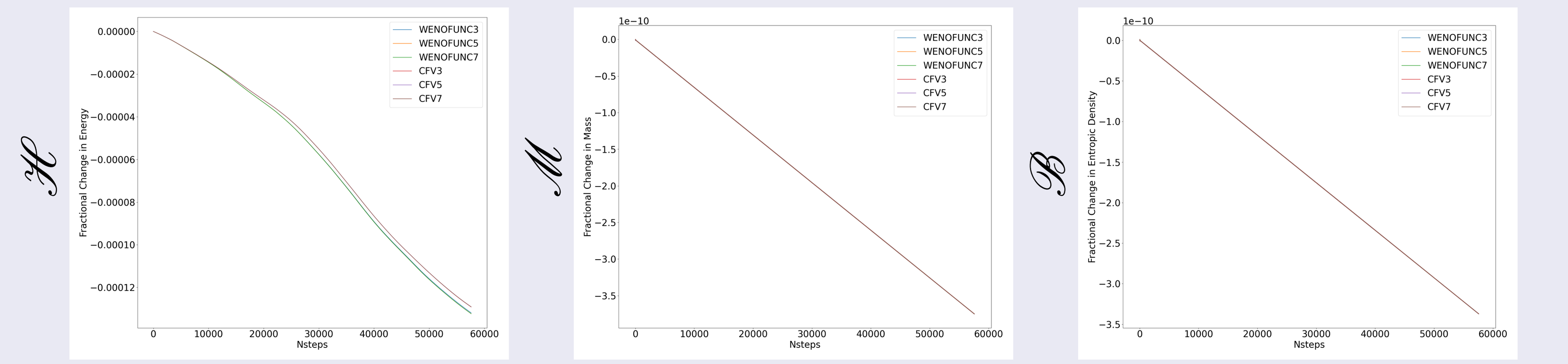


Potential temperature perturbation θ'



Results for q_v and θ' from the rising bubble (RB) test case for the moist compressible Euler (MCE) equations, comparing 3rd, 5th and 7th order WENO (top row in each figure) and CFV (bottom row in each figure) reconstructions. WENO eliminates spurious oscillations while retaining high resolution of small scale features (low dissipation). Increasing the order of accuracy with WENO decreases the dissipation and improves effective resolution, while with CFV this leads to noisier solutions.

(V) Conserved Quantities



Conservation of total energy $\mathscr{H}$ (left), total mass $\mathscr{M}$ (middle), and total entropy $\mathscr{B}$ (right) for the MCE RB test case. Using both CFV and WENO reconstructions, $\mathscr{M}$ and $\mathscr{B}$ are conserved to machine-precision, while $\mathscr{H}$ is conserved to time truncation error.

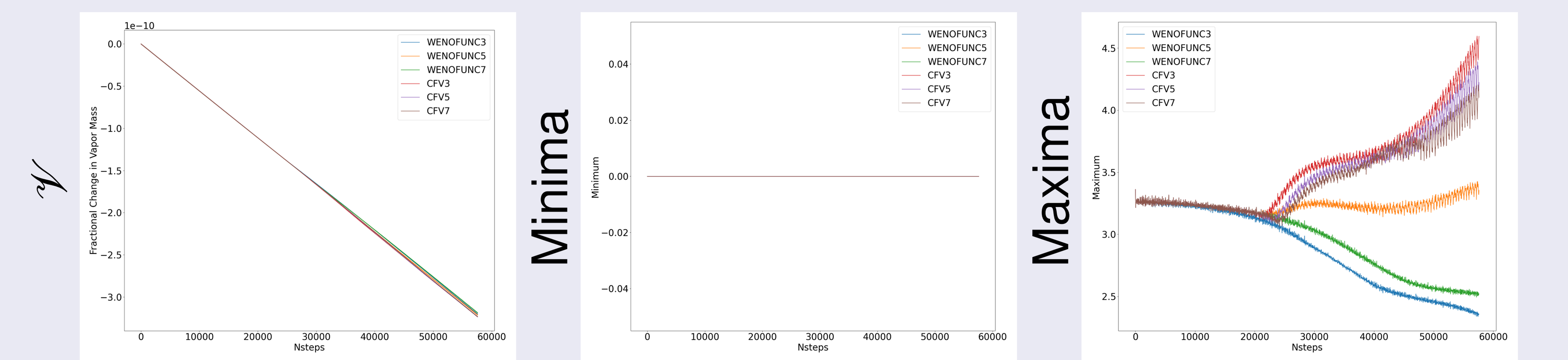
(VI) Adding monotonicity/positive-definiteness

- Monotonicity/positive-definiteness can be enforced by introducing flux-corrected transport (FCT) operators $\mathbf{\Phi}_k$ (could be identity for some $\tilde{D}_k^n$) that scales fluxes $\frac{\tilde{D}_k^e}{\tilde{\rho}^e}\tilde{F}^{n-1} = \tilde{D}_k^e\tilde{U}^{n-1}$ at grid cell edges:

$$\frac{\partial v^1}{\partial t} + \dots + \sum_k \mathbf{\Phi}_k\frac{\tilde{D}_k^e}{\tilde{\rho}^e}\mathbf{D}_1 B^0 = 0$$

$$\frac{\partial \tilde{D}_k^n}{\partial t} + \tilde{\mathbf{D}}_n\left(\mathbf{\Phi}_k\frac{\tilde{D}_k^e}{\tilde{\rho}^e}\tilde{F}^{n-1}\right) = 0$$

- This works well because WENO reconstructions are *essentially monotonic* ($\rightarrow$ positive-definite), therefore $\mathbf{\Phi}_k$ are close to identity



Conservation of total water vapor mass $\mathscr{V}$ (left) and ρ_v minima (left) / maxima (right) for the MCE RB test case. For both CFV and WENO reconstructions $\mathscr{V}$ is conserved to machine-precision and ρ_v is positive-definite, while WENO significantly limits overshoots in the ρ_v maxima compared to CFV.

(VII) Conclusions

- We have developed a structure-preserving, high-order and oscillation-limiting transport operator for densities, with an optional FCT-type approach to obtain monotonicity/positive-definiteness.
- Results from MCE RB test case demonstrate the effectiveness of WENO reconstructions compared to CFV reconstructions.

(VIII) Future Work

- Develop structure-preserving, high-order and oscillation-limiting transport operators (i.e. $\mathscr{L}_{\mathbf{u}} a$ and $\diamond$) for other types of real and (co)-tangent bundle-valued k-forms (e.x. scalars, vectors, tensors)
  - Useful for magnetohydrodynamics (MHD) and other charged fluid models, alternative GFD formulations, complex fluids, etc.
  - Already developed for "velocity self-advection" operator $q\mathbf{F}^T$ in 2D, a type of *interior product* (this is $\mathbf{Q}$ operator)
- Extend ideas to spacetime formulations for fluids
  - Can this lead to structure-preserving semi-Lagrangian approaches?

(IX) References

- C. Eldred, W. Bauer. **An interpretation of TRiSK-type schemes from a discrete exterior calculus perspective**, *in preparation*
- C. Eldred, M. Norman, M. Taylor. **Extending TRiSK with higher-order Hodge stars and WENO/FCT**, *in preparation*