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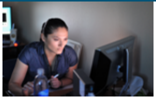
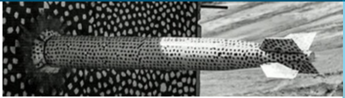
Multiscale geometric mechanics formulations for GFD parameterization





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The equations of GFD

- For fully resolved scales (micro/DNS scale, approx O(1) cm), the equations of GFD are well-understood*, ex. compressible Navier-Stokes-Fourier:

$$
\begin{aligned}
\frac{\partial \mathbf{v}}{\partial t} + \nabla \times \mathbf{v} \times \mathbf{u} + \alpha \nabla p + \nabla \phi &= \frac{1}{\rho} \nabla \cdot \sigma^{\mathrm{fr}} \\
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\
\frac{\partial S}{\partial t} + \nabla \cdot (S \mathbf{u}) &= \frac{1}{T} \left(\sigma^{\mathrm{fr}} : \nabla \mathbf{u} - \nabla \cdot (T \mathbf{j}_s) \right)
\end{aligned}
$$

- Key feature of these equations is **physical consistency**:
  - conservation of energy by both reversible and irreversible processes (1st law of thermodynamics)
  - conservation of thermodynamic entropy by reversible processes and generation of thermodynamic entropy by irreversible processes (2nd law of thermodynamics)

*- multi-component flows with condensed phases are still an area of active research

The problem of parameterization

- Cannot afford to run numerical models for GFD at fully resolved scales (O(1) cm): instead we run at O(100) m at best (usually much coarser)!
- Scale mismatch leads to problem of parameterization: how to represent the effects of unresolved scales on the resolved scales = multiscale models
- Some modern approaches in GFD:
  - superparameterization/multiscale modeling framework (MMF)
  - higer-order closure models such as SHOC/CLUBB
  - scale aware models such as eddy diffusivity/mass flux (EDMF)
- Unfortunately, these approaches to this problem break physical consistency

How can physically consistent parameterizations be developed?
Step back: what underlies physical consistency in fully resolved equations?

Geometric mechanics formulations

- Geometric mechanics formulations (Lagrangian/variational, Hamiltonian, single + double generator bracket, metriplectic, GENERIC) provides a framework to understand physical consistency
- The key elements are:
  - A set of degrees of freedom x
  - A *Lagrangian* $\mathscr{L}[x]$ with associated Hamiltonian $\mathscr{H}[x]$: (essentially) the sum of all the relevant energies in the system ex. kinetic, potential, internal, etc.
  - An entropy $\mathscr{S}[x]$: the sum of all the relevant entropies in the system
  - A dissipation potential $\Phi[x]$: The rate at which irreversible processes generate entropy
- These pieces can be combined to get both reversible and irreversible dynamics
- In the end they just express the exchange of energy and entropy between various reservoirs: kinetic, internal, potential, etc.

Physical consistency in geometric mechanics formulations

- Reversible dynamics come from a *variational principle* applied to Lagrangian $\mathscr{L}[x]$, with associated *Hamiltonian* formulation:

$$\delta \int_{t_1}^{t_2} \mathscr{L}[\mathbf{x}] = 0 \qquad \frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \{\mathscr{F}, \mathscr{H}\}$$

- Irreversible dynamics come from a *constrained variational principle* (by dissipation potential $\Phi[x]$) applied to Lagrangian $\mathscr{L}[x]$, with associated *bracket (single/double generator, metriplectic, GENERIC)* formulation:

$$\delta \int_{t_1}^{t_2} \mathscr{L}[\mathbf{x}] = 0 \qquad \frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \{\mathscr{F}, \mathscr{H}\} + (\mathscr{F}, \mathscr{S})$$

- Physical consistency is built in through symmetries in the Lagrangian $\mathscr{L}[x]$ and properties of $\Phi[x]$: ensures that Poisson brackets $\{,\}$ and metric brackets $(,)$ have the appropriate properties

These formulations describe all physically consistent equations in GFD, at fully resolved scales. What about multiscale approaches?

Multiscale geometric mechanics formulations

Key Idea: Introduce degrees of freedom to (partially) describe the unresolved (subgrid, represent subgrid variability) scales: x', use these to develop the key elements of geometric mechanics formulations: $\mathscr{L}$, $\mathscr{S}$, Φ

Specifically:

- Express physical quantities in terms of resolved $\bar{x}$ and unresolved x' parts
- Parameterize averaged $\hat{\mathscr{L}}[\bar{x}, x']$ Lagrangian and dissipation potential $\hat{\Phi}[\bar{x}, x']$ in terms of resolved $\bar{x}$ and unresolved x'
- Apply usual techniques (constrained variational principle) on $\hat{\mathscr{L}}[\bar{x}, x']$ and $\hat{\Phi}[\bar{x}, x']$ to get equations of motion for both resolved and unresolved dofs
- Physical consistency is "built in" if appropriate symmetries and properties are preserved in $\hat{\mathscr{L}}[\bar{x}, x']$ and $\hat{\Phi}[\bar{x}, x']$

Difficulty is in choice of appropriate $\bar{x}$ and x', and how to construct $\hat{\mathscr{L}}[\bar{x}, x']$ and $\hat{\Phi}[\bar{x}, x']$. Some ideas are given in the next few slides

0th Order Model

- No subgrid dofs: $x' = 0$
- No irreversible processes: $\hat{\Phi} = 0$
- Lagrangian takes same form as fully resolved case: $\hat{\mathscr{L}}[\bar{x}]$ is just $\mathscr{L}[x]$ with x replaced by $\bar{x}$

$$
\begin{aligned}
\frac{\partial \bar{\mathbf{v}}}{\partial t} + \nabla \times \bar{\mathbf{v}} \times \bar{\mathbf{u}} + \bar{\alpha} \nabla \bar{p} + \nabla \bar{\phi} &= 0 \\
\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}}) &= 0 \\
\frac{\partial \bar{S}}{\partial t} + \nabla \cdot (\bar{S} \bar{\mathbf{u}}) &= 0
\end{aligned}
$$

This is the usual starting point for dynamical cores in GFD, with "physics" added to the right-hand side in a somewhat arbitrary manner that breaks physical consistency and requires the use of fixers

1st Order Model

- No subgrid dofs: $x' = 0$
- Treat subgrid processes using same form as physically irreversible processes: $\hat{\Phi}[\bar{x}]$ is just $\Phi[x]$ with x replaced by $\bar{x}$
- Lagrangian takes same form as fully resolved case: $\hat{\mathscr{L}}[\bar{x}]$ is just $\mathscr{L}[x]$ with x replaced by $\bar{x}$

$$\frac{\partial \bar{\mathbf{v}}}{\partial t} + \nabla \times \bar{\mathbf{v}} \times \bar{\mathbf{u}} + \bar{\alpha} \nabla \bar{p} + \nabla \bar{\phi} = \frac{1}{\bar{\rho}} \nabla \cdot \bar{\sigma}^{\mathrm{fr}}$$

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

$$\frac{\partial \bar{S}}{\partial t} + \nabla \cdot (\bar{S} \bar{\mathbf{u}}) = \frac{1}{\bar{T}} \left(\bar{\sigma}^{\mathrm{fr}} : \nabla \bar{\mathbf{u}} - \nabla \cdot (\bar{T} \bar{\mathbf{j}}_s) \right)$$

with $\bar{\sigma}^{\mathrm{fr}}$ and $\bar{\mathbf{j}}_s$ parameterized in terms of $\bar{x}$ in essentially the same way as NSF equations (i.e. using *thermodynamic forces* adapted to vertical/horizontal split)

This is an approach pioneered by Almut Gassmann: the 1st (to my knowledge) physically consistent treatment of physics parameterizations

Issues with 1st Order Model and moving beyond it

- $\mathscr{L}$ (and entropy) are highly nonlinear functions of $\mathbf{x}$: $\overline{\mathscr{L}[\mathbf{x}]} \neq \mathscr{L}[\bar{\mathbf{x}}]$
- $\mathscr{L}[\bar{\mathbf{x}}]$ has only resolved energy reservoirs (similar for $\mathscr{S}[\bar{\mathbf{x}}]$)
- Most subgrid processes in the atmosphere and ocean are unresolved reversible processes: different mechanics and types of energy and entropy exchanges than irreversible processes
- Can we do better? We think so! How?
  - Add TKE and TPE to $\mathscr{L}[\bar{x}, x']$, parameterized in terms of new unresolved dofs that represent subgrid variability: ex. entropy variance $(\theta')^2$, moisture variance $(q_v')^2$, Reynolds stress tensor $\mathbf{R}$, etc.
  - Use a dissipation potential $\bar{\Phi}[\bar{x}, x']$ parameterzed in terms of these new unresolved dofs
  - Some important progress for kinetic energy, with Reynolds stress tensor $\mathbf{R}$ serving as new subgrid dof
  - Internal/potential energy parts are much trickier, subject of current work by Thomas and myself

Model with Stress Tensor

- Add turbulent kinetic energy $\rho\kappa$ to $\mathscr{L}$, with $\kappa = \frac{1}{2}\mathrm{Tr}\mathbf{R}$
- Assume **R** is advected (Lie-dragged) by the flow

$$\frac{\partial \bar{\mathbf{v}}}{\partial t} + \nabla \times \bar{\mathbf{v}} \times \bar{\mathbf{u}} + \bar{\alpha}\nabla\bar{p} + \nabla\bar{\phi} + \nabla\cdot\mathbf{R} = 0$$

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

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

$$\frac{\partial \mathbf{R}}{\partial t} + \nabla\cdot(\mathbf{R}\otimes\bar{v}) + (\mathbf{R}\cdot\nabla)\bar{v} + (\mathbf{R}^T\cdot\nabla)\bar{v} = 0$$

Progress: Now there is reversible exchange of energy between resolved reservoirs and turbulent/subgrid reservoir of TKE ($\rho\kappa$). This model is missing, however, irreversible source and diffusion terms on the rhs of the **R** equation, and corresponding terms in the entropy equation. These amount to adding a proper definition of dissipation potential Φ.

Summary and Conclusions

Ultimate goal: Multiscale formulation for (geophysical) fluid dynamics with consistent exchanges between resolved/unresolved reservoirs of energy and entropy = **a physically consistent approach to parameterization**

- Multiscale geometric mechanics formulations provide a powerful tool for realizing this goal
- Many questions and a lot of work remains, for example:
  - What are the appropriate choices of resolved and unresolved dofs?
  - How should Lagrangian $\hat{\mathscr{L}}$ and dissipation potential $\hat{\Phi}$ be formulated in terms of these dofs?
  - How much of $\hat{\Phi}$ should represent true physically irreversible processes and how much subgrid turbulent (=reversible) dynamics?
  - How does this approach connect to state of the art parameterizations such as the multiscale modeling framework (MMF) and higher-order closure schemes ex. SHOC/CLUBB?