Structure Preserving Discretisation of Kinetic and Gyrokinetic Equations

Discrete Geometric Field Theory in Plasma Physics

Michael Kraus (michael.kraus@ipp.mpg.de)

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Structure Preserving Integration Schemes

- Courant, Friedrichs, Lewy (1928): preserving first integrals of an equation during discretisation is advantageous for the stability of the resulting scheme

- preserving structural properties of an equation when performing a discretisation produces not only more stable schemes but more realistic and more accurate representations of the physical system at hand

- some geometric structures:
  - identities (e.g. $\mathbf{dd} = 0$, $\nabla \times \nabla = 0$, $\nabla \cdot \nabla \times = 0$, $\nabla \cdot \vec{E} = \rho$, $\nabla \cdot \vec{B} = 0$)
  - Casimirs, momentum maps, constants of motion (e.g.momentum, energy)
  - symplecticity, phasespace volume, incompressibility
  - symmetries (e.g. particle relabeling, gauge)

- while structure preserving integration schemes for ODEs have been known for several decades, the development of general methods for PDEs is a rather young and lively field of research

Variational Integrators (VIs)

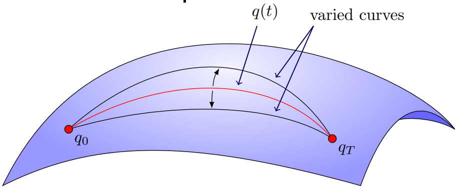
- common practice: discretisation of the Euler-Lagrange equations derived from a continuous Lagrangian via a variational principle
- VIs: discretise the Lagrangian and the accompanying Hamiltonian action principle to obtain discrete Euler-Lagrange equations
  - → automatically preserve symplecticity and discrete momenta associated to symmetries of the Lagrangian through a discrete Noether theorem
  - → good long-time energy behaviour (oscillating but bound error), no artificial numerical damping
  - → simultaneous discretisation in (phase)space and time
  - → easily applicable to different meshes (even unstructured)
- instead of solving the exact system approximately, we solve an approximate system exactly

VIs for Particle Dynamics (Discrete Mechanics)

Continuous Variational Principle

- action

$$\mathcal{A} = \int_0^T L\big(q(t), \dot{q}(t)\big)\, dt$$



- variation and partial integration (endpoints fixed: $\delta q(0) = \delta q(T) = 0$)

$$\delta\mathcal{A} = \int_0^T \left[\frac{\partial L}{\partial q} \cdot \delta q + \frac{\partial L}{\partial \dot{q}} \cdot \delta \dot{q} \right] dt = \int_0^T \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) \right] \cdot \delta q \, dt$$

- the variation of the action has to vanish for all δq, thus the integrand has to vanish, and we get the Euler-Lagrange equations

$$\frac{\partial L}{\partial q}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \right) = 0$$

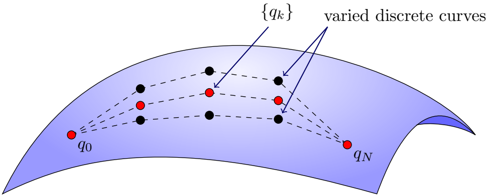
Discrete Variational Principle

- approximate q as the average of two neighbouring points

$$q \to \frac{q_k + q_{k+1}}{2}$$

and $\dot{q}$ with finite differences (timestep h)

$$\dot{q} \to \frac{q_{k+1} - q_k}{h}$$



- discrete action

$$\mathcal{A}_d = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}, h)$$

- discrete variational principle

$$\delta \mathcal{A}_d = \sum_{k=0}^{N-1} \left[D_1 L_d(q_k, q_{k+1}, h) \cdot \delta q_k + D_2 L_d(q_k, q_{k+1}, h) \cdot \delta q_{k+1} \right]$$

Discrete Variational Principle

- discrete variational principle

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- discrete partial integration (use $\delta q_0 = \delta q_N = 0$)

$$\begin{aligned} \delta \mathcal{A}_d &= D_1 L_d(q_0, q_1, h) \cdot \delta q_0 + \sum_{k=1}^{N-1} D_1 L_d(q_k, q_{k+1}, h) \cdot \delta q_k \\ &+ \sum_{k=1}^{N-1} D_2 L_d(q_{k-1}, q_k, h) \cdot \delta q_k + D_2 L_d(q_{N-1}, q_N, h) \cdot \delta q_N \\ &= \sum_{k=1}^{N-1} \big[D_1 L_d(q_k, q_{k+1}, h) + D_2 L_d(q_{k-1}, q_k, h) \big] \cdot \delta q_k \end{aligned}$$

Discrete Variational Principle

- discrete variational principle

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$$= \sum_{k=1}^{N-1} \big[D_1 L_d(q_k, q_{k+1}, h) + D_2 L_d(q_{k-1}, q_k, h) \big] \cdot \delta q_k$$

- the variation $\delta \mathcal{A}_d$ has to vanish for all δq_k, thus for all k we get the

Discrete Euler-Lagrange Equations

$$D_2 L_d(q_{k-1}, q_k, h) + D_1 L_d(q_k, q_{k+1}, h) = 0$$

VIs for Field Dynamics (Discrete Field Theory)

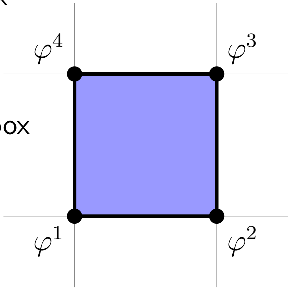
- average the fields over all vertices of a grid box

$$\varphi \to \bar{\varphi} = \frac{1}{4} \left(\varphi^1 + \varphi^2 + \varphi^3 + \varphi^4 \right)$$

- define derivatives along the edges of the grid box

$$\frac{\partial \varphi}{\partial x} \to \frac{1}{2} \left(\frac{\varphi^2 - \varphi^1}{h_x} + \frac{\varphi^3 - \varphi^4}{h_x} \right)$$

$$\frac{\partial \varphi}{\partial y} \to \frac{1}{2} \left(\frac{\varphi^4 - \varphi^1}{h_y} + \frac{\varphi^3 - \varphi^2}{h_y} \right)$$



- replace the continuous Lagrangian density with its discrete counterpart

$$L(\varphi, \varphi_x, \varphi_y) \to L_d(\varphi^1, \varphi^2, \varphi^3, \varphi^4)$$

$$\mathcal{A} = \int L(\varphi, \varphi_x, \varphi_y) \, dx \, dy \to \mathcal{A}_d = \sum_{\text{grid boxes}} L_d(\varphi^1, \varphi^2, \varphi^3, \varphi^4)$$

VIs for Field Dynamics (Discrete Field Theory)

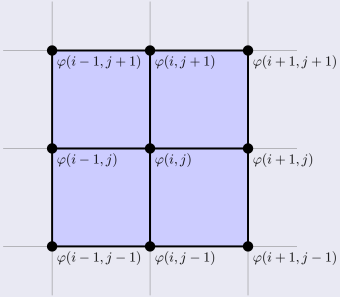
- apply discrete variational principle

$$\delta \mathcal{A}_d = \sum_{\text{grid boxes}} \frac{\partial L_d}{\partial \varphi^i}(\varphi^1, \varphi^2, \varphi^3, \varphi^4) \cdot \delta\varphi^i \qquad (1 \leq i \leq 4)$$

to obtain

Discrete Euler-Lagrange Field Equations

$$\begin{aligned} 0 = & \frac{\partial L_d}{\partial \varphi^1}\left(\varphi_{i,j}, \varphi_{i+1,j}, \varphi_{i+1,j+1}, \varphi_{i,j+1}\right) \\ & + \frac{\partial L_d}{\partial \varphi^2}\left(\varphi_{i-1,j}, \varphi_{i,j}, \varphi_{i,j+1}, \varphi_{i-1,j+1}\right) \\ & + \frac{\partial L_d}{\partial \varphi^3}\left(\varphi_{i-1,j-1}, \varphi_{i,j-1}, \varphi_{i,j}, \varphi_{i-1,j}\right) \\ & + \frac{\partial L_d}{\partial \varphi^4}\left(\varphi_{i,j-1}, \varphi_{i+1,j-1}, \varphi_{i+1,j}, \varphi_{i,j}\right) \end{aligned}$$



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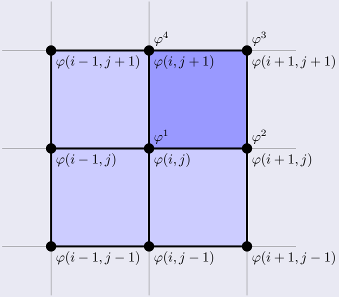

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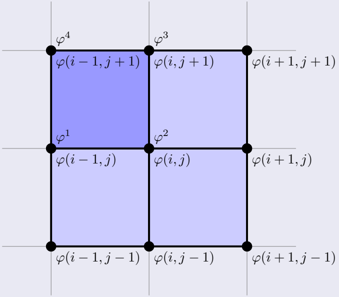

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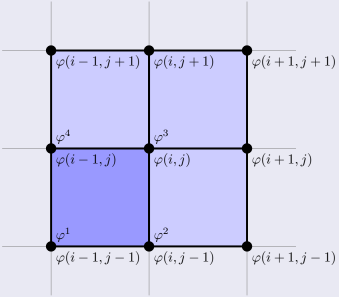

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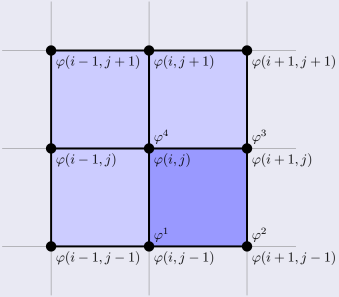

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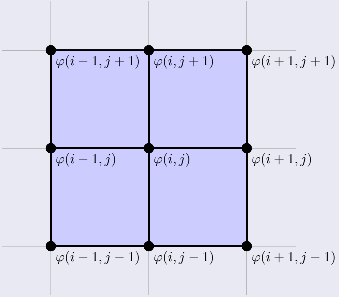

Kinetic and Gyrokinetic Theory

- Lagrangian formulations of gyrokinetics allow for rigorous proofs of energy and momentum conservation through Noether's theorem
- other conserved quantities: L1 and L2 norm of f, entropy

$$\int f \, d^3x \, d^3p, \quad \int f^2 \, d^3x \, d^3p, \quad \int f \, \log f \, d^3x \, d^3p$$

- test bed: the Vlasov-Poisson system in 1D
  - → the Vlasov equation determines the evolution of the distribution function f, which describes the state of a collisionless plasma

$$\frac{\partial f}{\partial t} + \frac{p}{m} \frac{\partial f}{\partial x} - q \frac{\partial \phi}{\partial x} \frac{\partial f}{\partial p} = 0$$

  - → the Poisson equation determines the electrostatic potential ϕ self-consistently w.r.t. the plasma's particle distribution f

$$\nabla^2 \phi = -e \int f \, dp$$

Kinetic and Gyrokinetic Theory

- to apply the discrete variational principle, we need a purely Eulerian field theoretic description of the Vlasov system

→ Eulerian action principles for the Vlasov-Poisson/Maxwell system?

- canonical Hamiltonian action principle

$$\mathcal{A}(f, g) = \int \left(\dot{f} g - \mathcal{H} \right) dt\, dx\, dp + \frac{1}{2} \int |\nabla \phi|^2 \, dt\, dx$$

→ the Vlasov-Poisson system is Hamiltonian but not canonical

→ there is only f but no canonical conjugate field variable g

- Clebsch parametrisation of $f = [\alpha, \beta]$

$$\mathcal{A}(\alpha, \beta) = \int \left(\alpha \dot{\beta} - \mathcal{H} \right) dt\, dx\, dp + \frac{1}{2} \int |\nabla \phi|^2 \, dt\, dx$$

→ α and β are canonical conjugate variables, but not well behaved (i.e. are not bounded or produce singularities in the velocity space)

Kinetic and Gyrokinetic Theory

→ Eulerian action principles for the Vlasov-Poisson/Maxwell system?

- Low's action using Lagrangian variables $f(x, v, t) = f(x_0, v_0)$

$$\mathcal{A}(x, \phi) = \int f(x_0, v_0) \left(\frac{m}{2} \dot{x}^2(x_0, v_0, t) - q\phi(x(x_0, v_0, t)) \right) dt \, dx_0 \, dv_0 + \ldots$$

- Cendra's reduced Euler-Poincaré action principle

$$\mathcal{A}(\vec{u}, f, \phi) = \int f \left(\frac{m}{2} \vec{u}_s^2 + \frac{m}{2} (\vec{u}_s - \vec{v})^2 - q\phi \right) dt \, dx \, dv + \ldots$$

$$\delta \vec{u} = \frac{\partial \vec{w}}{\partial t} + [\vec{u}, \vec{w}] \qquad \text{and} \qquad \delta f = -\nabla_{\vec{z}} \cdot (f \vec{w})$$

$\vec{u}$: phasespace velocity field, $\vec{w}$: virtual displacement in phasespace

→ transformation to Eulerian variables by employing invariance properties

→ analogous to incompressible fluid theory with Lin constraints

→ discretisation of the volume preserving diffeomorphism group

→ exact conservation of energy and phasespace volume, time-reversibility

Semidiscretisation

- semi-discretisation of the phasespace part (Poisson bracket)

→ idea: discrete functional derivative ↔ discrete variational derivative

$$\mathcal{E} = \int S\,[f,h]\,dx\,dp \quad \rightarrow \quad \frac{\delta \mathcal{E}}{\delta S} = [f,h] = -\frac{\partial f}{\partial t}$$

- to retain the antisymmetry properties of the bracket, one has to realise the equality of permutations in the integrand (by partial integration)

$$\int S\,[f,h]\,dx\,dp = \int f\,[h,S]\,dx\,dp = \int h\,[S,f]\,dx\,dp$$

- thus the energy functional can be written as $(\alpha + \beta + \gamma = 1)$

$$\mathcal{E} = \int \Big(\alpha\, S\,[f,h] + \beta\, f\,[h,S] + \gamma\, h\,[S,f] \Big)\; dx\,dp$$

- applying the variational integrator scheme to this functional with $\alpha = \beta = \gamma = 1/3$, one obtains the well-known Arakawa scheme
- discretising the derivatives on a triangular grid, the very same formalism produces Sadourney's scheme ("Arakawa on triangles")

- semi-discretisa bracket)

→ idea: discrete tional derivative

$$\mathcal{E} = \int S \quad \partial f / \partial t$$

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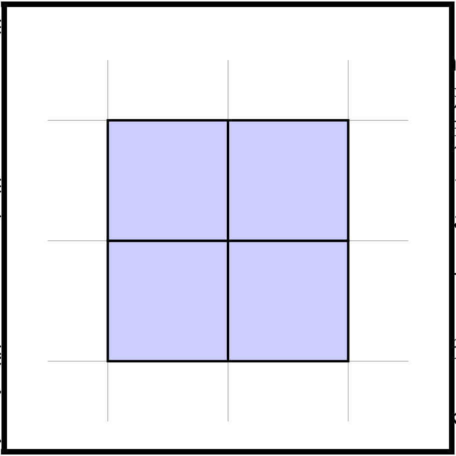

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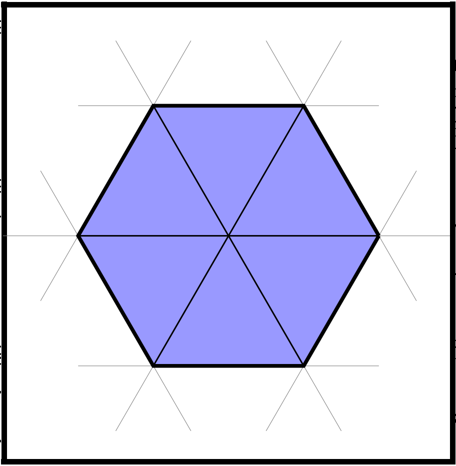

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Semidiscretisation

- generalise to a Nambu three bracket $\left((a,b,c) \in \{x,y,z\}\right)$

$$[f,g,h] \equiv \epsilon^{abc} f_{,a} \, g_{,b} \, h_{,c} = \frac{\partial f}{\partial x} \left[g,h\right]_{yz} + \frac{\partial f}{\partial y} \left[g,h\right]_{zx} + \frac{\partial f}{\partial z} \left[g,h\right]_{xy}$$

- the energy functional is completely analogous to the previous one

$$\begin{aligned} \mathcal{E} &= \int S\,[f,g,h]\, dx\, dy\, dz \\ &= \frac{1}{4} \int \Big(S\,[f,g,h] + f\,[S,h,g] + g\,[S,f,h] + h\,[S,g,f] \Big)\, dx\, dy\, dz \end{aligned}$$

- results in quite large integrators
  - $\rightarrow$ use scripts for the derivation
  - $\rightarrow$ easily adaptable to different meshes, discretisation schemes, and actions
  - $\rightarrow$ produces ready-to-use Fortran code

Semidiscretisation

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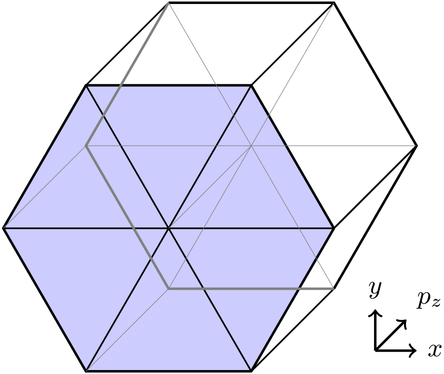
- application: gyrokinetic Vlasov equation on extruded triangular mesh

$$\frac{\partial f}{\partial t} + \frac{1}{\sqrt{g}\,B_{\|}^{*}}\left[h, f, A_{\varphi}^{*}\right]_{xyp_z} = 0$$



x, y	coordinates of the poloidal plane
p_z	parallel momentum
g	metric
f	distribution function
h	particle Hamiltonian
$\vec{A}^{*}$	$= \vec{A} + \frac{c}{e} p_z \vec{b}$
$B_{\|}^{*}$	$= \vec{b}\cdot(\nabla\times\vec{A}^{*})$

Summary and Outlook

Achievements:

- variational derivation of Arakawa's scheme: easily generalisable to higher dimensions, different meshes, and/or higher order
- antisymmetry-preserving discretisation of the three-bracket on an extruded triangular grid
- Nambu field bracket formulation of the noncanonical Hamiltonian description of the Vlasov equation (Lie-Poisson bracket) and application of antisymmetry-preserving semi-discretisation schemes

Next Steps:

- discretisation of Cendra's Euler-Poincaré action principle via discretisation of the volume preserving diffeomorphism group
- reduction of Sugama's gyrokinetic field action to Euler-Poincaré form
- discretisation of electromagnetic field action with discrete diff. forms
- numerical validation of the three-bracket discretisation
- further generalisation and exploration of the Nambu field bracket