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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

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

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

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

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

- definitions of charge density ρ and current density J in terms of f

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

- 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

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	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: calculus of differential forms (subset of tensor analysis)
- in three dimensional space Ω: 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 in Maxwell's equations as differential forms

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

Maxwell's Equations and the deRham Complex

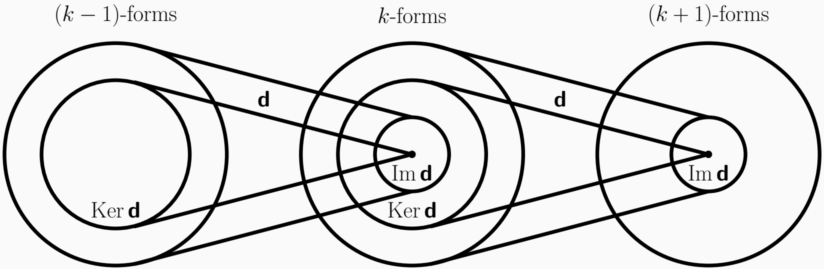
- the spaces of Maxwell's equations form a deRham complex

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

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

$$\mathbb{R} \rightarrow \Lambda^0(\Omega) \stackrel{\mathsf{d}}{\rightarrow} \Lambda^1(\Omega) \stackrel{\mathsf{d}}{\rightarrow} \Lambda^2(\Omega) \stackrel{\mathsf{d}}{\rightarrow} \Lambda^3(\Omega) \rightarrow 0$$

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



- in general $\mathsf{d} \circ \mathsf{d} = 0$, in particular $\text{curl}\,\text{grad} = 0$ and $\text{div}\,\text{curl} = 0$

Discrete deRham Complex

- discrete deRham complex

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

- discrete spaces $\Lambda_h^k \subset \Lambda^k$ are finite element spaces of differential forms with degrees of freedom in $\mathbb{R}^{N_k}$
- compatibility: projections π_h^k 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[1]

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[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

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

$$S_j^p(x) = w_j^p(x)\, S_j^{p-1}(x) + (1 - w_{j+1}^p(x))\, S_{j+1}^{p-1}(x), \qquad S_j^0(x) = \begin{cases} 1 & x \in [x_j, x_{j+1}), \\ 0 & \text{else}, \end{cases}$$

  where

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

  and the knot vector $\Xi = \{x_i\}_{1 \le i \le N+p}$ 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 $p-1$

$$\frac{\mathrm{d}}{\mathrm{d}x} S_j^p(x) = p \left(\frac{S_j^{p-1}(x)}{x_{j+p} - x_j} - \frac{S_{j+1}^{p-1}(x)}{x_{j+p+1} - x_{j+1}} \right)$$

Spline Differential Forms

- zero-form basis

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

- one-form basis

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

- two-form basis

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

- three-form basis

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

Discrete Poisson Brackets

Hamiltonian Systems and Poisson Brackets

- let $u(t,x) = (u^1,\, u^2,\, \dots,\, u^m)^T$ be the field variables of some system of partial differential equations, defined over the space Ω 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

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\}$$

- $\mathcal{H}$ 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

$$\{\mathcal{F}, \mathcal{G}\} = \int\limits_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i}\, \mathcal{J}^{ij}(u)\, \frac{\delta \mathcal{G}}{\delta u^j}\, \mathrm{d}z$$

where $\mathcal{F}$ and $\mathcal{G}$ are functionals of u and $\delta\mathcal{F}/\delta u^i$ is the functional derivative

$$\frac{d}{d\epsilon} \mathcal{F}\big[u^1,\, \dots,\, u^i + \epsilon v^i,\, \dots,\, u^m\big]\Big|_{\epsilon=0} = \int\limits_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i}\, v^i \, \mathrm{d}z$$

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 Φ, i.e., $\{\mathcal{H}, \Phi\} = 0$, then Φ 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)

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

- Vlasov–Maxwell noncanonical Hamiltonian structure

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}\}[f, E, B] = & \int f \left[\frac{\delta \mathcal{F}}{\delta f}, \frac{\delta \mathcal{G}}{\delta f} \right] \mathrm{d}x \mathrm{d}v + \int f \left(\frac{\partial}{\partial v} \frac{\delta \mathcal{F}}{\delta f} \cdot \frac{\delta \mathcal{G}}{\delta E} - \frac{\partial}{\partial v} \frac{\delta \mathcal{G}}{\delta f} \cdot \frac{\delta \mathcal{F}}{\delta E} \right) \mathrm{d}x \mathrm{d}v \\ & + \int f B \cdot \left(\frac{\partial}{\partial v} \frac{\delta \mathcal{F}}{\delta f} \times \frac{\partial}{\partial v} \frac{\delta \mathcal{G}}{\delta f} \right) \mathrm{d}x \mathrm{d}v + \int \left(\frac{\delta \mathcal{F}}{\delta E} \cdot \nabla \times \frac{\delta \mathcal{G}}{\delta B} - \frac{\delta \mathcal{G}}{\delta E} \cdot \nabla \times \frac{\delta \mathcal{F}}{\delta B} \right) \mathrm{d}x \end{aligned}$$

- 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

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

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

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

- 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,

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

  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

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

  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,

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

  become functions of the particle phasespace trajectories,

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

- replace functional derivatives with partial derivatives

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

- rewrite kinetic bracket as semi-discrete particle bracket

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

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

Discretisation of the Electrodynamic Fields

- semi-discrete electric field E_h and magnetic field B_h

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

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

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

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

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

with mass matrices

$$(\mathbb{M}_1)_{\alpha\beta} = \int \Lambda^1_\alpha(x)\, \Lambda^1_\beta(x)\, \mathrm{d}x, \qquad (\mathbb{M}_2)_{\alpha\beta} = \int \Lambda^2_\alpha(x)\, \Lambda^2_\beta(x)\, \mathrm{d}x$$

Semi-Discrete Poisson Bracket

- semi-discrete Poisson bracket

$$
\begin{aligned}
\{F, G\}_d[\boldsymbol{X}, \boldsymbol{V}, \boldsymbol{e}, \boldsymbol{b}] = {} & \frac{\partial F}{\partial \boldsymbol{X}} \mathbb{M}_p^{-1} \frac{\partial G}{\partial \boldsymbol{V}} - \frac{\partial G}{\partial \boldsymbol{X}} \mathbb{M}_p^{-1} \frac{\partial F}{\partial \boldsymbol{V}} \\
& + \left(\frac{\partial F}{\partial \boldsymbol{V}} \right)^\top \mathbb{M}_p^{-1} \mathbb{M}_q \mathbb{\Lambda}^1(\boldsymbol{X})^\top \mathbb{M}_1^{-1} \left(\frac{\partial G}{\partial \boldsymbol{e}} \right) - \left(\frac{\partial F}{\partial \boldsymbol{e}} \right)^\top \mathbb{M}_1^{-1} \mathbb{\Lambda}^1(\boldsymbol{X}) \mathbb{M}_q \mathbb{M}_p^{-1} \left(\frac{\partial G}{\partial \boldsymbol{V}} \right) \\
& + \left(\frac{\partial F}{\partial \boldsymbol{V}} \right)^\top \mathbb{M}_p^{-1} \mathbb{M}_q \mathbb{B}(\boldsymbol{X}, \boldsymbol{b}) \mathbb{M}_p^{-1} \left(\frac{\partial G}{\partial \boldsymbol{V}} \right) \\
& + \left(\frac{\partial F}{\partial \boldsymbol{e}} \right)^\top \mathbb{M}_1^{-1} \mathbb{C}^\top \left(\frac{\partial G}{\partial \boldsymbol{b}} \right) - \left(\frac{\partial F}{\partial \boldsymbol{b}} \right)^\top \mathbb{C} \mathbb{M}_1^{-1} \left(\frac{\partial G}{\partial \boldsymbol{e}} \right)
\end{aligned}
$$

- mass & charge matrices: $\mathbb{M}_p = M_p \otimes \mathbb{I}_3$, $\mathbb{M}_q = M_q \otimes \mathbb{I}_3$, $(M_p)_{aa} = m_a w_a$, $(M_q)_{aa} = q_a w_a$
- $\mathbb{\Lambda}^1(\boldsymbol{X})$ is the $3N_p \times N_1$ matrix with generic term $\boldsymbol{\Lambda}_i^1(\boldsymbol{x}_a)$ with $1 \leq a \leq N_p$, $1 \leq i \leq N_1$
- $\mathbb{B}(\boldsymbol{X}, \boldsymbol{b})$ is the $3N_p \times 3N_p$ block diagonal matrix with generic block

$$
\widehat{\boldsymbol{B}}_h(\boldsymbol{x}_a, t) = \sum_{i=1}^{N_2} b_i(t) \begin{pmatrix} 0 & \Lambda_i^{2,3}(\boldsymbol{x}_a) & -\Lambda_i^{2,2}(\boldsymbol{x}_a) \\ -\Lambda_i^{2,3}(\boldsymbol{x}_a) & 0 & \Lambda_i^{2,1}(\boldsymbol{x}_a) \\ \Lambda_i^{2,2}(\boldsymbol{x}_a) & -\Lambda_i^{2,1}(\boldsymbol{x}_a) & 0 \end{pmatrix}
$$

Semi-Discrete Poisson System

- with discrete Hamiltonian

$$H = \mathcal{H}(f_h, E_h, B_h) = \tfrac{1}{2}\, \boldsymbol{V}^\top \mathbb{M}_p \boldsymbol{V} + \tfrac{1}{2}\, \boldsymbol{e}^\top \mathbb{M}_1 \boldsymbol{e} + \tfrac{1}{2}\, \boldsymbol{b}^\top \mathbb{M}_2 \boldsymbol{b}.$$

- semi-discrete equations of motion

$$\dot{\boldsymbol{X}} = \{\boldsymbol{X}, H\}_d = \boldsymbol{V}, \qquad \frac{dx_s}{dt} = v_s,$$

$$\dot{\boldsymbol{V}} = \{\boldsymbol{V}, H\}_d = \mathbb{M}_p^{-1} \mathbb{M}_q \big(\mathbb{\Lambda}^1(\boldsymbol{X}) \boldsymbol{e} + \mathbb{B}(\boldsymbol{X}, \boldsymbol{b})\, \boldsymbol{V} \big), \qquad \frac{dv_s}{dt} = e_s \big(E(x_s) + v_s \times B(x_s) \big),$$

$$\dot{\boldsymbol{e}} = \{\boldsymbol{e}, H\}_d = \mathbb{M}_1^{-1} \big(\mathbb{C}^\top \mathbb{M}_2 \boldsymbol{b} - \mathbb{\Lambda}^1(\boldsymbol{X})^\top \mathbb{M}_q \boldsymbol{V} \big), \qquad \frac{\partial E}{\partial t} = \operatorname{curl} B - J,$$

$$\dot{\boldsymbol{b}} = \{\boldsymbol{b}, H\}_d = -\mathbb{C} \boldsymbol{e}, \qquad \frac{\partial B}{\partial t} = -\operatorname{curl} E$$

Semi-Discrete Poisson System

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

$$\{F, G\}_d = \mathrm{D}F^\top J(\boldsymbol{u})\,\mathrm{D}G$$

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

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

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

$$\operatorname{div} B_h(x, t) = 0 \qquad \text{and} \qquad \operatorname{curl} \boldsymbol{\Lambda}^1 = \mathbb{C}^\top \boldsymbol{\Lambda}^2$$

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

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

Casimir Invariants

- Casimir invariants: functionals $\mathcal{C}(f, E, B)$ which Poisson commute with every other functional $\mathcal{G}(f, E, B)$ so that $\{\mathcal{C}, \mathcal{G}\} = 0$
- integral of any real function h_s of each distribution function f_s

$$\mathcal{C}_s = \int h_s(f_s)\,\mathrm{d}x\mathrm{d}v$$

- Gauss' law

$$\mathcal{C}_E = \int h_E(x)\big(\operatorname{div} E - \rho\big)\,\mathrm{d}x, \qquad \mathbb{G}^\top M_1 \boldsymbol{e} = -\mathbb{\Lambda}^0(\boldsymbol{X})^\top \mathbb{M}_q \mathbb{1}_{N_p}$$

- divergence-free property of the magnetic field (pseudo-Casimir)

$$\mathcal{C}_B = \int h_B(x)\,\operatorname{div} B\,\mathrm{d}x, \qquad \mathbb{D}\boldsymbol{b}(t) = 0 \quad \text{if} \quad \mathbb{D}\boldsymbol{b}(0) = 0$$

(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

$$H_{V_i} = \frac{1}{2}\, \boldsymbol{V}_i^T \mathbb{M}_p \boldsymbol{V}_i, \qquad H_E = \frac{1}{2}\, \boldsymbol{e}^T \mathbb{M}_1 \boldsymbol{e}, \qquad H_B = \frac{1}{2}\, \boldsymbol{b}^T \mathbb{M}_2 \boldsymbol{b}$$

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

$$\dot{\boldsymbol{u}} = \{\boldsymbol{u}, H_{V_i}\}_d, \qquad \dot{\boldsymbol{u}} = \{\boldsymbol{u}, H_E\}_d, \qquad \dot{\boldsymbol{u}} = \{\boldsymbol{u}, H_B\}_d$$

- each subsystem can be solved exactly

$$\varphi_{t,E}(\boldsymbol{u}_0) = \boldsymbol{u}_0 + \int_0^t \{\boldsymbol{u}, H_E\}_d \, dt\,, \qquad \varphi_{t,B}(\boldsymbol{u}_0) = \boldsymbol{u}_0 + \int_0^t \{\boldsymbol{u}, H_B\}_d \, dt\,, \qquad \ldots$$

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[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.

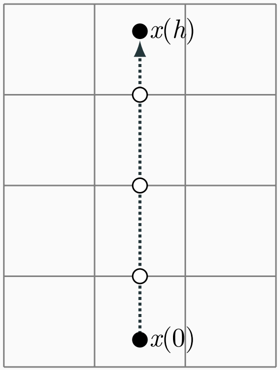
Splitting Methods

- for the exact solution of the kinetic subsystems

$$\varphi_{t,V_i}(\boldsymbol{u}_0) = \boldsymbol{u}_0 + \int_0^t \{\boldsymbol{u}, H_{V_i}\}_d \, dt$$

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

$$\begin{aligned}
\boldsymbol{X}_1(h) &= \boldsymbol{X}_1(0) + h\,\boldsymbol{V}_1(0), \\
\boldsymbol{V}_2(h) &= \boldsymbol{V}_2(0) + \int_0^h dt\,\boldsymbol{V}_3(0)\,\boldsymbol{b}(0)\,\Lambda^{2,1}(\boldsymbol{X}(t)), \\
\boldsymbol{V}_3(h) &= \boldsymbol{V}_3(0) - \int_0^h dt\,\boldsymbol{V}_2(0)\,\boldsymbol{b}(0)\,\Lambda^{2,1}(\boldsymbol{X}(t)), \\
\mathbb{M}_1\,\boldsymbol{e}(h) &= \mathbb{M}_1\,\boldsymbol{e}(0) - \int_0^h dt\,\Lambda^{1,1}(\boldsymbol{X}(t))\,\mathbb{M}_p\,\boldsymbol{V}_1(0)
\end{aligned}$$



→ solution is gauge invariant and charge conserving

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

Squire, Qin, Tang. Geometric integration of the Vlasov-Maxwell system with a variational particle-in-cell scheme. Physics of Plasmas 19, 084501, 2012.

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

$$H = H_{V_1} + H_{V_2} + H_{V_3} + H_E + H_B$$

- 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

$$\Psi_h = \varphi_{h/2,E} \circ \varphi_{h/2,B} \circ \varphi_{h/2,V_1} \circ \varphi_{h/2,V_2} \circ \varphi_{h,V_3} \circ \varphi_{h/2,V_2} \circ \varphi_{h/2,V_1} \circ \varphi_{h/2,B} \circ \varphi_{h/2,E}$$

Integral Preserving Methods

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 ($\operatorname{curl}\operatorname{grad} = 0$, $\operatorname{div}\operatorname{curl} = 0$)
  - 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 $\mathcal{F}$ of some field $f \in H^1(\Omega)$
- the functional derivative of $\mathcal{F}$ with respect to f is defined by

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

  where g is an element of the same space as f, that is $g \in H^1(\Omega)$, while the functional derivative $\delta\mathcal{F}/\delta f$ 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 φ_i

$$f_h(t, z) = \sum_{i=1}^{N} f_i(t)\, \varphi_i(z), \qquad \boldsymbol{f}(t) = \big(f_1(t), \dots, f_N(t)\big)^T \in \mathbb{R}^N$$

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

$$\mathcal{F}[f_h] = F(\boldsymbol{f})$$

Discretisation of Functional Derivatives

- in order to discretise brackets, we need to replace functional derivatives like $\delta\mathcal{F}/\delta f$ with partial derivative $\partial F/\partial \boldsymbol{f}$
- require that the pairing be equal to some finite-dimensional equivalent

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

where $\boldsymbol{g}(t) = \big(g_1(t), \dots, g_N(t)\big)^T \in \mathbb{R}^N$ 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 $\varphi = (\varphi_1, \dots, \varphi_N)^T$ by $\psi = (\psi_1, \dots, \psi_N)^T$

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

Discretisation of Functional Derivatives

- in the dual basis, the functional derivative can be written as

$$\frac{\delta \mathcal{F}[f_h]}{\delta f} = \sum_{i=1}^{N} a_i \, \psi_i(z)$$

- choose $\boldsymbol{g} = (0, \, \ldots, \, 0, \, 1, \, 0, \, \ldots, \, 0)^\top$ with 1 at the i-th position and 0 everywhere else, so that $g_h = \varphi_i$, we have

$$\left\langle \frac{\delta \mathcal{F}[f_h]}{\delta f} \, , g_h \right\rangle_{L^2} = \int_\Omega \sum_{j=1}^{N} a_j \, \psi_j(z) \, \varphi_i(z) \, dz = \frac{\partial F}{\partial f_i} = \left\langle \frac{\partial F}{\partial \boldsymbol{f}} \, , \, \boldsymbol{g} \right\rangle_{\mathbb{R}^N}$$

and thus find that

$$a_i = \frac{\partial F}{\partial f_i} \qquad \text{and therefore} \qquad \frac{\delta \mathcal{F}[f_h]}{\delta f} = \sum_{i=1}^{N} \frac{\partial F}{\partial f_i} \, \psi_i(z)$$

- express the dual basis ψ in terms of the primal basis φ as

$$\psi_i(z) = \sum_{j=1}^{N} \alpha_{ij} \, \varphi_j(z) \qquad \text{so that} \qquad \frac{\delta \mathcal{F}[f_h]}{\delta f} = \sum_{i,j=1}^{N} \frac{\partial F}{\partial f_i} \, \alpha_{ij} \, \varphi_j(z)$$

Discretisation of Functional Derivatives

- determine the unknown coefficients α_{ij} by the L_2 inner product

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

- denoting by $\mathbb{M}$ the mass matrix of the basis functions φ

$$\mathbb{M}_{jk} = \int\limits_{\Omega} \varphi_j(z) \, \varphi_k(z) \, dz,$$

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

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

so that

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

Numerical Examples

Nonlinear Landau Damping

- numerical example: nonlinear Landau damping

$$
\begin{aligned}
f(x, v, t=0) &= \exp\left(-\frac{v_1^2 + v_2^2}{2v_{\mathrm{th}}^2}\right)\big(1+\alpha\cos(kx)\big), \\
B_3(x, t=0) &= 0, \\
E_2(x, t=0) &= 0,
\end{aligned}
$$

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

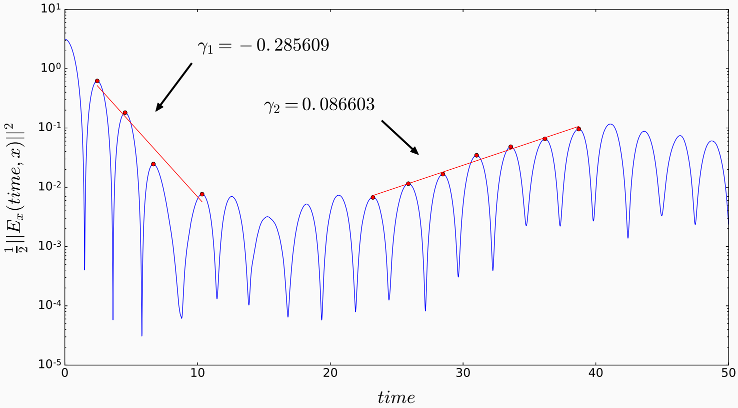
- numerical parameters: splines of degree 3 and 2

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

- physical parameters:

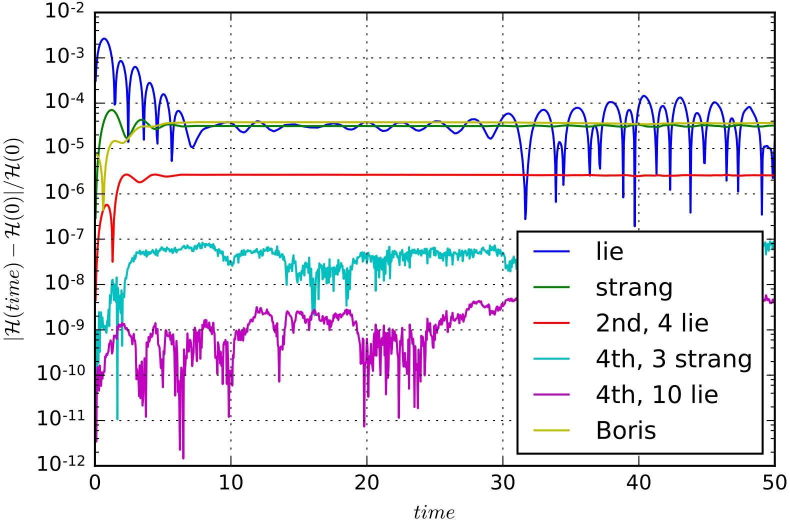
$$
v_{\mathrm{th}} = 1, \qquad k = 0.5, \qquad \alpha = 0.5
$$

Nonlinear Landau Damping



Integrator	γ_1	γ_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	$+0.086$

Nonlinear Landau Damping



Streaming Weibel Instability

- numerical example: streaming Weibel instability

$$
\begin{aligned}
f(x,v,t=0) &= \frac{1}{\pi v_{\mathrm{th}}} \exp\left(-\frac{1}{2}\frac{v_1^2}{v_{\mathrm{th}}^2}\right)\left(\delta \exp\left(-\frac{(v_2-v_{0,1})^2}{2v_{\mathrm{th}}^2}\right) + (1-\delta)\exp\left(-\frac{(v_2-v_{0,2})^2}{2v_{\mathrm{th}}^2}\right)\right),\\
B_3(x,t=0) &= \beta \sin(kx),\\
E_2(x,t=0) &= 0,
\end{aligned}
$$

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

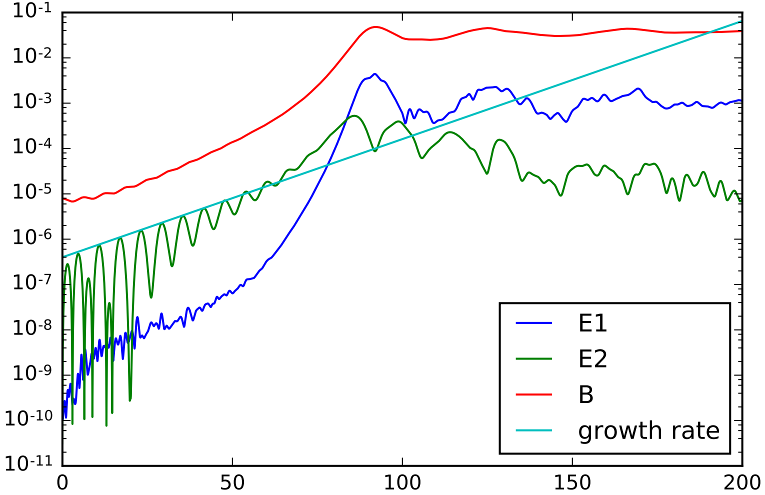
- numerical parameters: splines of degree 3 and 2

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

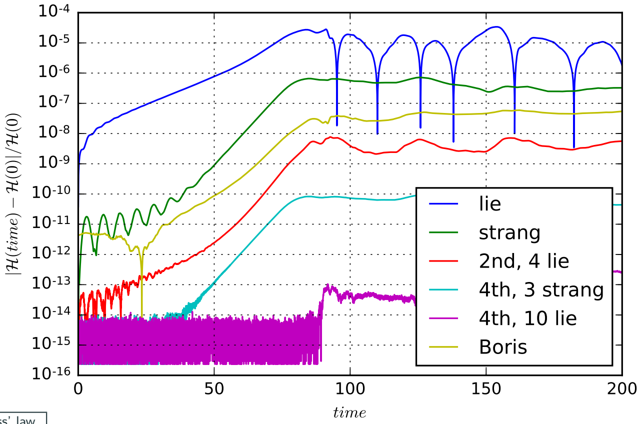
- physical parameters:

$$
v_{\mathrm{th}} = \frac{0.1}{\sqrt{2}}, \qquad k = 0.2, \qquad \beta = -10^{-3}, \qquad v_{0,1} = 0.5, \qquad v_{0,2} = -0.1, \qquad \delta = \frac{1}{6}
$$

Streaming Weibel Instability



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