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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 phasespace distribution function $f_s(t, x, v)$ of some particle species s in a collisionless plasma

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

- Maxwell's equations determine the evolution of the electromagnetic fields created by the charged particles of the plasma

$$\frac{\partial E}{\partial t} = \nabla \times B - J, \qquad \nabla \cdot E = -\rho, \qquad \rho(t, x) = \sum_s e_s \int dv\, f_s(t, x, v),$$

$$\frac{\partial B}{\partial t} = -\nabla \times E, \qquad \nabla \cdot B = 0, \qquad J(t, x) = \sum_s e_s \int dv\, f_s(t, x, v)\, v$$

f_s	distribution function of particle species s	E	electric field	ρ	charge density
e_s	charge of particle species s	B	magnetic field	J	current density

Geometric Structures of the Vlasov-Maxwell System

- the spaces of electrodynamics have a deRham complex structure
  - identities from vector calculus
  - generalised Stokes theorem
- Poisson structure
  - antisymmetric bracket satisfying the Jacobi identity
  - Casimir invariants
- Noether theorem
  - energy conservation (time translation invariance)
  - momentum conservation (spatial translation invariance)
  - charge conservation (gauge invariance)

Outline

Discrete Differential Forms

Differential Forms

- 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	V/m	1D path
magnetic flux density	B	$(\mathrm{Vs})/\mathrm{m}^2$	2D surface
charge density	ρ	$(\mathrm{As})/\mathrm{m}^3$	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

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

  in terms of differential forms

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

- exterior derivative $\mathsf{d} : \Lambda^k \to \Lambda^{k+1}$ (generalises grad, curl, div)
- complex property: $\mathsf{Im}\,\{\mathsf{d} : \Lambda^{k-1} \to \Lambda^k\} \subseteq \mathsf{Ker}\,\{\mathsf{d} : \Lambda^k \to \Lambda^{k+1}\}$
- specifically $\mathsf{Im}\,\{\text{grad}\} \subseteq \mathsf{Ker}\,\{\text{curl}\}$, $\mathsf{Im}\,\{\text{curl}\} \subseteq \mathsf{Ker}\,\{\text{div}\}$
- 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

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

- the discrete spaces $\Lambda_h^k \subset \Lambda^k$ are finite element spaces of differential forms
- complex property holds at the matrix level: $\mathrm{Im}\,\mathbb{G} \subseteq \mathrm{Ker}\,\mathbb{C}$, $\mathrm{Im}\,\mathbb{C} \subseteq \mathrm{Ker}\,\mathbb{D}$, $\mathbb{C}\mathbb{G} = 0$, $\mathbb{D}\mathbb{C} = 0$

$$\mathbb{R}^{N_0} \xrightarrow{\quad \mathbb{G} \quad} \mathbb{R}^{N_1} \xrightarrow{\quad \mathbb{C} \quad} \mathbb{R}^{N_2} \xrightarrow{\quad \mathbb{D} \quad} \mathbb{R}^{N_3}$$

- 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 compatibility and $\mathrm{d} \circ \mathrm{d} = 0$ 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.

Discrete Poisson Brackets

Morrison-Marsden-Weinstein Bracket

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

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

- Hamiltonian: sum of the kinetic energy of the particles, the electrostatic field energy and the magnetic field energy

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

- time evolution of any functional $F[f, E, B]$

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

Morrison-Marsden-Weinstein Bracket

- infinite dimensional fields f, E, B $\to$ finite-dimensional representation
- Vlasov-Maxwell noncanonical Hamiltonian structure $\to$ discretisation of the brackets

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

- Hamiltonian: sum of the kinetic energy of the particles, the electrostatic field energy and the magnetic field energy $\to$ discretisation of functionals

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

- time evolution of any functional $F[f, E, B]$ $\to$ time discretisation

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

Discretisation of the Fields

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

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

  with weights w_a, particle positions x_a and particle velocities v_a
- 1-form and 2-form spline basis functions (vector-valued)

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

- semi-discrete electric field E_h and magnetic field B_h

$$E_h(t, x) = \sum_{\alpha=1}^{N_1} e_\alpha(t) \, \Lambda^1_\alpha(x), \qquad B_h(t, x) = \sum_{\alpha=1}^{N_2} b_\alpha(t) \, \Lambda^2_\alpha(x),$$

  with coefficient vectors e and b

Discretisation of the Distribution Function

- functionals of the distribution function, $F[f]$, restricted to particle-like distribution functions,

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

  become functions of the particle phasespace trajectories,

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

- replace functional derivatives with partial derivatives

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

- rewrite kinetic bracket as semi-discrete particle bracket

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

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

Discretisation of the Electrodynamic Fields

- semi-discrete electric field E_h and magnetic field B_h

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

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

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

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

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

with mass matrices

$$(M_1)_{\alpha\beta} = \int dx\, \Lambda^1_\alpha(x)\, \Lambda^1_\beta(x), \qquad (M_2)_{\alpha\beta} = \int dx\, \Lambda^2_\alpha(x)\, \Lambda^2_\beta(x)$$

Semi-Discrete Poisson Bracket

- semi-discrete Poisson bracket

$$\begin{aligned}\{\hat F,\hat G\}_d[\mathbf{X},\mathbf{V},\mathbf{e},\mathbf{b}] = {} & \frac{\partial \hat F}{\partial \mathbf{X}}\mathbb{M}_p^{-1}\frac{\partial \hat G}{\partial \mathbf{V}} - \frac{\partial \hat G}{\partial \mathbf{X}}\mathbb{M}_p^{-1}\frac{\partial \hat F}{\partial \mathbf{V}} + \left(\frac{\partial \hat F}{\partial \mathbf{V}}\right)^\top \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{B}(\mathbf{X},\mathbf{b})\,\mathbb{M}_p^{-1}\left(\frac{\partial \hat G}{\partial \mathbf{V}}\right) \\ & + \left(\frac{\partial \hat F}{\partial \mathbf{V}}\right)^\top \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{\Lambda}^1(\mathbf{X})^\top M_1^{-1}\left(\frac{\partial \hat G}{\partial \mathbf{e}}\right) - \left(\frac{\partial \hat F}{\partial \mathbf{e}}\right)^\top M_1^{-1}\mathbb{\Lambda}^1(\mathbf{X})\,\mathbb{M}_q\mathbb{M}_p^{-1}\left(\frac{\partial \hat G}{\partial \mathbf{V}}\right) \\ & + \left(\frac{\partial \hat F}{\partial \mathbf{e}}\right)^\top M_1^{-1}\mathbb{C}^\top\left(\frac{\partial \hat G}{\partial \mathbf{b}}\right) - \left(\frac{\partial \hat F}{\partial \mathbf{b}}\right)^\top \mathbb{C}M_1^{-1}\left(\frac{\partial \hat G}{\partial \mathbf{e}}\right)\end{aligned}$$

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

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

Semi-Discrete Poisson System

- with discrete Hamiltonian

$$\hat{\mathcal{H}} = \tfrac{1}{2}\,\mathbf{V}^\top \mathbb{M}_p \mathbf{V} + \tfrac{1}{2}\,\mathbf{e}^\top M_1 \mathbf{e} + \tfrac{1}{2}\,\mathbf{b}^\top M_2 \mathbf{b}.$$

- semi-discrete equations of motion

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

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

$$\dot{\mathbf{e}} = \{\mathbf{e}, \hat{\mathcal{H}}\}_d = M_1^{-1}\big(\mathbb{C}^\top M_2 \mathbf{b} - \mathbb{\Lambda}^1(\mathbf{X})^\top \mathbb{M}_q \mathbf{V}\big), \qquad \frac{\partial E}{\partial t} = \operatorname{curl} B - J,$$

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

Semi-Discrete Poisson System

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

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

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

$$\mathcal{J}(\mathbf{u}) = \begin{pmatrix} 0 & \mathbb{M}_p^{-1} & 0 & 0 \\ -\mathbb{M}_p^{-1} & \mathbb{M}_p^{-1} \mathbb{M}_q \mathbb{B}(\mathbf{X}, \mathbf{b})\, \mathbb{M}_p^{-1} & \mathbb{M}_p^{-1} \mathbb{M}_q \mathbb{\Lambda}^1(\mathbf{X}) M_1^{-1} & 0 \\ 0 & -M_1^{-1} \mathbb{\Lambda}^1(\mathbf{X})^\top \mathbb{M}_q \mathbb{M}_p^{-1} & 0 & M_1^{-1} \mathbb{C}^\top \\ 0 & 0 & -\mathbb{C} M_1^{-1} & 0 \end{pmatrix}$$

- $\mathcal{J}$ is anti-symmetric and satisfies the Jacobi identity if

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

→ both conditions are satisfied due to the discrete deRham complex

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

Casimir Invariants

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

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

- Gauss' law

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

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

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

(h_E and h_B are arbitrary real functions of $\mathbf{x}$)

Splitting Methods

Splitting Methods

- Hamiltonian splitting[2]

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

with

$$\hat{\mathcal{H}}_{p_\mu} = \frac{1}{2}\,\mathbf{V}_\mu^\top M_p \mathbf{V}_\mu, \qquad \hat{\mathcal{H}}_E = \frac{1}{2}\,\mathbf{e}^\top M_1 \mathbf{e}, \qquad \hat{\mathcal{H}}_B = \frac{1}{2}\,\mathbf{b}^\top M_2 \mathbf{b}$$

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

$$\dot{\mathbf{u}} = \{\mathbf{u}, \hat{\mathcal{H}}_{p_\mu}\}_d, \qquad \dot{\mathbf{u}} = \{\mathbf{u}, \hat{\mathcal{H}}_E\}_d, \qquad \dot{\mathbf{u}} = \{\mathbf{u}, \hat{\mathcal{H}}_B\}_d$$

- each subsystem can be solved exactly

$$\varphi_{t,E}(\mathbf{u}_0) = \mathbf{u}_0 + \int_0^t \{\mathbf{u}, \hat{\mathcal{H}}_E\}_d \, dt\,, \qquad \varphi_{t,B}(\mathbf{u}_0) = \mathbf{u}_0 + \int_0^t \{\mathbf{u}, \hat{\mathcal{H}}_B\}_d \, dt\,, \qquad \ldots$$

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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”. Journal of Computational Physics 297, 721–723, 2015.

He, Qin, Sun, Xiao, Zhang, Liu. Hamiltonian integration methods for Vlasov–Maxwell equations. Physics of Plasmas 22, 124503, 2015.

Splitting Methods

- for the exact solution of the kinetic subsystems

$$\varphi_{t,p_\mu}(\mathbf{u}_0) = \mathbf{u}_0 + \int_0^t \{\mathbf{u}, \hat{\mathcal{H}}_{p_\mu}\}_d \, dt$$

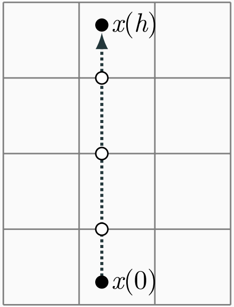
we have to compute line integrals exactly[3] (e.g. $i = 1$)

$$\mathbf{X}_1(\Delta t) = \mathbf{X}_1(0) + \Delta t \, \mathbf{V}_1(0),$$

$$M_p \mathbf{V}_2(\Delta t) = M_p \mathbf{V}_2(0) - \int_0^{\Delta t} M_q \mathbb{\Lambda}^2_3(\mathbf{b}(0), \mathbf{X}(t)) \, \mathbf{V}_1(0) \, \mathrm{d}t,$$

$$M_p \mathbf{V}_3(\Delta t) = M_p \mathbf{V}_3(0) + \int_0^{\Delta t} M_q \mathbb{\Lambda}^2_2(\mathbf{b}(0), \mathbf{X}(t)) \, \mathbf{V}_1(0) \, \mathrm{d}t,$$

$$M_1 \mathbf{e}(\Delta t) = M_1 \mathbf{e}(0) - \int_0^{\Delta t} \mathbb{\Lambda}^1_1(\mathbf{X}(t))^\top M_q \mathbf{V}_1(0) \, \mathrm{d}t$$



→ 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.

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

Splitting Methods

- the exact solution of each subsystem constitutes a Poisson map
- compositions of Poisson maps are themselves Poisson maps
- Poisson structure preserving integrators: composition of exact solutions of the subsystems
- first order time integrator: Lie-Trotter composition

$$\Psi_h = \varphi_{h,E} \circ \varphi_{h,B} \circ \varphi_{h,p_1} \circ \varphi_{h,p_2} \circ \varphi_{h,p_3}$$

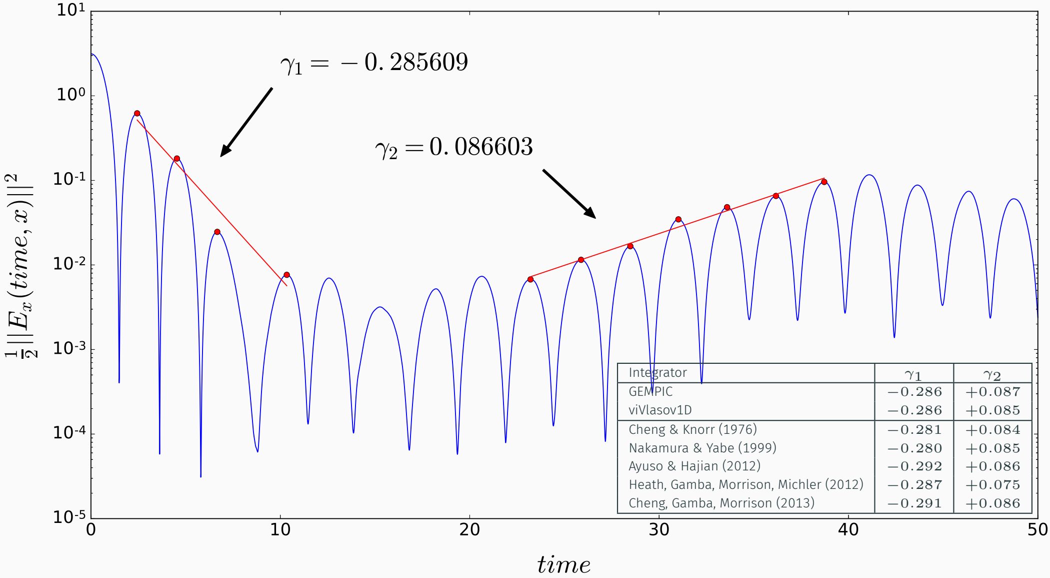
- second order time integrator: symmetric composition

$$\Psi_h = \varphi_{h/2,E} \circ \varphi_{h/2,B} \circ \varphi_{h/2,p_1} \circ \varphi_{h/2,p_2} \circ \varphi_{h,p_3} \circ \varphi_{h/2,p_2} \circ \varphi_{h/2,p_1} \circ \varphi_{h/2,B} \circ \varphi_{h/2,E}$$

- higher order time integrators: Baker-Campbell-Hausdorff formula
- backward error analysis confirms boundedness of energy error

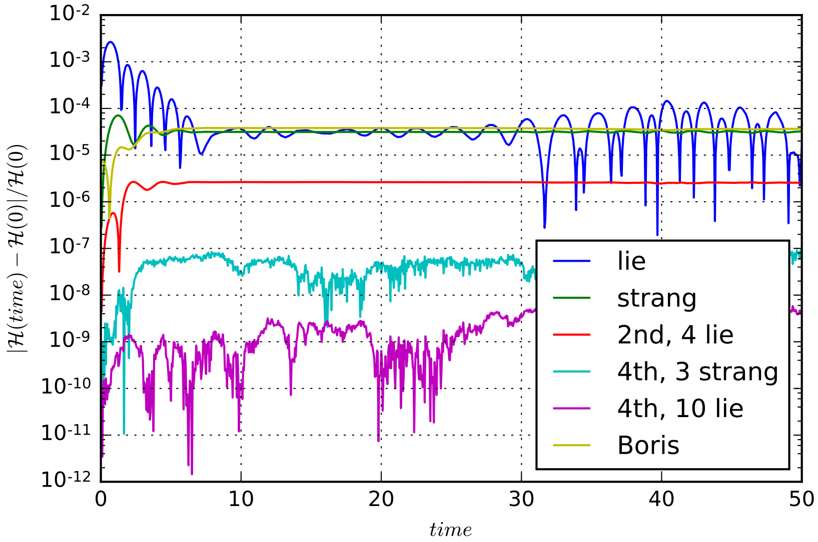
Numerical Examples

Nonlinear Landau Damping

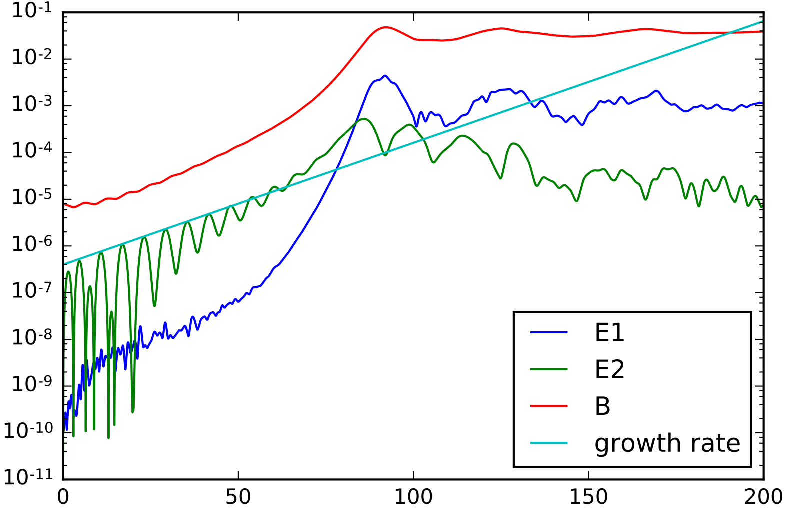


Integrator	γ_1	γ_2
GEMPIC	-0.286	$+0.087$
viVlasov1D	-0.286	$+0.085$
Cheng & Knorr (1976)	-0.281	$+0.084$
Nakamura & Yabe (1999)	-0.280	$+0.085$
Ayuso & Hajian (2012)	-0.292	$+0.086$
Heath, Gamba, Morrison, Michler (2012)	-0.287	$+0.075$
Cheng, Gamba, Morrison (2013)	-0.291	$+0.086$

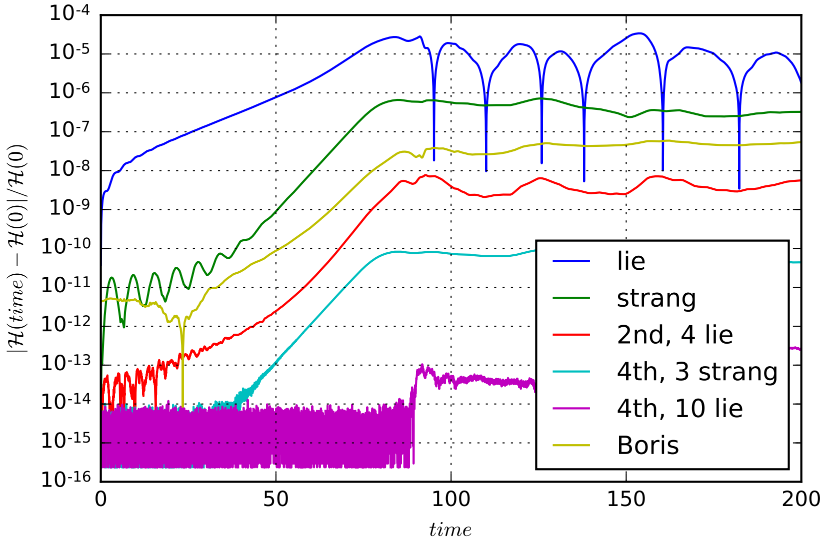
Nonlinear Landau Damping



Streaming Weibel Instability



Streaming Weibel Instability



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, virtual elements, mimetic spectral elements, mimetic finite differences, ...
  - exactly satisfy identities from vector calculus ($\mathbf{curl}\,\mathbf{grad} = 0$, $\mathbf{div}\,\mathbf{curl} = 0$)
  - stability: $\mathrm{d} \circ \mathrm{d} = 0$ and compatibility of the finite element deRham complex
- discrete Poisson brackets
  - Poisson structure is retained at the semi-discrete level (Jacobi identity, Casimir invariants)
  - splitting methods for Poisson time integration (good long-time energy behaviour, no dissipation)
  - gauge invariance guarantees exact charge conservation (Gauss' law)
  - computational cost comparable to traditional, non-conservative methods
- ongoing and future work
  - 3D3V, fully Eulerian discretisation, application to gyrokinetics and fluid models
  - new splitting methods or variational integrators for degenerate Lagrangians
  - integral-preserving time discretisation (average vector field method, continuous stage Runge-Kutta methods)

Spline Differential Forms

B-Splines

- 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

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

Spline Differential Forms

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

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

- zero-form basis

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

Spline Differential Forms

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

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

- one-form basis

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

Spline Differential Forms

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

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

- two-form basis

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

Spline Differential Forms

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

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

- three-form basis

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

Initial Conditions

Nonlinear Landau Damping

- numerical example: nonlinear Landau damping

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

$$B_3(x, t = 0) = 0,$$

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

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

- numerical parameters:

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

- physical parameters:

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

Streaming Weibel Instability

- numerical example: streaming Weibel instability

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

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

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

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

- numerical parameters: splines of degree 3 and 2

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

- physical parameters:

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