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**
  \[
  \dot{X}_s = V_s, \quad \dot{V}_s = e_s E(t, X_s) + \frac{e_s}{c} V_s \times B(t, X_s)
  \]
  \[
  f_s(t, X_s(t), V_s(t)) = f_s(X_s(0), V_s(0))
  \]

- **Maxwell’s equations in Eulerian coordinates**
  \[
  \frac{\partial E}{\partial t} = \nabla \times B - J, \quad \nabla \cdot E = -\rho, \quad \rho(t, x) = \sum_s e_s \int dv f_s(t, x, v),
  \]
  \[
  \frac{\partial B}{\partial t} = -\nabla \times E, \quad \nabla \cdot B = 0, \quad J(t, x) = \sum_s e_s \int dv f_s(t, x, v) v
  \]

- 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)
Discrete Poisson Brackets
Morrison-Marsden-Weinstein Bracket

- **Vlasov-Maxwell noncanonical Hamiltonian structure**

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

- **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

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

- 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 \( a \),

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

with weights \( w_a \), particle positions \( x_a \) and particle velocities \( v_a \)

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

\[
\Lambda_\alpha^1(x) = \begin{pmatrix} \Lambda_\alpha^{1,1}(x) \\ \Lambda_\alpha^{1,2}(x) \\ \Lambda_\alpha^{1,3}(x) \end{pmatrix}, \quad \Lambda_\alpha^2(x) = \begin{pmatrix} \Lambda_\alpha^{2,1}(x) \\ \Lambda_\alpha^{2,2}(x) \\ \Lambda_\alpha^{2,3}(x) \end{pmatrix}
\]

- semi-discrete electric field \( E_h \) and magnetic field \( B_h \)

\[
E_h(t, x) = \sum_{\alpha=1}^{N_{dof}} e_\alpha(t) \Lambda_\alpha^1(x), \quad B_h(t, x) = \sum_{\alpha=1}^{N_{dof}} b_\alpha(t) \Lambda_\alpha^2(x)
\]

with coefficient vectors \( e \) and \( b \)
Discretisation of the Distribution Function

- functionals of the distribution function, $F[f]$, restricted to particle-like distribution functions,
\[
  f_h(x, v, t) = \sum_{a=1}^{N_p} w_a \delta(x - x_a(t)) \delta(v - v_a(t)),
\]
become functions of the particle phasespace trajectories,
\[
  F[f_h] = \hat{F}(x_a, v_a)
\]
- replace functional derivatives with partial derivatives
\[
  \frac{\partial \hat{F}}{\partial x_a} = w_a \frac{\partial}{\partial x} \frac{\delta F}{\delta f} \bigg|_{(x_a, v_a)} \quad \text{and} \quad \frac{\partial \hat{F}}{\partial v_a} = w_a \frac{\partial}{\partial v} \frac{\delta F}{\delta f} \bigg|_{(x_a, v_a)}
\]
- 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 $B_h$

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

- 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

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

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

$$\frac{\delta F[E_h]}{\delta E} = \sum_{\alpha,\beta} \frac{\partial \hat{F}(e)}{\partial e_\alpha} (M^{-1}_1)_{\alpha\beta} \Lambda^1_\beta(x), \quad \frac{\delta F[B_h]}{\delta B} = \sum_{\alpha,\beta} \frac{\partial \hat{F}(b)}{\partial b_\alpha} (M^{-1}_2)_{\alpha\beta} \Lambda^2_\beta(x)$$

with mass matrices

$$(M_1)_{\alpha\beta} = \int dx \Lambda^1_\alpha(x) \Lambda^1_\beta(x), \quad (M_2)_{\alpha\beta} = \int dx \Lambda^2_\alpha(x) \Lambda^2_\beta(x)$$
Semi-Discrete Poisson Bracket

semi-discrete Poisson bracket

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

rotation matrix (decomposable into mass matrix \( M_2 \) and incidence matrix \( I \))

\[
R_{\alpha \beta} = \int dx \Lambda_\alpha^2(x) \cdot \nabla \times \Lambda_\beta^1(x), \quad R = M_2 I
\]
Semi-Discrete Poisson System

- semi-discrete equations of motion

\[ \dot{x}_p = \{x_p, \hat{H}\}_d, \quad \dot{v}_p = \{v_p, \hat{H}\}_d, \quad \dot{e} = \{e, \hat{H}\}_d, \quad \dot{b} = \{b, \hat{H}\}_d \]

with discrete Hamiltonian

\[ \hat{H} = \frac{1}{2} v_p^T(t) M_p v_p(t) + \frac{1}{2} e^T(t) M_1 e(t) + \frac{1}{2} b^T(t) M_2 b(t) \]

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

\[
\frac{d}{dt} \begin{pmatrix} x_p \\ v_p \\ e \\ b \end{pmatrix} = \begin{pmatrix} 0 & M_p^{-1} & 0 & 0 \\ -M_p^{-1} & \hat{B}_h^T(t, x_p) M_p^{-1} & (\Lambda^1(x_p))^T M_1^{-1} & 0 \\ 0 & -M_1^{-1}(\Lambda^1(x_p)) & 0 & M_1^{-1}I^T \\ 0 & 0 & -IM_1^{-1} & 0 \end{pmatrix} \begin{pmatrix} \partial \hat{H}/\partial x_p \\ \partial \hat{H}/\partial v_p \\ \partial \hat{H}/\partial e \\ \partial \hat{H}/\partial b \end{pmatrix}
\]

where \( \hat{B}_h(t, x_p) \) is the \( 3N_p \times 3N_p \) anti-symmetric block-diagonal matrix,

\[
\hat{B}_h(t, x_p) = \sum_{\alpha} b_{\alpha}(t) \hat{\Lambda}_{\alpha}^2(x_p), \quad \hat{\Lambda}_{\alpha}^2(x_p) = \begin{pmatrix} \hat{\Lambda}_{\alpha}^2(x_1) \\ \hat{\Lambda}_{\alpha}^2(x_2) \\ \vdots \\ \hat{\Lambda}_{\alpha}^2(x_{N_p}) \end{pmatrix}
\]
Semi-Discrete Poisson System

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

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

- $P$ is anti-symmetric and satisfies the Jacobi identity if $\nabla \cdot B_h(x_a) = 0 \ \forall a$ and

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

- recursion relation for splines, evaluated at all particle positions $x_a$

\[
\nabla \times \Lambda^1 = \hat{\Lambda}^2 \mathcal{I}, \quad \hat{\Lambda}^2_\alpha(x_a) = \begin{pmatrix} 0 & -\Lambda^{2,3}_\alpha(x_a) & \Lambda^{2,2}_\alpha(x_a) \\ \Lambda^{2,3}_\alpha(x_a) & 0 & -\Lambda^{2,1}_\alpha(x_a) \\ -\Lambda^{2,2}_\alpha(x_a) & \Lambda^{2,1}_\alpha(x_a) & 0 \end{pmatrix}
\]
Splitting Methods

- Hamiltonian splitting\(^1\)

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

with

\[ \hat{\mathcal{H}}_{p_i} = \frac{1}{2} v_{p_i}^T M_p v_{p_i}, \quad \hat{\mathcal{H}}_E = \frac{1}{2} e^T M_1 e, \quad \hat{\mathcal{H}}_B = \frac{1}{2} b^T M_2 b \]

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

\[ \dot{y} = \{ y, \hat{\mathcal{H}}_{p_i} \}_d, \quad \dot{y} = \{ y, \hat{\mathcal{H}}_E \}_d, \quad \dot{y} = \{ y, \hat{\mathcal{H}}_B \}_d \]

- each subsystem can be solved exactly

\[ \varphi_{t,E}(y_0) = y_0 + \int_0^t \{ y, \hat{\mathcal{H}}_E \}_d dt, \quad \varphi_{t,B}(y_0) = y_0 + \int_0^t \{ y, \hat{\mathcal{H}}_B \}_d dt, \quad \ldots \]

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Splitting Methods

- for the exact solution of the kinetic subsystems

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

we have to compute line integrals exactly\(^2\) (e.g. \(i = 1\))

\[ x_{p}^1(h) = x_{p}^1(0) + h v_{p}^1(0), \]
\[ v_{p}^2(h) = v_{p}^2(0) + \int_0^h dt \, v_{p}^3(0) \, b(0) \, \Lambda^{2,1}(x_{p}(t)), \]
\[ v_{p}^3(h) = v_{p}^3(0) - \int_0^h dt \, v_{p}^2(0) \, b(0) \, \Lambda^{2,1}(x_{p}(t)), \]
\[ M_1 e(h) = M_1 e(0) - \int_0^h dt \, \Lambda^{1,1}(x_{p}(t)) \, M_p v_{p}^1(0) \]

→ solution is gauge invariant and therefore charge conserving

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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

\[
\Psi_h = \varphi_{h/2,E} \circ \varphi_{h/2,B} \circ \varphi_{h/2,p_1} \circ \varphi_{h/2,p_2} \circ \varphi_{h,p_3} \circ \varphi_{h/2,p_2} \circ \varphi_{h/2,p_1} \circ \varphi_{h/2,B} \circ \varphi_{h/2,E}
\]
Nonlinear Landau Damping

- numerical example: Nonlinear Landau Damping

\[ f(x, v) = f_M \left(1 + A \cos(kx)\right), \quad f_M(x, v) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2} \frac{v^2}{v_{th}^2}\right\} \]

- numerical parameters:
  \[ x^1 \in [0, 2\pi/k), \quad v \in \mathbb{R}^2, \quad h_t = 0.01, \quad n_x = 32 \]

- physical parameters:
  \[ v_{th} = 1, \quad k = 0.5, \quad A = 0.5 \]
\[ |E_x(t, x)|^2 \]

- \( \gamma_1 = -0.287246 \)
- \( \gamma_2 = 0.086020 \)

<table>
<thead>
<tr>
<th>Integrator</th>
<th>( \gamma_1 )</th>
<th>( \gamma_2 )</th>
</tr>
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<tbody>
<tr>
<td>PoissonPIC</td>
<td>-0.287</td>
<td>+0.086</td>
</tr>
<tr>
<td>viVlasov1D</td>
<td>-0.286</td>
<td>+0.085</td>
</tr>
<tr>
<td>Cheng &amp; Knorr (1976)</td>
<td>-0.281</td>
<td>+0.084</td>
</tr>
<tr>
<td>Nakamura &amp; Yabe (1999)</td>
<td>-0.280</td>
<td>+0.085</td>
</tr>
<tr>
<td>Ayuso &amp; Hajian (2012)</td>
<td>-0.292</td>
<td>+0.086</td>
</tr>
<tr>
<td>Heath, Gamba, et al. (2012)</td>
<td>-0.287</td>
<td>+0.075</td>
</tr>
</tbody>
</table>
Nonlinear Landau Damping

\[
\frac{(E(t) - E(0))}{E(0)}
\]

\(1e-6\)
Nonlinear Landau Damping

\[
\frac{E(t) - E(0)}{E(0)}
\]

\(10^6\)

<table>
<thead>
<tr>
<th>t</th>
<th>(E(t) - E(0))/E(0)</th>
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</tr>
<tr>
<td>20</td>
<td>3.55</td>
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<td>90</td>
<td>3.90</td>
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<tr>
<td>100</td>
<td>3.95</td>
</tr>
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</table>
Summary and Outlook
Summary and Outlook

- discrete electrodynamics (also fluid dynamics, magnetohydrodynamics, ...)
  - discrete differential forms and discrete deRham complexes of compatible spaces: splines, mixed finite elements, mimetic spectral elements, virtual elements
  - exactly satisfy identities from vector calculus ($\text{curl}\ \text{grad} = 0$, $\text{div}\ \text{curl} = 0$)
  - 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 ($\rightarrow$ toroidal momentum transport)
  - general: logical or physical coordinates, discretisation techniques, various systems

- ongoing and future work
  - Casimir Invariants, Hamiltonian Noether theorem, fully Eulerian discretisation, extension towards discrete metriplectic and double brackets for dissipative systems
Summary and Outlook

ongoing and future work


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

variational integrators for degenerate Lagrangians

- multi-step methods featuring parasitic modes or one-step methods for an extended system drifting off the constraint submanifold

  various solutions:

  - projection of variational integrators enforcing the constraint
  - Lagrange d’Alembert integrators enforcing secondary constraint
  - pullback of extended system with continuous Legendre transform
  - conjugate-symplectic variational integrators based on formal Lagrangians

  very good long-time stability and conservation of energy and momentum maps

ongoing work

- gauge invariant integrators of arbitrary order in spline fields
Teaser
Passing Particle 4D, \( h = \frac{T_b}{50}, \ n_b = 10^6, \ n_t = 5 \times 10^7 \)

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
Summary and Outlook

- ongoing and future work
  - new splitting methods or variational integrators for degenerate Lagrangians (or covariant Poisson brackets)

- variational integrators for degenerate Lagrangians
  - multi-step methods featuring parasitic modes or one-step methods for an extended system drifting off the constraint submanifold
  - various solutions:
    - projection of variational integrators enforcing the constraint
    - Lagrange d’Alembert integrators enforcing secondary constraint
    - pullback of extended system with continuous Legendre transform
    - conjugate-symplectic variational integrators based on formal Lagrangians
  - very good long-time stability and conservation of energy and momentum maps

- ongoing work
  - gauge invariant integrators of arbitrary order in spline fields
Discrete Differential Forms
Maxwell’s equations

\[ \frac{\partial E}{\partial t} = \nabla \times B - J, \quad \nabla \cdot E = -\rho, \]
\[ \frac{\partial B}{\partial t} = -\nabla \times E, \quad \nabla \cdot B = 0 \]

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

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Unit</th>
<th>Integration along</th>
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<tbody>
<tr>
<td>scalar electric potential</td>
<td>(\phi)</td>
<td>V</td>
<td>0D point</td>
</tr>
<tr>
<td>electric field intensity</td>
<td>(E)</td>
<td>V/m</td>
<td>1D path</td>
</tr>
<tr>
<td>magnetic flux density</td>
<td>(B)</td>
<td>(Vs)/m(^2)</td>
<td>2D surface</td>
</tr>
<tr>
<td>charge density</td>
<td>(\rho)</td>
<td>(As)/m(^3)</td>
<td>3D volume</td>
</tr>
</tbody>
</table>

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 $\Lambda^0$: scalar quantities (functions)
  - 1-forms $\Lambda^1$: vectorial quantities (line elements)
  - 2-forms $\Lambda^2$: vectorial quantities (surface elements)
  - 3-forms $\Lambda^3$: scalar quantities (volume elements)

- electromagnetic fields as differential forms
  \[ \phi \in \Lambda^0(\Omega), \quad A, E \in \Lambda^1(\Omega), \quad B, J \in \Lambda^2(\Omega), \quad \rho \in \Lambda^3(\Omega) \]

- exterior derivative $d : \Lambda^k \rightarrow \Lambda^{k+1}$ (generalises grad, curl, div)

- hodge $\star : \Lambda^k \rightarrow \Lambda^{n-k}$ (isomorphism on metric spaces)

- Maxwell's equations with differential forms
  \[ \frac{\partial E}{\partial t} = \star d \star B - \star J, \quad d \star E = -\rho, \]
  \[ \frac{\partial B}{\partial t} = -dE, \quad dB = 0 \]
Maxwell’s Equations and the deRham Complex

- the spaces of Maxwell’s equations form a deRham complex
- for geometers
  \[ \mathbb{R} \to \Lambda^0(\Omega) \xrightarrow{d} \Lambda^1(\Omega) \xrightarrow{d} \Lambda^2(\Omega) \xrightarrow{d} \Lambda^3(\Omega) \to 0 \]
- for analysts
  \[ \mathbb{R} \to H^1(\Omega) \xrightarrow{\text{grad}} H(\text{curl}, \Omega) \xrightarrow{\text{curl}} H(\text{div}, \Omega) \xrightarrow{\text{div}} L^2(\Omega) \to 0 \]
- complex: \( \text{Im} \{d : \Lambda^{k-1} \to \Lambda^k\} \subseteq \text{Ker} \{d : \Lambda^k \to \Lambda^{k+1}\} \)
discrete deRham complex

\[ \mathbb{R} \rightarrow \Lambda^0(\Omega) \xrightarrow{d} \Lambda^1(\Omega) \xrightarrow{d} \Lambda^2(\Omega) \xrightarrow{d} \Lambda^3(\Omega) \rightarrow 0 \]

\[ \downarrow \pi_h^0 \quad \downarrow \pi_h^1 \quad \downarrow \pi_h^2 \quad \downarrow \pi_h^3 \]

\[ \mathbb{R} \rightarrow \Lambda^0_h(\Omega) \xrightarrow{d} \Lambda^1_h(\Omega) \xrightarrow{d} \Lambda^2_h(\Omega) \xrightarrow{d} \Lambda^3_h(\Omega) \rightarrow 0 \]

- the discrete spaces \( \Lambda^k_h \subset \Lambda^k \) are finite element spaces of differential forms, building a deRham complex
- exactness: \( \text{Im} \{ d : \Lambda^{k-1} \rightarrow \Lambda^k \} = \text{Ker} \{ d : \Lambda^k \rightarrow \Lambda^{k+1} \} \)
- compatibility: projections \( \pi^k_h \) commute with exterior derivative \( d \)
- 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.\(^3\)

---


Spline Differential Forms

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

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

- zero-form basis

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

- 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 \( E_h \in \Lambda^1_h(\Omega) \)

\[
E_h(t, x) = \sum_{i,j,k} e_{i,j,k}(t) \Lambda_{i,j,k}^1(x)
\]

- One-form basis

\[
\Lambda^1_h(\Omega) = \text{span} \left\{ \begin{pmatrix}
D^p_i(x^1) & S^p_j(x^2) & S^p_k(x^3) \\
0 & 0 & 0 \\
0 & 0 & 0 \\
S^p_i(x^1) & D^p_j(x^2) & S^p_k(x^3) \\
0 & 0 & 0 \\
S^p_i(x^1) & S^p_j(x^2) & D^p_k(x^3)
\end{pmatrix}, \begin{pmatrix}
D^p_i(x^1) & S^p_j(x^2) & S^p_k(x^3) \\
0 & 0 & 0 \\
0 & 0 & 0 \\
S^p_i(x^1) & D^p_j(x^2) & S^p_k(x^3) \\
0 & 0 & 0 \\
S^p_i(x^1) & S^p_j(x^2) & D^p_k(x^3)
\end{pmatrix}, \begin{pmatrix}
D^p_i(x^1) & S^p_j(x^2) & S^p_k(x^3) \\
0 & 0 & 0 \\
0 & 0 & 0 \\
S^p_i(x^1) & D^p_j(x^2) & S^p_k(x^3) \\
0 & 0 & 0 \\
S^p_i(x^1) & S^p_j(x^2) & D^p_k(x^3)
\end{pmatrix} \right\}
\]

- Spline differentials

\[
\frac{d}{dx} S^p_i(x) = D^p_i(x) - D^p_{i+1}(x), \quad D^p_i(x) = p \frac{S^p_{i-1}(x)}{x_{i+p} - x_i}
\]
Spline Differential Forms

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

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

- two-form basis

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

- spline differentials

$$\frac{d}{dx} S_i^p(x) = D^p_i(x) - D^p_{i+1}(x), \quad D^p_i(x) = p \frac{S^p_{i-1}(x)}{x_{i+p} - x_i}$$
Spline Differential Forms

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

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

- three-form basis

$$\Lambda^3_h(\Omega) = \text{span} \left\{ D^p_i(x^1) D^p_j(x^2) D^p_k(x^3) \right\}$$

- spline differentials

$$\frac{d}{dx} S^p_i(x) = D^p_i(x) - D^p_{i+1}(x), \quad D^p_i(x) = p \frac{S^p_{i-1}(x)}{x_{i+p} - x_i}$$
Variational Integrators and Noether Theorem
Continuous Action Principle for Vlasov-Maxwell

- variations of the action

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

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

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

\[ E = -\nabla \phi - \frac{\partial A}{\partial t}, \quad B = \nabla \times A \]

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

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

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,

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

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

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 $x = (t, x)$ and $y = (x_a, v_a, \phi, A)^4$

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

with

$$ \xi|_{\epsilon=0} = \text{id} \quad \text{and} \quad \eta|_{\epsilon=0} = \text{id} $$

- symmetry: action is invariant under transformation

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

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

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

→ 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 $(\phi, A)$ 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

\[ V = V^\mu \frac{\partial}{\partial x^\mu} + V^\alpha \frac{\partial}{\partial y^\alpha} \]
\[ V^\mu = \frac{\partial \xi^\mu}{\partial \epsilon} \bigg|_{\epsilon = 0} \]
\[ V^\alpha = \frac{\partial \eta^\alpha}{\partial \epsilon} \bigg|_{\epsilon = 0} \]

- prolongation: action of the transformation on derivatives of fields

\[ \text{pr} \ V = V^\mu \frac{\partial}{\partial x^\mu} + V^\alpha \frac{\partial}{\partial y^\alpha} + \left( \frac{\partial V^\alpha}{\partial x^\mu} + y^\alpha_\nu \frac{\partial V^\nu}{\partial x^\mu} + y^\beta_\mu \frac{\partial V^\alpha}{\partial y^\beta} \right) \frac{\partial}{\partial y^\alpha} \]

- symmetry condition in terms of the generating vector field

\[ \text{pr} \ V(\mathcal{L}) + \mathcal{L} \ \text{div} \ V = 0, \]
\[ \bar{V} = V^\mu \frac{\partial}{\partial x^\mu} \]

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

\[ \text{div} \ \mathcal{J} = \frac{\partial}{\partial x^\mu} \left[ \frac{\partial \mathcal{L}}{\partial y^\alpha_\mu} (x, y, y^\mu) \cdot (V^\alpha - y^\alpha_\nu V^\nu) + V^\mu \mathcal{L} \right] = 0 \]
Symmetries and the Noether Theorem

- generating vector field

\[ V = V^\mu \frac{\partial}{\partial x^\mu} + V^\alpha \frac{\partial}{\partial y^\alpha}, \quad V^\mu = \left. \frac{\partial \xi^\mu}{\partial \epsilon} \right|_{\epsilon=0}, \quad V^\alpha = \left. \frac{\partial \eta^\alpha}{\partial \epsilon} \right|_{\epsilon=0} \]

- prolongation: action of the transformation on derivatives of fields

\[ \text{pr} V = V^\mu \frac{\partial}{\partial x^\mu} + V^\alpha \frac{\partial}{\partial y^\alpha} + \left( \frac{\partial V^\alpha}{\partial x^\mu} + y^\alpha \frac{\partial V^\nu}{\partial x^\mu} + y^\beta \frac{\partial V^\alpha}{\partial y^\beta} \right) \frac{\partial}{\partial y^\alpha} \]

- generalisation: divergence symmetries

\[ \text{pr} V(\mathcal{L}) + \mathcal{L} \text{ div } \overline{V} = \text{div } \mathcal{C} \]

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

\[ \text{div}(J - \mathcal{C}) = \frac{\partial}{\partial x^\mu} \left[ \frac{\partial \mathcal{L}}{\partial y^a_{\mu}}(x, y, y_{\mu}) \cdot (V^a - y^a_{\nu} V^\nu) + V^\mu \mathcal{L} - \mathcal{C}^\mu \right] = 0 \]
Symmetries and the Noether Theorem

- generating vector field

\[ V = V^\mu \frac{\partial}{\partial x^\mu} + V^\alpha \frac{\partial}{\partial y^\alpha}, \quad V^\mu = \frac{\partial \xi^\mu}{\partial \epsilon} \bigg|_{\epsilon=0}, \quad V^\alpha = \frac{\partial \eta^\alpha}{\partial \epsilon} \bigg|_{\epsilon=0} \]

- prolongation: action of the transformation on derivatives of fields

\[ \text{pr} \, V = V^\mu \frac{\partial}{\partial x^\mu} + V^\alpha \frac{\partial}{\partial y^\alpha} + \left( \frac{\partial V^\alpha}{\partial x^\mu} + y^\alpha_\nu \frac{\partial V^\nu}{\partial x^\mu} + y^\beta_\mu \frac{\partial V^\alpha}{\partial y^\beta} \right) \frac{\partial}{\partial y^\alpha_\mu} \]

- generalisation: divergence symmetries

\[ \text{pr} \, V(\mathcal{L}) + \mathcal{L} \text{ div } \bar{V} = \text{ div } \mathcal{C} \]

- conservation law: time derivative of Noether charge vanishes

\[ \frac{d}{dt} \int \left[ \frac{\partial \mathcal{L}}{\partial y^\alpha_t}(x, y, y_\mu) \cdot (V^\alpha - y^\alpha_\nu V^\nu) + V^t \mathcal{L} - C^t \right] \, dx = 0 \]
Conservation Laws of the Vlasov-Maxwell System

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

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

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

- energy conservation: translation of time

$$t \rightarrow t + \epsilon, \quad V = \frac{\partial}{\partial t}, \quad \text{pr} V = \frac{\partial}{\partial t}$$

- equivariance condition satisfied: \(\text{pr} V(\mathcal{L}) + \mathcal{L} \text{ div } \overline{V} = 0\)

- conservation law

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

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

- momentum conservation: translation of space ($u \in \mathbb{R}^3$)
  
  $x \rightarrow x + \epsilon u, \quad x_a \rightarrow x_a + \epsilon u, \quad V = u \frac{\partial}{\partial x} + u \frac{\partial}{\partial x_a}, \quad \text{pr} V = u \frac{\partial}{\partial x} + u \frac{\partial}{\partial x_a}$

- equivariance condition satisfied: $\text{pr} V(\mathcal{L}) + \mathcal{L} \ \text{div} \ \vec{V} = 0$

- conservation law
  \[
  \frac{d}{dt} \left[ \sum_a w_a \left[ m_a v_a + e_a A(t, x) \right] \cdot u \right] = 0
  \]
Conservation Laws of the Vlasov-Maxwell System

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

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

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

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

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

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

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

$$\mathcal{C}^x = \sum_a w_a e_a \psi(x_a(t)) \delta(x - x_a(t)) \dot{x}_a(t)$$
Conservation Laws of the Vlasov-Maxwell System

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

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

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

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

\[
A \rightarrow A + \epsilon \nabla \psi, \quad V = \nabla \psi \frac{\partial}{\partial A}, \quad \text{pr} \ V = \nabla \psi \frac{\partial}{\partial A} + (\partial_\mu \nabla \psi) \frac{\partial}{\partial A_\mu}
\]

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

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

\[
+ \frac{\partial}{\partial t} \left( \sum_a w_a e_a \psi(x_a(t)) \delta(x - x_a(t)) \right)
\]

\[
+ \nabla \cdot \left( \sum_a w_a e_a \psi(x_a(t)) \delta(x - x_a(t)) \dot{x}_a(t) \right) = 0
\]
Conservation Laws of the Vlasov-Maxwell System

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

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

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

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

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

- Conservation law: $\text{div} \ \tilde{\mathcal{J}} = \text{div}(\mathcal{J} - \mathcal{C}) = 0$ 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 $A_h = \int dt L_h$ with $L_h = \int L_h \, dx$,

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

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

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

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

- the semi-discrete action retains temporal and gauge invariance, but loses momentum conservation, except for axisymmetric fields
Semi-Discrete Action Principle for Vlasov-Maxwell

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

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

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

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

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

- 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 \( y_h(t) = (x_a(t), v_a(t), A_\alpha(t), \phi_\alpha(t)) \)

\[
L_h(y_h, \dot{y}_h) = \sum_a w_a \left[ \left( m_a v_a + e_a A_h(t, x_a(t)) \right) \cdot \dot{x}_a(t) - \left( \frac{m_a}{2} v_a^2 + e_a \phi_h(t, x_a(t)) \right) \right] \\
+ \frac{1}{2} \int \left[ \left| -\nabla \phi_h(t, x) - \frac{\partial A_h}{\partial t}(t, x) \right|^2 - |\nabla \times A_h(t, x)|^2 \right] \, dx
\]

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

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

- fully discrete action

\[
A_d = \sum_{n=1}^{n_t-1} L_d(y_n, y_{n+1}), \quad L_d(y_n, y_{n+1}) = \int_{t_n}^{t_{n+1}} L_h(y_d(t), \dot{y}_d(t)) \, dt
\]

- lose energy conservation, but symplectic (energy error bounded)
Gauge Invariance of the Discrete Vlasov-Maxwell Action

- discrete Lagrangian

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

- variations of fully discrete action

\[ \delta \int_{t_n}^{t_{n+1}} dt A_h(t, x_a(t)) \cdot \dot{x}_a(t) = \int_{t_n}^{t_{n+1}} dt \sum_{l,m=1}^{s} \delta X^m_{a,n} \cdot \nabla A_h(t, x_a(t)) \cdot X^l_{a,n} \dot{\varphi}^l_n(t) \varphi^m_n(t) \]

\[ + \int_{t_n}^{t_{n+1}} dt \sum_{m=1}^{s} A_h(t, x_a(t)) \cdot \delta X^m_{a,n} \dot{\varphi}^m_n(t) + \ldots \]

\[ = \int_{t_n}^{t_{n+1}} dt \sum_{l,m=1}^{s} \delta X^m_{a,n} \cdot \nabla A_h(t, x_a(t)) \cdot X^l_{a,n} \dot{\varphi}^l_n(t) \varphi^m_n(t) \]

\[ - \int_{t_n}^{t_{n+1}} dt \sum_{l,m=1}^{s} X^l_{a,n} \cdot \nabla A_h(t, x_a(t)) \cdot \delta X^m_{a,n} \dot{\varphi}^l_n(t) \varphi^m_n(t) + \ldots \]
Gauge Invariance of the Discrete Vlasov-Maxwell Action

- **discrete Lagrangian**

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

- **variations of fully discrete action**

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

\[
+ \int_{t_n}^{t_{n+1}} dt \sum_{m=1}^s A_h(t, x_a(t)) \cdot \delta X_{a,n}^m \varphi_{n}^m(t) + \ldots
\]

\[
= \int_{t_n}^{t_{n+1}} dt \ \sum_{l,m=1}^s \delta X_{a,n}^m \cdot \hat{B}_h(t, x_a(t)) \cdot X_{a,n}^l \varphi_{n}^l(t) \varphi_{n}^m(t) + \ldots
\]
Remark: Semi-Discrete Particle-in-Fourier Lagrangian

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

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

\[ + \frac{1}{2} \int_0^T dt \int dx \ |\nabla \phi_h(t, x)|^2 \]

where

\[ \phi_h(t, x) = \sum_{k \neq 0} \frac{1}{(ik)^2} \ b_k(t) \ \exp \left\{ - ikx \right\} \]

Euler-Lagrange equation for the Fourier coefficients \( b_k \)

\[ b_k(t) = \sum_a w_a \ \exp \left\{ ikx_a(t) \right\} \]

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

\[ \exp \left\{ - ik\tilde{x}_b + ik\tilde{x}_a \right\} = \exp \left\{ - ikx_b + ikx_a \right\} \]
Guiding Centre Dynamics
Guiding Centre Dynamics

- charged particle phasespace Lagrangian
  \[ L(x, \dot{x}, v, \dot{v}) = (A(x) + v) \cdot \dot{x} - \frac{1}{2} v^2 \]

- coordinate transformation
  \[ (x^i, v^i) \rightarrow (X^i, \theta, u, \mu) \]
  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
  \[ L(q, \dot{q}) = (A(X + \rho) + ub(X + \rho)) \cdot (\dot{X} + \dot{\rho}) + \mu \dot{\theta} - \frac{1}{2} u^2 - \mu B(X + \rho) \]

- strong magnetic fields: neglect finite gyroradius effects
- guiding centre Lagrangian \((q = (X^i, u) \text{ and } \mu \text{ a parameter})\)
  \[ L(q, \dot{q}) = (A(X) + ub(X)) \cdot \dot{X} - \frac{1}{2} u^2 - \mu B(X) \]
Variational Guiding Centre Integrators

- guiding centre Lagrangian

\[ L(q, \dot{q}) = (A(X) + ub(X)) \cdot \dot{X} - \frac{1}{2} u^2 - \mu B(X), \quad q = (X^i, u) \]

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

\[
p_k = -D_1 L_d(q_k, q_{k+1}), \\
p_{k+1} = D_2 L_d(q_k, q_{k+1})
\]

- use continuous Legendre transform to obtain the second initial condition

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

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

\[
\phi(p, q) = p - \alpha(q) = 0 \quad \text{(Dirac constraint)}
\]

- variational integrators will in general not satisfy the constraint

- geometric interpretation for appearance of parasitic modes
Passing Particle 2D, \( h = \frac{\tau_b}{50} \), \( n_b = 10.000 \)
**Orthogonal Projection**

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

\[
\begin{align*}
\tilde{z}_{n+1} &= \Psi_h(z_n) \\
z_{n+1} &= \tilde{z}_{n+1} + \Omega^{-1} \nabla \phi^T(\tilde{z}_{n+1}) \lambda_{n+1} \\
0 &= \phi(z_{n+1})
\end{align*}
\]

with \( \Omega \) the canonical symplectic matrix

\[
\Omega = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}
\]
Passing and Trapped Particle 2D, $h = \frac{\tau_b}{50}$, $n_b = 25.000$

Variational Runge-Kutta 2

Orthogonal Projection
Symmetric Projection

- Symmetric symplectic projection of primary constraint, \( z = (p, q) \)

\[
\begin{align*}
\tilde{z}_k &= z_k + \Omega^{-1} \nabla \phi^T(z_k) \lambda_{k+1} \\
\tilde{z}_{k+1} &= \Psi_h(\tilde{z}_k) \\
\tilde{z}_{k+1} &= \tilde{z}_{k+1} + \Omega^{-1} \nabla \phi^T(z_{k+1}) \lambda_{k+1} \\
0 &= \phi(z_{k+1}).
\end{align*}
\]

with \( \Omega \) the canonical symplectic matrix

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\Omega = \begin{pmatrix} 0 & -1 \\ 1 & 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 and Trapped Particle 2D, $h = \frac{\tau_b}{50}$, $n_b = 25.000$

Explicit RK4

Variational RK4 (2 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
Implementation in Gyrokinetic Application Codes

- First results from conjugate symplectic particle integrators in NEMORB

- Runtime increased by 20% ~ 30% but no dissipation of energy