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Metriplectic Integrators for the Landau Collision Operator

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Outline

The Vlasov–Maxwell–Landau System

The Vlasov–Maxwell System

- the Vlasov–Maxwell system determines the evolution of the distribution function $f_s(t, x, v)$ of some particle species s with mass m_s and charge e_s in a collisionless plasma

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

  and the associated electromagnetic fields $E(t, x)$ and $B(t, x)$

$$\frac{1}{c^2}\frac{\partial E}{\partial t}(t, x) = \nabla \times B(t, x) - j(t, x), \qquad \nabla \cdot E(t, x) = -\frac{1}{\varepsilon_0}\rho(t, x),$$

$$\frac{\partial B}{\partial t}(t, x) = -\nabla \times E(t, x), \qquad \nabla \cdot B(t, x) = 0$$

- definitions of charge density ρ and current density j in terms of f

$$\rho(t, x) = \sum_s e_s \int f_s(t, x, v)\, \mathrm{d}v, \qquad j(t, x) = \sum_s e_s \int f_s(t, x, v)\, v\, \mathrm{d}v$$

The Vlasov–Maxwell–Landau System

- the Vlasov–Maxwell–Landau system determines the evolution a collisional plasma and the associated electromagnetic fields

$$\frac{\partial f_s}{\partial t}(t,x,v) + e_s\, v \cdot \frac{\partial f_s}{\partial x}(t,x,v) + \frac{e_s}{m_s}\big(E(t,x) + v \times B(t,x)\big) \cdot \frac{\partial f_s}{\partial v}(t,x,v) = C[f_s]$$

$$\frac{1}{c^2}\frac{\partial E}{\partial t}(t,x) = \nabla \times B(t,x) - j(t,x), \qquad \nabla \cdot E(t,x) = -\frac{1}{\varepsilon_0}\rho(t,x),$$

$$\frac{\partial B}{\partial t}(t,x) = -\nabla \times E(t,x), \qquad \nabla \cdot B(t,x) = 0$$

- the Landau collision operator $C[f_s]$ is given by

$$C[f_s](v) = \sum_{s'} \frac{c_{ss'}}{m_s}\frac{\partial}{\partial v} \cdot \int_{\Omega_v} U(v,v') \cdot J_{ss'}(v,v')\, \mathrm{d}v', \qquad c_{ss'} = \frac{e_s^2\, e_{s'}^2 \ln \Lambda}{8\pi\varepsilon_0^2}$$

with e_s and m_s the charge and mass of particles of species s, ε_0 the vacuum permittivity, and $\ln \Lambda$ the Coulomb logarithm

The Landau Collision Operator

- the Landau collision operator $C[f_s]$ is given by

$$C[f_s](v) = \sum_{s'} \frac{c_{ss'}}{m_s} \frac{\partial}{\partial v} \cdot \int_{\Omega_v} U(v, v') \cdot J_{ss'}(v, v') \, \mathrm{d}v', \qquad c_{ss'} = \frac{e_s^2 e_{s'}^2 \ln \Lambda}{8\pi \varepsilon_0^2}$$

- the antisymmetric vector $J_{ss'}(v, v') = -J_{s's}(v', v)$ depends on f_s and $f_{s'}$ and is defined as

$$J_{ss'}(v, v') = \frac{f_{s'}(v')}{m_s} \frac{\partial f_s(v)}{\partial v} - \frac{f_s(v)}{m_{s'}} \frac{\partial f_{s'}(v')}{\partial v'}$$

- the Landau tensor $U(v, v')$ is a scaled projection matrix of the relative velocity $v - v'$ between the colliding particles, valid at non-relativistic energies,

$$U_{ij}(v, v') = \frac{1}{|v - v'|} \left(\delta_{ij} - \frac{(v_i - v'_i)(v_j - v'_j)}{|v - v'|^2} \right)$$

Geometric Structures of the Vlasov–Maxwell–Landau System

- the spaces of electrodynamics have a deRham complex structure
- Poisson structure of the Vlasov–Maxwell system
  (antisymmetric bracket satisfying the Jacobi identity)
- metriplectic structure of the Vlasov–Maxwell–Landau system
  (metric bracket for the collision operator)
- conservation of mass, momentum, energy, charge, laws of thermodynamics

Poisson and Metriplectic Brackets

Hamiltonian Systems and Poisson Brackets

- let $u(t,x) = (u^1,\, u^2,\, ...,\, u^m)^T$ be the dynamical variables of some system of partial differential equations, defined over the space Ω with coordinates x, and $\mathcal{F}$ an arbitrary functional of u
- if the system is Hamiltonian the evolution of such functionals $\mathcal{F}$ is given by

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\}$$

- $\mathcal{H}$ is the Hamiltonian functional, usually the total energy of the system
- the Poisson bracket $\{\cdot,\cdot\}$ is an bilinear, anti-symmetric bracket of the form

$$\{\mathcal{F}, \mathcal{G}\} = \int_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i} \, \mathcal{J}^{ij}(u) \, \frac{\delta \mathcal{G}}{\delta u^j} \, \mathrm{d}z$$

where $\mathcal{F}$ and $\mathcal{G}$ are functionals of u and $\delta\mathcal{F}/\delta u^i$ is the functional derivative

$$\frac{d}{d\epsilon} \mathcal{F}\big[u^1,\, ...,\, u^i + \epsilon v^i,\, ...,\, u^m\big]\Big|_{\epsilon=0} = \int_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i} \, v^i \, \mathrm{d}z$$

Hamiltonian Systems and Poisson Brackets

- the Poisson bracket $\{\cdot,\cdot\}$ is an bilinear, anti-symmetric bracket of the form

$$\{\mathcal{F},\mathcal{G}\} = \int\limits_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i} \, \mathcal{J}^{ij}(u) \, \frac{\delta \mathcal{G}}{\delta u^j} \, \mathrm{d}z$$

- the Poisson bracket $\{\cdot,\cdot\}$ satisfies Leibniz' rule and the Jacobi identity

$$\{\{\mathcal{F},\mathcal{G}\},\mathcal{H}\} + \{\{\mathcal{G},\mathcal{H}\},\mathcal{F}\} + \{\{\mathcal{H},\mathcal{F}\},\mathcal{G}\} = 0$$

  for arbitrary functionals $\mathcal{F},\mathcal{G},\mathcal{H}$ of u

- $\mathcal{J}(u)$ is an anti-self-adjoint operator, which has the property that

$$\sum_{l=1}^{m} \left(\frac{\partial \mathcal{J}^{ij}(u)}{\partial u^l} \, \mathcal{J}^{lk}(u) + \frac{\partial \mathcal{J}^{jk}(u)}{\partial u^l} \, \mathcal{J}^{li}(u) + \frac{\partial \mathcal{J}^{ki}(u)}{\partial u^l} \, \mathcal{J}^{lj}(u) \right) = 0$$

  for $1 \leq i,j,k \leq m$, ensuring that the bracket $\{\cdot,\cdot\}$ satisfies the Jacobi identity

- apart from that, $\mathcal{J}(u)$ is not required to be of any particular form and is allowed to depend on the fields u in an arbitrarily complicated way (nonlinear, differential and integral operators)

Hamiltonian Systems and Poisson Brackets

- the Poisson bracket $\{\cdot, \cdot\}$ is an bilinear, anti-symmetric bracket of the form

$$\{\mathcal{F}, \mathcal{G}\} = \int_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i} \, \mathcal{J}^{ij}(u) \, \frac{\delta \mathcal{G}}{\delta u^j} \, \mathrm{d}z$$

- Poisson systems preserve energy due to anti-symmetry of the bracket

$$\frac{d\mathcal{H}}{dt} = \{\mathcal{H}, \mathcal{H}\} = -\{\mathcal{H}, \mathcal{H}\} = 0$$

- if the Hamiltonian is constant along the flow of some functional Φ, i.e., $\{\mathcal{H}, \Phi\} = 0$, then Φ is a momentum map that is preserved by the flow of $\mathcal{H}$

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

- if $\mathcal{J}(u)$ has a non-empty nullspace, there exist so-called Casimir invariants, that is functionals $\mathcal{C}$ for which $\{\mathcal{F}, \mathcal{C}\} = 0$ for all functionals $\mathcal{F}$

Morrison–Marsden–Weinstein Bracket for the Vlasov–Maxwell System

- infinite dimensional fields f, E, B
- Vlasov–Maxwell noncanonical Hamiltonian structure

$$\{\mathcal{F},\mathcal{G}\}[f,E,B] = \sum_s \int \frac{f_s}{m_s} \left[\frac{\delta \mathcal{F}}{\delta f}, \frac{\delta \mathcal{G}}{\delta f} \right] \mathrm{d}z + \frac{1}{\varepsilon_0} \sum_s \frac{q_s}{m_s} \int f_s \left(\frac{\partial}{\partial v} \frac{\delta \mathcal{F}}{\delta f_s} \cdot \frac{\delta \mathcal{G}}{\delta E} - \frac{\partial}{\partial v} \frac{\delta \mathcal{G}}{\delta f_s} \cdot \frac{\delta \mathcal{F}}{\delta E} \right) \mathrm{d}z$$
$$+ \sum_s \frac{q_s}{m_s^2} \int f_s B \cdot \left(\frac{\partial}{\partial v} \frac{\delta \mathcal{F}}{\delta f_s} \times \frac{\partial}{\partial v} \frac{\delta \mathcal{G}}{\delta f_s} \right) \mathrm{d}z + \frac{1}{\varepsilon_0} \int \left(\frac{\delta \mathcal{F}}{\delta E} \cdot \nabla \times \frac{\delta \mathcal{G}}{\delta B} - \frac{\delta \mathcal{G}}{\delta E} \cdot \nabla \times \frac{\delta \mathcal{F}}{\delta B} \right) \mathrm{d}x$$

- Hamiltonian: functional of f, E, B (sum of the kinetic energy of the particles, the electrostatic field energy and the magnetic field energy)

$$\mathcal{H} = \frac{1}{2} \sum_s \int |v|^2 \, f_s(x,v) \, \mathrm{d}x \mathrm{d}v + \frac{1}{2} \int \left(\varepsilon_0 \, |E(x)|^2 + \mu_0^{-1} \, |B(x)|^2 \right) \mathrm{d}x$$

- time evolution of any functional $\mathcal{F}[f,E,B]$

$$\frac{d}{dt} \mathcal{F}[f,E,B] = \{\mathcal{F},\mathcal{H}\}$$

Casimir Invariants of the Morrison–Marsden–Weinstein Bracket

- momentum maps:
  - linear momentum

$$\mathcal{P} = \sum_s m_s \int_\Omega v f_s(t,z)\,\mathrm{d}z + \varepsilon_0 \int_{\Omega_x} E \times B \,\mathrm{d}x$$

- Casimir invariants:
  - integral of any real function h_s of each distribution function f_s

$$\mathcal{C}_s = \int h_s(f_s)\,\mathrm{d}z, \qquad \text{e.g.} \qquad \mathcal{M}_s = \int f_s\,\mathrm{d}z, \quad \mathcal{L}_s^2 = \frac{1}{2}\int \big|f_s\big|^2\,\mathrm{d}z, \quad \mathcal{S}_s = \int f_s \ln f_s \,\mathrm{d}z$$

  - divergence constraints of the electromagnetic fields (h_E and h_B are arbitrary real functions of x)

$$\mathcal{C}_E = \int h_E(x)\big(\operatorname{div} E - \rho\big)\,\mathrm{d}x,$$

$$\mathcal{C}_B = \int h_B(x)\,\operatorname{div} B\,\mathrm{d}x$$

Metriplectic Systems

- metriplectic dynamics describes systems that have a Hamiltonian part, determined by an anti-symmetric bracket $\{\cdot, \cdot\}$, and a dissipative part, determined by a symmetric bracket $(\cdot, \cdot)$
- the evolution of any functional $\mathcal{F}$ of the field variables u is given by

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

- $\mathcal{G} = \mathcal{H} - \mathcal{S}$ a generalised free energy functional with Hamiltonian $\mathcal{H}$ and entropy $\mathcal{S}$
- the symmetric bracket $(\cdot, \cdot)$ is given by

$$(\mathcal{F}, \mathcal{G}) = \int\limits_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i} \, \mathcal{K}^{ij}(u) \, \frac{\delta \mathcal{G}}{\delta u^j} \, \mathrm{d}z$$

- $\mathcal{K}(u)$ is a self-adjoint, negative semi-definite operator
- $\mathcal{S}$ is a Casimir invariant of the Poisson bracket $\{\cdot, \cdot\}$, such that $\{\mathcal{S}, \mathcal{F}\} = 0$ for all functionals $\mathcal{F}$
- $\mathcal{H}$ is a Casimir invariant of the metric bracket $(\cdot, \cdot)$, such that $(\mathcal{H}, \mathcal{F}) = 0$ for all functionals $\mathcal{F}$

Metriplectic Systems

- metriplectic dynamics
  - preserves energy

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \{\mathcal{H}, \mathcal{G}\} + (\mathcal{H}, \mathcal{G}) = \{\mathcal{H}, -\mathcal{S}\} = 0$$

  - produces entropy

$$\frac{\mathrm{d}\mathcal{S}}{\mathrm{d}t} = \{\mathcal{S}, \mathcal{G}\} + (\mathcal{S}, \mathcal{G}) = -(\mathcal{S}, \mathcal{S}) \geq 0$$

  - dissipates the free energy

$$\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}t} = \{\mathcal{G}, \mathcal{G}\} + (\mathcal{G}, \mathcal{G}) = (\mathcal{G}, \mathcal{G}) \leq 0$$

  - drives the solution towards a well-defined and unique equilibrium state

→ metriplectic dynamics satisfies an H-theorem and reproduces the laws of thermodynamics

Metriplectic Systems: Energy Principle and Equilibrium State

- for an equilibrium state u_{eq}, the time evolution of any functional $\mathcal{F}$ stalls, the free-energy functional $\mathcal{G}$ reaches its minimum, and the entropy functional $\mathcal{S}$ reaches its maximum

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t}[u_{eq}] = 0, \qquad \frac{\mathrm{d}\mathcal{G}}{\mathrm{d}t}[u_{eq}] = 0, \qquad \frac{\mathrm{d}\mathcal{S}}{\mathrm{d}t}[u_{eq}] = 0$$

- the equilibrium state satisfies an energy principle
  - the first variation of the free energy vanishes

$$\delta\mathcal{G}[u_{eq}] = 0$$

  - the second variation of the free energy is strictly positive

$$\delta^2\mathcal{G}[u_{eq}] > 0$$

Metriplectic Systems: Energy–Casimir Principle and Equilibrium State

- if Casimir invariants $\mathcal{C}_i$ exist, the equilibrium state becomes degenerate, and the energy principle must be modified to account for the Casimirs (usually mass, momentum and energy)
- energy–Casimir principle: the the equilibrium state satisfies

$$\delta\mathcal{G}[u_{eq}] + \sum_i \lambda_i \, \delta\mathcal{C}_i[u_{eq}] = 0,$$

  where λ_i act as Lagrange multipliers that are determined uniquely from the values of the Casimirs $\mathcal{C}_i[u_0]$ at the initial conditions u_0
- uniqueness: for each $x \in \Omega$ the equilibrium state of the free-energy functional $\mathcal{G}$ is unique

$$\delta^2 (\mathcal{G}[u_{eq}] + \sum_i \lambda_i \mathcal{C}_i[u_{eq}]) > 0$$

  (convexity argument: if Ω is a convex domain and $\mathcal{G}$ is strictly convex, then $\mathcal{G}$ has at most one critical point [Giaquinta and Hildebrandt, Calculus of Variations I, 2004])

Metric Bracket for Collision Operators

- various collision operators, including the Landau collision operator, can be obtained from a general metric bracket of the form

$$(\mathcal{F}, \mathcal{G}) = \int_{\Omega} \int_{\Omega} \left(\frac{\partial}{\partial v'} \frac{\delta \mathcal{F}}{\delta f(z')} - \frac{\partial}{\partial v''} \frac{\delta \mathcal{F}}{\delta f(z'')} \right) \cdot T(z'; z'') \cdot \left(\frac{\partial}{\partial v'} \frac{\delta \mathcal{G}}{\delta f(z')} - \frac{\partial}{\partial v''} \frac{\delta \mathcal{G}}{\delta f(z'')} \right) \mathrm{d}z' \, \mathrm{d}z''$$

  where $z = (x, v)$, $T(z'; z'') = W(z'; z'') \, \delta(x' - x'')$ and W a symmetric positive semi-definite matrix with a null eigenvector $v' - v''$

- different collision operators follow from different choices for the matrix W and the entropy $\mathcal{S}$

- the bracket satisfies conservation of mass, momentum and energy if W is restricted to the form

$$W_{ij}(z', z'') = \nu_c \, U_{ij}(z', z'') \, M(f(z')) \, M(f(z''))/2,$$

  with M an arbitrary function of f and U having the following symmetries

$$U_{ij}(z', z'') = U_{ji}(z', z''), \qquad U_{ij}(z', z'') = U_{ij}(z'', z'), \qquad (v'_i - v''_i) \, U_{ij} = 0$$

Metric Bracket for the Landau Collision Operator

- the entropy functional $\mathcal{S}$ is assumed to be of the form

$$\mathcal{S} = \int_{\Omega} s(f)\, \mathrm{d}z,$$

with s an arbitrary function of the distribution function f

- choosing $s(f) = f \ln f$ and $M(f) = f$ the metriplectic bracket becomes

$$(\mathcal{F}, \mathcal{G}) = \frac{\nu_c}{2} \int_{\Omega_x} \int_{\Omega_v} \int_{\Omega_v} \left(\frac{\partial}{\partial v'} \frac{\delta \mathcal{F}}{\delta f(x', v')} - \frac{\partial}{\partial v''} \frac{\delta \mathcal{F}}{\delta f(x', v'')} \right)$$

$$\cdot\, U(v', v'') \cdot \left(f(x', v'') \frac{\partial f(x', v')}{\partial v'} - f(x', v') \frac{\partial f(x', v'')}{\partial v''} \right) \mathrm{d}x' \, \mathrm{d}v' \, \mathrm{d}v''$$

- the Landau collision operator $C[f_s]$ is obtained as metric bracket $(\mathcal{F}, \mathcal{G})$ with

$$U_{ij}(v, v') = \frac{1}{|v - v'|} \left(\delta_{ij} - \frac{(v_i - v_i')(v_j - v_j')}{|v - v'|^2} \right)$$

Metric Bracket for the Landau Collision Operator

- the Landau bracket preserves mass, momentum and kinetic energy, as

$$(\mathcal{M}_s, \mathcal{F}) = 0, \qquad (\mathcal{P}, \mathcal{F}) = 0, \qquad (\mathcal{E}, \mathcal{F}) = 0,$$

  for arbitrary functionals $\mathcal{F}$, with

$$\mathcal{M}_s = m_s \int\limits_{\Omega} f_s(t,z)\,\mathrm{d}z, \qquad \mathcal{P} = \sum_s m_s \int\limits_{\Omega} v f_s(t,z)\,\mathrm{d}z, \qquad \mathcal{E} = \sum_s \frac{m_s}{2} \int\limits_{\Omega} |v|^2 f_s(t,z)\,\mathrm{d}z$$

- the equilibrium state obeys the energy-Casimir principle

$$\left(\frac{\delta \mathcal{S}}{\delta f_s} + \lambda_s \frac{\delta \mathcal{M}_s}{\delta f_s} + \lambda_{\mathcal{P}} \cdot \frac{\delta \mathcal{P}}{\delta f_s} + \lambda_{\mathcal{E}} \frac{\delta \mathcal{E}}{\delta f_s} \right) \bigg|_{f_s = f_{s,eq}} = 0, \quad \text{for all } s,$$

  which leads to the following condition for the equilibrium distribution functions

$$-\big(1 + \ln f_{s,eq}(t,z)\big) + \lambda_s m_s + \lambda_{\mathcal{P}} \cdot m_s v + \lambda_{\mathcal{E}} \frac{m_s}{2} |v|^2 = 0, \quad \text{for all } s$$

- the equilibrium distributions are thus identified as Maxwellians with each species having common temperature and flow velocity but possibly different densities

The Vlasov–Maxwell–Landau System

- the Vlasov–Maxwell–Landau system is a metriplectic system, whose equations are given by

$$\frac{d}{dt}\mathcal{F}[f, E, B] = \{\mathcal{F}, \mathcal{G}\} + (\mathcal{F}, \mathcal{G}), \qquad \mathcal{G} = \mathcal{H} - \mathcal{S},$$

- the entropy functional $\mathcal{S}$ is given by

$$\mathcal{S} = -T \sum_s \int_\Omega f_s(t, z) \ln f_s(t, z) \, \mathrm{d}z,$$

with T a normalisation constant in units of energy density

- the metriplectic bracket preserves mass, momentum and total energy

$$\mathcal{M}_s = m_s \int_\Omega f_s(t, z) \, \mathrm{d}z, \qquad \mathcal{P} = \sum_s m_s \int_\Omega v f_s(t, z) \, \mathrm{d}z + \varepsilon_0 \int_{\Omega_x} E \times B \, \mathrm{d}x,$$

$$\mathcal{H} = \sum_s \frac{m_s}{2} \int_\Omega |v|^2 f_s(t, z) \, \mathrm{d}z + \frac{1}{2} \int_{\Omega_x} \left(\varepsilon_0 \, |E(x)|^2 + \mu_0^{-1} \, |B(x)|^2 \right) \mathrm{d}x$$

The Vlasov–Maxwell–Landau System

- the equilibrium state is obtained from the energy–Casimir principle,

$$\delta\mathcal{G} + \sum_s \lambda_s \, \delta\mathcal{M}_s = \sum_s \left(\frac{\delta\mathcal{H}}{\delta f_s} - \frac{\delta\mathcal{S}}{\delta f_s} + \lambda_s \frac{\delta\mathcal{M}_s}{\delta f_s} \right) \delta f_{s,eq} + \frac{\delta\mathcal{H}}{\delta E} \cdot \delta E_{eq} + \frac{\delta\mathcal{H}}{\delta B} \cdot \delta B_{eq} = 0.$$

- for arbitrary variations $\delta f_{s,eq}$, δE_{eq} and δB_{eq}, the principle leads to the conditions

$$-T\big(1 + \ln f_{s,eq}\big) = \frac{m_s}{2} |v|^2 + \lambda_s m_s, \qquad E_{eq}(x) = 0, \qquad B_{eq}(x) = 0,$$

- $f_{s,eq}$ describe Maxwellian distribution functions with zero flow and equal uniform temperature

- the Lagrange multipliers λ_s are uniquely determined from the initial conditions by

$$\int_\Omega f_{s,0}(z) \, dz = \int_\Omega f_{s,eq}(z) \, dz$$

Discrete Brackets

Discretisation of the Landau Bracket

- finite-dimensional representation f_h of the distribution function f:
  finite element approximation f_h of f with respect to a basis φ_i

$$f_h(t, z) = \sum_{i=1}^{N} f_i(t) \, \varphi_i(z)$$

- discretisation of functionals:
  apply the functional $\mathcal{F}$ to f_h, so that $\mathcal{F}$ becomes a function F of the degrees of freedom $\boldsymbol{f}$

$$\mathcal{F}[f_h] = F(\boldsymbol{f}), \qquad \boldsymbol{f}(t) = \big(f_1(t), \ldots, f_N(t) \big)^T \in \mathbb{R}^N$$

- discretisation of brackets: replace functional derivatives $\delta\mathcal{F}/\delta f$ with partial derivatives $\partial F/\partial \boldsymbol{f}$

$$\frac{\delta \mathcal{F}[f_h]}{\delta f} = \sum_{i,j=1}^{N} \frac{\partial F}{\partial f_i} \, (\mathbb{M}^{-1})_{ij} \, \varphi_j(z), \qquad \mathbb{M}_{jk} = \int_\Omega \varphi_j(z) \, \varphi_k(z) \, \mathrm{d}z$$

- time discretisation: splitting methods, integral preserving methods

Discrete Metric Bracket

- restricting the metric bracket to the space of functionals on the finite element space, we can replace the functional derivatives with partial derivatives and compute the remaining integrals,

$$(A, B)_h = \sum_{i,j,k,\ell=1}^{N} \frac{\partial A}{\partial f_i} \, (\mathbb{M}^{-1})_{ij} \, \mathbb{L}_{jk}(\boldsymbol{f}) \, (\mathbb{M}^{-1})_{k\ell} \frac{\partial B}{\partial f_\ell}$$

  with the symmetric matrix $\mathbb{L}(\boldsymbol{f})$ given by

$$\mathbb{L}_{ij}(\boldsymbol{f}) = -\frac{1}{2} \int_\Omega \int_\Omega \left(\frac{\partial \varphi_i(v')}{\partial v'} - \frac{\partial \varphi_i(v'')}{\partial v''} \right) \cdot M(f_h(v')) \, U(v'; v'') \, M(f_h(v'')) \cdot \left(\frac{\partial \varphi_j(v')}{\partial v'} - \frac{\partial \varphi_j(v'')}{\partial v''} \right) \mathrm{d}v' \, \mathrm{d}v''$$

- the discrete bracket remains negative semi-definite, with a sufficient but not necessary condition provided by the positive semi-definiteness of $M(f_h)$

Discrete Metric Bracket

- the action of the discrete metric bracket on two functions, $A(\boldsymbol{f}) = \mathcal{A}[f_h]$ and $B(\boldsymbol{f}) = \mathcal{B}[f_h]$, can be expressed as

$$(A, B)_h = \nabla A^T \mathbb{K}(\boldsymbol{f}) \, \nabla B,$$

where the gradient ∇ is to be taken with respect to the degrees of freedom $\boldsymbol{f}$ and the matrix operator $\mathbb{K}$ is given by

$$\mathbb{K}(\boldsymbol{f}) = \mathbb{M}^{-1} \, \mathbb{L}(\boldsymbol{f}) \, \mathbb{M}^{-1}$$

- inserting $\boldsymbol{f}$ and $G(\boldsymbol{f}) = \mathcal{G}[f_h]$, denoting the discrete free energy, into the bracket, the semi-discrete equations of motion for $\boldsymbol{f}$ read

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}t} = (\boldsymbol{f}, G(\boldsymbol{f}))_h = \mathbb{K}(\boldsymbol{f}) \, \nabla G(\boldsymbol{f})$$

Conservation Properties of the Discrete Metric Bracket

- the mass, momentum and kinetic energy carried by the discrete distribution function f_h are

$$M(\boldsymbol{f}) \equiv \mathcal{M}[f_h] = \sum_{i=1}^{N} f_i \int_{\Omega} \varphi_i(v)\,\mathrm{d}v = \mathbb{1}^T \mathbb{M}\,\boldsymbol{f},$$

$$P(\boldsymbol{f}) \equiv \mathcal{P}[f_h] = \sum_{i=1}^{N} f_i \int_{\Omega} v\,\varphi_i(v)\,\mathrm{d}v = \widehat{v}^T \mathbb{M}\,\boldsymbol{f},$$

$$E(\boldsymbol{f}) \equiv \mathcal{E}[f_h] = \frac{m}{2} \sum_{i=1}^{N} f_i \int_{\Omega} |v|^2\,\varphi_i(v)\,\mathrm{d}v = \frac{m}{2}\,\widehat{\varepsilon}^T \mathbb{M}\,\boldsymbol{f}$$

where $\mathbb{1}$ denotes the vector in $\mathbb{R}^N$ with all elements 1 and $\widehat{v}$ and $\widehat{\varepsilon}$ denote coefficients, s.th.

$$\sum_{i=1}^{N} \widehat{v}_i \varphi_i(v) = v, \qquad \sum_{i=1}^{N} \widehat{\varepsilon}_i \varphi_i(v) = v^2$$

Conservation Properties of the Discrete Metric Bracket

- when using a basis that can represent v and v^2 exactly, e.g., quadratic Lagrange finite elements, mass, momentum and kinetic energy are Casimir invariants of the discrete metric bracket as

$$
\begin{aligned}
(M, F)_h &= \mathbb{1}^T \mathbb{M} G(\boldsymbol{f}) \, \nabla \widehat{F} = \mathbb{1}^T \mathbb{L}(\boldsymbol{f}) \mathbb{M}^{-1} \nabla F = 0, \\
(P, F)_h &= \widehat{v}^T \mathbb{M} G(\boldsymbol{f}) \, \nabla \widehat{F} = \widehat{v}^T \mathbb{L}(\boldsymbol{f}) \mathbb{M}^{-1} \nabla F = 0, \\
(E, F)_h &= \widehat{\varepsilon}^T \mathbb{M} G(\boldsymbol{f}) \, \nabla \widehat{F} = \hat{\varepsilon}^T \mathbb{L}(\boldsymbol{f}) \mathbb{M}^{-1} \nabla F = 0,
\end{aligned}
$$

  for arbitrary functions F

- this follows directly from the properties of the Landau matrix $\mathbb{L}$, namely

$$
\mathbb{1}^T \mathbb{L}(\boldsymbol{f}) \equiv 0, \qquad \hat{v}^T \mathbb{L}(\boldsymbol{f}) \equiv 0, \qquad \hat{\varepsilon}^T \mathbb{L}(\boldsymbol{f}) \equiv 0 \qquad \text{for any } \boldsymbol{f}
$$

Semi-discrete H-Theorem

- the time evolution of the discrete entropy

$$\widehat{S}(\boldsymbol{f}) \equiv \mathcal{S}[f_h] = \int_\Omega s\left(\sum_j f_j \phi_j(v) \right) \mathrm{d}v,$$

is given by the action of the discrete metric bracket as

$$\frac{\mathrm{d}S}{\mathrm{d}t} = (S, G)_h = (S, E - S)_h = -(S, S)_h \geq 0, \qquad G = E(\boldsymbol{f}) - S(\boldsymbol{f}) = \mathcal{E}[f_h] - \mathcal{S}[f_h]$$

- we used that the kinetic energy E is in the nullspace of the discrete bracket
- the last inequality follows from the fact that $\mathbb{L}(\boldsymbol{f})$, and thus the discrete bracket, is negative semi-definite as long as $M(f_h)$ remains positive semi-definite
- the semi-discrete entropy evolves monotonically in time

Semi-discrete H-Theorem

- as in the continuous case, the equilibrium state is determined by the energy-Casimir method,

$$\delta S(\boldsymbol{f}_{eq}) + \delta \sum_i \lambda_i C_i(\boldsymbol{f}_{eq}) = 0,$$

specifically,

$$\left[\delta S + \lambda_M \delta(\mathbb{1}^T \mathbb{M} \boldsymbol{f}) + \lambda_P \delta(\widehat{v}^T \mathbb{M} \boldsymbol{f}) + \lambda_E \delta\left(\frac{m}{2} \widehat{\varepsilon}^T \mathbb{M} \boldsymbol{f}\right)\right]\Bigg|_{\boldsymbol{f}=\boldsymbol{f}_{eq}} = 0$$

- we obtain the following condition for the discrete equilibrium state $\boldsymbol{f}_{eq}$,

$$\sum_i \left[\nabla_i S(\boldsymbol{f}_{eq}) + \sum_j \left(\lambda_M \mathbb{M}_{ji} + \lambda_P \hat{v}_j \mathbb{M}_{ji} + \frac{m}{2} \lambda_E \hat{\varepsilon}_j \mathbb{M}_{ji}\right)\right] \delta f_{eq,i} = 0,$$

where the gradient of the discrete entropy function,

$$\nabla_i S(\boldsymbol{f}) = \int_\Omega \phi_i(v)\, s_f\left(\sum_j f_j \phi_j(v)\right) \mathrm{d}v,$$

corresponds to a projection of $s_f(f_h)$ onto the finite element space

Semi-discrete H-Theorem

- the equilibrium state is determined by the energy-Casimir method

$$\delta S(\boldsymbol{f}_{eq}) + \delta \sum_i \lambda_i C_i(\boldsymbol{f}_{eq}) = 0$$

- in order to obtain the discrete equilibrium state, we have to solve

$$\nabla S(\boldsymbol{f}_{eq}) + \lambda_M \mathbb{M}\mathbb{1} + \lambda_P \mathbb{M}\widehat{v} + \frac{m}{2} \lambda_E \mathbb{M}\widehat{\varepsilon} = 0$$

- by matching the mass, momentum and kinetic energy of the equilibrium and the initial condition, we can determine the multipliers λ_M, λ_P and λ_E

$$\mathbb{1}^T \mathbb{M} \boldsymbol{f}_{eq} = \mathbb{1}^T \mathbb{M} \boldsymbol{f}_0, \qquad \widehat{v}^T \mathbb{M} \boldsymbol{f}_{eq} = \widehat{v}^T \mathbb{M} \boldsymbol{f}_0, \qquad \frac{m}{2} \widehat{\varepsilon}^T \mathbb{M} \boldsymbol{f}_{eq} = \frac{m}{2} \widehat{\varepsilon}^T \mathbb{M} \boldsymbol{f}_0$$

- uniqueness of the semi-discrete equilibrium state $\boldsymbol{f}_{eq}$ follows from the same convexity argument as in the continuous case

Time Discretisation

Integral Preserving Methods

- consider a system of ordinary differential equations in the form

$$\frac{du}{dt} = \mathbb{S}(u)\, \nabla I(u)$$

where $\mathbb{S}(u)$ can be an anti-symmetric matrix for conservative systems, a symmetric matrix for dissipative systems, or a combination thereof for metriplectic systems, and $I \colon \mathbb{R}^N \to \mathbb{R}$ is a differentiable function

- discrete gradients: discrete analogues of the gradient of a function

$$\frac{u_{n+1} - u_n}{\Delta t} = \overline{\mathbb{S}}(u_n, u_{n+1})\, \overline{\nabla} I(u_n, u_{n+1})$$

- example: average discrete gradient

$$\overline{\nabla} I(u_n, u_{n+1}) = \int\limits_0^1 \nabla I\big((1-\xi) u_n + \xi u_{n+1}\big)\, d\xi$$

Integral Preserving Methods

- discrete gradients: discrete analogues of the gradient of a function

$$\frac{u_{n+1} - u_n}{\Delta t} = \overline{\mathbb{S}}(u_n, u_{n+1})\, \overline{\nabla} I(u_n, u_{n+1})$$

- $\overline{\mathbb{S}}(u_n, u_{n+1})$ is any symmetric, anti-symmetric or metriplectic matrix that approaches $\mathbb{S}(u)$ in the limit of $u_{n+1} \to u_n$ and $\Delta t \to 0$
- $\overline{\nabla} I(u_n, u_{n+1})$ is a discrete gradient, that is a vector valued continuous function of (u_n, u_{n+1}), satisfying

$$(u_{n+1} - u_n) \cdot \overline{\nabla} I(u_n, u_{n+1}) = I(u_{n+1}) - I(u_n), \qquad \overline{\nabla} I(u_n, u_n) = \nabla I(u_n)$$

- using discrete gradients for the temporal discretisation leads to algorithms that preserve mass, momentum and energy exactly and exhibit the correct monotonic behaviour of the entropy

Discrete Conservation Laws

- for the discrete metric system, the matrix $\mathbb{S}$ is given by the matrix operator $\mathbb{K}$ of the metric bracket, that is

$$\mathbb{S}(\boldsymbol{f}) = \mathbb{K}(\boldsymbol{f}) = \mathbb{M}^{-1}\,\mathbb{L}(\boldsymbol{f})\,\mathbb{M}^{-1},$$

  and I corresponds to the discrete free energy $G(\boldsymbol{f}) = E(\boldsymbol{f}) - S(\boldsymbol{f}) = \mathcal{E}[f_h] - \mathcal{S}[f_h]$

- the difference of the energy at consecutive points in time is obtained from

$$\begin{aligned}\hat{\varepsilon}^T \mathbb{M}(\hat{f}_{n+1} - \hat{f}_n) &= \Delta t\, \widehat{\varepsilon}^T\, \mathbb{M}\, \overline{\mathbb{K}}(\boldsymbol{f}_n, \boldsymbol{f}_{n+1})\, G(\boldsymbol{f}_n, \boldsymbol{f}_{n+1}) \\ &= \Delta t\, \widehat{\varepsilon}^T\, \mathbb{M}\, \mathbb{M}^{-1}\, \overline{\mathbb{L}}(\boldsymbol{f}_n, \boldsymbol{f}_{n+1})\, \mathbb{M}^{-1}\, \overline{\nabla} G(\boldsymbol{f}_n, \boldsymbol{f}_{n+1})\end{aligned}$$

- the right-hand side vanishes exactly since $\widehat{\varepsilon}^T \mathbb{M}\mathbb{M}^{-1} \overline{\mathbb{L}}(\boldsymbol{f}_n, \boldsymbol{f}_{n+1}) = \widehat{\varepsilon}^T \overline{\mathbb{L}}(\boldsymbol{f}_n, \boldsymbol{f}_{n+1}) = 0$
- we thus have that $\widehat{\varepsilon}^T \mathbb{M} \boldsymbol{f}_{n+1} = \widehat{\varepsilon}^T \mathbb{M} \boldsymbol{f}_n$, i.e., the energy at time t_{n+1} equals the energy at time t_n
- mass and momentum conservation are proved in full analogy

Discrete Entropy Production

- the monotonic increase of entropy can be seen by considering the difference of the entropy at two consecutive points in time

$$S(\boldsymbol{f}_{n+1}) - S(\boldsymbol{f}_n) = \big(E(\boldsymbol{f}_{n+1}) - G(\boldsymbol{f}_{n+1})\big) - \big(E(\boldsymbol{f}_n) - G(\boldsymbol{f}_n)\big),$$

where the discrete energy function E is conserved, so that $E(\boldsymbol{f}_{n+1}) = E(\boldsymbol{f}_n)$

- using the defining property of the discrete gradient, we have

$$\begin{aligned} S(\boldsymbol{f}_{n+1}) - S(\boldsymbol{f}_n) &= -\big(G(\boldsymbol{f}_{n+1}) - G(\boldsymbol{f}_n)\big) \\ &= -\Delta t \, \overline{\nabla} G^T(\boldsymbol{f}_n, \boldsymbol{f}_{n+1}) \, \mathbb{M}^{-1} \, \overline{\mathbb{L}}(\boldsymbol{f}_n, \boldsymbol{f}_{n+1}) \, \mathbb{M}^{-1} \, \overline{\nabla} G(\boldsymbol{f}_n, \boldsymbol{f}_{n+1}) \\ &\geq 0, \end{aligned}$$

as $\overline{\mathbb{L}}$ is symmetric negative semi-definite matrix and $\mathbb{M}$ is a symmetric matrix

Summary and Outlook

Summary and Outlook

	Particle-in-Cell	Grid Based
Poisson Integrators	GEMPIC	?
Metriplectic Integrators	?	Current Work

Reference: Physics of Plasmas, Volume 24, 102311, 2017, arXiv:1707.01801

Appendix: Discrete Functional Derivatives

Discretisation of Functional Derivatives

- the functional derivative of a functional $\mathcal{F}[f]$ with respect to f is defined by

$$\frac{d}{d\epsilon}\mathcal{F}\big[f + \epsilon g\big]\Big|_{\epsilon=0} = \left\langle \frac{\delta \mathcal{F}}{\delta f} \, , \, g \right\rangle_{L^2} = \int\limits_{\Omega} \frac{\delta \mathcal{F}}{\delta f} \, g(z) \, \mathrm{d}z,$$

  where g is an element of the same space as f, e.g., $f, g \in L^2(\Omega)$, while the functional derivative $\delta\mathcal{F}/\delta f$ is an element of the dual space and $\langle \cdot \, , \, \cdot \rangle$ denotes the appropriate pairing

- require that the pairing be equal to some finite-dimensional equivalent

$$\left\langle \frac{\delta \mathcal{F}[f_h]}{\delta f} \, , \, g_h \right\rangle_{L^2} = \left\langle \frac{\partial F}{\partial \boldsymbol{f}} \, , \, \boldsymbol{g} \right\rangle_{\mathbb{R}^N} = \sum_{i=1}^{N} \frac{\partial F}{\partial f_i} \, g_i$$

  where $\boldsymbol{g}(t) = \big(g_1(t), \dots, g_N(t)\big)^T \in \mathbb{R}^N$ denotes the degrees of freedom of g_h

$$g_h(t, z) = \sum_{i=1}^{N} g_i(t) \, \varphi_i(z)$$

Discretisation of Functional Derivatives

- denote the dual basis to $\varphi = (\varphi_1, \dots, \varphi_N)^T$ by $\psi = (\psi_1, \dots, \psi_N)^T$

$$\langle \psi_i \, , \, \varphi_j \rangle_{L^2} = \int_\Omega \psi_i(z) \, \varphi_j(z) \, \mathrm{d}z = \delta_{ij} \qquad \text{for} \qquad 1 \leq i, j \leq N$$

- in the dual basis, the functional derivative can be written as

$$\frac{\delta \mathcal{F}[f_h]}{\delta f} = \sum_{i=1}^{N} a_i \, \psi_i(z)$$

- choose $\boldsymbol{g} = (0, \, \dots, \, 0, \, 1, \, 0, \, \dots, \, 0)^\top$ with 1 at the i-th position and 0 else, s.th. $g_h = \varphi_i$ and

$$\left\langle \frac{\delta \mathcal{F}[f_h]}{\delta f} \, , \, g_h \right\rangle_{L^2} = \int_\Omega \sum_{j=1}^{N} a_j \, \psi_j(z) \, \varphi_i(z) \, \mathrm{d}z = \frac{\partial F}{\partial f_i} = \left\langle \frac{\partial F}{\partial \boldsymbol{f}} \, , \, \boldsymbol{g} \right\rangle_{\mathbb{R}^N}$$

- we thus find that

$$a_i = \frac{\partial F}{\partial f_i} \qquad \text{and therefore} \qquad \frac{\delta \mathcal{F}[f_h]}{\delta f} = \sum_{i=1}^{N} \frac{\partial F}{\partial f_i} \, \psi_i(z)$$

Discretisation of Functional Derivatives

- express the dual basis ψ in terms of the primal basis φ as

$$\psi_i(z) = \sum_{j=1}^{N} \mathbb{A}_{ij}\, \varphi_j(z) \qquad \text{so that} \qquad \frac{\delta \mathcal{F}[f_h]}{\delta f} = \sum_{i,j=1}^{N} \frac{\partial F}{\partial f_i}\, \mathbb{A}_{ij}\, \varphi_j(z)$$

- determine the unknown coefficients $\mathbb{A}_{ij}$ by the L_2 inner product

$$\langle \psi_i \,,\, \varphi_k \rangle_{L^2} = \int_\Omega \sum_{j=1}^{N} \mathbb{A}_{ij}\, \varphi_j(z)\, \varphi_k(z)\, \mathrm{d}z = \sum_{j=1}^{N} \mathbb{A}_{ij} \int_\Omega \varphi_j(z)\, \varphi_k(z)\, \mathrm{d}z$$

- denoting by $\mathbb{M}$ the mass matrix of the basis functions φ

$$\mathbb{M}_{jk} = \int_\Omega \varphi_j(z)\, \varphi_k(z)\, \mathrm{d}z,$$

  and using $\langle \psi_i \,,\, \varphi_k \rangle_{L^2} = \delta_{ik}$, we obtain the relation

$$\mathbb{1} = \mathbb{A}\mathbb{M} \qquad \text{and thus} \qquad \mathbb{A} = \mathbb{M}^{-1} \qquad \text{so that} \qquad \frac{\delta \mathcal{F}[f_h]}{\delta f} = \sum_{i,j=1}^{N} \frac{\partial F}{\partial f_i}\, (\mathbb{M}^{-1})_{ij}\, \varphi_j(z)$$