Geometric Finite-Element Particle-in-Cell Methods for the Vlasov-Maxwell System

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Geometric Structures of the Vlasov-Maxwell System

- Vlasov equation in Lagrangian coordinates

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

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

- 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 satisfying the Jacobi identity)
- variational structure (Hamilton's action principle)
- energy, momentum and charge conservation (Noether theorem)

Outline

1. Discrete Differential Forms
2. Discrete Poisson Brackets
3. Variational Integrators and Noether Theorem
4. Summary and Outlook

Discrete Differential Forms

Differential Forms

- Maxwell's equations

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

- mathematical language of vector analysis too limited to provide an intuitive description of electrodynamics (only two types of objects)

Quantity	Symbol	Unit	Integration along
scalar electric potential	ϕ	V	0D point
electric field intensity	E	$\mathrm{V/m}$	1D path
magnetic flux density	B	$\mathrm{(Vs)/m^2}$	2D surface
charge density	ρ	$\mathrm{(As)/m^3}$	3D volume

- alternative: 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

Differential Forms

- in three dimensional space: four types of forms
  - 0-forms Λ^0: scalar quantities (functions)
  - 1-forms Λ^1: vectorial quantities (line elements)
  - 2-forms Λ^2: vectorial quantities (surface elements)
  - 3-forms Λ^3: scalar quantities (volume elements)
- 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 $\mathbf{d} : \Lambda^k \to \Lambda^{k+1}$ (generalises grad, curl, div)
- hodge $\star : \Lambda^k \to \Lambda^{n-k}$ (isomorphism on metric spaces)
- Maxwell's equations with differential forms

$$\frac{\partial E}{\partial t} = \star \mathbf{d} \star B - \star J, \qquad \mathbf{d} \star E = -\rho,$$
$$\frac{\partial B}{\partial t} = -\mathbf{d} E, \qquad \mathbf{d} B = 0$$

Maxwell's Equations and the deRham Complex

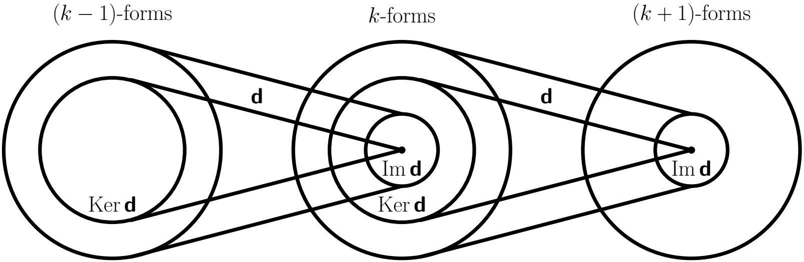
- the spaces of Maxwell's equations form a deRham complex
- for geometers

$$\mathbb{R} \;\rightarrow\; \Lambda^0(\Omega) \;\xrightarrow{\mathbf{d}}\; \Lambda^1(\Omega) \;\xrightarrow{\mathbf{d}}\; \Lambda^2(\Omega) \;\xrightarrow{\mathbf{d}}\; \Lambda^3(\Omega) \;\rightarrow\; 0$$

- for analysts

$$\mathbb{R} \;\rightarrow\; H^1(\Omega) \;\xrightarrow{\text{grad}}\; H(\text{curl}, \Omega) \;\xrightarrow{\text{curl}}\; H(\text{div}, \Omega) \;\xrightarrow{\text{div}}\; L^2(\Omega) \;\rightarrow\; 0$$

- complex: $\text{Im}\,\{\mathbf{d} : \Lambda^{k-1} \rightarrow \Lambda^k\} \subseteq \text{Ker}\,\{\mathbf{d} : \Lambda^k \rightarrow \Lambda^{k+1}\}$



$$\mathbf{d} \circ \mathbf{d} = 0, \qquad \text{curl}\,\text{grad} = 0, \qquad \text{div}\,\text{curl} = 0$$

Discrete deRham Complex

- discrete deRham complex

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

- the discrete spaces $\Lambda_h^k \subset \Lambda^k$ are finite element spaces of differential forms, building a deRham complex
- exactness: $\text{Im}\,\{\mathbf{d} : \Lambda^{k-1} \rightarrow \Lambda^k\} = \text{Ker}\,\{\mathbf{d} : \Lambda^k \rightarrow \Lambda^{k+1}\}$
- compatibility: projections π_h^k commute with exterior derivative $\mathbf{d}$
- 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[1]

[1] 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 $\phi_h \in \Lambda^0_h(\Omega)$

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

- zero-form basis

$$\Lambda^0_h(\Omega) = \operatorname{span}\left\{ S^p_i(x^1)\, S^p_j(x^2)\, S^p_k(x^3) \right\}$$

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

$$S^p_i(x) = \frac{x - x_i}{x_{i+p-1} - x_i}\, S^{p-1}_i(x) + \frac{x_{i+p} - x}{x_{i+p} - x_{i+1}}\, S^{p-1}_{i+1}(x)$$

where

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

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

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

- 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

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

Discrete Poisson Brackets

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 spline 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

$$E_h(t, x) = \sum_{\alpha=1}^{N_{\text{dof}}} e_\alpha(t) \, \Lambda^1_\alpha(x), \qquad B_h(t, x) = \sum_{\alpha=1}^{N_{\text{dof}}} b_\alpha(t) \, \Lambda^2_\alpha(x)$$

  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

$$E_h(x) = \sum_\alpha e_\alpha(t)\, \Lambda^1_\alpha(x), \qquad B_h(x) = \sum_\alpha b_\alpha(t)\, \Lambda^2_\alpha(x)$$

- 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 $\hat{F}(b)$,

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

  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 $\mathcal{I}$)

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

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

$$\hat{\mathcal{H}} = \tfrac{1}{2}\, v_p^T(t)\, M_p v_p(t) + \tfrac{1}{2}\, e^T(t)\, M_1 e(t) + \tfrac{1}{2}\, b^T(t)\, M_2 b(t)$$

- 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 $\nabla \cdot B_h(x_a) = 0 \; \forall a$ and

$$\frac{\partial \Lambda^{1,i}_{\alpha}}{\partial x^j}(x_a) - \frac{\partial \Lambda^{1,j}_{\alpha}}{\partial x^i}(x_a) = \sum_{\beta} \left(\widehat{\Lambda}^2_{\beta}(x_a)\right)_{ij} \mathcal{I}_{\beta\alpha} \quad \text{for all} \quad a, \alpha \quad \text{and} \quad 1 \leq i, j \leq 3$$

→ recursion relation for splines ($\mathbf{d}\Lambda^1 = \widehat{\Lambda}^2 \mathcal{I}$), evaluated at all particle positions x_a

Splitting Methods

- Hamiltonian splitting[2]

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

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

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

- each subsystem can be solved exactly

$$\varphi_{t,E}(y_0) = y_0 + \int_0^t \{y, \hat{\mathcal{H}}_E\}_d dt, \qquad \varphi_{t,B}(y_0) = y_0 + \int_0^t \{y, \hat{\mathcal{H}}_B\}_d dt, \qquad \dots$$

[2] 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

- for the exact solution of the kinetic subsystems

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

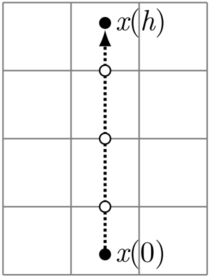
we have to compute line integrals exactly[3] (e.g. $i = 1$)

$$x_p^1(h) = x_p^1(0) + h v_p^1(0),$$

$$v_p^2(h) = v_p^2(0) + \int_0^h dt \, v_p^3(0) \, b(0) \, \Lambda^{2,1}(x_p(t)),$$

$$v_p^3(h) = v_p^3(0) - \int_0^h dt \, v_p^2(0) \, b(0) \, \Lambda^{2,1}(x_p(t)),$$

$$M_1 e(h) = M_1 e(0) - \int_0^h dt \, \Lambda^{1,1}(x_p(t)) \, M_p v_p^1(0)$$



3 Campos Pinto, Jund, Salmon, Sonnendrücker. Charge-conserving FEM-PIC schemes on general grids. Comptes Rendus Mécanique 342, 570–582, 2014.

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Moon, Teixeira, Omelchenko. Exact charge-conserving scatter–gather algorithm for particle-in-cell simulations on unstructured grids. CPC 194, 43–53, 2015.

Splitting Methods

- Hamiltonian splitting

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

- the exact solution of each subsystem constitutes a Poisson map
- 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 and Noether Theorem

Continuous Action Principle for Vlasov-Maxwell

- variations of the action

$$\mathcal{A} = \sum_s \int dt \int dX \int dV \Big[f_s(t,X,V) \Big(m_s V + e_s A(t,X) \Big) \cdot \dot{X} - \Big(\frac{m_s}{2} V^2 + e_s \phi(t,X) \Big) \Big]$$

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

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

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

- 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

Continuous Action Principle for Vlasov-Maxwell

- the action of the particle-field system,

$$\mathcal{A} = \sum_a w_a \int dt \int dx \left[\Big(m_a v_a + e_a A(t,x) \Big) \cdot \dot{x}_a(t) - \left(\frac{m_a}{2} v_a^2 + e_a \phi(t,x) \right) \right] \delta(x - x_a)$$

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

  is invariant under temporal, spatial and gauge transformations

→ energy conservation

$$\frac{d}{dt} \left[\sum_a w_a \left(\frac{m_a}{2} v_a^2 + e_a \phi(t, x_a) \right) + \frac{1}{2} \int dx \left(|E(t,x)|^2 + |B(t,x)|^2 \right) \right] = 0$$

→ momentum conservation

$$\frac{d}{dt} \left[\sum_a w_a m_a v_a \right] = 0$$

→ charge conservation

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

Symmetries and the Noether Theorem

- consider a transformation of $\mathrm{x} = (t, x)$ and $\mathrm{y} = (x_a, v_a, \phi, A)$[4]

$$(\mathrm{x}, \mathrm{y}) \to (\tilde{\mathrm{x}}, \tilde{\mathrm{y}}) = (\xi(\mathrm{x}, \epsilon),\ \eta(\mathrm{x}, \mathrm{y}(\mathrm{x}), \epsilon))$$

  with

$$\xi\big|_{\epsilon=0} = \mathrm{id} \qquad \text{and} \qquad \eta\big|_{\epsilon=0} = \mathrm{id}$$

- symmetry: action is invariant under transformation

$$\int_{\tilde{\Omega}} \mathcal{L}\big(\tilde{\mathrm{x}}, \tilde{\mathrm{y}}, \tilde{\mathrm{y}}_\mu\big)\, d\tilde{\mathrm{x}} = \int_{\Omega} \mathcal{L}\big(\mathrm{x}, \mathrm{y}, \mathrm{y}_\mu\big)\, d\mathrm{x}$$

- equivalent to infinitesimal equivariance condition on the Lagrangian $\mathcal{L}$

$$\frac{d}{d\epsilon} \int_{\tilde{\Omega}} \mathcal{L}\big(\tilde{\mathrm{x}}, \tilde{\mathrm{y}}, \tilde{\mathrm{y}}_\mu\big)\, d\tilde{\mathrm{x}}\bigg|_{\epsilon=0} = 0 \qquad \Leftrightarrow \qquad \mathrm{pr}\, V(\mathcal{L}) + \mathcal{L}\ \mathrm{div}\, \overline{V} = 0$$

→ variation of $\mathcal{L}$ in the direction of the vector field V vanishes

[4] Caution: The simplified notation used here hides the fact that (x_a, v_a) depend only on t while (ϕ, A) depend on both, t and x. The appropriate setting of jet bundles is more rigorous but technically more involved.

Symmetries and the Noether Theorem

- generating vector field

$$V = V^{\mu} \frac{\partial}{\partial \mathrm{x}^{\mu}} + V^{\alpha} \frac{\partial}{\partial \mathrm{y}^{\alpha}}, \qquad V^{\mu} = \frac{\partial \xi^{\mu}}{\partial \epsilon}\bigg|_{\epsilon=0}, \qquad V^{\alpha} = \frac{\partial \eta^{\alpha}}{\partial \epsilon}\bigg|_{\epsilon=0}$$

- prolongation: action of the transformation on derivatives of fields

$$\mathrm{pr}\, V = V^{\mu} \frac{\partial}{\partial \mathrm{x}^{\mu}} + V^{\alpha} \frac{\partial}{\partial \mathrm{y}^{\alpha}} + \left(\frac{\partial V^{\alpha}}{\partial \mathrm{x}^{\mu}} + \mathrm{y}^{\alpha}_{\nu} \frac{\partial V^{\nu}}{\partial \mathrm{x}^{\mu}} + \mathrm{y}^{\beta}_{\mu} \frac{\partial V^{\alpha}}{\partial \mathrm{y}^{\beta}} \right) \frac{\partial}{\partial \mathrm{y}^{\alpha}_{\mu}}$$

- symmetry condition in terms of the generating vector field

$$\mathrm{pr}\, V(\mathcal{L}) + \mathcal{L}\ \mathrm{div}\, \overline{V} = 0, \qquad \overline{V} = V^{\mu} \frac{\partial}{\partial \mathrm{x}^{\mu}}$$

- conservation law: divergence of the Noether current $\mathcal{J}$ vanishes

$$\mathrm{div}\, \mathcal{J} = \frac{\partial}{\partial \mathrm{x}^{\mu}} \left[\frac{\partial \mathcal{L}}{\partial \mathrm{y}^{\alpha}_{\mu}} (\mathrm{x}, \mathrm{y}, \mathrm{y}_{\mu}) \cdot (V^{\alpha} - \mathrm{y}^{\alpha}_{\nu} V^{\nu}) + V^{\mu} \mathcal{L} \right] = 0$$

Symmetries and the Noether Theorem

- generating vector field

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- generalisation: divergence symmetries

$$\mathrm{pr}\, V(\mathcal{L}) + \mathcal{L}\, \mathrm{div}\, \overline{V} = \mathrm{div}\, \mathcal{C}$$

- divergence of the generalised Noether current $\tilde{\mathcal{J}} = \mathcal{J} - \mathcal{C}$ vanishes

$$\mathrm{div}(\mathcal{J} - \mathcal{C}) = \frac{\partial}{\partial \mathrm{x}^{\mu}} \left[\frac{\partial \mathcal{L}}{\partial \mathrm{y}^{a}_{\mu}}(\mathrm{x}, \mathrm{y}, \mathrm{y}_{\mu}) \cdot (V^{a} - \mathrm{y}^{a}_{\nu} V^{\nu}) + V^{\mu} \mathcal{L} - \mathcal{C}^{\mu} \right] = 0$$

Symmetries and the Noether Theorem

- generating vector field

$$V = V^{\mu} \frac{\partial}{\partial \mathrm{x}^{\mu}} + V^{\alpha} \frac{\partial}{\partial \mathrm{y}^{\alpha}}, \qquad V^{\mu} = \frac{\partial \xi^{\mu}}{\partial \epsilon} \bigg|_{\epsilon=0}, \qquad V^{\alpha} = \frac{\partial \eta^{\alpha}}{\partial \epsilon} \bigg|_{\epsilon=0}$$

- prolongation: action of the transformation on derivatives of fields

$$\mathrm{pr}\, V = V^{\mu} \frac{\partial}{\partial \mathrm{x}^{\mu}} + V^{\alpha} \frac{\partial}{\partial \mathrm{y}^{\alpha}} + \left(\frac{\partial V^{\alpha}}{\partial \mathrm{x}^{\mu}} + \mathrm{y}^{\alpha}_{\nu} \frac{\partial V^{\nu}}{\partial \mathrm{x}^{\mu}} + \mathrm{y}^{\beta}_{\mu} \frac{\partial V^{\alpha}}{\partial \mathrm{y}^{\beta}} \right) \frac{\partial}{\partial \mathrm{y}^{\alpha}_{\mu}}$$

- generalisation: divergence symmetries

$$\mathrm{pr}\, V(\mathcal{L}) + \mathcal{L}\, \mathrm{div}\, \overline{V} = \mathrm{div}\, \mathcal{C}$$

- conservation law: time derivative of Noether charge vanishes

$$\frac{d}{dt} \int \left[\frac{\partial \mathcal{L}}{\partial \mathrm{y}^{a}_{t}} (\mathrm{x}, \mathrm{y}, \mathrm{y}_{\mu}) \cdot \left(V^{a} - \mathrm{y}^{a}_{\nu} V^{\nu} \right) + V^{t} \mathcal{L} - \mathcal{C}^{t} \right] dx = 0$$

Conservation Laws of the Vlasov-Maxwell System

- Lagrange density $\mathcal{L}$ so that $\mathcal{A} = \int dt \int dx \, \mathcal{L}$,

$$\mathcal{L} = \sum_a w_a \left[\Big(m_a v_a + e_a A(t,x) \Big) \cdot \dot{x}_a(t) - \left(\frac{m_a}{2} v_a^2 + e_a \phi(t,x) \right) \right] \delta(x - x_a) + \frac{1}{2} \left[\left| -\nabla\phi(t,x) - \frac{\partial A}{\partial t}(t,x) \right|^2 - |\nabla \times A(t,x)|^2 \right],$$

- energy conservation: translation of time

$$t \to t + \epsilon, \qquad V = \frac{\partial}{\partial t}, \qquad \mathrm{pr}\, V = \frac{\partial}{\partial t}$$

- equivariance condition satisfied: $\mathrm{pr}\, V(\mathcal{L}) + \mathcal{L} \, \mathrm{div}\, \overline{V} = 0$
- conservation law

$$\frac{d}{dt} \left[\sum_a w_a \left[\frac{m_a}{2} v_a^2 + e_a \phi(t, x_a) \right] + \frac{1}{2} \int dx \left(|E(t,x)|^2 + |B(t,x)|^2 \right) \right] = 0$$

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- momentum conservation: translation of space ($u \in \mathbb{R}^3$)

$$x \to x + \epsilon u, \quad x_a \to x_a + \epsilon u, \quad V = u \frac{\partial}{\partial x} + u \frac{\partial}{\partial x_a}, \quad \mathrm{pr}\, V = u \frac{\partial}{\partial x} + u \frac{\partial}{\partial x_a}$$

- equivariance condition satisfied: $\mathrm{pr}\, V(\mathcal{L}) + \mathcal{L} \, \mathrm{div}\, \overline{V} = 0$
- conservation law

$$\frac{d}{dt} \bigg[\sum_a w_a \Big[m_a v_a + e_a A(t,x) \Big] \cdot u \bigg] = 0$$

Conservation Laws of the Vlasov-Maxwell System

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- charge conservation: gauge transformation ($\psi = \psi(x)$)

$$A \to A + \epsilon \nabla\psi, \quad V = \nabla\psi \, \frac{\partial}{\partial A}, \quad \mathrm{pr}\, V = \nabla\psi \, \frac{\partial}{\partial A} + (\partial_\mu \nabla\psi) \, \frac{\partial}{\partial A_\mu}$$

- divergence symmetry: $\mathrm{pr}\, V(\mathcal{L}) + \mathcal{L} \, \mathrm{div} \, \overline{V} = \mathrm{div} \, \mathcal{C}$

$$\mathcal{C}^t = \sum_a w_a e_a \, \psi(x_a(t)) \, \delta(x - x_a(t))$$

$$\mathcal{C}^x = \sum_a w_a e_a \, \psi(x_a(t)) \, \delta(x - x_a(t)) \, \dot{x}_a(t)$$

Conservation Laws of the Vlasov-Maxwell System

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- conservation law: $\operatorname{div} \widetilde{\mathcal{J}} = \operatorname{div}(\mathcal{J} - \mathcal{C}) = 0$

$$\operatorname{div} \widetilde{\mathcal{J}} = \left[-\frac{\partial E(t,x)}{\partial t} + \nabla \times B(t,x) - \sum_a w_a e_a \, \delta(x - x_a(t)) \, \dot{x}_a(t) \right] \cdot \nabla \psi(x) + \frac{\partial}{\partial t} \left(\sum_a w_a e_a \, \psi(x_a(t)) \, \delta(x - x_a(t)) \right) + \nabla \cdot \left(\sum_a w_a e_a \, \psi(x_a(t)) \, \delta(x - x_a(t)) \, \dot{x}_a(t) \right) = 0$$

Conservation Laws of the Vlasov-Maxwell System

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- conservation law: $\operatorname{div} \widetilde{\mathcal{J}} = \operatorname{div}(\mathcal{J} - \mathcal{C}) = 0$ with $\psi(x) = 1$

$$\frac{\partial \rho(t,x)}{\partial t} + \nabla \cdot J(t,x) = 0,$$

$$\rho(t,x) = \sum_a w_a e_a \, \delta(x - x_a(t)), \quad J(t,x) = \sum_a w_a e_a \, \delta(x - x_a(t)) \, \dot{x}_a(t)$$

Semi-Discrete Action Principle for Vlasov-Maxwell

- variations of the semi-discrete action $\mathcal{A}_h = \int dt\, L_h$ with $L_h = \int \mathcal{L}_h\, dx$,

$$\mathcal{L}_h = \sum_a w_a \Big[\Big(m_a v_a + e_a A_h(t,x) \Big) \cdot \dot{x}_a(t) - \Big(\frac{m_a}{2} v_a^2 + e_a \phi_h(t,x) \Big) \Big] \, \delta(x - x_a)$$
$$+ \frac{1}{2} \left[\left| -\nabla \phi_h(t,x) - \frac{\partial A_h}{\partial t}(t,x) \right|^2 - |\nabla \times A_h(t,x)|^2 \right],$$

leads to same equations of motion as semi-discrete Poisson bracket upon

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

- the semi-discrete action retains temporal and gauge invariance, but loses momentum conservation, except for axisymmetric fields

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

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- the semi-discrete action retains temporal and gauge invariance, but loses momentum conservation, except for axisymmetric fields

Fully Discrete Vlasov-Maxwell Action

- semi-discrete Lagrangian $(y_h(t) = (x_a(t), v_a(t), A_\alpha(t), \phi_\alpha(t)))$

$$L_h(y_h, \dot{y}_h) = \sum_a w_a \Big[\Big(m_a v_a + e_a A_h(t, x_a(t)) \Big) \cdot \dot{x}_a(t) - \Big(\frac{m_a}{2} v_a^2 + e_a \phi_h(t, x_a(t)) \Big) \Big]$$

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

- time discretisation (e.g., Lagrange polynomials $l(t)$)

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

- fully discrete action

$$\mathcal{A}_d = \sum_{n=1}^{n_t - 1} L_d(y_n, y_{n+1}), \qquad L_d(y_n, y_{n+1}) = \int_{t_n}^{t_{n+1}} L_h(y_d(t), \dot{y}_d(t)) \, dt$$

- lose energy conservation, but symplectic (energy error bounded)

Gauge Invariance of the Discrete Vlasov-Maxwell Action

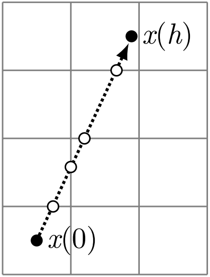
- discrete Lagrangian

$$L_d(y_n, y_{n+1}) = \int_{t_n}^{t_{n+1}} dt \sum_a w_a e_a A_h(t, x_a(t)) \cdot \dot{x}_a(t) + \dots$$

- variations of fully discrete action

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

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



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

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

Gauge Invariance of the Discrete Vlasov-Maxwell Action

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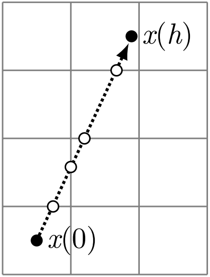
$$+ \int_{t_n}^{t_{n+1}} dt \sum_{m=1}^{s} A_h(t, x_a(t)) \cdot \delta X_{a,n}^m \, \dot{\varphi}_n^m(t) + \dots$$

$$= \int_{t_n}^{t_{n+1}} dt \sum_{l,m=1}^{s} \delta X_{a,n}^m \cdot \widehat{B}_h(t, x_a(t)) \cdot X_{a,n}^l \, \dot{\varphi}_n^l(t)\, \varphi_n^m(t) + \dots$$



Remark: Semi-Discrete Particle-in-Fourier Lagrangian

- semi-discrete Particle-in-Fourier action (Vlasov-Poisson)

$$\mathcal{A}_h = \sum_a \int_0^T dt\, w_a \Big[m_a v_a(t) \cdot \dot{x}_a(t) - \tfrac{1}{2} m_a \, |v_a(t)|^2 - e_a \phi_h(t, x_a(t)) \Big] + \frac{1}{2} \int_0^T dt \int dx \, |\nabla \phi_h(t,x)|^2$$

where

$$\phi_h(t,x) = \sum_{k \neq 0} \frac{1}{(ik)^2} \, b_k(t) \, \exp\big\{ - ikx \big\}$$

- Euler-Lagrange equation for the Fourier coefficients b_k

$$b_k(t) = \sum_a w_a \, \exp\big\{ ikx_a(t) \big\}$$

- symmetric under translations $\tilde{x}_a = x_a + \epsilon u$ as $\tilde{\phi}_h(\tilde{x}_b) = \phi_h(x_b)$ due to

$$\exp\big\{ - ik\tilde{x}_b + ik\tilde{x}_a \big\} = \exp\big\{ - ikx_b + ikx_a \big\}$$

Summary and Outlook

Summary and Outlook

- discrete electrodynamics
  - discrete differential forms and discrete deRham complexes: 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 symplectic time integration
  - gauge invariance guarantees charge conservation
  - general: logical or physical coordinates, discretisation techniques, various systems
- ongoing and future work
  - Hamiltonian Noether theorem, fully Eulerian discretisation, extension towards discrete metriplectic and double brackets for dissipative systems
  - application to Hamiltonian fluid systems and the *Hamiltonian Gyrokinetic Vlasov–Maxwell System* (Burby et al., Physics Letters A, 379, 2073–2077, 2015)

→ new splitting methods or variational integrators for degenerate Lagrangians (or covariant Poisson brackets)