Towards Geometric Finite-Element Particle-in-Cell Schemes for Gyrokinetics

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Outline

1. Geometric Numerical Integration
2. Discrete Differential Forms
3. Discrete Poisson Brackets
4. Variational Integrators
5. Summary and Outlook
6. Guiding Centre Dynamics

Structure-Preserving Discretisation

- geometric structure: global property of differential equations, which can be defined independently of particular coordinate representations [1]

  e.g., topology, conservation laws, symmetries, constraints, identities

- preservation of geometric properties is advantageous for numerical stability and crucial for long time simulations
- bounds global error growth and reduces numerical artifacts
- various families
  - Lie group integrators, discrete Euler-Poincaré methods
  - integral preserving schemes, discrete variational derivative method, discrete gradients
  - discrete differential forms and mimetic methods
  - symplectic and multisymplectic methods
  - variational and Poisson integrators

[1] Christiansen, Munthe-Kaas, Owren: Topics in Structure-Preserving Discretization, Acta Numerica 2011

Geometric Structures of the Vlasov-Maxwell System

- Vlasov equation in Lagrangian coordinates

$$\dot{X}_s = V_s, \qquad \dot{V}_s = e_s E(t, X_s) + \frac{e}{c} V_s \times B(t, X_s)$$

$$f_s(t, X_s(t), V_s(t)) = f_s(X_s(0), V_s(0))$$

- Maxwell's equations in Eulerian coordinates

$$\frac{\partial E}{\partial t} = \nabla \times B - j, \qquad \nabla \cdot E = -\rho, \qquad \rho(t, x) = \sum_s e_s \int dv\, f_s(t, x, v),$$

$$\frac{\partial B}{\partial t} = -\nabla \times E, \qquad \nabla \cdot B = 0, \qquad j(t, x) = \sum_s e_s \int dv\, f_s(t, x, v)\, v$$

- the spaces of electrodynamics have a deRham complex structure
- Poisson structure (antisymmetric bracket, Jacobi identity)
- variational structure (Hamilton's action principle)
- energy, momentum and charge conservation (Noether theorem)

Differential Forms

- mathematical language of vector analysis too limited to provide an intuitive description of electrodynamics (only two types of objects)
  - ϕ: scalar field
  - E: change of the electric potential over an infinitesimal path element
  - B: flux density (integrated over a two-dimensional surface)
  - ρ: charge density (integrated over a three-dimensional volume)
- tensor analysis is concise and general, but very abstract
- subset of tensor analysis: calculus of differential forms, combining much of the generality of tensors with the simplicity of vectors
- in three dimensional space: four types of forms
  - 0-forms Λ^0: scalar quantities (scalar field)
  - 1-forms Λ^1: vectorial quantities (field intensity)
  - 2-forms Λ^2: vectorial quantities (flux density)
  - 3-forms Λ^3: scalar quantities (scalar density)

Maxwell's Equations and the deRham Complex

- electromagnetic fields as differential forms

$$\phi \in \Lambda^0(\Omega), \qquad A, E \in \Lambda^1(\Omega), \qquad B, J \in \Lambda^2(\Omega), \qquad \rho \in \Lambda^3(\Omega)$$

- exterior derivative $\mathbf{d} : \Lambda^i \to \Lambda^{i+1}$ generalises grad, curl, div
- the spaces of Maxwell's equations build an exact deRham sequence
- for geometers

$$0 \to \Lambda^0(\Omega) \xrightarrow{\mathbf{d}} \Lambda^1(\Omega) \xrightarrow{\mathbf{d}} \Lambda^2(\Omega) \xrightarrow{\mathbf{d}} \Lambda^3(\Omega) \to 0$$

- for analysts

$$0 \to H^1(\Omega) \xrightarrow{\mathrm{grad}} H(\mathrm{curl}, \Omega) \xrightarrow{\mathrm{curl}} H(\mathrm{div}, \Omega) \xrightarrow{\mathrm{div}} L^2(\Omega) \to 0$$

- exactness: the range of $\mathbf{d}^i : \Lambda^i \to \Lambda^{i+1}$ equals the kernel of $\mathbf{d}^{i+1}$

$$\mathbf{dd}\bullet = 0, \qquad \mathrm{curl}\,\mathrm{grad}\,\bullet = 0, \qquad \mathrm{div}\,\mathrm{curl}\,\bullet = 0$$

Discrete deRham Complex

- discrete deRham complex

$$\begin{array}{ccccccccccccc} 0 & \rightarrow & \Lambda^0(\Omega) & \xrightarrow{\mathbf{d}} & \Lambda^1(\Omega) & \xrightarrow{\mathbf{d}} & \Lambda^2(\Omega) & \xrightarrow{\mathbf{d}} & \Lambda^3(\Omega) & \rightarrow & 0 \\ & & \downarrow \pi_h^0 & & \downarrow \pi_h^1 & & \downarrow \pi_h^2 & & \downarrow \pi_h^3 & & \\ 0 & \rightarrow & \Lambda_h^0(\Omega) & \xrightarrow{\mathbf{d}} & \Lambda_h^1(\Omega) & \xrightarrow{\mathbf{d}} & \Lambda_h^2(\Omega) & \xrightarrow{\mathbf{d}} & \Lambda_h^3(\Omega) & \rightarrow & 0 \end{array}$$

- the discrete spaces $\Lambda_h^i \subset \Lambda^i$ are finite element spaces of differential forms, building an exact deRham sequence
- compatibility: projections commuted with the exterior derivative
- by translating geometrical and topological tools, which are used in the analysis of stability and well-posedness of PDEs, to the discrete level one can show that exactness and compatibility guarantee stability[2]

[2] Arnold, Falk, Winther: Finite element exterior calculus, homological techniques, and applications. Acta Numerica 15, 1–155, 2006.

Arnold, Falk, Winther: Finite Element Exterior Calculus: From Hodge Theory to Numerical Stability, Bulletin of the AMS 47, 281-354, 2010.

Spline Differential Forms

- electrostatic potential $\phi_h \in \Lambda_h^0(\Omega)$

$$\phi_h(t, x) = \sum_{i,j,k} \phi_{i,j,k}(t)\, \Lambda^0_{i,j,k}(x)$$

- zero-form basis

$$\Lambda_h^0(\Omega) = \operatorname{span}\left\{ S_i^p(x^1)\, S_j^p(x^2)\, S_k^p(x^3) \right\}$$

- the i-th basic splines (B-spline) of order p is defined by

$$S_i^p(x) = \frac{x - x_i}{x_{i+p-1} - x_i}\, S_i^{p-1}(x) + \frac{x_{i+p} - x}{x_{i+p} - x_{i+1}}\, S_{i+1}^{p-1}(x)$$

where

$$S_i^1(x) = \begin{cases} 1 & x \in [x_j, x_{j+1}) \\ 0 & \text{else} \end{cases}$$

Spline Differential Forms

- electric field intensity $E_h \in \Lambda_h^1(\Omega)$

$$E_h(t,x) = \sum_{i,j,k} e_{i,j,k}(t)\, \Lambda^1_{i,j,k}(x)$$

- one-form basis

$$\Lambda_h^1(\Omega) = \operatorname{span}\left\{ \begin{pmatrix} D_i^p(x^1)\, S_j^p(x^2)\, S_k^p(x^3) \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ S_i^p(x^1)\, D_j^p(x^2)\, S_k^p(x^3) \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ S_i^p(x^1)\, S_j^p(x^2)\, D_k^p(x^3) \end{pmatrix} \right\}$$

- spline differentials

$$\frac{d}{dx} S_i^p(x) = D_i^p(x) - D_{i+1}^p(x), \qquad D_i^p(x) = p\, \frac{S_i^{p-1}(x)}{x_{i+p} - x_i}$$

Spline Differential Forms

- magnetic flux density $B_h \in \Lambda_h^2(\Omega)$

$$B_h(t,x) = \sum_{i,j,k} b_{i,j,k}(t)\, \Lambda^2_{i,j,k}(x)$$

- two-form basis

$$\Lambda_h^2(\Omega) = \text{span}\left\{ \begin{pmatrix} S_i^p(x^1)\, D_j^p(x^2)\, D_k^p(x^3) \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ D_i^p(x^1)\, S_j^p(x^2)\, D_k^p(x^3) \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ D_i^p(x^1)\, D_j^p(x^2)\, S_k^p(x^3) \end{pmatrix} \right\}$$

- spline differentials

$$\frac{d}{dx} S_i^p(x) = D_i^p(x) - D_{i+1}^p(x), \qquad D_i^p(x) = p\, \frac{S_i^{p-1}(x)}{x_{i+p} - x_i}$$

Spline Differential Forms

- charge density $\rho_h \in \Lambda_h^3(\Omega)$

$$\rho_h(t,x) = \sum_{i,j,k} \rho_{i,j,k}(t)\, \Lambda^3_{i,j,k}(x)$$

- three-form basis

$$\Lambda_h^3(\Omega) = \operatorname{span}\left\{ D_i^p(x^1)\, D_j^p(x^2)\, D_k^p(x^3) \right\}$$

- spline differentials

$$\frac{d}{dx} S_i^p(x) = D_i^p(x) - D_{i+1}^p(x), \qquad D_i^p(x) = p\,\frac{S_i^{p-1}(x)}{x_{i+p} - x_i}$$

Morrison-Marsden-Weinstein Bracket

- Vlasov-Maxwell noncanonical Hamiltonian structure

$$\{F, G\}[f, E, B] = \int dx\, dv\, f \left[\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f}\right] + \int dx\, dv\, f \left(\frac{\partial}{\partial v}\frac{\delta F}{\delta f} \cdot \frac{\delta G}{\delta E} - \frac{\partial}{\partial v}\frac{\delta G}{\delta f} \cdot \frac{\delta F}{\delta E}\right)$$
$$+ \int dx\, dv\, f\, B \cdot \left(\frac{\partial}{\partial v}\frac{\delta F}{\delta f} \times \frac{\partial}{\partial v}\frac{\delta G}{\delta f}\right) + \int dx \left(\frac{\delta F}{\delta E} \cdot \nabla \times \frac{\delta G}{\delta B} - \frac{\delta G}{\delta E} \cdot \nabla \times \frac{\delta F}{\delta B}\right)$$

- Hamiltonian: sum of the kinetic energy of the particles, the electrostatic field energy and the magnetic field energy

$$\mathcal{H} = \frac{1}{2}\int |v|^2\, f(x, v)\, dx\, dv + \frac{1}{2}\int \left(|E(x)|^2 + |B(x)|^2 \right) dx$$

- time evolution of any functional $F[f, E, B]$

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

Discretisation of the Vlasov-Maxwell Poisson System

- finite-dimensional representation of the fields f, E, B
- discretisation of the brackets

$$\{F, G\}[f, E, B] = \int dx\, dv\, f \left[\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right] + \int dx\, dv\, f \left(\frac{\partial}{\partial v} \frac{\delta F}{\delta f} \cdot \frac{\delta G}{\delta E} - \frac{\partial}{\partial v} \frac{\delta G}{\delta f} \cdot \frac{\delta F}{\delta E} \right)$$
$$+ \int dx\, dv\, f\, B \cdot \left(\frac{\partial}{\partial v} \frac{\delta F}{\delta f} \times \frac{\partial}{\partial v} \frac{\delta G}{\delta f} \right) + \int dx \left(\frac{\delta F}{\delta E} \cdot \nabla \times \frac{\delta G}{\delta B} - \frac{\delta G}{\delta E} \cdot \nabla \times \frac{\delta F}{\delta B} \right)$$

- discretisation of functionals

$$\mathcal{H} = \frac{1}{2} \int |v|^2\, f(x, v)\, dx\, dv + \frac{1}{2} \int \left(|E(x)|^2 + |B(x)|^2 \right) dx$$

- time discretisation

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

Discretisation of the Fields

- particle-like distribution function for N_p particles labeled by a,

$$f_h(x, v, t) = \sum_{a=1}^{N_p} w_a \, \delta\big(x - x_a(t)\big) \, \delta\big(v - v_a(t)\big),$$

  with weights w_a, particle positions x_a and particle velocities v_a

- 1-form and 2-form basis functions (vector-valued)

$$\Lambda^1_\alpha(x) = \begin{pmatrix} \Lambda^{1,1}_\alpha(x) \\ \Lambda^{1,2}_\alpha(x) \\ \Lambda^{1,3}_\alpha(x) \end{pmatrix}, \qquad \Lambda^2_\alpha(x) = \begin{pmatrix} \Lambda^{2,1}_\alpha(x) \\ \Lambda^{2,2}_\alpha(x) \\ \Lambda^{2,3}_\alpha(x) \end{pmatrix}$$

- semi-discrete electric field E_h and magnetic field B_h

$$E_h(t, x) = \sum_{\alpha \in \mathbb{Z}^3} e_\alpha(t) \, \Lambda^1_\alpha(x), \qquad B_h(t, x) = \sum_{\alpha \in \mathbb{Z}^3} b_\alpha(t) \, \Lambda^2_\alpha(x)$$

  with coefficient vectors e and b

Discretisation of the Distribution Function

- functionals of the distribution function, $F[f]$, restricted to particle-like distribution functions,

$$f_h(x, v, t) = \sum_{a=1}^{N_p} w_a \, \delta\big(x - x_a(t)\big) \, \delta\big(v - v_a(t)\big),$$

  become functions of the particle phasespace trajectories,

$$F[f_h] = \hat{F}(x_a, v_a)$$

- replace functional derivatives with partial derivatives

$$\frac{\partial \hat{F}}{\partial x_a} = w_a \frac{\partial}{\partial x} \frac{\delta F}{\delta f} \bigg|_{(x_a, v_a)} \qquad \text{and} \qquad \frac{\partial \hat{F}}{\partial v_a} = w_a \frac{\partial}{\partial v} \frac{\delta F}{\delta f} \bigg|_{(x_a, v_a)}$$

- rewrite kinetic bracket as semi-discrete particle bracket

$$\int dx \, dv \, f \left[\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right] = \sum_a w_a \left(\frac{\partial}{\partial x} \frac{\delta F}{\delta f} \cdot \frac{\partial}{\partial v} \frac{\delta G}{\delta f} - \frac{\partial}{\partial v} \frac{\delta F}{\delta f} \cdot \frac{\partial}{\partial x} \frac{\delta G}{\delta f} \right) \bigg|_{(x_a, v_a)}$$

$$= \sum_a \frac{1}{w_a} \left(\frac{\partial \hat{F}}{\partial x_a} \cdot \frac{\partial \hat{G}}{\partial v_a} - \frac{\partial \hat{G}}{\partial x_a} \cdot \frac{\partial \hat{F}}{\partial v_a} \right)$$

Discretisation of the Electrodynamic Fields

- semi-discrete electric field E_h and magnetic field B_h

$$E_h(x) = \sum_{\alpha \in \mathbb{Z}^3} e_\alpha(t)\, \Lambda^1_\alpha(x), \qquad B_h(x) = \sum_{\alpha \in \mathbb{Z}^3} b_\alpha(t)\, \Lambda^2_\alpha(x)$$

- functionals $F[E]$ and $F[B]$, restricted to the semi-discrete fields E_h and B_h, can be considered as functions $\hat{F}(e)$ and $\hat{F}(b)$ of the finite element coefficients

$$F[E_h] = \hat{F}(e), \qquad F[B_h] = \hat{F}(b)$$

- functional derivatives of linear and quadratic functionals $F[E_h]$ and $F[B_h]$ can be replaced with partial derivatives of $\hat{F}(e)$ and $\hat{F}(b)$,

$$\frac{\delta F[E_h]}{\delta E} = \sum_{\alpha,\beta} \frac{\partial \hat{F}(e)}{\partial e_\alpha}\, (M_1^{-1})_{\alpha\beta}\, \Lambda^1_\beta(x), \quad \frac{\delta F[B_h]}{\delta B} = \sum_{\alpha,\beta} \frac{\partial \hat{F}(b)}{\partial b_\alpha}\, (M_2^{-1})_{\alpha\beta}\, \Lambda^2_\beta(x)$$

  with mass matrices

$$(M_1)_{\alpha\beta} = \int dx\, \Lambda^1_\alpha(x)\, \Lambda^1_\beta(x), \qquad (M_2)_{\alpha\beta} = \int dx\, \Lambda^2_\alpha(x)\, \Lambda^2_\beta(x)$$

Semi-Discrete Poisson Bracket

- semi-discrete Poisson bracket

$$
\begin{aligned}
\{\hat{F}, \hat{G}\}_d[x_a, v_a, e_\alpha, b_\alpha] = & \sum_a \frac{1}{w_a} \left(\frac{\partial \hat{F}}{\partial x_a} \cdot \frac{\partial \hat{G}}{\partial v_a} - \frac{\partial \hat{G}}{\partial x_a} \cdot \frac{\partial \hat{F}}{\partial v_a} \right) \\
& + \sum_a \sum_{\alpha,\beta} \left(\frac{\partial \hat{F}}{\partial v_a} \cdot \frac{\partial \hat{G}}{\partial e_\alpha} (M_1^{-1})_{\alpha\beta} \, \Lambda^1_\beta(x_a) - \frac{\partial \hat{G}}{\partial v_a} \cdot \frac{\partial \hat{F}}{\partial e_\alpha} (M_1^{-1})_{\alpha\beta} \, \Lambda^1_\beta(x_a) \right) \\
& + \sum_a \sum_\alpha b_\alpha(t) \, \Lambda^2_\alpha(x_a) \cdot \left(\frac{1}{w_a} \frac{\partial \hat{F}}{\partial v_a} \times \frac{\partial \hat{G}}{\partial v_a} \right) \\
& + \sum_{\alpha,\beta,\gamma,\eta} \left(\frac{\partial \hat{F}}{\partial e_\alpha} (M_1^{-1})_{\alpha\beta} \, R^T_{\beta\eta} \, (M_2^{-1})_{\eta\gamma} \, \frac{\partial \hat{G}}{\partial b_\gamma} - \frac{\partial \hat{G}}{\partial e_\alpha} (M_1^{-1})_{\alpha\beta} \, R^T_{\beta\eta} \, (M_2^{-1})_{\eta\gamma} \, \frac{\partial \hat{F}}{\partial b_\gamma} \right)
\end{aligned}
$$

- rotation matrix (decomposable into mass matrix M_2 and incidence matrix $\mathcal{I}$)

$$
R_{\alpha\beta} = \int dx \, \Lambda^2_\alpha(x) \cdot \nabla \times \Lambda^1_\beta(x), \qquad R = M_2 \mathcal{I}
$$

Semi-Discrete Poisson System

- semi-discrete equations of motion

$$\dot{x}_p = \{x_p, \hat{\mathcal{H}}\}_d, \qquad \dot{v}_p = \{v_p, \hat{\mathcal{H}}\}_d, \qquad \dot{e} = \{e, \hat{\mathcal{H}}\}_d, \qquad \dot{b} = \{b, \hat{\mathcal{H}}\}_d$$

  with discrete Hamiltonian

$$\hat{\mathcal{H}} = \frac{1}{2} \sum_a |v_a|^2 \; w_a + \frac{1}{2} \sum_{\alpha,\beta} e_\alpha(t) \, (M_1)_{\alpha\beta} \; e_\beta(t) + \frac{1}{2} \sum_{\alpha,\beta} b_\alpha(t) \, (M_2)_{\alpha\beta} \; b_\beta(t)$$

- Poisson system: $\dot{y} = P(y) \, \nabla \hat{\mathcal{H}}(y)$ with $y = (x_p, v_p, e, b)$

$$\frac{d}{dt} \begin{pmatrix} x_p \\ v_p \\ e \\ b \end{pmatrix} = \begin{pmatrix} 0 & M_p^{-1} & 0 & 0 \\ -M_p^{-1} & \widehat{B}_h^T(t, x_p) \, M_p^{-1} & (\Lambda^1(x_p))^T M_1^{-1} & 0 \\ 0 & -M_1^{-1}(\Lambda^1(x_p)) & 0 & M_1^{-1}\mathcal{I}^T \\ 0 & 0 & -\mathcal{I} M_1^{-1} & 0 \end{pmatrix} \begin{pmatrix} \partial\hat{\mathcal{H}}/\partial x_p \\ \partial\hat{\mathcal{H}}/\partial v_p \\ \partial\hat{\mathcal{H}}/\partial e \\ \partial\hat{\mathcal{H}}/\partial b \end{pmatrix}$$

- P is anti-symmetric and satisfies the Jacobi identity if $\operatorname{div} B_h = 0$ and

$$\frac{\partial \Lambda^1_{ki}(x_a)}{\partial x_a^j} - \frac{\partial \Lambda^1_{kj}(x_a)}{\partial x_a^i} = \sum_\alpha \left(\widehat{\Lambda}^2_\alpha(x_a) \right)_{ij} \mathcal{I}_{\alpha k} \quad \text{for all} \quad a, i, j, k,$$

→ recursion relation for splines, evaluated at all particle positions

Splitting Methods

- Hamiltonian splitting[3]

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{p_1} + \hat{\mathcal{H}}_{p_2} + \hat{\mathcal{H}}_{p_3} + \hat{\mathcal{H}}_E + \hat{\mathcal{H}}_B$$

with

$$\hat{\mathcal{H}}_{p_i} = \frac{1}{2}\,(v_p^i)^T M_p v_p^i, \qquad \hat{\mathcal{H}}_E = \frac{1}{2}\,e^T M_1\,e, \qquad \hat{\mathcal{H}}_B = \frac{1}{2}\,b^T M_2\,b$$

- split semi-discrete Vlasov-Maxwell equations into five subsystems

$$\dot{y} = \{y, \hat{\mathcal{H}}_{p_i}\}_d, \qquad \dot{y} = \{y, \hat{\mathcal{H}}_E\}_d, \qquad \dot{y} = \{y, \hat{\mathcal{H}}_B\}_d$$

- the exact solution of each subsystem constitutes a Poisson map

$$\varphi_{t,p_i}(y_0) = y_0 + \int_0^t \{y, \hat{\mathcal{H}}_{p_i}\}_d dt, \quad \varphi_{t,E}(y_0) = y_0 + \int_0^t \{y, \hat{\mathcal{H}}_E\}_d dt, \quad \ldots$$

[3] Crouseilles, Einkemmer, Faou. Hamiltonian splitting for the Vlasov– Maxwell equations. Journal of Computational Physics 283, 224–240, 2015.
Qin, He, Zhang, Liu, Xiao, Wang. Comment on “Hamiltonian splitting for the Vlasov–Maxwell equations”. arXiv:1504.07785, 2015.
He, Qin, Sun, Xiao, Zhang, Liu. Hamiltonian integration methods for Vlasov–Maxwell equations. arXiv:1505.06076, 2015.

Splitting Methods

- Hamiltonian splitting

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{p_1} + \hat{\mathcal{H}}_{p_2} + \hat{\mathcal{H}}_{p_3} + \hat{\mathcal{H}}_{E} + \hat{\mathcal{H}}_{B}$$

- compositions of Poisson maps are themselves Poisson maps
- construct Poisson structure preserving integration methods by composition of exact solutions of the subsystems
- first order time integrator: Lie-Trotter composition

$$\Psi_h = \varphi_{h,E} \circ \varphi_{h,B} \circ \varphi_{h,p_1} \circ \varphi_{h,p_2} \circ \varphi_{h,p_3}$$

- second order time integrator: symmetric composition

$$\Psi_h = \varphi_{h/2,E} \circ \varphi_{h/2,B} \circ \varphi_{h/2,p_1} \circ \varphi_{h/2,p_2} \circ \varphi_{h,p_3} \circ \varphi_{h/2,p_2} \circ \varphi_{h/2,p_1} \circ \varphi_{h/2,B} \circ \varphi_{h/2,E}$$

Variational Integrators

- systematic way to derive structure-preserving discretisation schemes for Lagrangian and Hamiltonian dynamical systems
- preserved structures
  - discrete symplectic structure

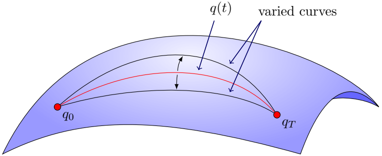
  $\rightarrow$ good long-time energy behaviour (bounded error)
  - discrete momenta related to symmetries of the discrete Lagrangian

  $\rightarrow$ discrete Noether theorem provides discrete symmetry condition and discrete form of conservation laws
- idea
  - discretisation of the Lagrangian and Hamilton's principle of stationary action
  - application of the discrete action principle to the discrete Lagrangian to obtain discrete Euler-Lagrange equations directly
- allow for straight-forward derivation of integrators for coupled systems (e.g., coupling of particles and fields for particle-in-cell schemes)

Continuous and Discrete Action Principle

- action: functional of a curve $q(t)$

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



- Hamilton's principle of stationary action: among all possible trajectories the system follows the one that makes the action integral $\mathcal{A}$ stationary

$$\delta \mathcal{A} = 0 \qquad \rightarrow \qquad \frac{\partial L}{\partial q}(q, \dot{q}) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q})\right) = 0$$

- approximate Lagrangian with finite differences and quadrature formula

$$L_d(q_n, q_{n+1}) = h\, L\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h}\right)$$

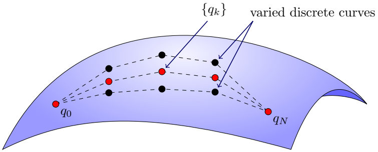
- stationarity of the discrete action: discrete Euler-Lagrange equations

$$\delta \mathcal{A}_d = \delta \sum_{n=0}^{N-1} L_d(q_n, q_{n+1}) = 0 \quad \rightarrow \quad D_2 L_d(q_{n-1}, q_n) + D_1 L_d(q_n, q_{n+1}) = 0$$

Continuous and Discrete Action Principle

- action: functional of a curve $q(t)$

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



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$$\delta \mathcal{A} = 0 \qquad \rightarrow \qquad \frac{\partial L}{\partial q}(q, \dot{q}) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q})\right) = 0$$

- approximate Lagrangian with finite differences and quadrature formula

$$L_d(q_n, q_{n+1}) = h\, L\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h}\right)$$

- stationarity of the discrete action: discrete Euler-Lagrange equations

$$\delta \mathcal{A}_d = \delta \sum_{n=0}^{N-1} L_d(q_n, q_{n+1}) = 0 \quad \rightarrow \quad D_2 L_d(q_{n-1}, q_n) + D_1 L_d(q_n, q_{n+1}) = 0$$

Continuous Action Principle for Vlasov-Maxwell

- variations of the action

$$\mathcal{A} = \sum_s \int dt \int dX \int dV f_s(t, X, V) \left[m V + e_s A(t, X) \right] \cdot \dot{X} - \left[\tfrac{1}{2} m \, |V|^2 + e_s \phi(t, X) \right]$$
$$+ \frac{1}{2} \int dt \int dx \left[\left| \nabla \phi(t, x) - \frac{\partial A}{\partial t}(t, x) \right|^2 - |\nabla \times A(t, x)|^2 \right]$$

lead to the same equations of motion as the Poisson bracket upon

$$E = -\nabla \phi - \frac{\partial A}{\partial t}, \qquad B = \nabla \times A$$

- the Vlasov-Maxwell action is (weakly) gauge invariant

$$\mathcal{A}[x, v, A + \nabla \psi, \phi] = \mathcal{A}[x, v, A, \phi] + \text{boundary terms}$$

- corresponding conservation law: charge conservation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot j = 0$$

Semi-Discrete Action Principle for Vlasov-Maxwell

- semi-discrete action (particles, splines, time-continuous)

$$\mathcal{A}_h = \frac{1}{N} \sum_a \int_0^T dt \left[m_a v_a(t) + e_a A_h(t, x_a(t)) \right] \cdot \dot{x}_a(t) - \left[\tfrac{1}{2} m_a \left| v_a(t) \right|^2 + e_a \phi_h(t, x_a(t)) \right]$$

$$+ \frac{1}{2} \int_0^T dt \int dx \left[\left| \nabla \phi_h(t, x) - \frac{\partial A_h}{\partial t}(t, x) \right|^2 - \left| \nabla \times A_h(t, x) \right|^2 \right]$$

→ same equations of motion as the semi-discrete Poisson bracket, upon

$$E_h = -\nabla \phi_h - \frac{\partial A_h}{\partial t}, \qquad B_h = \nabla \times A_h$$

- the semi-discrete action is still (weakly) gauge invariant

$$\mathcal{A}_h \left[x, v, A_h + \nabla \psi_h, \phi_h \right] = \mathcal{A}_h \left[x, v, A_h, \phi_h \right] + \text{boundary terms}$$

- corresponding conservation law: charge conservation

$$\frac{\partial \rho_h}{\partial t} + \nabla \cdot j_h = 0$$

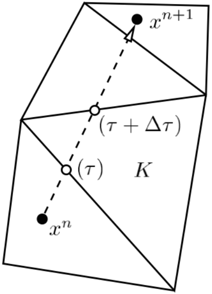
Gauge Invariance of the Discrete Action

- time discretisation (e.g., Lagrange polynomials)

$$y_h(t)\big|_{[t_n,t_{n+1}]} = \sum_{m=1}^{s} Y_{n,m}\,\varphi_n^m(t), \qquad \varphi_n^m(t) = l^m\big((t-t_n)/(t_{n+1}-t_n)\big)$$

- variations of fully discrete action

$$\delta \int_{t_n}^{t_{n+1}} dt\, A_h(t, x_h(t)) \cdot \dot{x}_h(t) = \int_{t_n}^{t_{n+1}} dt \sum_{l,m=1}^{s} \delta X_{n,m} \cdot \nabla A_h(t, x_h(t)) \cdot X_{n,l}\, \dot{\varphi}_n^l(t)\, \varphi_n^m(t)$$



$$+ \int_{t_n}^{t_{n+1}} dt \sum_{m=1}^{s} A_h(t, x_h(t)) \cdot \delta X_{n,m}\, \dot{\varphi}_n^m(t) + \ldots$$

$$= \int_{t_n}^{t_{n+1}} dt \sum_{l,m=1}^{s} \delta X_{n,m} \cdot \nabla A_h(t, x_h(t)) \cdot X_{n,l}\, \dot{\varphi}_n^l(t)\, \varphi_n^m(t)$$

$$- \int_{t_n}^{t_{n+1}} dt \sum_{l,m=1}^{s} X_{n,l} \cdot \nabla A_h(t, x_h(t)) \cdot \delta X_{n,m}\, \dot{\varphi}_n^l(t)\, \varphi_n^m(t) + \ldots$$

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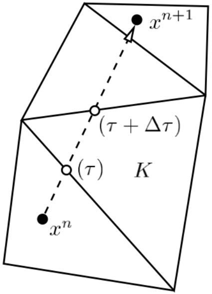


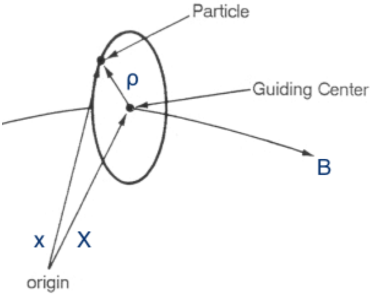
$$+ \int_{t_n}^{t_{n+1}} dt \sum_{m=1}^{s} A_h(t, x_h(t)) \cdot \delta X_{n,m}\, \dot{\varphi}_n^m(t) + \ldots$$

$$= \int_{t_n}^{t_{n+1}} dt \sum_{l,m=1}^{s} \delta X_{n,m} \cdot B_h(t, x_h(t)) \cdot X_{n,l}\, \dot{\varphi}_n^l(t)\, \varphi_n^m(t) + \ldots$$

Summary and Outlook

- Maxwell equations
  - discrete differential forms (discrete exterior calculus, mimetic discretisation): splines, mixed finite elements, mimetic spectral elements, virtual elements
  - stability: exactness and compatibility of the finite element deRham complex
- discrete Poisson brackets and variational integrators
  - Poisson structure is retained at the semi-discrete level
  - splitting methods or variational integrators for time integration
  - gauge invariance guarantees charge conservation
- variational integrators for degenerate Lagrangians
  - multi-step methods featuring parasitic modes or one-step methods for an extended system drifting off the constraint submanifold
  - projection of variational integrators for the unconstrained extended system
  - very good long-time stability and conservation of energy and momentum maps
- ongoing work
  - application to the *Hamiltonian Gyrokinetic Vlasov–Maxwell System* (Burby et al., Physics Letters A, 379, pp. 2073–2077, 2015)
  - extension towards discrete metriplectic brackets for dissipative systems

Guiding Centre Dynamics



- charged particle phasespace Lagrangian

$$L(x, \dot{x}, v, \dot{v}) = (A(x) + v) \cdot \dot{x} - \tfrac{1}{2} v^2$$

- coordinate transformation

$$(x^i, v^i) \quad \rightarrow \quad (X^i, \theta, u, \mu)$$

with $\rho = b \times v_\perp / |B|$ and

$$u = b \cdot \dot{X}, \quad v_\perp = v - ub, \quad \mu = v_\perp^2 / 2\,|B|\,, \quad B = \nabla \times A, \quad b = B/\,|B|$$

so that the Lagrangian becomes

$$L(q, \dot{q}) = \big(A(X+\rho) + ub(X+\rho)\big) \cdot \big(\dot{X} + \dot{\rho}\big) + \mu\dot{\theta} - \tfrac{1}{2} u^2 - \mu B(X+\rho)$$

- strong magnetic fields: neglect finite gyroradius effects
- guiding centre Lagrangian ($q = (X^i, u)$ and μ a parameter)

$$L(q, \dot{q}) = (A(X) + ub(X)) \cdot \dot{X} - \tfrac{1}{2} u^2 - \mu B(X)$$

Variational Guiding Centre Integrators

- guiding centre Lagrangian

$$L(q,\dot{q}) = (A(X) + ub(X)) \cdot \dot{X} - \tfrac{1}{2}u^2 - \mu B(X), \qquad q = (X^i, u)$$

  is degenerate (linear in velocities), that is

$$\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} = 0$$

  and therefore leads to first order ordinary differential equations

- straight-forward application of the discrete action principle leads to multi-step variational integrators

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

→ we need two sets of initial data even though we have first order ODEs

→ support parasitic modes, not long-time stable

Variational Guiding Centre Integrators

- use discrete Legendre transform to obtain position-momentum form

$$\begin{aligned} p_k &= -D_1 L_d(q_k, q_{k+1}), \\ p_{k+1} &= D_2 L_d(q_k, q_{k+1}) \end{aligned}$$

- use continuous Legendre transform to obtain the second initial condition

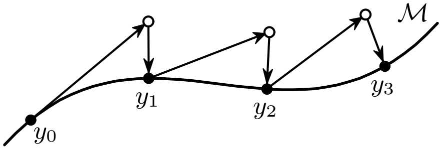
$$p_0 = \frac{\partial L}{\partial \dot{q}}(q_0) = \alpha(q_0), \qquad \alpha(q) = A(X) + u\, b(X)$$

- one-step method for an extended dynamical system (p, q) whose dynamics is constrained to a subspace defined by

$$\phi(p, q) = p - \alpha(q) = 0 \qquad \text{(Dirac constraint)}$$

- variational integrators will in general not satisfy the constraint
- geometric interpretation for appearance of parasitic modes

Orthogonal Projection



- orthogonal symplectic projection of primary constraint, $z = (p, q)$

$$\tilde{z}_{n+1} = \Psi_h(z_n) \qquad \text{apply variational one-step method}$$

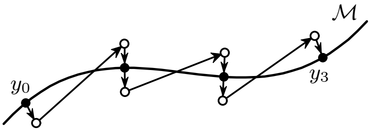
$$z_{n+1} = \tilde{z}_{n+1} + \Omega^{-1} \nabla \phi^T(z_{n+1}) \lambda_{n+1} \qquad \text{project on constraint submanifold}$$

$$0 = \phi(z_{n+1})$$

with Ω the canonical symplectic matrix

$$\Omega = \begin{pmatrix} \mathbb{0} & -\mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}$$

Symmetric Projection



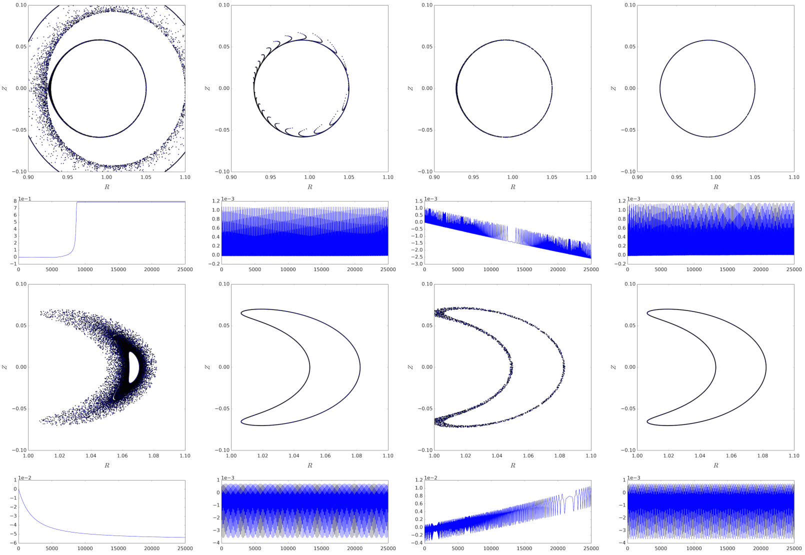
- symmetric symplectic projection of primary constraint, $z = (p, q)$

$$
\begin{aligned}
\tilde{z}_k &= z_k + \Omega^{-1} \nabla \phi^T(z_k)\, \lambda_{k+1} && \text{perturb initial data} \\
\tilde{z}_{k+1} &= \Psi_h(\tilde{z}_k) && \text{apply variational one-step method} \\
z_{k+1} &= \tilde{z}_{k+1} + \Omega^{-1} \nabla \phi^T(z_{k+1}) \lambda_{k+1} && \text{project on constraint submanifold} \\
0 &= \phi(z_{k+1}).
\end{aligned}
$$

with Ω the canonical symplectic matrix

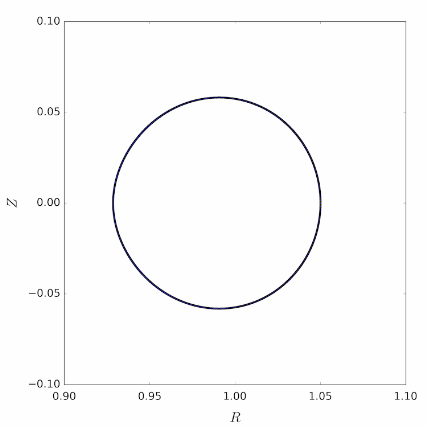
$$
\Omega = \begin{pmatrix} \mathbb{0} & -\mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}
$$

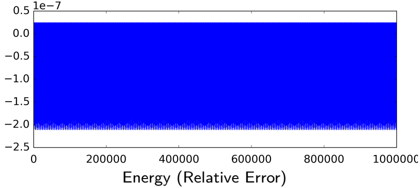
Passing and Trapped Particle 2D, $h = \frac{\tau_b}{50}$, $n_b = 25.000$

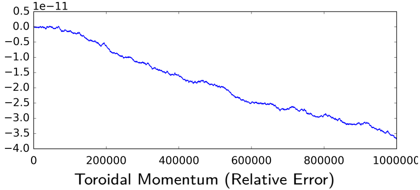


Explicit RK4 | Variational RK2 (1 stage) | Orthogonal Projection | Symmetric Projection

Passing Particle 4D, $h = \frac{\tau_b}{50}$, $n_b = 10^6$, $n_t = 5 \times 10^7$

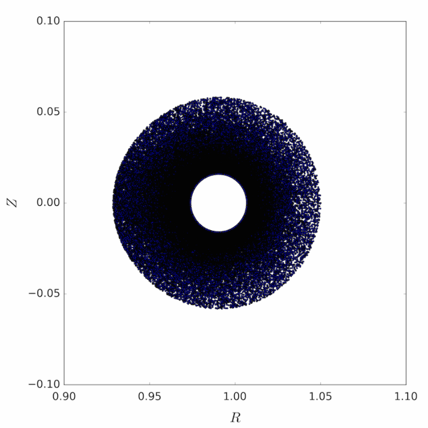


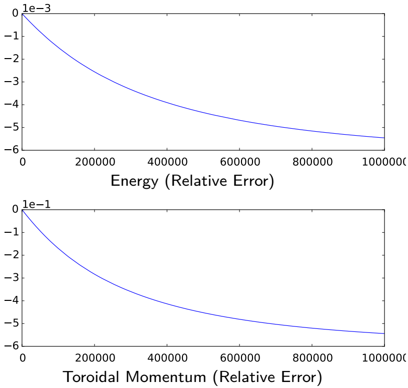




Variational Runge-Kutta, 2 stages, order 4, symmetric projection

Passing Particle 4D, $h = \frac{\tau_b}{50}$, $n_b = 10^6$, $n_t = 5 \times 10^7$





Explicit Runge-Kutta, order 4