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Write equations of motion as

$$\frac{\partial \mathbf{x}}{\partial t} + \mathbb{J}(\mathbf{x}) \frac{\delta \mathcal{H}}{\delta \mathbf{x}} = 0 \tag{1}$$

Why?

$$\mathbb{J} = -\mathbb{J}^T \qquad \mathbb{J} \frac{\delta \mathcal{C}}{\delta \mathbf{x}} = 0 \tag{2}$$

Exposes conservation properties: energy (anti-symmetry), Casimirs (mass, entropy, potential vorticity, enstrophy, etc.)

Discrete conservation ↔ preserve properties of $\mathbb{J}$
How? Mimetic (structure-preserving) discretizations!

Works for reversible (entropy-conserving) dynamics

example: shallow water equations

$$\begin{aligned} \frac{\partial h}{\partial t} + \nabla \cdot (h\mathbf{v}) &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + q(h\mathbf{v})^T + \nabla(\frac{\mathbf{v}\cdot\mathbf{v}}{2} + gh) &= 0 \end{aligned}$$

Energy (=Hamiltonian)

$$\mathcal{H}[h, \mathbf{v}] = \int g\frac{h^2}{2} + h\frac{\mathbf{v}\cdot\mathbf{v}}{2}$$

$$\frac{\delta\mathcal{H}}{\delta h} = gh + \frac{\mathbf{v}\cdot\mathbf{v}}{2} \qquad \frac{\delta\mathcal{H}}{\delta\mathbf{v}} = h\mathbf{v}$$

So

$$\begin{aligned} \frac{\partial h}{\partial t} + \nabla \cdot (\frac{\delta\mathcal{H}}{\delta\mathbf{v}}) &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + q(\frac{\delta\mathcal{H}}{\delta\mathbf{v}})^T + \nabla(\frac{\delta\mathcal{H}}{\delta h}) &= 0 \end{aligned}$$

Quasi-Hamiltonian Numerical Models

Well-established approach to dynamical core design, can combine with time integration

- Shallow water (momentum and vorticity-divergence): Salmon (2004, 2005, 2007), Eldred (2017)
- Dry, fully compressible, Eulerian : Gassmann (2013)
- Lagrangian & mass-based, deep-atmosphere quasi-hydrostatic: Tort & Dubos (2015), Tort et. al 2015
- Compatible finite elements : Cotter, Thuburn, Shipton, Eldred, Wimmer, Bauer, Lee (2012+)
- Moist non-hydrostatic, non-Eulerian coordinate, spectral elements / mimetic finite differences : Taylor et. al (2019)
- Energy-conserving time stepping : Eldred (2019)

Big question: what about physics parameterizations and irreversible processes?

Physical processes conserve energy and either conserve entropy (**reversible**) or generate entropy (**irreversible**)

ex. reversible: transport/advection
ex. irreversible: viscous dissipation, phase changes

What is the geometric structure that underlies irreversible processes? → Metriplectic

Hamiltonian (reversible) and Metric, dissipation (irreversible)

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbb{J}(\mathbf{x})\frac{\delta \mathcal{H}}{\delta \mathbf{x}}(\mathbf{x}) + \mathbb{M}(\mathbf{x})\frac{\delta \mathcal{S}}{\delta \mathbf{x}}(\mathbf{x})$$

Applies to many areas of physics i.e. complex fluids, MHD, electrodynamics, multicomponent/multiphase fluids

Consider a single component fluid undergoing viscous dissipation and heat conduction. The dynamics are described by the compressible Navier-Stokes-Fourier (NSF) equations:

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} + \nabla\Phi + \frac{1}{\rho}\nabla p - \frac{1}{\rho}\nabla\cdot\sigma_{fr} &= 0 \\ \frac{\partial S}{\partial t} + \nabla\cdot(\rho s\mathbf{v}) + \frac{1}{T}\nabla\cdot\mathbf{j}_h - \frac{1}{T}\nabla\mathbf{u} : \sigma_{fr} &= 0 \\ \frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) &= 0 \end{aligned}$$

The stress tensor σ_{fr} and heat flux $\mathbf{j}_h$ are given by

$$\sigma_{fr} = \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + (\zeta - \frac{2}{3}\mu)(\nabla\cdot\mathbf{u})\mathbb{I} \qquad \mathbf{j}_h = -\kappa\nabla T$$

with thermal conductivity κ, shear viscosity μ and bulk viscosity ζ.

Navier-Stokes-Fourier equations are DNS scale: Actual geophysical models use resolutions that are much lower! What do we do?

One approach: Treat subgrid-scale parameterizations by analogy with parameterization of molecular-scale irreversible processes

examples: finite-differences Gassmann (2015, 2018), compatible FE + energy-conserving time integration Eldred (current)

Limitations:

- Only resolved scale energy and entropy
- No memory: immediate (single time step) energy conversions and entropy generation
- Local: subgrid-scale processes affect only a single grid cell

Can we do better? How?

What are the big questions here?

- How do existing parameterizations fit (or not fit) into a geometric framework?
- Can this inform the development of energetically and thermodynamically consistent versions of these parameterizations? Novel approaches?
- Can we write down a single set of equations that is used consistently for the entire model (physics and dynamics)? For all scales?
- Resolved vs. unresolved reservoirs of energy and entropy, flows of various types of energy (and entropy) through reservoirs?
- Should parameterizations be purely irreversible? Or involve reversible processes as well?

Physics-Dynamics ~~Coupling~~ Decoupling

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