GEMKIN : Geometric Methods for Kinetic Equations

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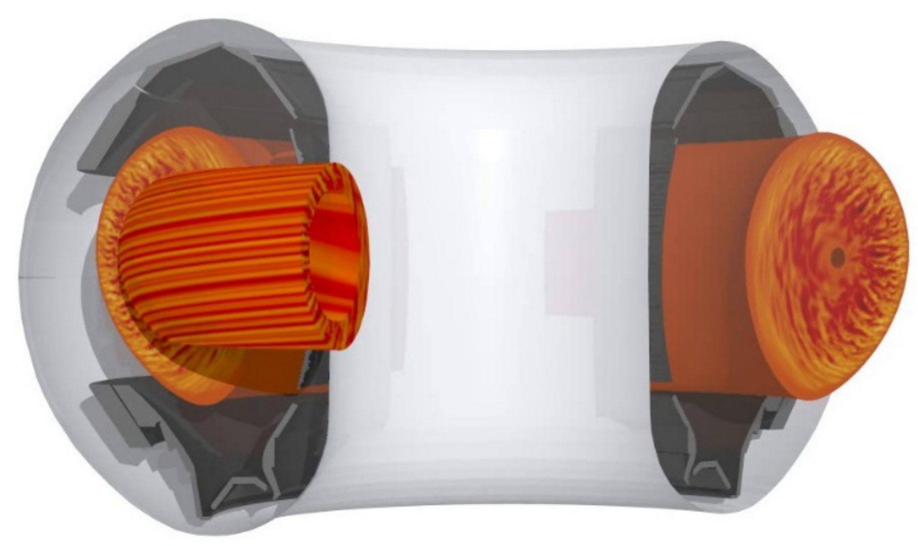
Geometric Discretization Methods

- Courant, Friedrichs and Lewy noticed already in 1928 that preserving first integrals of an equation during discretisation is advantageous for the stability of the resulting scheme
- preserving such geometric structures results not only in more stable schemes but also in more realistic and more accurate representations of the physical system at hand
- geometric structure: global property of some system of partial differential equations, which can be defined independently of a particular coordinate representation, e.g., topology, conservation laws, symmetries, constraints, identities
- Geometric discretization methods enable correct long time simulation of complex systems, like tokamaks



Hamiltonian dynamics

Hamiltonian dynamics is a mathematical formalism to describe the equations of a physical system. The equations of motion of such systems are given by

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{F, \mathcal{H}\}.$$

Here, $\mathcal{H}$ is the Hamiltonian which corresponds to the total energy of the system and $\{.,.\}$ is a Poisson bracket, a skew-symmetric operator satisfying the Leibniz rule and the Jacobi identity.
A Casimir invariant is a functional C which Poisson commutes with every functional F:

$$\{F, C\} = 0.$$

A second family of conserved quantities are momentum maps, Φ, along whose flow the Hamiltonian is constant, i.e.

$$\{\mathcal{H}, \Phi\} = 0 \Rightarrow \frac{d\Phi}{dt} = 0.$$

Kinetic models of plasma dynamics

The Vlasov equation,

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_s = 0,$$

describes the evolution of the probability distribution function of a plasma.
It is coupled to the Maxwell equations, which describe the evolution of the electromagnetic fields,

$$\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \mathbf{J}, \qquad \nabla \cdot \mathbf{E} = \rho,$$
$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \qquad \nabla \cdot \mathbf{B} = 0,$$

by the source terms $\mathbf{J}$ and ρ, the first two moments of the particle distribution function f_s:

$$\mathbf{J} = \sum_s q_s \int f_s \mathbf{v}\, \mathrm{d}\mathbf{v}, \qquad \rho = \sum_s q_s \int f_s\, \mathrm{d}\mathbf{v}.$$

The system satisfies the following conservation law

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \mathbf{J} = 0.$$

The Hamiltonian is given by

$$\mathcal{H} = \sum_s \frac{m_s}{2} \int |\mathbf{v}|^2 f_s\, \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{v} + \frac{1}{2} \int \left(|\mathbf{E}|^2 + |\mathbf{B}|^2\right) \mathrm{d}\mathbf{x}.$$

The Poisson bracket for the Vlasov-Maxwell system has the following form

$$\begin{aligned}\{F, G\}(f_s, \mathbf{E}, \mathbf{B}) = & \sum_s \int \left[\frac{\delta F}{\delta f_s}, \frac{\delta G}{\delta f_s}\right] \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{v} \\ & + \sum_s \frac{q_s}{m_s} \int f_s \left(\nabla_{\mathbf{v}} \frac{\delta F}{\delta f_s} \cdot \frac{\delta G}{\delta \mathbf{E}} - \nabla_{\mathbf{v}} \frac{\delta G}{\delta f_s} \cdot \frac{\delta F}{\delta \mathbf{E}}\right) \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{v} \\ & + \sum_s \frac{q_s}{m_s^2} \int f_s \mathbf{B} \cdot \left(\nabla_{\mathbf{v}} \frac{\delta F}{\delta f_s} \times \nabla_{\mathbf{v}} \frac{\delta G}{\delta f_s}\right) \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{v} \\ & + \int \left(\operatorname{curl} \frac{\delta F}{\delta \mathbf{E}} \cdot \frac{\delta G}{\delta \mathbf{B}} - \operatorname{curl} \frac{\delta G}{\delta \mathbf{E}} \cdot \frac{\delta F}{\delta \mathbf{B}}\right) \mathrm{d}\mathbf{x}.\end{aligned}$$

The Casimir invariants of this bracket are

$$C_E = \int h_E(\mathbf{x})(\operatorname{div} \mathbf{E} - \rho)\, \mathrm{d}\mathbf{x}, \qquad C_B = \int h_B(\mathbf{x}) \operatorname{div} \mathbf{B}\, \mathrm{d}\mathbf{x},$$

which are equivalent to two of the Maxwell's equations.

A momentum map is the total momentum:

$$P = \sum_s \int m_s \mathbf{v} f_s\, \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{v} + \int \mathbf{E} \times \mathbf{B}\, \mathrm{d}\mathbf{x}.$$

Geometric discretisation of Vlasov-Maxwell

- Maxwell's equation are discretized in the framework of Finite Element Exterior Calculus (FEEC), based on a continuous and discrete complex involving compatible Finite Element spaces:

$$\begin{array}{ccccccc} H^1(\Omega) & \xrightarrow{\mathbf{grad}} & H(\mathbf{curl}, \Omega) & \xrightarrow{\mathbf{curl}} & H(\operatorname{div}, \Omega) & \xrightarrow{\operatorname{div}} & L^2(\Omega) \\ \downarrow \Pi_0 & & \downarrow \Pi_1 & & \downarrow \Pi_2 & & \downarrow \Pi_3 \\ V_0 & \xrightarrow{\mathbf{grad}} & V_1 & \xrightarrow{\mathbf{curl}} & V_2 & \xrightarrow{\operatorname{div}} & V_3 \end{array}$$

  - $\mathbf{curl}\,\mathbf{grad} = 0$ and $\operatorname{div} \mathbf{curl} = 0$ exactly preserved at discrete level
  - Commuting diagram is an essential piece:

$$\Pi_1 \mathbf{grad} \psi = \mathbf{grad} \Pi_0 \psi, \quad \Pi_2 \mathbf{curl} \mathbf{A} = \mathbf{curl} \Pi_1 \mathbf{A}, \quad \Pi_3 \operatorname{div} \mathbf{A} = \operatorname{div} \Pi_2 \mathbf{A}.$$

- The Vlasov equation is discretized with a Particle in Cell method (PIC):

$$f_h(\mathbf{x}, \mathbf{v}, t) = \sum_{p=1}^{Np} w_p \delta(\mathbf{x} - \mathbf{x}_p(t)) \delta(\mathbf{v} - \mathbf{v}_p(t)).$$

- Plugging these approximations in the Poisson bracket and the hamiltonian a Finite Dimensional Poisson bracket and Hamiltonian are obtained.
- Time discretisation based on Hamiltonian splitting or Discrete Gradient method.
- Implemented with spline Finite Elements in arbitrary curvilinear coordinates.

Adding the collision operator

- Vlasov-Maxwell-Landau kinetic model
  - Conserves energy $\mathcal{H} = \frac{m}{2} \int f v^2 \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{v} + \frac{\epsilon_0}{2} \int E^2 \mathrm{d}\mathbf{x} + \frac{1}{2\mu_0} \int B^2 \mathrm{d}\mathbf{x}$
  - Dissipates entropy $\mathcal{S} = \int f \ln f \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{v}$
- Fits into the metriplectic framework, involving a Hamiltonian and a dissipative part

$$\frac{d}{dt}\mathcal{F} = \{\mathcal{F}, \mathcal{H}\} + (\mathcal{F}, \mathcal{S})$$

- The metriplectic bracket of the Vlasov-Maxwell-Landau system preserves mass, momentum, total energy, the divergence constraints on E and B, and satisfies an H-theorem (monotonic dissipation of entropy, unique equilibrium state)
- many systems in plasma physics (e.g., XMHD, kinetic, hybrid) possess a similar structure consisting of a Hamiltonian part $\{\cdot, \cdot\}$ and an entropy-dissipating part $(\cdot, \cdot)$.
- discretisation of the brackets instead of the dynamical equation guarantees these properties at the discrete level for different numerical methods (FEM, DG, PIC, ...)

Nonlinear Landau Collision Operator

- FEM, DG, PIC discretizations of the metric bracket formulation of the Landau operator
- temporal discretisation via discrete gradient methods
- exact conservation of mass, momentum, energy and discrete H-theorem
- Outlook:
  - PIC and DG discretisation of the full 6D Vlasov-Maxwell-Landau system
  - low-rank tensor approximation for more efficient computations