

Discretization I

What do you have to say about a numerical model/scheme ?

- Nice !
- Ugly !
- I like it !
- I hate it !

Hmm... let's try and be more factual

- Accurate
- Conservative
- Dispersive
- Dissipative / diffusive
- Positive / monotone
- Stable
- Explicit vs Implicit
- Local vs global
- We care about these properties because they are present in the continuous laws of motion
- Can we obtain them in a discretized model ? How ?
- All ? Independently ? Incompatibilities ?
- Implications for performance / parallelism ?

Context : Cartesian geometry

- Conservation laws for continuous models
- From the continuous to the discrete, and what you lose
- Numerical dispersion : illustration with the rotating shallow-water equations

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What they are

- Lagrangian vs integral
- Adiabatic vs diabatic
- Robust vs fragile

Where they come from

- Kinematics vs dynamics
- Variational principles, symmetries and dynamical conservation laws

What they imply

stability

Conservation laws for continous models

Integral conservation law : $\mathcal{M} = \int \rho dx dy dz$ $\frac{d\mathcal{M}}{dt} =$ boundary terms • Mass Total water / other species $\mathcal{H} = \int \left(\frac{u^2 + v^2 + w^2}{2} + gz + e\left(\frac{1}{\rho}, s, r\right)\right) \rho \mathrm{d}x \mathrm{d}y \mathrm{d}z$ Energy • (angular) momentum • Potential enstrophy $\mathcal{L} = \int a^2 \cos^2 \Phi \left(\Omega + \dot{\lambda} \right) \mu \mathrm{d}\lambda \mathrm{d}\phi \mathrm{d}z$ $\mathcal{Z} = \int \rho q^2 \mathrm{d}x \mathrm{d}y \mathrm{d}z$ $\frac{Ds}{Dt} = 0 \qquad \frac{Dq}{Dt} = 0$ Lagrangian conservation law : examples • Entropy

- Water / other species
- Potential vorticity

Lagrangian conservation laws => infinitely many integral conservation laws

Example : potential vorticity => potential enstrophy

$$\frac{\mathrm{d}}{\mathrm{d}t} \int f(q,s)\rho \mathrm{d}x \mathrm{d}y \mathrm{d}z = boundary \text{ terms}}$$

Conservation laws : adiabatic vs diabatic

- irreversible processus => extra source / flux terms
 - total energy : heating
 - momentum : viscous stresses (boundary)
- Exception : mass

Actual physics are irreversible but very little : frictionless limit Relevant conservation laws ? cf Thuburn, JCP 2008

https://wiki.ucar.edu/download/attachments/25037023/14-Thuburn-Conservation.pdf?api=v2

Focus on adiabatic conservation laws, i.e. those that hold when irreversible physics is neglected

Conservation laws : kinematic vs dynamical

 Kinematic conservation law : true for any equation of motion (e.g. Hydrostatic vs nonhydrostatic)

$$\mathcal{M} = \int \rho \mathrm{d}x \mathrm{d}y \mathrm{d}z$$

$$\frac{Ds}{Dt} = 0$$



• Dynamical conservation law : depends on the equation of motion ...

$$\mathcal{L} = \int a^2 \cos^2 \Phi \left(\Omega + \dot{\lambda} \right) \mu d\lambda d\phi dz$$
$$\mathcal{H} = \int \left(\frac{u^2 + v^2 + w^2}{2} + gz + e\left(\frac{1}{\rho}, s, r \right) \right) \rho dx dy dz$$

Back to the origin of dynamical conservation laws



Lagrangian least action principle for fluid flow (Eckart, 1960; Morrison, 1998)

inertia Coriolis pressure gravity

$$\frac{D\dot{\mathbf{x}}}{Dt} + 2\mathbf{\Omega} \times \dot{\mathbf{x}} + \frac{1}{\rho}\nabla p + \nabla \Phi = 0$$

$$\delta \int \mathcal{L}dt = 0$$

$$\mathbf{L} = \mathcal{K} + \mathcal{C} - \mathcal{P} = \int L(\mathbf{x}, \dot{\mathbf{x}}, \rho, s)dm$$

$$\mathcal{K} = \frac{1}{2}\int \dot{\mathbf{x}} \cdot \dot{\mathbf{x}}dm$$

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$$\mathcal{L} = \int (\mathbf{U} \cdot \mathbf{x}) \cdot \dot{\mathbf{x}} + gz - e(\frac{1}{\rho}, s)$$

$$L(\mathbf{x}, \dot{\mathbf{x}}, \rho, s) = \frac{\dot{\mathbf{x}} \cdot \dot{\mathbf{x}}}{2} + (\mathbf{\Omega} \times \mathbf{x}) \cdot \dot{\mathbf{x}} - gz - e\left(\frac{1}{\rho}, s\right)$$

$$\frac{D}{Dt} \frac{\partial L}{\partial \dot{\mathbf{x}}} = \frac{1}{\rho} \nabla \left(\rho^2 \frac{\partial L}{\partial \rho}\right) + \frac{\partial L}{\partial \mathbf{x}}$$

$$E = \dot{\mathbf{x}} \cdot \mathbf{v} - L$$
energy
$$\frac{\partial}{\partial t} \left(\rho \mathbf{v}\right) - \nabla \left(\rho^2 \frac{\partial L}{\partial \rho}\right) + \operatorname{div} \left[\rho \dot{\mathbf{x}} \otimes \mathbf{v}\right] = \rho \frac{\partial L}{\partial \mathbf{x}}$$
Flux-form momentum budget
$$B = \mathbf{v} \cdot \dot{\mathbf{x}} - \rho \frac{\partial L}{\partial \rho} - L$$
Bernoulli function
$$\frac{\partial \mathbf{v}}{\partial t} + \frac{\nabla \times \mathbf{v}}{\rho} \times \rho \mathbf{u} + \nabla B - T \nabla s = 0$$

$$q = \frac{1}{\rho} (\nabla \times \mathbf{v}) \cdot \nabla s$$

$$\frac{Dq}{Dt} = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \frac{\nabla \times \mathbf{v}}{\rho} \times \rho \mathbf{u} + \nabla B - T \nabla s = 0$$

Crocco's theorem = curl-form

Potential vorticity

Conservation laws for continous models

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What they imply

• stability

$$\int f(q,s)\rho \mathrm{d}x \mathrm{d}y \mathrm{d}z$$

Casimir (kinematic) invariants

$$\mathcal{H} = \int \left(\frac{u^2 + v^2 + w^2}{2} + gz + e\left(\frac{1}{\rho}, s, r\right)\right) \rho \mathrm{d}x \mathrm{d}y \mathrm{d}z$$
 Energy

$$\mathcal{L} = \int a^2 \cos^2 \Phi \left(\Omega + \dot{\lambda} \right) \mu \mathrm{d}\lambda \mathrm{d}\phi \mathrm{d}z$$

Absolute angular momentum (AAM)

Conservation laws for continous models : what they imply Energy-Casimir stability theory

• consider some integral invariant

$$\mathcal{E} = \mathcal{H} - \int f(s)\rho \mathrm{d}x \mathrm{d}y \mathrm{z}$$
pseudo-energy



- suppose that
- => stationary and stable flow !

$$\delta \mathcal{E} = 0$$



Sufficient stability criterion

Conservation laws for continous models : what they imply Energy-Casimir stability theory

$$\mathcal{E} = \mathcal{H} - \int f(s) \rho \mathrm{d}x \mathrm{d}y \mathrm{z}$$

pseudo-energy

$$\delta \mathcal{E} = \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \int \left(\frac{1}{2} \left(\mathbf{u} + \varepsilon \delta \mathbf{u}\right)^2 + gz + e - f\right) \rho \mathrm{d}x \mathrm{d}y \mathrm{d}z$$
$$= \int \mathbf{u} \cdot \delta \mathbf{u} \rho \mathrm{d}x \mathrm{d}y \mathrm{d}z \qquad \mathbf{u} = \mathbf{0}$$

$$gz + h = f(s)$$

Montgomery potential

$$T = \frac{\mathrm{d}f}{\mathrm{d}s}$$

$$\begin{split} \delta \mathcal{E} &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \int \left(gz + e\left(\rho + \varepsilon\delta\rho, s\right) - f(s)\right) \left(\rho + \varepsilon\delta\rho\right) \mathrm{d}x \mathrm{d}y \mathrm{d}z \\ &= \int \left(gz + e + \frac{p}{\rho} - f\right) \delta\rho \mathrm{d}x \mathrm{d}y \mathrm{d}z \\ \delta \mathcal{E} &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \int \left(gz + e\left(\rho, s + \varepsilon\delta s\right) - f(s + \varepsilon\delta s)\right) \rho \mathrm{d}x \mathrm{d}y \mathrm{d}z \\ &= \int \left(T - \frac{\mathrm{d}f}{\mathrm{d}s}\right) \delta s\rho \mathrm{d}x \mathrm{d}y \mathrm{d}z \end{split}$$

$$\delta \mathcal{E}=0$$
Hydrostatic balance

$$\delta^2 \mathcal{E} > 0$$
Static stability ds/dz > 0

Conservation laws for continous and discrete models

More conserved integral invariants, more guarantees of stability

$$\int f(q, s)\rho dx dy dz \qquad \qquad \text{Casimir (kinematic) invariants}$$

$$\mathcal{H} = \int \left(\frac{u^2 + v^2 + w^2}{2} + gz + e\left(\frac{1}{\rho}, s, r\right)\right) \rho dx dy dz \qquad \qquad \text{Energy}$$

$$\mathcal{L} = \int a^2 \cos^2 \Phi \left(\Omega + \dot{\lambda}\right) \mu d\lambda d\phi dz \qquad \qquad \text{Absolute angular momentum (AAM)}$$

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Discrete degrees of freedom

- Discrete representations of scalar and vector fields
- Interpolation/reconstruction/projection ; order of accuracy
- Immediate consequences : (non-)preservation of algebraic identities

We assume that the following has already been done :

A set of equations has been chosen :

thermodynamics, geometry, hydrostatic/NH/Boussinesq

- A flow representation has been chosen : Eulerian vs non-Eulerian vertical coordinate
- Prognostic variables have been chosen
- It is known how to obtain diagnostic variables : local or non-local (e.g. elliptic) problem

Now we want to represent each field (prognostic, diagnostic) by a large but finite set of numbers.

- How to do it ? basic examples
- How to apply operations (algebraic, differential) to these discrete representations ?
- Consequences for the properties of the scheme ?

Simplest idea :

- Sample field(s) at a number of points
- Those points usually form a *mesh*
- Interpolate between these points as needed





Charney et al., 1950

Interpolation is a *reconstruction* problem :

- Data : M values of function f at points xi
- Unknown : function g in D-dimensional space with the same values as f at xi
- If D>M : over-conditioned problem => least-squares
- Once g has been found, use it instead of f to compute values and derivatives where needed



Geophysical flow fields not very smooth : high-order (>4) interpolation probably not worth the cost (see Mavriplis, 2011)

Typical spaces for g :

- Polynomials
- Splines
- Radial basis functions (RBF)
- ..

Interpolation is a *reconstruction* problem :

- Data : M values of function f at points xi
- Unknown : function g in D-dimensional space with the same values as f at xi
- If M>D : over-conditioned problem => least-squares
- Once g has been found, use it instead of f to compute values and derivatives where needed



- 2 data enough for 1D linear interpolation
- Interpolated values 2nd-order accurate
- gradient 1st-order accurate
- except at midpoint : second-order accurate gradient
- superconvergence : extra accuracy at some special points

Simplest idea : interpolation

- Sample field(s) at a number of points
- Those points usually form a *mesh*
- Interpolate between these points as needed

Another idea : « histopolation »

- Data = field integrated over each mesh cells
- Use cell data and nearest neighbors to reconstruct field
- Typical of finite volume methods



Multidimensional reconstruction

10 Quadratic

20 Cubic



D 1 Constant x y x² xy y² x³ x²y xy² y³ 3 Linear 6 Quadratic 10 Cubic **15 Quartic** D Constant 1 4 Linear

3D

хуz $x^2 y^2 z^2 xy xz yz$ $x^{3}y^{3}z^{3}x^{2}yx^{2}z^{2}y^{2}xy^{2}z^{2}z^{2}xz^{2}yxyz$

for order-n reconstruction

1D : D ≥ n $2D : D \ge n(n+1)/2$

 $3D: D \ge (d+1)^3/3$

N local DxD linear systems to solve (pre-computation) Store NxD weights

High-order reconstruction rapidly very costly !

Cartesian or 2Dx1D meshes more efficient

Representation of vector fields



Different quantities possibly placed at different places : *staggered meshes*

Representation of vector fields

Strong recent trend in various fields of computational physics : *discrete differential geometry (see Thuburn & Cotter, 2012)*

- Describe fields through their integrals over geometric objects
- Match geometric object (point, line, surface, volume) and « nature » of field



 Scalar field 0D scalar field pointwise value Momentum line integral 1D covariant ٠ integral across surface 2D Flux contravariant ٠ integral over cell 3D • Density mass-weighted scalar field

Representation of scalars and vectors : implications

No shortage of discrete representations of scalar and vector fields

- Which algebraic identities survive/fail at the discrete level ?
- How to analyse the behavior that *emerges* from a certain combination of choices ?

$$\nabla f(a,b) = \frac{\partial f}{\partial a} \nabla a + \frac{\partial f}{\partial b} \nabla b$$
$$\operatorname{div}(f\mathbf{u}) = \mathbf{u} \cdot \nabla f + f \operatorname{div} \mathbf{u}$$

$$\int \mathbf{u} \cdot \nabla f + \int f \operatorname{div} \mathbf{u} = 0$$

$$\int_{\Omega} \mathrm{div} \, \mathbf{F} \mathrm{d}\Omega = \int_{\partial \Omega} \mathbf{F} \cdot \mathrm{d} \mathbf{\Sigma}$$

usually *fails*

usually fails ... but

often **doable :** compatible discretizations of grad and div Taylor, 2010

often **works** : with flux-form, yields conservation of linear integral invariants **Finite-volume approach**

> Enough for conservation of nonlinear invariants ? More later ...



Which algebraic identities survive/fail at the discrete level ?

$$\int_{\Omega} \operatorname{div} \mathbf{F} d\Omega = \int_{\partial \Omega} \mathbf{F} \cdot d\mathbf{\Sigma}$$
$$\int_{\Sigma} (\nabla \times \mathbf{v}) \cdot d\mathbf{\Sigma} = \oint_{\partial \Sigma} \mathbf{v} \cdot d\mathbf{l}$$
$$\int_{AB} \nabla f \cdot d\mathbf{l} = f(B) - f(A)$$
$$\nabla \times (\nabla f) = 0$$
$$\operatorname{div} (\nabla \times \mathbf{v}) = 0$$

often **works** : together with flux-form, yields *conservation of linear invariants* **Finite-volume approach**

often easy using discrete differential geometry

important for vorticity dynamics



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Why analyze the RSW equations rather than the full 3D equations ?

- Simpler
- Disentangle issues related to vertical and horizontal discretization
- 3D hydrostatic modes separate into vertical structure equation and horizontal propagation problem

Basic idea : wave propagation reveals how the different fields are coupled to each other

- Hopefully numerical wave propagation resembles physical wave propagation ...
- Many bad surprises ahead !
- If equations include many effects (forces), hard to have all couplings right
- Damage control : do at least the fast waves well



 $\frac{\partial v'}{\partial t} + f(y)u' + \frac{\partial p'}{\partial u} = 0$

$$w' = \frac{1}{gH_n} \frac{\partial p'}{\partial t} \qquad \Rightarrow$$

-200u -1,5

RSW : exact dispersion relationship



$$\omega^2(k) = f^2 + K^2 c^2$$
Inertia Gravity

Recap : waves in 3D stratified Boussinesq

Vertical density profile (stratification) determines N(z), eigenvalues c⁻² and baroclinic structure W(z)

$$N^{-2}(z)\frac{\mathrm{d}W}{\mathrm{d}z^2} + c^{-2}W = 0$$

$$\partial_t p' + c^2 \left(\partial_x u' + \partial_y v' \right) = 0$$

$$\partial_t u' - fv' + \partial_x p' = 0$$

$$\partial_t v' + fu' + \partial_x p' = 0$$

 $N^2 = -\frac{g}{\rho} \frac{\mathrm{d}\rho}{\mathrm{d}z}$

$$\begin{array}{l} p'\sim \exp i\left(kx+ly-\omega t\right)\\ \omega^2(k)=f^2+K^2c^2 \qquad K^2=k^2+l^2\\ \text{Rossby radius } \mathsf{R}_{d}\text{=c/f} \end{array}$$



Do the waves propagate numerically as in the continuous model ?

- Numerical integrations in time
- Look for eigenmodes and frequencies
 - Regular mesh (Cartesian / Hexagonal / Triangular) : Fourier transform => analytic dispersion relationship (*Randall, 1994*)
 - Unstructured mesh : numerical (Weller et al., 2012)

RSW : numerical dispersion relationship



Usually better to *stagger* a field and its derivative Or dissipate high spatial frequencies (but reduces effective model resolution)

RSW : numerical dispersion relationship

i+1

Usually better to *stagger* a field and its derivative => C-grid



- Looks much better
- Gravity-waves propagate physically due to velocity – mass staggering
- But:
 - u and v at different sites
 - Coriolis term requires averaging
 - Rossby radius unresolved => Inertial waves too slow



(Randall, 1994)



C-grid staggering on unstructured mesh

RSW : numerical dispersion relationship

Gravity waves want u-v staggered ; inertial waves want u-v collocated => many possible trade-offs



Excellent dispersion but must solve Poisson problems

Regular polygonal C-grids



Imbalance in the number of degrees of freedom => numerical branches in the dispersion relationship

General polygonal grids : more possibilities, more problems ...



(h) Voronoi cube, 864 cells, 3,192 DOFs

... and solutions : see Thuburn (2008), Thuburn et al. (2009, 2014), ...

(g) 960 kites, 2,880 DOFs





(d) rotated skipped, 866 cells, $\Delta t = 3600 \text{ sec}$ (e) hexagonal, 642 cells, $\Delta t = 3600 \text{ sec}$ (f) 1,280 triangles, $\Delta t = 3600 \text{ sec}$. $\ell_2(q) = 4.4 \times 10^{-6}$ $\ell_2(q) = 1.8 \times 10^{-6}$ $\ell_2(q) = 3.1 \times 10^{-7}$



FIG. 7. Relative vorticity on the dual grid after 5 days for the linearized shallow water equations simulating a linearized version of Williamson et al. (1992), test case 2.

Conservation laws

- Generic due to variational principle underlying the adiabatic equations of motion
- Nonlinear integral invariants guarantee stability close to certain base flows
- *Linear* integral invariants (mass, species) can be preserved by a *finite-volume* approach

From the continuous to the discrete, and what you lose

- Many ways to *represent* prognostic and diagnostic fields
- Determines to a great extent how they *couple* to each other
- Most algebraic identities lost
- Certain important vector-differential identities can be preserved
- Care required to avoid bad surprises with numerical dispersion unphysical branches unphysical propagation of small-scale modes propagative => stationary but also stationary => propagative

References

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