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On the Structure-Preserving Discretisation of Poisson and Leibniz Brackets

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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 in a collisionless plasma

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

f_s phasespace density distribution function of plasma particle species s
e_s charge of particle species s
E electric field
B magnetic field

- Maxwell's equations

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

- 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

- Vlasov equation in Lagrangian coordinates
  - characteristics

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

  - reconstruction of the phasespace density distribution

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

- Maxwell's equations in Eulerian coordinates
  - dynamical equations

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

  - constraints

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

  - definitions of charge density and current density 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)
- metriplectic structure of the Vlasov–Maxwell–Fokker–Planck system (metric bracket for the collision operator)

Hamiltonian Systems and Poisson Brackets

- let $u(t,x) = (u^1, u^2, ..., u^m)^T$ 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

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

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

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

- the Poisson bracket $\{\cdot, \cdot\}$ satisfies Leibniz' rule and the Jacobi identity

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 $\mathcal{H}$

Morrison–Marsden–Weinstein Bracket

- infinite dimensional fields f, E, B
- Vlasov–Maxwell noncanonical Hamiltonian structure

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

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

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

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

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

Leibniz Brackets

- denote by $u(t,x) = (u^1,\, u^2,\, ...,\, u^m)^T$ the field variables of some system of PDEs, defined over the space Ω with coordinates $z = (x,v)$
- a Leibniz bracket is the sum of a skew-symmetric Poisson bracket $\{\cdot,\cdot\}$ and a symmetric bracket $(\cdot,\cdot)$ accounting for dissipative effects
- the evolution of some functional $\mathcal{F}$ of the field variables u is given by

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F},\mathcal{G}\} + (\mathcal{F},\mathcal{G})$$

  with $\mathcal{G}$ e.g. the Hamiltonian or some generalised free energy functional
- the bracket $(\cdot,\cdot)$ is a bilinear, symmetric bracket, satisfying Leibniz' rule

$$(\mathcal{F},\mathcal{G}) = \int\limits_{\Omega} \frac{\delta\mathcal{F}}{\delta u^i}\,\mathcal{K}^{ij}(u)\,\frac{\delta\mathcal{G}}{\delta u^j}\,dz$$

- $\mathcal{K}(u)$ is a self-adjoint, semi-definite operator

Double Bracket Dynamics

- double bracket dynamics describes systems that have a Hamiltonian part $\{\cdot, \cdot\}$ and an energy dissipating part $(\cdot, \cdot)_{\mathcal{H}}$
- the evolution of some functional $\mathcal{F}$ of the field variables u is given by

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\} + (\mathcal{F}, \mathcal{H})_{\mathcal{H}}$$

- $\mathcal{H}$ is the Hamiltonian functional, usually the total energy of the system
- the double bracket $(\cdot, \cdot)_{\mathcal{H}}$ is a symmetric bracket

$$(\mathcal{F}, \mathcal{G})_{\mathcal{H}} = \int_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i} \, \mathcal{K}^{ij}(u) \, \frac{\delta \mathcal{G}}{\delta u^j} \, dz \qquad \text{with} \qquad \mathcal{K} = \mathcal{J}^2$$

- double bracket dynamics preserves Casimir invariants and dissipates energy

$$\frac{d\mathcal{C}}{dt} = 0, \qquad \frac{d\mathcal{H}}{dt} \leq 0$$

- applications: geometric relaxation methods for the computation of kinetic and magnetohydrodynamic equilibria

Metriplectic Systems and Leibniz Brackets

- metriplectic dynamics describes systems that have a Hamiltonian part $\{\cdot,\cdot\}$ and an Casimir (entropy) dissipating part $(\cdot,\cdot)_{\mathcal{S}}$
- the evolution of some functional $\mathcal{F}$ of the field variables u is given by

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F},\mathcal{G}\} + (\mathcal{F},\mathcal{G})_{\mathcal{S}}$$

- $\mathcal{G} = \mathcal{H} - \mathcal{S}$ a generalised free energy functional with entropy functional $\mathcal{S}$, which is a Casimir invariant of the Poisson bracket $\{\cdot,\cdot\}$
- the metriplectic bracket $(\cdot,\cdot)_{\mathcal{S}}$ is a symmetric bracket

$$(\mathcal{F},\mathcal{G})_{\mathcal{S}} = \int\limits_{\Omega} \frac{\delta\mathcal{F}}{\delta u^i}\,\mathcal{K}^{ij}(u)\,\frac{\delta\mathcal{G}}{\delta u^j}\,dz$$

- $\mathcal{K}(u)$ is a self-adjoint operator with appropriate nullspace s.th. $(\mathcal{H},\mathcal{G})_{\mathcal{S}} = 0$
- metriplectic dynamics preserves energy and dissipates entropy (H-theorem)

$$\frac{d\mathcal{H}}{dt} = 0, \qquad \frac{d\mathcal{S}}{dt} \leq 0$$

The Landau Collision Operator

- various collision operators, including the Landau collision operator as well as other small-angle Coulomb collision operators relevant for plasmas, can be obtained from a general metric bracket

$$(\mathcal{F}, \mathcal{G})_{\mathcal{S}} = \int_{\Omega} \int_{\Omega} \left(\frac{\partial}{\partial v'} \frac{\delta \mathcal{F}}{\delta f(z')} - \frac{\partial}{\partial v''} \frac{\delta \mathcal{F}}{\delta f(z'')} \right) \cdot T(z'; z'') \cdot \left(\frac{\partial}{\partial v'} \frac{\delta \mathcal{G}}{\delta f(z')} - \frac{\partial}{\partial v''} \frac{\delta \mathcal{G}}{\delta f(z'')} \right) dz' \, dz''$$

  where $T(z'; z'') = W(z'; z'') \, \delta(x' - x'')$ with W a symmetric positive semi-definite matrix with a null eigenvector $v' - v''$

- different collision operators follow from different choices for the matrix W and the entropy functional $\mathcal{S}$, which is of the form

$$\mathcal{S} = \int_{\Omega} s(f) \, dz,$$

  with s an arbitrary function of the distribution function f

The Landau Collision Operator

- restricting W to be of the form

$$W_{ij}(z', z'') = \nu_c \, U_{ij}(z', z'') \, K(f(z')) \, K(f(z''))/2,$$

with K an arbitrary function of f and U with the following symmetries,

$$U_{ij}(z', z'') = U_{ji}(z', z''), \qquad U_{ij}(z', z'') = U_{ij}(z'', z'), \qquad (v'_i - v''_i) \, U_{ij} = 0$$

the bracket always satisfies the required symmetry properties so that mass, momentum and energy are preserved

- choosing $s(f) = f \ln f$ and $K(f) = f$ the metriplectic bracket becomes

$$(\mathcal{F}, \mathcal{G})_{\mathcal{S}} = \frac{\nu_c}{2} \int\limits_{\Omega_x} \int\limits_{\Omega_v} \int\limits_{\Omega_v} \left(\frac{\partial}{\partial v'} \frac{\delta \mathcal{F}}{\delta f(x', v')} - \frac{\partial}{\partial v''} \frac{\delta \mathcal{F}}{\delta f(x', v'')} \right)$$

$$\cdot \, U(v', v'') \cdot \left(f(x', v'') \frac{\partial f(x', v')}{\partial v'} - f(x', v') \frac{\partial f(x', v'')}{\partial v''} \right) dx' \, dv' \, dv''$$

The Vlasov–Maxwell–Fokker–Planck System

- the Vlasov–Maxwell–Fokker–Planck system determines the evolution a collisional plasma and the associated electromagnetic fields

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

$$\begin{aligned} E_t(t,x) &= \nabla \times B(t,x) - J(t,x), & \nabla \cdot E(t,x) &= -\rho(t,x), \\ B_t(t,x) &= -\nabla \times E(t,x), & \nabla \cdot B(t,x) &= 0 \end{aligned}$$

- the Landau collision operator $C[f_s]$ is given by the metric bracket $(\mathcal{F}, \mathcal{G})_{\mathcal{S}}$ with

$$U_{ij}(v,v') = \frac{1}{|v - v'|} \left(\delta_{ij} - \frac{(v_i - v'_i)(v_j - v'_j)}{|v - v'|^2} \right)$$

- the dynamics can thus be described by the metriplectic evolution equation

$$\frac{d}{dt}\mathcal{F}[f, E, B] = \{\mathcal{F}, \mathcal{H} - \mathcal{S}\} + (\mathcal{F}, \mathcal{H} - \mathcal{S})_{\mathcal{S}}$$

Discrete Brackets

Discretisation of the Vlasov-Maxwell Poisson System

- finite-dimensional representation f_h, E_h, B_h of the fields f, E, B
- discretisation of functionals

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

- discretisation of the brackets: 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 discretisation: splitting methods, integral preserving methods

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

Discrete Brackets

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

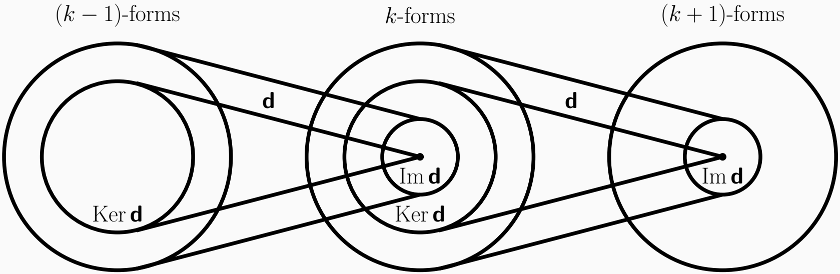
- the spaces of Maxwell's equations form a deRham complex

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

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

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

- 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

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

- the discrete spaces $\Lambda_h^k \subset \Lambda^k$ are finite element spaces of differential forms with degrees of freedom in $\mathbb{R}^{N_k}$
- complex property holds at the matrix level: $\operatorname{Im}\mathbb{G} \subseteq \operatorname{Ker}\mathbb{C}$, $\operatorname{Im}\mathbb{C} \subseteq \operatorname{Ker}\mathbb{D}$

$$
\mathbb{R}^{N_0} \xrightarrow{\quad \mathbb{G} \quad} \mathbb{R}^{N_1} \xrightarrow{\quad \mathbb{C} \quad} \mathbb{R}^{N_2} \xrightarrow{\quad \mathbb{D} \quad} \mathbb{R}^{N_3} \qquad \text{with} \quad \mathbb{C}\mathbb{G} = 0,\ \mathbb{D}\mathbb{C} = 0
$$

- 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]

[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 order p is recursively 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 derivatives

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

where

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

Spline Differential Forms

- zero-form basis

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

- one-form basis

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

Spline Differential Forms

- two-form basis

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

- three-form basis

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

Spline Differential Forms

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

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

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

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

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

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

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

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

Discrete Brackets

Discrete Functional Derivatives

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

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

- 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

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

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 $\boldsymbol{e}$ and $\boldsymbol{b}$

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

$$\begin{aligned} \int dx \, dv \, f \left[\frac{\delta \mathcal{F}}{\delta f}, \frac{\delta \mathcal{G}}{\delta f} \right] &= \sum_a w_a \left(\frac{\partial}{\partial x} \frac{\delta \mathcal{F}}{\delta f} \cdot \frac{\partial}{\partial v} \frac{\delta \mathcal{G}}{\delta f} - \frac{\partial}{\partial v} \frac{\delta \mathcal{F}}{\delta f} \cdot \frac{\partial}{\partial x} \frac{\delta \mathcal{G}}{\delta f} \right) \bigg|_{(x_a, v_a)} \\ &= \sum_a \frac{1}{w_a} \left(\frac{\partial F}{\partial x_a} \cdot \frac{\partial G}{\partial v_a} - \frac{\partial G}{\partial x_a} \cdot \frac{\partial F}{\partial v_a} \right) \end{aligned}$$

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 $F(\boldsymbol{b})$

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

with mass matrices

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

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 $1 \le a \le N_p$, $1 \le i \le N_1$
- $\mathbb{B}(\boldsymbol{X}, \boldsymbol{b})$ 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

$$H = \tfrac{1}{2}\, \boldsymbol{V}^\top \mathbb{M}_p \boldsymbol{V} + \tfrac{1}{2}\, \boldsymbol{e}^\top \mathbb{M}_1 \boldsymbol{e} + \tfrac{1}{2}\, \boldsymbol{b}^\top \mathbb{M}_2 \boldsymbol{b}.$$

- 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 functionals 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

Integral Preserving Methods

Integral Preserving Methods

- consider a system of ordinary differential equations in the form

$$\frac{du}{dt} = J(u)\,\nabla H(u)$$

where $J(u)$ can be an anti-symmetric matrix for conservative systems, a symmetric matrix for dissipative systems, or a combination thereof for metriplectic systems, and $H : \mathbb{R}^N \to \mathbb{R}$ is a differentiable function

- discrete gradients: discrete analogues of the gradient of a function

$$\frac{u_{n+1} - u_n}{t_{n+1} - t_n} = \bar{J}(u_n, u_{n+1})\,\bar{\nabla} H(u_n, u_{n+1}),$$

- $\bar{J}(u_n, u_{n+1})$ is any symmetric or anti-symmetric matrix that approaches $J(u)$ in the limit of $u_{n+1} \to u_n$ and $\Delta t \to 0$
- $\bar{\nabla} H(u_n, u_{n+1})$ is a discrete gradient, that is a vector valued continuous function of (u_n, u_{n+1}), satisfying

$$(u_{n+1} - u_n) \cdot \bar{\nabla} H(u_n, u_{n+1}) = H(u_{n+1}) - H(u_n), \quad \bar{\nabla} H(u_n, u_n) = \nabla H(u_n)$$

Integral Preserving Methods

- midpoint discrete gradient ($u_{n+1/2} = \frac{1}{2}(u_n + u_{n+1})$)

$$\bar{\nabla} H(u_n, u_{n+1}) = \nabla H(u_{n+1/2}) + (u_{n+1} - u_n) \frac{H(u_{n+1}) - H(u_n) - (u_{n+1} - u_n) \cdot \nabla H(u_{n+1/2})}{\left| u_{n+1} - u_n \right|^2}$$

- average discrete gradient (c.f. average vector field method)

$$\bar{\nabla} H(u_n, u_{n+1}) = \int_0^1 \nabla H\big((1-\xi) u_n + \xi u_{n+1}\big) \, d\xi$$

- generalised collocation methods ($h = t_{n+1} - t_n$, $0 \le c_i \le 1$, $1 \le i \le s$)

$$\dot{u}_h(t_n + c_i h) = J\big(u_h(t_n + c_i h)\big) \int_0^1 \frac{l^{s,i}(\tau)}{b_i} \nabla H\big(u_h(t_n + \tau h)\big) \, d\tau$$

$$u_{n+1} = u_h(t_{n+1})$$

Time Integration

Splitting Methods

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

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

[2] Crouseilles, Einkemmer, Faou. Hamiltonian splitting for the Vlasov-Maxwell equations. Journal of Computational Physics 283, 224–240, 2015.

Qin, He, Zhang, Liu, Xiao, Wang. Comment on "Hamiltonian splitting for the Vlasov–Maxwell equations". arXiv:1504.07785, 2015.

He, Qin, Sun, Xiao, Zhang, Liu. Hamiltonian integration methods for Vlasov–Maxwell equations. arXiv:1505.06076, 2015.

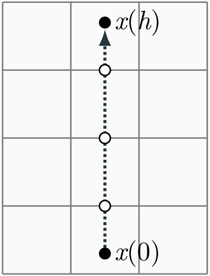
Splitting Methods

- for the exact solution of the kinetic subsystems

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

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

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

- second order time integrator: symmetric composition

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

Time Integration

Numerical Examples

Nonlinear Landau Damping

- numerical example: nonlinear Landau damping

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

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

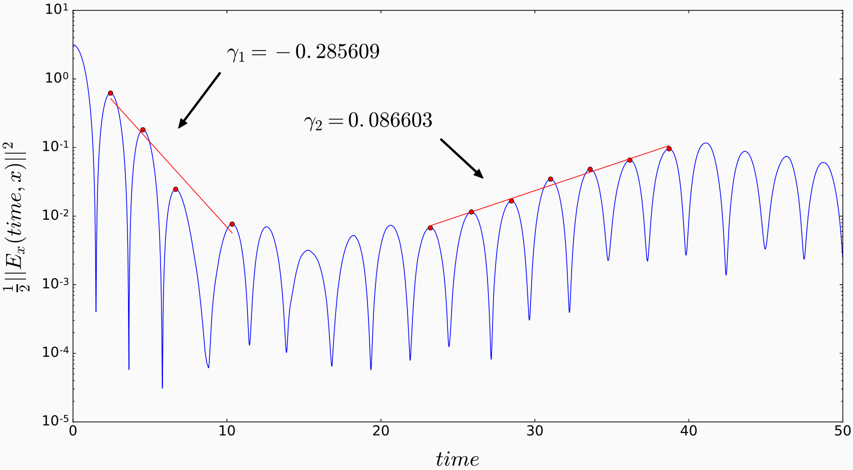
- numerical parameters:

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

- physical parameters:

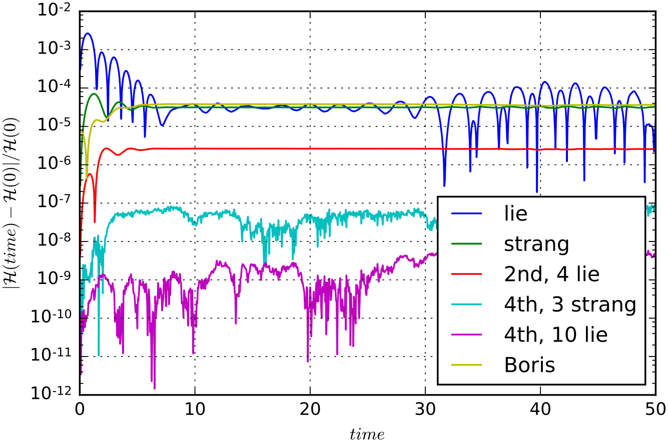
$$
v_{\mathrm{th}} = 1, \qquad k = 0.5, \qquad \alpha = 0.5
$$

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

$$f(x,v,t=0) = \frac{1}{\pi v_{\text{th}}} \exp\left(-\frac{1}{2}\frac{v_1^2}{v_{\text{th}}^2}\right)\left(\delta \exp\left(-\frac{(v_2 - v_{0,1})^2}{2v_{\text{th}}^2}\right) + (1-\delta)\exp\left(\right.\right.$$

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

$$E_2(x,t=0) = 0,$$

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

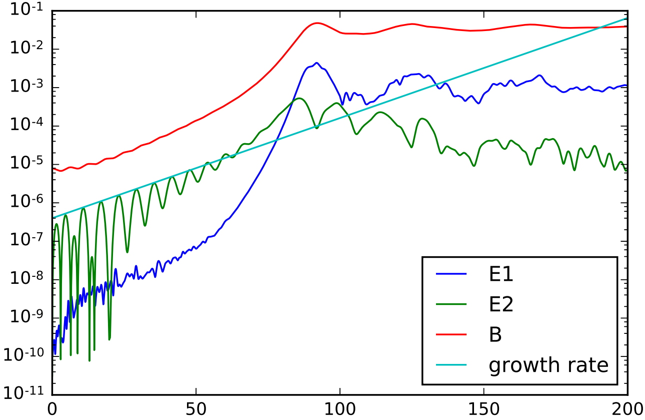
- numerical parameters: splines of degree 3 and 2

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

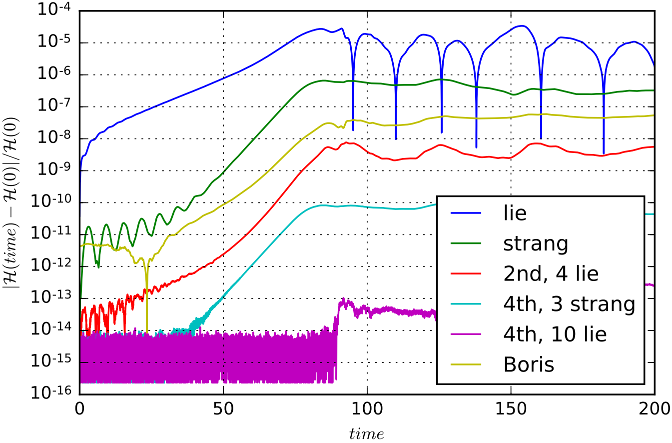
- physical parameters:

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

Streaming Weibel Instability



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

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 ($\operatorname{curl}\operatorname{grad} = 0$, $\operatorname{div}\operatorname{curl} = 0$)
    - 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
    - general: logical or physical coordinates, discretisation techniques, various systems
- ongoing and future work
    - Casimir Invariants, Hamiltonian Noether theorem, fully Eulerian discretisation
    - new splitting methods or variational integrators for degenerate Lagrangians
    - integral-preserving time discretisation (discrete gradients, average vector field method, generalised collocation methods)
    - metriplectic integrators for the Landau collision operator