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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

$$\begin{array}{lll} \dfrac{\partial E}{\partial t} = \nabla \times B - J, & \nabla \cdot E = -\rho, & \rho(t, x) = \displaystyle\sum_s e_s \int dv\, f_s(t, x, v), \\ \dfrac{\partial B}{\partial t} = -\nabla \times E, & \nabla \cdot B = 0, & J(t, x) = \displaystyle\sum_s e_s \int dv\, f_s(t, x, v)\, v \end{array}$$

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 (canonical and noncanonical)
  - antisymmetric bracket satisfying the Jacobi identity
  - Casimir invariants

- variational structure
  - Hamilton's principle of stationary action
  - symplectic structure

- Noether theorem
  - energy conservation (time translation invariance)
  - momentum conservation (spatial translation invariance)
  - charge conservation (gauge invariance)

Outline

1. Discrete Differential Forms
2. Discrete Poisson Brackets
3. Splitting Methods
4. Numerical Examples
5. Summary and Outlook

Discrete Differential Forms

Differential Forms

- mathematical language of calculus 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	$(\mathrm{Vs})/\mathrm{m}^2$	2D surface
charge density	ρ	$(\mathrm{As})/\mathrm{m}^3$	3D volume

- alternative: exterior calculus and differential forms
- 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 d : $\Lambda^k \to \Lambda^{k+1}$ (generalises grad, curl, div)
- complex property: Im $\{$d : $\Lambda^{k-1} \to \Lambda^k\} \subseteq$ Ker $\{$d : $\Lambda^k \to \Lambda^{k+1}\}$
- specifically Im $\{\text{grad}\} \subseteq$ Ker $\{\text{curl}\}$, Im $\{\text{curl}\} \subseteq$ Ker $\{\text{div}\}$
- in general d $\circ$ d $= 0$, in particular $\text{curl}\,\text{grad} = 0$ and $\text{div}\,\text{curl} = 0$

Discrete deRham Complex

- discrete deRham complex

$$\begin{tikzcd}
\mathbb{R} \arrow[r] & \Lambda^0(\Omega) \arrow[r, "\mathrm{d}"] \arrow[d, "\pi_h^0"] & \Lambda^1(\Omega) \arrow[r, "\mathrm{d}"] \arrow[d, "\pi_h^1"] & \Lambda^2(\Omega) \arrow[r, "\mathrm{d}"] \arrow[d, "\pi_h^2"] & \Lambda^3(\Omega) \arrow[r] \arrow[d, "\pi_h^3"] & 0 \\
\mathbb{R} \arrow[r] & \Lambda_h^0(\Omega) \arrow[r, "\mathrm{d}"] & \Lambda_h^1(\Omega) \arrow[r, "\mathrm{d}"] & \Lambda_h^2(\Omega) \arrow[r, "\mathrm{d}"] & \Lambda_h^3(\Omega) \arrow[r] & 0
\end{tikzcd}$$

- the discrete spaces $\Lambda_h^k \subset \Lambda^k$ are finite element spaces of differential forms
- 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]

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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.

Discrete deRham Complex

- weak formulation of Ampère's equation and Gauss' law

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega E\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} = \int_\Omega B\cdot\operatorname{curl}\mathbf{v}\,\mathrm{d}\mathbf{x} - \int_\Omega J\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} \qquad \forall\mathbf{v}\in H(\operatorname{curl},\Omega),$$

$$\int_\Omega E\cdot\nabla v\,\mathrm{d}\mathbf{x} = -\int_\Omega \rho v\,\mathrm{d}\mathbf{x} \qquad \forall v\in H^1(\Omega),$$

- project all fields to finite dimensional subspaces, e.g.,

$$E_h(t,x) = \sum_{\alpha=1}^{N_1}\sum_{i=1}^{3} e_{\alpha,i}(t)\,\mathbf{\Lambda}^1_{\alpha,i}(x), \qquad B_h(t,x) = \sum_{\alpha=1}^{N_2}\sum_{i=1}^{3} b_{\alpha,i}(t)\,\mathbf{\Lambda}^2_{\alpha,i}(x),$$

  with mass matrices M_1 and M_2 given by

$$(M_1)_{\alpha,\beta} = \int_\Omega \mathbf{\Lambda}^1_\alpha\cdot\mathbf{\Lambda}^1_\beta\,\mathrm{d}\mathbf{x}, \qquad (M_2)_{\alpha,\beta} = \int_\Omega \mathbf{\Lambda}^2_\alpha\cdot\mathbf{\Lambda}^2_\beta\,\mathrm{d}\mathbf{x},$$

  and coefficient vectors $\mathbf{e} = (e_{1,1}, e_{1,2}, \dots, e_{N_1,3})^\top$ and $\mathbf{b} = (b_{1,1}, b_{1,2}, \dots, b_{N_2,3})^\top$

Discrete deRham Complex

- weak formulation of Ampère's equation and Gauss' law

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega E_h \cdot \mathbf{v}_h \,\mathrm{d}\mathbf{x} &= \int_\Omega B_h \cdot \operatorname{curl} \mathbf{v}_h \,\mathrm{d}\mathbf{x} - \int_\Omega J_h \cdot \mathbf{v}_h \,\mathrm{d}\mathbf{x} && \forall \mathbf{v} \in \Lambda_h^1(\Omega), \\ \int_\Omega E_h \cdot \nabla v_h \,\mathrm{d}\mathbf{x} &= - \int_\Omega \rho_h v_h \,\mathrm{d}\mathbf{x} && \forall v \in \Lambda_h^0(\Omega), \end{aligned}$$

- finite dimensional Maxwell's equations

$$\begin{aligned} M_1 \frac{\mathrm{d}\mathbf{e}}{\mathrm{d}t} - \mathbb{C}^\top M_2 \mathbf{b} &= -\mathbf{j}, & \mathbb{G}^\top M_1 \mathbf{e} &= \boldsymbol{\varrho}, \\ \frac{\mathrm{d}\mathbf{b}}{\mathrm{d}t} + \mathbb{C}\mathbf{e} &= 0, & \mathbb{D}\mathbf{b} &= 0 \end{aligned}$$

- complex property holds at the matrix level: $\mathbb{C}\mathbb{G} = 0$, $\mathbb{D}\mathbb{C} = 0$

$$\mathbb{R}^{N_0} \xrightarrow{\mathbb{G}} \mathbb{R}^{N_1} \xrightarrow{\mathbb{C}} \mathbb{R}^{N_2} \xrightarrow{\mathbb{D}} \mathbb{R}^{N_3} \qquad \text{with} \qquad \operatorname{Im} \mathbb{G} \subseteq \operatorname{Ker} \mathbb{C}, \ \operatorname{Im} \mathbb{C} \subseteq \operatorname{Ker} \mathbb{D}$$

B-Splines

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

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

  where

$$S_i^0(x) = \begin{cases} 1 & x \in [x_j, x_{j+1}) \\ 0 & \text{else} \end{cases}$$

- 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

$$\Lambda_h^0(\Omega) = \operatorname{span}\left\{ S^p(x)\, S^p(y)\, S^p(z) \right\}$$

$$\Lambda_h^1(\Omega) = \operatorname{span}\left\{ \begin{pmatrix} S^{p-1}(x)\, S^p(y)\, S^p(z) \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ S^p(x)\, S^{p-1}(y)\, S^p(z) \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ S^p(x)\, S^p(y)\, S^{p-1}(z) \end{pmatrix} \right\}$$

$$\Lambda_h^2(\Omega) = \operatorname{span}\left\{ \begin{pmatrix} S^p(x)\, S^{p-1}(y)\, S^{p-1}(z) \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ S^{p-1}(x)\, S^p(y)\, S^{p-1}(z) \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ S^{p-1}(x)\, S^{p-1}(y)\, S^p(z) \end{pmatrix} \right\}$$

$$\Lambda_h^3(\Omega) = \operatorname{span}\left\{ S^{p-1}(x)\, S^{p-1}(y)\, S^{p-1}(z) \right\}$$

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 → finite-dimensional representation
- Vlasov-Maxwell noncanonical Hamiltonian structure → discretisation of the brackets

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

- Hamiltonian: sum of the kinetic energy of the particles, the electrostatic field energy and the magnetic field energy → 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 $F[f, E, B]$ → 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

- semi-discrete electric field E_h and magnetic field B_h

$$E_h(t, x) = \sum_{\alpha=1}^{N_1} \sum_{i=1}^{3} e_{\alpha,i}(t) \, \mathbf{\Lambda}^1_{\alpha,i}(x), \qquad B_h(t, x) = \sum_{\alpha=1}^{N_2} \sum_{i=1}^{3} b_{\alpha,i}(t) \, \mathbf{\Lambda}^2_{\alpha,i}(x),$$

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

$$\mathbf{\Lambda}^m_{\alpha,1} = \begin{pmatrix} \Lambda^{m,1}_\alpha \\ 0 \\ 0 \end{pmatrix}, \qquad \mathbf{\Lambda}^m_{\alpha,2} = \begin{pmatrix} 0 \\ \Lambda^{m,2}_\alpha \\ 0 \end{pmatrix}, \qquad \mathbf{\Lambda}^m_{\alpha,1} = \begin{pmatrix} 0 \\ 0 \\ \Lambda^{m,3}_\alpha \end{pmatrix}, \qquad m = 1, 2,$$

  and coefficient vectors $\mathbf{e}$ and $\mathbf{b}$

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

$$E_h(t,x) = \sum_{\alpha=1}^{N_1} \sum_{i=1}^{3} e_{\alpha,i}(t)\, \mathbf{\Lambda}^1_{\alpha,i}(x), \qquad B_h(t,x) = \sum_{\alpha=1}^{N_2} \sum_{i=1}^{3} b_{\alpha,i}(t)\, \mathbf{\Lambda}^2_{\alpha,i}(x),$$

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

$$\begin{aligned} \dot{\mathbf{X}} &= \{\mathbf{X}, \hat{\mathcal{H}}\}_d = \mathbf{V}, \\ \dot{\mathbf{V}} &= \{\mathbf{V}, \hat{\mathcal{H}}\}_d = \mathbb{M}_p^{-1} \mathbb{M}_q \big(\mathbb{\Lambda}^1(\mathbf{X}) \mathbf{e} + \mathbb{B}(\mathbf{X}, \mathbf{b}) \mathbf{V} \big), \\ \dot{\mathbf{e}} &= \{\mathbf{e}, \hat{\mathcal{H}}\}_d = M_1^{-1} \big(\mathbb{C}^\top M_2 \mathbf{b} - \mathbb{\Lambda}^1(\mathbf{X})^\top \mathbb{M}_q \mathbf{V} \big), \\ \dot{\mathbf{b}} &= \{\mathbf{b}, \hat{\mathcal{H}}\}_d = -\mathbb{C} \mathbf{e}, \end{aligned}$$

$$\begin{aligned} \frac{dx_s}{dt} &= v_s, \\ \frac{dv_s}{dt} &= e_s \big(E(x_s) + v_s \times B(x_s) \big), \\ \frac{\partial E}{\partial t} &= \operatorname{curl} B - J, \\ \frac{\partial B}{\partial t} &= - \operatorname{curl} E \end{aligned}$$

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 $\mathcal{G}(f, E, B)$ so that $\{\mathcal{C}, \mathcal{G}\} = 0$
- integral of any real function h_s of each distribution function f_s

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

- Gauss' law

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

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

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

(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

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

- 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.

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Splitting Methods

- for the exact solution of the kinetic subsystems

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

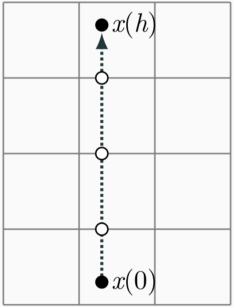
we have to compute line integrals exactly[3] (e.g. $i = 1$)

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

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

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

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



→ solution is gauge invariant and therefor charge conserving

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[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

- 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

Implementation

- 1D2V implementation in SeLaLib (`http://selalib.gforge.inria.fr/`)

  modular library for the kinetic and gyrokinetic simulation of tokamak plasmas by semi-Lagrangian or particle-in-cell methods

- finite element basis: spline differential forms of order 2/3 or 4/5

- various splitting schemes of order 1, 2, 4

- computational cost comparable with standard methods (e.g. Boris-Yee)

Nonlinear Landau Damping

- numerical example: nonlinear Landau damping

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

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

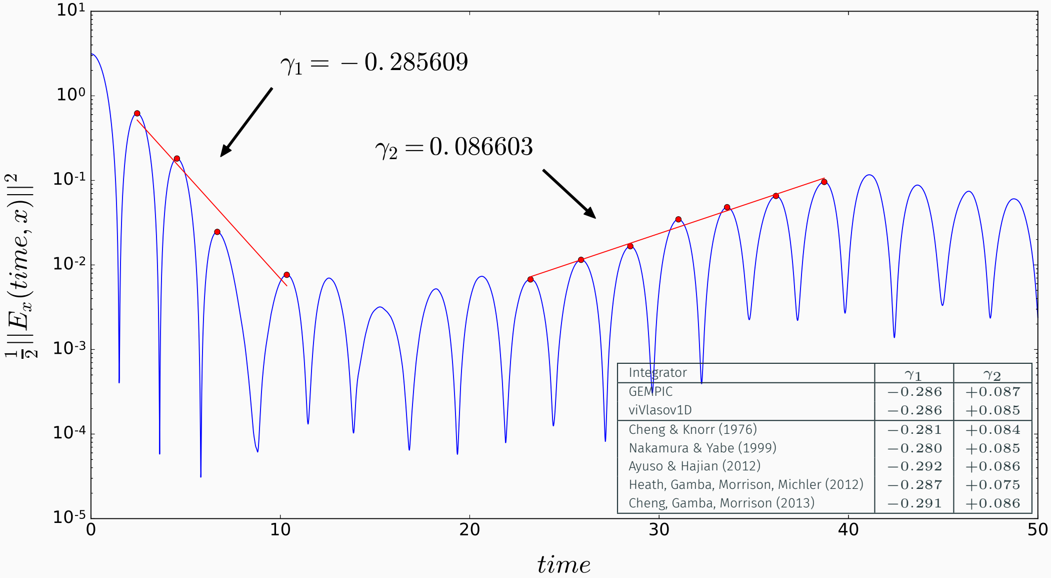
- numerical parameters:

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

- physical parameters:

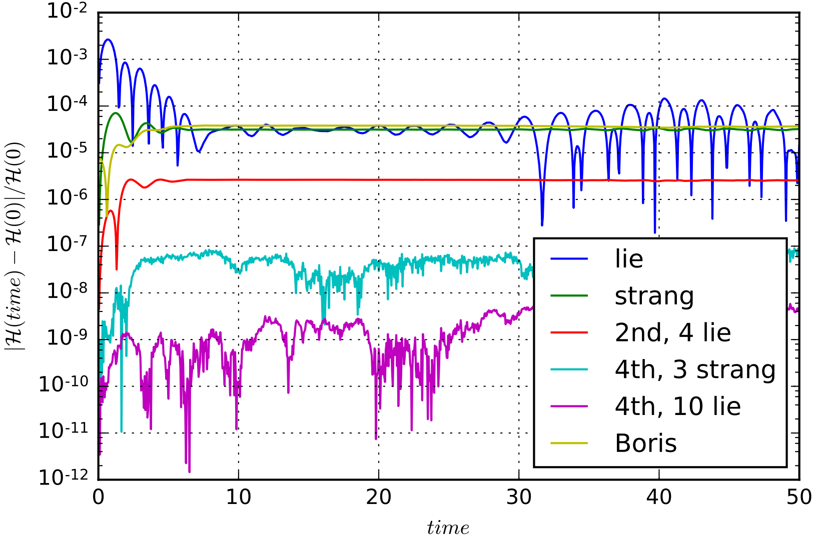
$$
v_{\text{th}} = 1, \qquad k = 0.5, \qquad \alpha = 0.5
$$

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

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

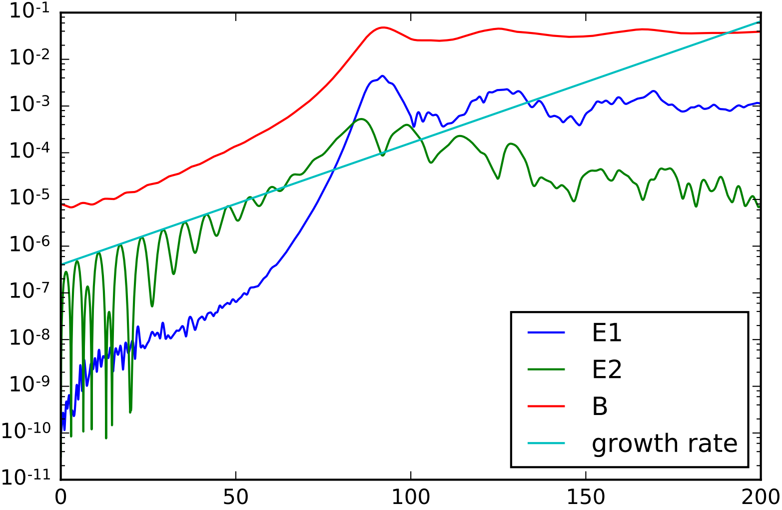
  and $E_1(x, t=0)$ is computed from Poisson's equation
- numerical parameters: splines of degree 3 and 2

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

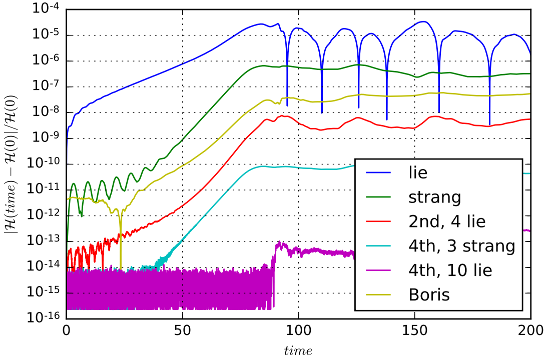
- physical parameters:

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

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

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 ($\mathrm{curl}\, \mathrm{grad} = 0$, $\mathrm{div}\, \mathrm{curl} = 0$)
  - 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
  - 2D2V, 2D3V, 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)