Structure-preserving continuum gyrokinetic modeling for improved data locality

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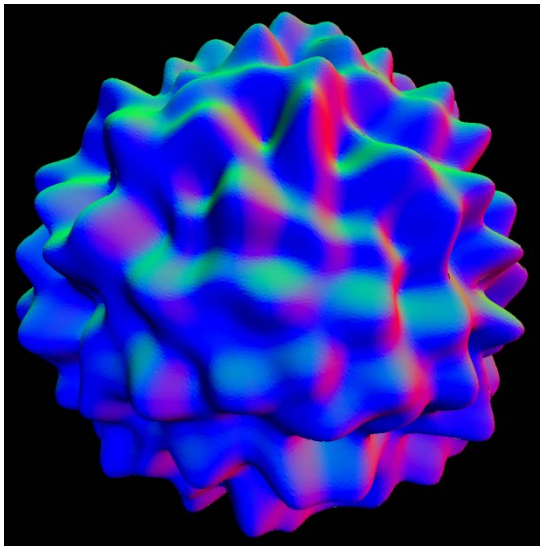
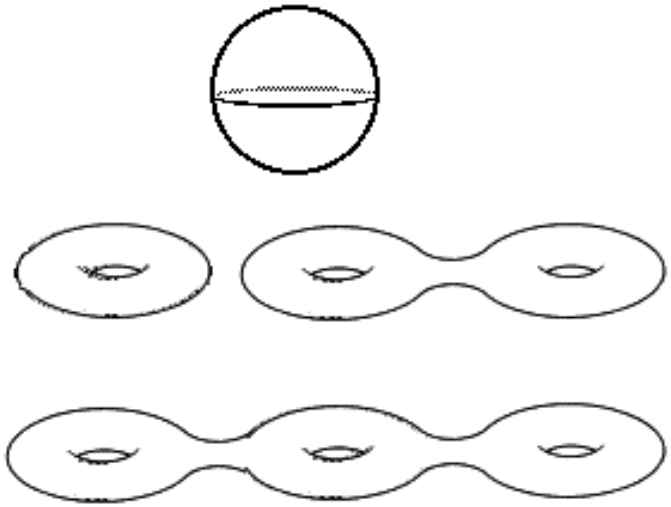
Q: What is "Structure?"

A: Qualitative (as opposed to quantitiative) properties of our mathematical description of nature

Example:



there are many surfaces



Structural property of surfaces: classification theorem

Structure comes in many shapes and sizes

Examples of structure in dynamical laws:

- Energy & momentum conservation
- Symplectic form conservation
- Topology of space of solutions
- Variational formulation
- PDE type, i.e. hyperbolic, elliptic, parabolic

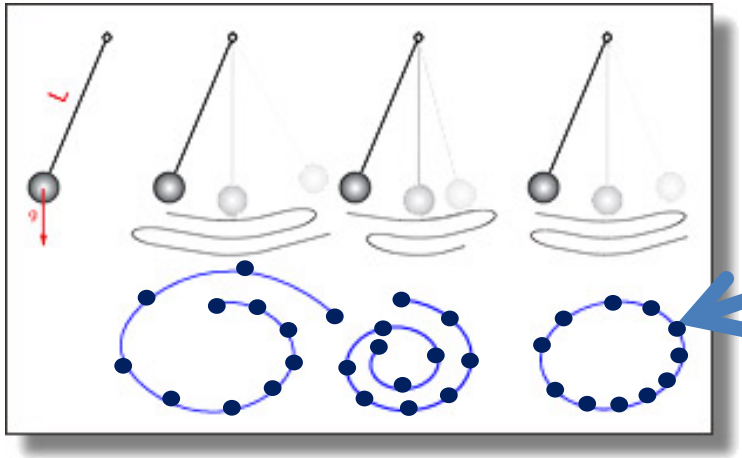
Q: What is a structure-preserving simulation?

A: A simulation based on a discrete model of nature that shares some structural properties with our ``fundamental" model of nature

Example:

$$\ddot{\theta} = -\frac{g}{\ell}\sin\theta$$

Structural property: closed orbits in phase space



Structure preserving simulation

Q: How is a structure-preserving simulation designed?

A:

1. Identify structure in our fundamental natural laws
2. Develop a reduced (continuum) model with same structure
3. Discretize reduced model without violating structural constraints

Note: Basic theory plays an indispensable role in structure-preserving simulation design

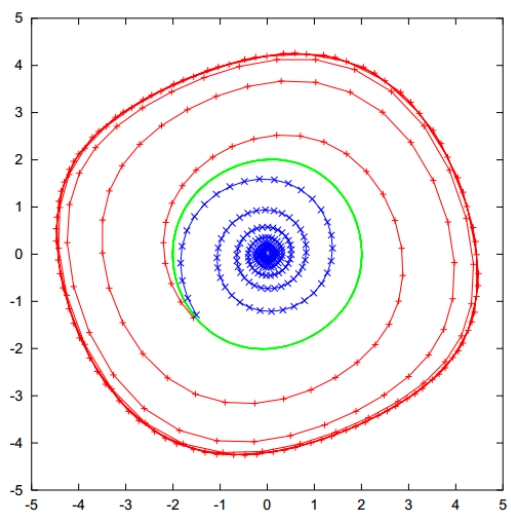
- Steps 1+2 fall under the purview of what Phil identified as basic theory
  - Step 1 example: identifying the Morrison-Marsden-Weinstein Poisson bracket for Vlasov-Maxwell equations
  - Step 2 example: Brizard and Sugama's field-theoretic formulation of gyrokinetics
- Step 3 involves interaction between basic theory and computer science

Q: Why are structure-preserving simulations desirable?

A: Stability, Verifiability, Scalability

We want simulations that are stable

- Long-time stability of simulated dynamics can be poor even for convergent methods
  - This issue is mitigated by using a simulation that preserves conservation laws; at least the behavior of *some* observables is stable forever



Explicit Euler (gains energy)

Implicit Euler (loses energy)

Exact phase diagram solution (ideal harmonic oscillator)

We want simulations that are verifiable

- We generally know very little about the behavior of our reduced model *other than its structure*
  - The more structure the reduced model has, the more comprehensive our verification efforts can become

If you want to verify your pistol is working correctly, it's good to know which end the bullet is supposed to come out of.

We want simulations that are scalable

- Non-local Communication is public enemy #1 on modern supercomputers
  - Fundamental plasma models tend to be expressed as hyperbolic PDEs, which naturally lead to algorithms with only nearest-neighbor communication
  - Preserving this hyperbolic nature in a reduced model will therefore naturally lead to algorithms that profit from both nearest-neighbor communication and dynamical reduction

An example of structure-preserving simulation design: simulating magnetized plasma microturbulence

Step 1: identify structure in fundamental model

- The fundamental (classical) model of collisionless magnetized plasma microturbulence is the Vlasov-Maxwell system

$$\partial_t f_s + v \cdot \nabla f_s + \frac{q_s}{m_s}(E + v \times B/c) \cdot \nabla_v f_s = 0$$

$$\frac{1}{c}\partial_t B = -\nabla \times E$$

$$\frac{1}{c}\partial_t E = \nabla \times B - \frac{4\pi}{c}\sum_s q_s \int v f_s \, d^3v$$

$$\nabla \cdot B = 0$$

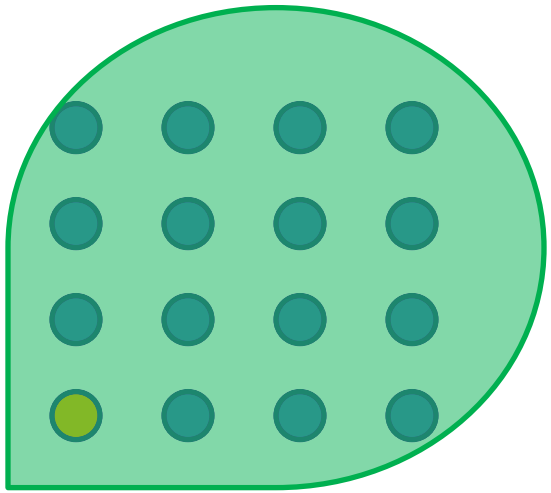
$$\nabla \cdot E = 4\pi \sum_s q_s \int f_s \, d^3v$$

Notable structure

- Variational principle
- Gauge invariance
- Hyperbolic field equations

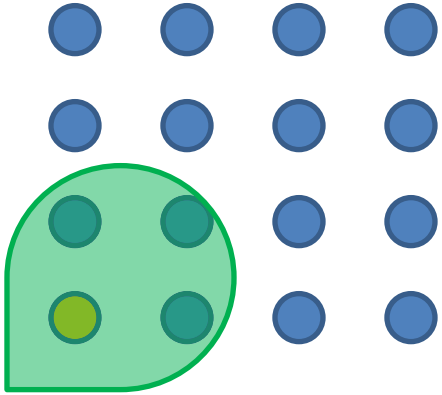
Why are elliptic field solves bothersome?

NON-LOCALITY!



global vs local domain of dependence

(circles = grid points)



$$\Delta\phi = -\rho$$

$$\partial_t^2\phi = \Delta\phi$$

What about local iterative methods like SOR?

- There are iterative methods for elliptic equations that only require nearest-neighbor operations
  - ❑ Which is faster: hyperbolic+FDTD or elliptic+SOR?

$$\frac{T_{\text{wall}}^{\text{hyperbolic}}}{T_{\text{wall}}^{\text{elliptic}}} = \frac{\Delta x_{\text{grid}}}{L_{\text{system}}} \frac{v_{\text{hyperbolic}}}{v_{\text{elliptic}}} \frac{1}{\log(\text{tol}_{\text{elliptic}})}$$

  - ✓ Favorable scaling with resolution
  - ✓ Bruce Scott has had success replacing elliptic solves with hyperbolic in gyrofluid sims

Step 2: develop structure-preserving reduced model

- We would like to avoid resolving the gyromotion of particles because $\omega_* \ll \omega_c$
  - ➢ We want a gyrokinetic model

- The first gyrokinetic model that is gauge invariant, variational, hyperbolic is given in

J. W. Burby, A. J. Brizard, P. J. Morrison, and H. Qin, Phys. Lett. A **379**, 2073 (2015).

J. W. Burby, A. J. Brizard, P. J. Morrison, and H. Qin, arXiv:1411.1790 (2015).

Important feature of reduced model: light speed is reduced by gyrocenter polarization effects

$$D = \varepsilon \cdot E$$

$$\Rightarrow v_{\text{phase}} \approx c/\sqrt{\varepsilon} \approx v_{\text{A}}$$

Large ε is consistent with the notion of the ``gyrokinetic vacuum”

Step 3: develop structure preserving discretization

Conclusions

- Structure-preserving simulations are stable, verifiable, scalable
- Basic theory plays an integral role in all phases of structure-preserving simulation design
  1. Identify structure in fundamental mathematical model
  2. Develop structure preserving reduced models
  3. Discretize reduced model without violating structural constraints

Grand challenges

- Discretization challenge: How can we harness the full power of next-generation heterogeneous massively-parallel supercompupters to study plasma physics?

- Reduced modeling challenge: Can classical gyrokinetic field theory be extended to quantum gyrokinetic field theory?