GEMPIC: Geometric ElectroMagnetic Particle-in-Cell Methods for the Vlasov-Maxwell System

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The Vlasov–Maxwell System

- the Vlasov equation determines the evolution of the distribution function $f_s(t, x, v)$ of some particle species $s$ with charge $e_s$ in a collisionless plasma

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

- Maxwell’s equations for electric field $E$ and magnetic induction $B$

$$E_t(t, x) = \nabla \times B(t, x) - J(t, x), \quad \nabla \cdot E(t, x) = -\rho(t, x),$$

$$B_t(t, x) = -\nabla \times E(t, x), \quad \nabla \cdot B(t, x) = 0$$

- definitions of charge density $\rho$ and current density $J$ in terms of $f$

$$\rho(t, x) = \sum_s e_s \int dv f_s(t, x, v), \quad J(t, x) = \sum_s e_s \int dv f_s(t, x, v) v$$

- geometric structures of the Vlasov–Maxwell System
  - 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. Time Integration

4. Summary and Outlook
Discrete Differential Forms
Differential Forms

- the mathematical language of vector analysis is too limited to provide an intuitive description of electrodynamics (only two types of objects: scalars and vectors)

| Quantity                  | Symbol | Unit     | Integration along |
|---------------------------|--------|----------|-------------------|
| scalar electric potential | $\phi$ | V        | 0D point          |
| electric field intensity  | $E$    | V/m      | 1D path           |
| magnetic flux density     | $B$    | (Vs)/m$^2$ | 2D surface       |
| charge density            | $\rho$ | (As)/m$^3$ | 3D volume        |

- alternative: calculus of differential forms (subset of tensor analysis)

- in three dimensional space $\Omega$: 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 in Maxwell’s equations as differential forms
  \[
  \phi \in \Lambda^0(\Omega), \quad A, E \in \Lambda^1(\Omega), \quad B, J \in \Lambda^2(\Omega), \quad \rho \in \Lambda^3(\Omega)
  \]
Maxwell’s Equations and the deRham Complex

- the spaces of Maxwell’s equations form a deRham complex

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

in terms of differential forms and the exterior derivative \( d : \Lambda^k \rightarrow \Lambda^{k+1} \)

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

- complex: \( \text{Im} \{ d : \Lambda^{k-1} \rightarrow \Lambda^k \} \subseteq \text{Ker} \{ d : \Lambda^k \rightarrow \Lambda^{k+1} \} \)

\[ \begin{array}{ccc}
(k-1)-\text{forms} & & \text{Ker} d \\
\text{d} & & \text{Im} d \\
\text{Ker} d & & \text{Im} d \\
& k\text{-forms} & \text{(k+1)-forms} \\
& \text{d} & \text{d} \\
\end{array} \]

- in general \( d \circ d = 0 \), in particular \( \text{curl} \text{ grad} = 0 \) and \( \text{div} \text{ curl} = 0 \)
Discrete deRham Complex

- discrete deRham complex

\[
\begin{align*}
\mathbb{R} & \rightarrow \Lambda^0(\Omega) \xrightarrow{d} \Lambda^1(\Omega) \xrightarrow{d} \Lambda^2(\Omega) \xrightarrow{d} \Lambda^3(\Omega) \rightarrow 0 \\
\downarrow \pi_h^0 & \downarrow \pi_h^1 \downarrow \pi_h^2 \downarrow \pi_h^3 \\
\mathbb{R} & \rightarrow \Lambda^0_h(\Omega) \xrightarrow{d} \Lambda^1_h(\Omega) \xrightarrow{d} \Lambda^2_h(\Omega) \xrightarrow{d} \Lambda^3_h(\Omega) \rightarrow 0
\end{align*}
\]

- discrete spaces \( \Lambda^k_h \subset \Lambda^k \) are finite element spaces of differential forms with degrees of freedom in \( \mathbb{R}^{N_k} \)

- 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 the complex property and compatibility guarantee stability

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**Spline Differential Forms**

- the $i$-th basic splines (B-spline) of degree $p$ is recursively defined by

$$S^p_j(x) = w^p_j(x) S^{p-1}_j(x) + (1 - w^p_{j+1}(x)) S^{p-1}_{j+1}(x), \quad S^0_j(x) = \begin{cases} 1 & x \in [x_j, x_{j+1}), \\ 0 & \text{else}, \end{cases}$$

where

$$w^p_j(x) = \frac{x - x_j}{x_{j+p} - x_j},$$

and the knot vector $\Xi = \{x_i\}_{1 \leq i \leq N+p}$ is a non-decreasing sequence of points

- the derivative of a spline of degree $p$ can be computed as the difference of two splines of degree $p - 1$

$$\frac{d}{dx} S^p_j(x) = p \left( \frac{S^{p-1}_j(x)}{x_{j+p} - x_j} - \frac{S^{p-1}_{j+1}(x)}{x_{j+p+1} - x_{j+1}} \right)$$
Spline Differential Forms

- zero-form basis

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

- one-form basis

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

- two-form basis

\[ \Lambda^2_h(\Omega) = \text{span} \left\{ \begin{pmatrix} S^p_i(x^1) & S^{p-1}_j(x^2) & S^{p-1}_k(x^3) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ S^p_i(x^1) & S^{p-1}_j(x^2) & S^{p-1}_k(x^3) \end{pmatrix} \right\} \]

- three-form basis

\[ \Lambda^3_h(\Omega) = \text{span} \left\{ \begin{pmatrix} S^{p-1}_i(x^1) & S^{p-1}_j(x^2) & S^{p-1}_k(x^3) \end{pmatrix} \right\} \]
Discrete Poisson Brackets
Hamiltonian Systems and Poisson Brackets

- let \( u(t, x) = (u^1, u^2, \ldots, u^m)^T \) be the field variables of some system of partial differential equations, defined over the space \( \Omega \) with coordinates \( z = (x, v) \)
- let \( \mathcal{F} \) denote an arbitrary functional of the field variables \( u \)
- if the system is Hamiltonian the evolution of \( \mathcal{F} \) is given by
  \[
  \frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\}
  \]
  where \( \mathcal{H} \) is the Hamiltonian functional, usually the total energy of the system
- the Poisson bracket \( \{\cdot, \cdot\} \) is an bilinear, anti-symmetric bracket of the form
  \[
  \{\mathcal{F}, \mathcal{G}\} = \int_\Omega \frac{\delta \mathcal{F}}{\delta u^i} \mathcal{J}^{ij}(u) \frac{\delta \mathcal{G}}{\delta u^j} \, dz
  \]
  where \( \mathcal{F} \) and \( \mathcal{G} \) are functionals of \( u \) and \( \delta \mathcal{F}/\delta u^i \) is the functional derivative
  \[
  \left. \frac{d}{d\epsilon} \mathcal{F}[u^1, \ldots, u^i + \epsilon v^i, \ldots, u^m] \right|_{\epsilon=0} = \int_\Omega \frac{\delta \mathcal{F}}{\delta u^i} v^i \, dz
  \]
Hamiltonian Systems and Poisson Brackets

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

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

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

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

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

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

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

- if the Hamiltonian is constant along the flow of some functional $\Phi$, i.e., $\{\mathcal{H}, \Phi\} = 0$, then $\Phi$ is a momentum map that is preserved by the flow of $\mathcal{H}$ (Noether's theorem)
Morrison–Marsden–Weinstein Bracket

- infinite dimensional fields \( f, E, B \)

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

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

- Vlasov–Maxwell noncanonical Hamiltonian structure

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

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

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

\[
\frac{d}{dt} \mathcal{F}[f, E, B] = \{ \mathcal{F}, \mathcal{H} \}
\]
**Morrison–Marsden–Weinstein Bracket**

- Infinite dimensional fields $f, E, B \rightarrow$ finite-dimensional representation $f_h, E_h, B_h$

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

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

- Vlasov–Maxwell noncanonical Hamiltonian structure $\rightarrow$ discrete functional derivatives

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

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

- Time evolution of any functional $\mathcal{F}[f, E, B] \rightarrow$ time discretisation: splitting methods, integral preserving methods

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

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

- semi-discrete electric field $E_h$ and magnetic field $B_h$

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

with coefficient vectors $e$ and $b$
Discretisation of the Distribution Function

- functionals of the distribution function, $\mathcal{F}[f]$, 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,

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

- replace functional derivatives with partial derivatives

$$\frac{\partial F}{\partial x_a} = w_a \left. \frac{\partial}{\partial x} \delta f \right|_{(x_a, v_a)} \quad \text{and} \quad \frac{\partial F}{\partial v_a} = w_a \left. \frac{\partial}{\partial v} \delta f \right|_{(x_a, v_a)}$$

- rewrite kinetic bracket as semi-discrete particle bracket

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

$$= \sum_a \frac{1}{w_a} \left( \frac{\partial F}{\partial x_a} \cdot \frac{\partial G}{\partial v_a} - \frac{\partial G}{\partial x_a} \cdot \frac{\partial F}{\partial v_a} \right)$$
Discretisation of the Electrodynamic Fields

- semi-discrete electric field $E_h$ and magnetic field $B_h$

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

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

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

- replace functional derivatives of $\mathcal{F}[E_h]$ and $\mathcal{F}[B_h]$ with partial derivatives of $F(e)$ and $F(b)$

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

with mass matrices

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

- semi-discrete Poisson bracket

\[
\{ F, G \}_d[\mathbf{X}, \mathbf{V}, \mathbf{e}, \mathbf{b}] = \frac{\partial F}{\partial \mathbf{X}} M_p^{-1} \frac{\partial G}{\partial \mathbf{V}} - \frac{\partial G}{\partial \mathbf{X}} M_p^{-1} \frac{\partial F}{\partial \mathbf{V}} \\
+ \left( \frac{\partial F}{\partial \mathbf{V}} \right)^T M_p^{-1} M_q \Lambda^1(\mathbf{X}) M_1^{-1} \left( \frac{\partial G}{\partial \mathbf{e}} \right) - \left( \frac{\partial F}{\partial \mathbf{e}} \right)^T M_1^{-1} \Lambda^1(\mathbf{X}) M_q M_p^{-1} \left( \frac{\partial G}{\partial \mathbf{V}} \right) \\
+ \left( \frac{\partial F}{\partial \mathbf{V}} \right)^T M_p^{-1} M_q B(\mathbf{X}, \mathbf{b}) M_p^{-1} \left( \frac{\partial G}{\partial \mathbf{V}} \right) \\
+ \left( \frac{\partial F}{\partial \mathbf{e}} \right)^T M_1^{-1} C^T \left( \frac{\partial G}{\partial \mathbf{b}} \right) - \left( \frac{\partial F}{\partial \mathbf{b}} \right)^T C M_1^{-1} \left( \frac{\partial G}{\partial \mathbf{e}} \right)
\]

- mass & charge matrices: 
  \[ M_p = M_p \otimes \mathbb{1}_3, \ M_q = M_q \otimes \mathbb{1}_3, \ (M_p)_{aa} = m_a w_a, \ (M_q)_{aa} = q_a w_a \]

- \( \Lambda^1(\mathbf{X}) \) is the \( 3N_p \times N_1 \) matrix with generic term \( \Lambda^1_i(x_a) \) with \( 1 \leq a \leq N_p, \ 1 \leq i \leq N_1 \)

- \( B(\mathbf{X}, \mathbf{b}) \) is the \( 3N_p \times 3N_p \) block diagonal matrix with generic block

\[
\hat{B}_h(x_a, t) = \sum_{i=1}^{N_2} b_i(t) \begin{pmatrix}
0 & \Lambda^{2,3}_i(x_a) & -\Lambda^{2,2}_i(x_a) \\
-\Lambda^{2,3}_i(x_a) & 0 & \Lambda^{2,1}_i(x_a) \\
\Lambda^{2,2}_i(x_a) & -\Lambda^{2,1}_i(x_a) & 0
\end{pmatrix}
\]
Semi-Discrete Poisson System

- with discrete Hamiltonian

\[ H = \mathcal{H}(f_h, E_h, B_h) = \frac{1}{2} V^\top M_p V + \frac{1}{2} e^\top M_1 e + \frac{1}{2} b^\top M_2 b. \]

- semi-discrete equations of motion

\[
\begin{align*}
\dot{X} &= \{ X, H \}_d = V, & \frac{dx_s}{dt} &= v_s, \\
\dot{V} &= \{ V, H \}_d = M_p^{-1} M_q (\Lambda^1(X) e + B(X, b) V), & \frac{dv_s}{dt} &= e_s (E(x_s) + v_s \times B(x_s)), \\
\dot{e} &= \{ e, H \}_d = M_1^{-1} (C^\top M_2 b - \Lambda^1(X)^\top M_q V), & \frac{\partial E}{\partial t} &= \text{curl } B - J, \\
\dot{b} &= \{ b, H \}_d = -C e, & \frac{\partial B}{\partial t} &= -\text{curl } E
\end{align*}
\]
Semi-Discrete Poisson System

- action of the discrete bracket on functions $F$ and $G$ of $u = (X, V, e, b)^\top$

$$\{F, G\}_d = DF^\top J(u) DG$$

- Poisson system: $\dot{u} = J(u) \nabla H(u)$ with $u = (X, V, e, b)^\top$ and

$$J(u) = \begin{pmatrix}
0 & M^{-1}_p & 0 & 0 \\
- M^{-1}_p & M^{-1}_p M_q B(X, b) M^{-1}_p & M^{-1}_p M_q A^1(X) M^{-1}_1 & 0 \\
0 & - M^{-1}_1 A^1(X)^\top M_q M^{-1}_p & 0 & M^{-1}_1 C^\top \\
0 & 0 & - C M^{-1}_1 & 0
\end{pmatrix}$$

- $J$ is anti-symmetric and satisfies the Jacobi identity if

$$\text{div } B_h(x, t) = 0 \text{ and } \text{curl } A^1 = C^\top A^2$$

→ both conditions are satisfied due to the discrete deRham complex structure

→ choosing initial conditions such that $\text{div } B_h(x, 0) = 0$ we have $\text{div } B_h(x, t) = 0$ for all times $t$
Casimir Invariants

- Casimir invariants: functionals $C(f, E, B)$ which Poisson commute with every other functional $G(f, E, B)$ so that $\{C, G\} = 0$

- integral of any real function $h_s$ of each distribution function $f_s$
  $$C_s = \int h_s(f_s) \, dx \, dv$$

- Gauss' law
  $$C_E = \int h_E(x) (\text{div } E - \rho) \, dx,$$
  $$\mathcal{C}^\top M_1 e = -\Lambda^0(X)^\top M_q \mathbb{1}_N$$

- divergence-free property of the magnetic field (pseudo-Casimir)
  $$C_B = \int h_B(x) \text{ div } B \, dx,$$
  $$\mathbb{D} b(t) = 0 \text{ if } \mathbb{D} b(0) = 0$$
  ($h_E$ and $h_B$ are arbitrary real functions of $x$)

→ the semi-discrete system, satisfying the Jacobi identity and preserving all Casimir invariants, is a Hamiltonian system of ODEs
Time Integration
Splitting Methods

- Hamiltonian splitting\(^2\)

\[ H = H_{V_1} + H_{V_2} + H_{V_3} + H_E + H_B \]

with

\[ H_{V_i} = \frac{1}{2} V_i^T M_i V_i, \quad H_E = \frac{1}{2} e^T M_1 e, \quad H_B = \frac{1}{2} b^T M_2 b \]

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

\[ \dot{u} = \{u, H_{V_i}\}_d, \quad \dot{u} = \{u, H_E\}_d, \quad \dot{u} = \{u, H_B\}_d \]

- each subsystem can be solved exactly

\[ \phi_{t,E}(u_0) = u_0 + \int_0^t \{u, H_E\}_d dt, \quad \phi_{t,B}(u_0) = u_0 + \int_0^t \{u, H_B\}_d dt, \quad \ldots \]

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Splitting Methods

- for the exact solution of the kinetic subsystems

\[ \varphi_t, V_i(u_0) = u_0 + \int_0^t \{ u, H_{V_i} \} \, dt \]

we have to compute line integrals exactly\(^3\) (e.g. \(i = 1\))

\[ X_1(h) = X_1(0) + h V_1(0), \]
\[ V_2(h) = V_2(0) + \int_0^h dt \, V_3(0) b(0) \Lambda^{2,1}(X(t)), \]
\[ V_3(h) = V_3(0) - \int_0^h dt \, V_2(0) b(0) \Lambda^{2,1}(X(t)), \]
\[ M_1 e(h) = M_1 e(0) - \int_0^h dt \Lambda^{1,1}(X(t)) M_p V_1(0) \]

→ solution is gauge invariant and charge conserving

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Splitting Methods

- Hamiltonian splitting

\[ H = H_{V_1} + H_{V_2} + H_{V_3} + H_E + H_B \]

- the exact solution of each subsystem constitutes a Poisson map

- compositions of Poisson maps are themselves Poisson maps

- construction of Poisson structure preserving integrators by composition of exact solutions of the subsystems

- first order time integrator: Lie-Trotter composition

\[ \Psi_h = \varphi_{h,E} \circ \varphi_{h,B} \circ \varphi_{h,V_1} \circ \varphi_{h,V_2} \circ \varphi_{h,V_3} \]

- second order time integrator: symmetric composition

\[ \Psi_h = \varphi_{h/2,E} \circ \varphi_{h/2,B} \circ \varphi_{h/2,V_1} \circ \varphi_{h/2,V_2} \circ \varphi_{h/2,V_3} \circ \varphi_{h/2,V_2} \circ \varphi_{h/2,V_1} \circ \varphi_{h/2,B} \circ \varphi_{h/2,E} \]
See Talk by Eric Sonnendrücker...
Summary and Outlook
Summary and Outlook

- discrete electrodynamics (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 follows from exactness and compatibility of the finite element deRham complex

- discrete Poisson brackets
  - Poisson structure is retained at the semi-discrete level
  - gauge invariance, charge conservation, Casimir conservation
  - construction of Poisson time integrators by Hamiltonian splitting methods
  - construction of energy-preserving time integrators by discrete gradients (c.f. talk by Eric Sonnendrücker)

- ongoing and future work
  - Eulerian discretisation, boundary conditions, geometry, delta-f, collisions, ...
  - gyrokinetics, magnetohydrodynamics, kinetic-fluid hybrid models, ...
  - metriplectic integrators for the Landau collision operator (arXiv:1707.01801, accepted by PoP)
Appendix
Discretisation of Functional Derivatives

- consider some functional $F$ of some field $f \in H^1(\Omega)$
- the functional derivative of $F$ with respect to $f$ is defined by

$$
\frac{d}{d\epsilon} F[f + \epsilon g] \bigg|_{\epsilon=0} = \left\langle \frac{\delta F}{\delta f} , g \right\rangle_{L^2} = \int_{\Omega} \frac{\delta F}{\delta f} g(z) \, dz
$$

where $g$ is an element of the same space as $f$, that is $g \in H^1(\Omega)$, while the functional derivative $\delta F/\delta f$ is an element of the dual space of $H^1(\Omega)$, and $\langle \cdot , \cdot \rangle$ denotes the appropriate pairing

- consider a finite element approximation $f_h$ of $f$ with respect to a basis $\varphi_i$

$$
f_h(t, z) = \sum_{i=1}^{N} f_i(t) \varphi_i(z), \quad \mathbf{f}(t) = (f_1(t), \ldots, f_N(t))^T \in \mathbb{R}^N
$$

- if we apply the functional $F$ to $f_h$, then $F$ becomes a function $F$ of the degrees of freedom $\mathbf{f}$

$$
F[f_h] = F(\mathbf{f})
$$
Discretisation of Functional Derivatives

- In order to discretise brackets, we need to replace functional derivatives like $\delta F/\delta f$ with partial derivative $\partial F/\partial f$

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

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

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

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

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

$$\langle \psi_i, \varphi_j \rangle_{L^2} = \int_{\Omega} \psi_i(z) \varphi_j(z) \, dz = \delta_{ij} \quad \text{for} \quad 1 \leq i, j \leq N$$
Discretisation of Functional Derivatives

- in the dual basis, the functional derivative can be written as
  \[
  \frac{\delta F[f_h]}{\delta f} = \sum_{i=1}^{N} a_i \psi_i(z)
  \]

- choose \( g = (0, \ldots, 0, 1, 0, \ldots, 0)^\top \) with 1 at the \( i \)-th position and 0 everywhere else, so that \( g_h = \varphi_i \), we have
  \[
  \langle \frac{\delta F[f_h]}{\delta f}, g_h \rangle_{L^2} = \int_{\Omega} \sum_{j=1}^{N} a_j \psi_j(z) \varphi_i(z) \, dz = \frac{\partial F}{\partial f_i} = \langle \frac{\partial F}{\partial f}, g \rangle_{\mathbb{R}^N}
  \]
  and thus find that
  \[
  a_i = \frac{\partial F}{\partial f_i}
  \]
  and therefore
  \[
  \frac{\delta F[f_h]}{\delta f} = \sum_{i=1}^{N} \frac{\partial F}{\partial f_i} \psi_i(z)
  \]

- express the dual basis \( \psi \) in terms of the primal basis \( \varphi \) as
  \[
  \psi_i(z) = \sum_{j=1}^{N} \alpha_{ij} \varphi_j(z)
  \]
  so that
  \[
  \frac{\delta F[f_h]}{\delta f} = \sum_{i,j=1}^{N} \frac{\partial F}{\partial f_i} \alpha_{ij} \varphi_j(z)
  \]
Discretisation of Functional Derivatives

- determine the unknown coefficients $\alpha_{ij}$ by the $L_2$ inner product

$$\langle \psi_i, \varphi_k \rangle_{L^2} = \int_{\Omega} \sum_{j=1}^{N} \alpha_{ij} \varphi_j(z) \varphi_k(z) \, dz = \sum_{j=1}^{N} \alpha_{ij} \int_{\Omega} \varphi_j(z) \varphi_k(z) \, dz.$$  

- denoting by $M$ the mass matrix of the basis functions $\varphi$

$$M_{jk} = \int_{\Omega} \varphi_j(z) \varphi_k(z) \, dz,$$

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

$$\mathbb{1} = \alpha M \quad \text{and thus} \quad \alpha = M^{-1}$$

so that

$$\frac{\delta F[f_h]}{\delta f} = \sum_{i,j=1}^{N} \frac{\partial F}{\partial f_i} (M^{-1})_{ij} \varphi_j(z).$$
Numerical Examples
Nonlinear Landau Damping

- numerical example: nonlinear Landau damping

\[ f(x, v, t = 0) = \exp \left( -\frac{v_1^2 + v_2^2}{2v_{th}^2} \right) \left( 1 + \alpha \cos(kx) \right), \]

\[ B_3(x, t = 0) = 0, \]

\[ E_2(x, t = 0) = 0, \]

and \( E_1(x, t = 0) \) is computed from Poisson's equation

- numerical parameters: splines of degree 3 and 2

\[ x \in [0, 2\pi/k), \quad v \in \mathbb{R}^2, \quad \Delta t = 0.05, \quad n_x = 32, \quad n_p = 100,000 \]

- physical parameters:

\[ v_{th} = 1, \quad k = 0.5, \quad \alpha = 0.5 \]
Nonlinear Landau Damping

\[ \frac{1}{2} \|E_x(t, x)\|^2 \]

\[ \gamma_1 = -0.285609 \]

\[ \gamma_2 = 0.086603 \]

| Integrator                        | $\gamma_1$   | $\gamma_2$   |
|----------------------------------|--------------|--------------|
| GEMPIC                           | -0.286       | +0.087       |
| viVlasov1D                       | -0.286       | +0.085       |
| Cheng & Knorr (1976)             | -0.281       | +0.084       |
| Nakamura & Yabe (1999)           | -0.280       | +0.085       |
| Ayuso & Hajian (2012)            | -0.292       | +0.086       |
| Heath, Gamba, Morrison, Michler (2012) | -0.287       | +0.075       |
| Cheng, Gamba, Morrison (2013)    | -0.291       | +0.086       |
Streaming Weibel Instability

- numerical example: streaming Weibel instability

\[ f(x, v, t = 0) = \frac{1}{\pi v_{th}} \exp \left( - \frac{1}{2} \frac{v^2}{v_{th}^2} \right) \left( \delta \exp \left( - \frac{(v_2 - v_{0,1})^2}{2v_{th}^2} \right) + (1 - \delta) \exp \left( - \frac{(v_2 - v_{0,2})^2}{2v_{th}^2} \right) \right), \]

\[ B_3(x, t = 0) = \beta \sin(kx), \]

\[ E_2(x, t = 0) = 0, \]

and \( E_1(x, t = 0) \) is computed from Poisson’s equation

- numerical parameters: splines of degree 3 and 2

\[ x \in [0, 2\pi/k), \quad v \in \mathbb{R}^2, \quad \Delta t = 0.01, \quad n_x = 128, \quad n_p = 2,000,000 \]

- physical parameters:

\[ v_{th} = \frac{0.1}{\sqrt{2}}, \quad k = 0.2, \quad \beta = -10^{-3}, \quad v_{0,1} = 0.5, \quad v_{0,2} = -0.1, \quad \delta = \frac{1}{6} \]
Streaming Weibel Instability

The graph shows the growth rate of different fields denoted as E1, E2, and B, with a line indicating the growth rate. The x-axis represents a range from 0 to 200, and the y-axis shows the growth rate on a logarithmic scale from $10^{-11}$ to $10^{1}$.
Streaming Weibel Instability

Propagator | total energy | Gauss’ law
---|---|---
Lie | 6.4E-5 | 8.3E-15
Strang | 1.4E-6 | 1.4E-14
2nd, 4 Lie | 1.5E-8 | 2.0E-14
4th, 3 Strang | 1.7E-10 | 9.4E-15
4th, 10 Lie | 5.7E-13 | 1.0E-14
Boris | 1.1E-7 | 5.8E-4

| time |
|---|
| 0 | 50 | 100 | 150 | 200 |
| \(10^{-16}\) | \(10^{-15}\) | \(10^{-14}\) | \(10^{-13}\) | \(10^{-12}\) | \(10^{-11}\) | \(10^{-10}\) | \(10^{-9}\) | \(10^{-8}\) | \(10^{-7}\) | \(10^{-6}\) | \(10^{-5}\) | \(10^{-4}\) |

\[ \frac{|H(t) - H(0)|}{H(0)} \]