

Structure and Computation of Magnetofluid and Other Matter Models

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Survey Hamiltonian structure of matter models; viz. magnetofluids
and Vlasov. Describe GEMPIC a Poisson integrator.

Overview

- Hamiltonian Structure. Background material.
- Extended MHD. Aesthetically pleasing.
- Vlasov Computation. Pleasing and practical.

Über die Ausbreitung von Wellen in einem Plasma

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Zusammenfassung

Einleitend wird kurz auf die Bedeutung und die Anwendungsmöglichkeiten hingewiesen, die die Wellen in einem Plasma für verschiedene Gebiete der Physik und der Astrophysik haben können (Abschnitt 1). Die Grundgleichungen für ein nicht quasineutrales Plasma werden in Abschnitt 2 abgeleitet, wobei

Die Differenz der Gln. (2.3) und (2.4) ergibt nach Division durch m_i bzw. m_e und nach einigen weiteren Umformungen die „Diffusionsgleichung“, die auch als das verallgemeinerte OHMSche Gesetz bezeichnet wird:

$$\begin{aligned} \frac{1}{e^2} \frac{m_i m_e}{n_i m_e + n_e m_i} \left\{ \frac{d_2 \mathbf{j}}{dt} + \mathbf{N}_2 \right\} + \frac{1}{\sigma} (\mathbf{j} - \lambda \mathbf{v}) = \mathbf{E} + \frac{\varrho}{n_i m_e + n_e m_i} \frac{1}{c} [\mathbf{v} \mathbf{B}] + \\ + \frac{1}{e(n_i m_e + n_e m_i)} \left\{ (m_e - m_i) \frac{1}{c} [\mathbf{j} \mathbf{B}] - m_e \operatorname{grad} p_i + m_i \operatorname{grad} p_e \right\}. \quad (2.11) \end{aligned}$$

nicht mehr auftritt [2]. Weiterhin ist auf der linken Seite $\lambda \mathbf{v}$ der Konvektionsstrom infolge der elektrischen Raumladungsdichte. Schließlich ist

$$\begin{aligned} \frac{d_2 \mathbf{j}}{dt} &\equiv \frac{\partial \mathbf{j}}{\partial t} + \frac{\varrho}{m^2} \left(\frac{m_e}{n_i} + \frac{m_i}{n_e} \right) \{ (\mathbf{v} \operatorname{grad}) \mathbf{j} + (\mathbf{j} \operatorname{grad}) \mathbf{v} \} + \\ &+ \frac{1}{e m^2} \left(\frac{m_e^2}{n_i} - \frac{m_i^2}{n_e} \right) (\mathbf{j} \operatorname{grad}) \mathbf{j} + \frac{1}{e m^2} \left\{ \mathbf{j} \operatorname{grad} \left(\frac{m_e^2}{n_i} - \frac{m_i^2}{n_e} \right) \right\} \mathbf{j} + \\ &+ \frac{1}{m^2} \varrho \left\{ \mathbf{v} \operatorname{grad} \left(\frac{m_e}{n_i} + \frac{m_i}{n_e} \right) \right\} \mathbf{j} + \\ &+ \frac{1}{m} \left\{ m_e n_i \frac{\partial}{\partial t} \left(\frac{1}{n_i} \right) + m_i n_e \frac{\partial}{\partial t} \left(\frac{1}{n_e} \right) \right\} \quad (2.13) \end{aligned}$$

und

$$\begin{aligned} \mathbf{N}_2 &\equiv \frac{e}{m} \left\{ m_e n_i \frac{\partial}{\partial t} \left(\frac{n_e}{n_i} \right) - m_i n_e \frac{\partial}{\partial t} \left(\frac{n_i}{n_e} \right) \right\} \mathbf{v} + \frac{e \varrho^2}{m^2} \left(\frac{1}{n_i} - \frac{1}{n_e} \right) (\mathbf{v} \operatorname{grad}) \mathbf{v} + \\ &+ \frac{e \varrho}{m} \left\{ \mathbf{v} \operatorname{grad} \left(m_e \frac{n_e}{n_i} - m_i \frac{n_i}{n_e} \right) \right\} \mathbf{v} + \frac{1}{m^2} \left\{ \mathbf{j} \operatorname{grad} \left(m_e^2 \frac{n_e}{n_i} + m_i^2 \frac{n_i}{n_e} \right) \right\} \mathbf{v}. \quad (2.14) \end{aligned}$$

Auch hier ist die Aufspaltung zwischen $\frac{d_2 \mathbf{j}}{dt}$ und \mathbf{N}_2 wieder so vorgenommen worden, daß \mathbf{N}_2 verschwindet, wenn man Quasineutralität annimmt. \mathbf{N}_2 ist

Hamilton's Equations

Canonical Momentum: $p_i = \frac{\partial L}{\partial \dot{q}^i}$ ← inverse function theorem

Legendre Transform: $H(q, p) = p_i \dot{q}^i - L(\dot{q}, q)$

$$\dot{p}_i = -\frac{\partial H}{\partial q^i}, \quad \dot{q}^i = \frac{\partial H}{\partial p_i},$$

Phase Space Coordinates: $z = (q, p), \quad \alpha, \beta = 1, 2, \dots, 2N$

$$\dot{z}^\alpha = J_c^{\alpha\beta} \frac{\partial H}{\partial z^\beta} = \{z^\alpha, H\}, \quad (J_c^{\alpha\beta}) = \begin{pmatrix} 0_N & I_N \\ -I_N & 0_N \end{pmatrix},$$

$J_c :=$ Poisson tensor, Hamiltonian bi-vector, cosymplectic form

symplectic 2-form = (cosymplectic form) $^{-1}$: $\omega_{\alpha\beta}^c J_c^{\beta\gamma} = \delta_\alpha^\gamma,$

Noncanonical Hamiltonian Definition

A phase space \mathcal{P} diff. manifold with binary bracket operation on $C^\infty(\mathcal{P})$ functions $f, g: \mathcal{P} \rightarrow \mathbb{R}$, s.t. $\{\cdot, \cdot\}: C^\infty(\mathcal{P}) \times C^\infty(\mathcal{P}) \rightarrow C^\infty(\mathcal{P})$ satisfies

- Bilinear: $\{f + \lambda g, h\} = \{f, h\} + \lambda\{g, h\}, \quad \forall f, g, h \text{ and } \lambda \in \mathbb{R}$
- Antisymmetric: $\{f, g\} = -\{g, f\}, \quad \forall f, g$
- Jacobi: $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} \equiv 0, \quad \forall f, g, h$
- Leibniz: $\{fg, h\} = f\{g, h\} + \{f, h\}g, \quad \forall f, g, h.$

Above is a Lie algebra realization on functions. Take fg to be pointwise multiplication.

Eqs. Motion: $\frac{\partial \Psi}{\partial t} = \{\Psi, H\}, \Psi \text{ an observable \& } H \text{ a Hamiltonian.}$

Example: flows on Poisson manifolds, e.g. Weinstein 1983

Noncanonical Hamiltonian Dynamics

Sophus Lie (1890)

Noncanonical Coordinates:

$$\dot{z}^\alpha = J^{\alpha\beta} \frac{\partial H}{\partial z^\beta} = \{z^\alpha, H\}, \quad \{f, g\} = \frac{\partial f}{\partial z^\alpha} J^{\alpha\beta}(z) \frac{\partial g}{\partial z^\beta}, \quad \alpha, \beta = 1, 2, \dots M$$

Poisson Bracket Properties:

antisymmetry $\rightarrow \{f, g\} = -\{g, f\},$

Jacobi identity $\rightarrow \{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$

G. Darboux: $\det J \neq 0 \implies J \rightarrow J_c$ Canonical Coordinates

Sophus Lie: $\det J = 0 \implies$ Canonical Coordinates plus Casimirs

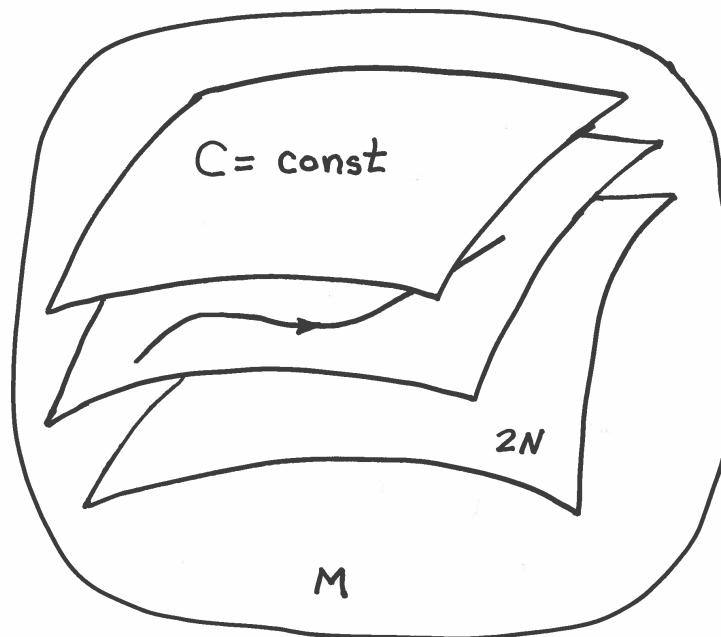
$$J \rightarrow J_d = \begin{pmatrix} 0_N & I_N & 0 \\ -I_N & 0_N & 0 \\ 0 & 0 & 0_{M-2N} \end{pmatrix}.$$

Poisson Manifold \mathcal{M} Cartoon

Degeneracy in $J \Rightarrow$ Casimirs:

$$\{f, C\} = 0 \quad \forall f : \mathcal{M} \rightarrow \mathbb{R}$$

Lie-Darboux Foliation by Casimir (symplectic) leaves:



Leaf vector fields, $Z_f = \{z, f\} = Jdf$ are tangent to leaves.

Lie-Poisson Brackets

Coordinates:

$$J^{\alpha\beta} = c_{\gamma}^{\alpha\beta} z^{\gamma}$$

where $c_{\gamma}^{\alpha\beta}$ are the structure constants for some Lie algebra.

Examples:

- 3-dimensional Bianchi algebras for free rigid body, Kida vortex, & rattleback toy.
- Infinite-dimensional theories - matter models: Ideal fluid flow, MHD, shearflow, extended MHD, Vlasov-Maxwell, BBGKY, etc.

Magnetohydrodynamics (MHD)

Equations of Motion:

Force	$\rho \frac{\partial \mathbf{v}}{\partial t} = -\rho \mathbf{v} \cdot \nabla \mathbf{v} - \nabla p + \frac{1}{c} \mathbf{J} \times \mathbf{B}$
Density	$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v})$
Entropy	$\frac{\partial s}{\partial t} = -\mathbf{v} \cdot \nabla s$
Ohm's Law	$\mathbf{E} + \mathbf{v} \times \mathbf{B} = \eta \mathbf{J} \approx 0$
Magnetic Field	$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} = \nabla \times (\mathbf{v} \times \mathbf{B})$

Energy:

$$H = \int_D d^3x \left(\frac{1}{2} \rho |\mathbf{v}|^2 + \rho U(\rho, s) + \frac{1}{2} |\mathbf{B}|^2 \right)$$

Thermodynamics:

$$p = \rho^2 \frac{\partial U}{\partial \rho} \quad s = \frac{\partial U}{\partial s}$$

Noncanonical Lie-Poisson Bracket (pjm & Greene 1980):

$$\begin{aligned}
 \{F, G\} = & - \int_D d^3x \left[M_i \left(\frac{\delta F}{\delta M_j} \frac{\partial}{\partial x^j} \frac{\delta G}{\delta M_i} - \frac{\delta G}{\delta M_j} \frac{\partial}{\partial x^j} \frac{\delta F}{\delta M_i} \right) \right. \\
 & + \rho \left(\frac{\delta F}{\delta \mathbf{M}} \cdot \nabla \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta \mathbf{M}} \cdot \nabla \frac{\delta F}{\delta \rho} \right) + \sigma \left(\frac{\delta F}{\delta \mathbf{M}} \cdot \nabla \frac{\delta G}{\delta \sigma} - \frac{\delta G}{\delta \mathbf{M}} \cdot \nabla \frac{\delta F}{\delta \sigma} \right) \\
 & + \mathbf{B} \cdot \left[\frac{\delta F}{\delta \mathbf{M}} \cdot \nabla \frac{\delta G}{\delta \mathbf{B}} - \frac{\delta G}{\delta \mathbf{M}} \cdot \nabla \frac{\delta F}{\delta \mathbf{B}} \right] \\
 & \left. + \mathbf{B} \cdot \left[\nabla \left(\frac{\delta F}{\delta \mathbf{M}} \right) \cdot \frac{\delta G}{\delta \mathbf{B}} - \nabla \left(\frac{\delta G}{\delta \mathbf{M}} \right) \cdot \frac{\delta F}{\delta \mathbf{B}} \right] \right],
 \end{aligned}$$

Dynamics:

$$\frac{\partial \rho}{\partial t} = \{\rho, H\}, \quad \frac{\partial s}{\partial t} = \{s, H\}, \quad \frac{\partial \mathbf{v}}{\partial t} = \{\mathbf{v}, H\}, \text{ and } \frac{\partial \mathbf{B}}{\partial t} = \{\mathbf{B}, H\}.$$

Densities:

$$\mathbf{M} := \rho \mathbf{v} \qquad \qquad \sigma := \rho s$$

Casimir Invariants

Helicities are Casimir Invariants:

$$\{F, C\}^{MHD} = 0 \quad \forall \text{ functionals } F.$$

Casimirs Invariants (helicities):

$$C_B = \int d^3x \mathbf{B} \cdot \mathbf{A}, \quad C_V = \int d^3x \mathbf{B} \cdot \mathbf{v}$$

Topological content, linking etc.

Cf. William Irvine, ...

Extended MHD (X**MHD)**

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Extended MHD

Ohm's Law:

$$\begin{aligned} \mathbf{E} + \frac{\mathbf{V} \times \mathbf{B}}{c} = & \frac{m_e}{e^2 n} \left(\frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot (\mathbf{V} \mathbf{J} + \mathbf{J} \mathbf{V}) \right) \\ & - \frac{m_e}{e^2 n} (\mathbf{J} \cdot \nabla) \left(\frac{\mathbf{J}}{n} \right) + \frac{(\mathbf{J} \times \mathbf{B})}{enc} - \frac{\nabla p_e}{en}. \end{aligned}$$

Momentum:

$$\begin{aligned} nm \left(\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} \right) = & -\nabla p + \frac{\mathbf{J} \times \mathbf{B}}{c} \\ & - \frac{m_e}{e^2} (\mathbf{J} \cdot \nabla) \left(\frac{\mathbf{J}}{n} \right). \end{aligned}$$

XMHD

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XMH D Scaled

Ohm's Law:

$$\begin{aligned} \mathbf{E} + \mathbf{V} \times \mathbf{B} = & \frac{d_e^2}{\rho} \left(\frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot (\mathbf{V} \mathbf{J} + \mathbf{J} \mathbf{V} - \frac{d_i}{\rho} \mathbf{J} \mathbf{J}) \right) \\ & + \frac{d_i}{\rho} (\mathbf{J} \times \mathbf{B} - \nabla p_e). \end{aligned}$$

Momentum:

$$\begin{aligned} \rho \left(\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} \right) = & -\nabla p + \mathbf{J} \times \mathbf{B} \\ & - d_e^2 \mathbf{J} \cdot \nabla \left(\frac{\mathbf{J}}{\rho} \right). \end{aligned}$$

Two parameters, $d_e = \frac{c}{\omega_{pe} L}$ measures electron inertia and $d_i = \frac{c}{\omega_{pi} L}$ accounts for current carried by electrons mostly

Energy Conservation

Candidate Hamiltonian:

$$H = \int d^3x \left[\rho \frac{|\mathbf{V}|^2}{2} + \rho U(\rho) + \frac{|\mathbf{B}|^2}{2} + d_e^2 \frac{|\mathbf{J}|^2}{2\rho} \right]$$

Kimura and pjm 2014 on energy conservation

H is conserved. Pressure, $p = \rho^2 \partial U / \partial \rho$.

What is the Poisson bracket? Casimirs? Helicities?

XMHD Hamiltonian Structure

Yoshida, Abdelhamid, Kawazura, pjm, Lingam, Miloshevich, D'Avignon

Poisson Bracket:

$$\begin{aligned}\{F, G\}^{XMHD} &= \{F, G\}^{MHD} \\ &+ d_e^2 \int_D d^3x \left[\frac{\nabla \times \mathbf{V}}{\rho} \cdot \left((\nabla \times F_{\mathbf{B}^\star}) \times (\nabla \times G_{\mathbf{B}^\star}) \right) \right] \\ &+ d_i \int_D d^3x \frac{\mathbf{B}^\star}{\rho} \cdot \left[(\nabla \times F_{\mathbf{B}}^\star) \times (\nabla \times G_{\mathbf{B}}^\star) \right]\end{aligned}$$

where we introduce the ‘inertial’ magnetic field

$$\mathbf{B}^\star = \mathbf{B} + d_e^2 \nabla \times \left(\frac{\nabla \times \mathbf{B}}{\rho} \right),$$

Hamiltonian:

$$H = \int_D d^3x \left[\frac{\rho |\mathbf{V}|^2}{2} + \rho U(\rho) + \frac{\mathbf{B} \cdot \mathbf{B}^\star}{2} \right].$$

XMHD Hamiltonian Structure (cont)

Casimirs;

$$C_{XMHD}^{\pm} = \int_D d^3x (\mathbf{V} + \lambda_{\pm} \mathbf{A}^{\star}) \cdot (\nabla \times \mathbf{V} + \lambda_{\pm} \mathbf{B}^{\star}) ,$$

where

$$\lambda_{\pm} = \frac{-d_i \pm \sqrt{d_i^2 + 4d_e^2}}{2d_e^2} .$$

Jacobi Identity:

Directly Abdelhamid et al.; remarkable transformations Lingam et al. which lead to **normal fields**.

Normal Fields

Normal Fields:

$$\mathcal{B}_\pm := \mathbf{B} + d_e^2 \nabla \times \left[\frac{\nabla \times \mathbf{B}}{\rho} \right] + \lambda_\pm \nabla \times \mathbf{V}$$

XMHD remarkably yields:

$$\frac{\partial \mathcal{B}_\pm}{\partial t} + \mathcal{L}_{V_\pm} \mathcal{B}_\pm = 0 \quad \leftarrow \quad \text{Lie dragging of 2-forms} \Rightarrow \text{frozen fluxes}$$

Dragging velocities:

$$\mathbf{V}_\pm = \mathbf{V} - \lambda_\mp \nabla \times \mathbf{B} / \rho$$

Helicities:

$$K_\pm = \int A_\pm \wedge dA_\pm, \quad \mathcal{B}_\pm = \nabla \times A_\pm \sim dA_\pm$$

Extended MHD

Ohm's Law:

$$\begin{aligned} \mathbf{E} + \frac{\mathbf{V} \times \mathbf{B}}{c} = & \frac{m_e}{e^2 n} \left(\frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot (\mathbf{V} \mathbf{J} + \mathbf{J} \mathbf{V}) \right) \\ & - \frac{m_e}{e^2 n} (\mathbf{J} \cdot \nabla) \left(\frac{\mathbf{J}}{n} \right) + \frac{(\mathbf{J} \times \mathbf{B})}{enc} - \frac{\nabla p_e}{en}. \end{aligned}$$

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$$\begin{aligned} nm \left(\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} \right) = & -\nabla p + \frac{\mathbf{J} \times \mathbf{B}}{c} \\ & - \frac{m_e}{e^2} (\mathbf{J} \cdot \nabla) \left(\frac{\mathbf{J}}{n} \right). \end{aligned}$$

Ohm's Laws

Normal Potentials:

$$\mathbf{E}_\pm = -\nabla\phi_\pm - \frac{1}{c}\frac{\partial\mathbf{A}_\pm}{\partial t}$$

Ohms Laws:

$$\mathbf{E}_\pm + \frac{\mathbf{v}_\pm \times \mathbf{B}_\pm}{c} = \nabla\gamma_\pm$$

Maxwell-Vlasov

Maxwell Part

$$\frac{\partial \mathbf{B}}{\partial t} = -c \nabla \times \mathbf{E}$$

$$\frac{\partial \mathbf{E}}{\partial t} = c \nabla \times \mathbf{B} - 4\pi \mathbf{J}_e$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = 4\pi \rho_e$$

$$\mathbf{E}(x,t), \mathbf{B}(x,t), \rho_e(x,t), \mathbf{J}_e(x,t)$$

Coupling to Vlasov

$$\frac{\partial f_s}{\partial t} = -\mathbf{v} \cdot \nabla f_s - \frac{e_s}{m_s} \left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right) \cdot \frac{\partial f_s}{\partial \mathbf{v}}$$

$$\rho_e(\mathbf{x}, t) = \sum_s e_s \int f_s(\mathbf{x}, \mathbf{v}, t) d^3v, \quad \mathbf{J}_e(\mathbf{x}, t) = \sum_s e_s \int \mathbf{v} f_s(\mathbf{x}, \mathbf{v}, t) d^3v$$

$f_s(\mathbf{x}, \mathbf{v}, t)$ is a phase space density for particles of species s with charge and mass, e_s, m_s .

An inclusive matter field theory that includes point particles and fluids as exact reductions.

Maxwell-Vlasov Structure

Hamiltonian:

$$H = \sum_s \frac{m_s}{2} \int |\mathbf{v}|^2 f_s d^3x d^3v + \frac{1}{8\pi} \int (|\mathbf{E}|^2 + |\mathbf{B}|^2) d^3x ,$$

Bracket:

$$\begin{aligned} \{F, G\} &= \sum_s \int \left(\frac{1}{m_s} f_s \left(\nabla F_{f_s} \cdot \partial_{\mathbf{v}} G_{f_s} - \nabla G_{f_s} \cdot \partial_{\mathbf{v}} F_{f_s} \right) \right. \\ &\quad + \frac{e_s}{m_s^2 c} f_s \mathbf{B} \cdot \left(\partial_{\mathbf{v}} F_{f_s} \times \partial_{\mathbf{v}} G_{f_s} \right) \\ &\quad + \left. \frac{4\pi e_s}{m_s} f_s \left(G_{\mathbf{E}} \cdot \partial_{\mathbf{v}} F_{f_s} - F_{\mathbf{E}} \cdot \partial_{\mathbf{v}} G_{f_s} \right) \right) d^3x d^3v \\ &\quad + 4\pi c \int (F_{\mathbf{E}} \cdot \nabla \times G_{\mathbf{B}} - G_{\mathbf{E}} \cdot \nabla \times F_{\mathbf{B}}) d^3x , \end{aligned}$$

where $\partial_{\mathbf{v}} := \partial/\partial \mathbf{v}$, F_{f_s} means functional derivative of F with respect to f_s etc.

pjm5,9 1980,1982; Marsden and Weinstein 1982

Maxwell-Vlasov Structure (cont)

Equations of Motion:

$$\frac{\partial f_s}{\partial t} = \{f_s, H\}, \quad \frac{\partial \mathbf{E}}{\partial t} = \{\mathbf{E}, H\}, \quad \frac{\partial \mathbf{B}}{\partial t} = \{\mathbf{B}, H\}.$$

Casimirs invariants:

$$\begin{aligned}\mathcal{C}_s^f[f_s] &= \int \mathcal{C}_s(f_s) d^3x d^3v \\ \mathcal{C}^E[\mathbf{E}, f_s] &= \int h^E(x) \left(\nabla \cdot \mathbf{E} - 4\pi \sum_s e_s \int f_s d^3v \right) d^3x, \\ \mathcal{C}^B[\mathbf{B}] &= \int h^B(x) \nabla \cdot \mathbf{B} d^3x,\end{aligned}$$

where \mathcal{C}_s , h^E and h^B are arbitrary functions of their arguments.
These satisfy the degeneracy conditions

$$\{F, C\} = 0 \quad \forall F.$$

GEMPIC

A Maxwell-Vlasov structure preserving particle-in-cell algorithm.

A Poisson integrator.

Michael Kraus, Katharina Kormann, pjm, and Eric Sonnendrücker,
Journal of Plasma Physics **83**, 905830401 (2017).

Discretizing the Noncanonical Maxwell-Vlasov Hamiltonian Structure

- Discretize fields f, E, B
- Discretize Vlasov-Maxwell noncanonical Poisson bracket
- Discretize Hamiltonian $\hat{\mathcal{H}}$
- Obtain finite-dimensional Hamiltonian system for

$$z = (z^1, z^2, \dots, z^N) = (X, V, E, B)$$

$$\dot{z}^i = \{z^i, \hat{\mathcal{H}}\}_d$$

with N very large.

de Rham complex

- ▶ Spaces of electromagnetics form a de Rham complex

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

with $\phi \in H^1(\Omega)$, $\mathbf{E}, \mathbf{A} \in H(\text{curl}, \Omega)$, $\mathbf{B}, \mathbf{J} \in H(\text{div}, \Omega)$, $\rho \in L_2(\Omega)$.

- ▶ Equivalent formulation of de Rham complex with differential forms

$$H\Lambda^0(\Omega) \xrightarrow{d} H\Lambda^1(\Omega) \xrightarrow{d} H\Lambda^2(\Omega) \xrightarrow{d} H\Lambda^3(\Omega)$$

Form	integrands	quantity	unit
0-form	point evaluation	ϕ	V
1-form	line integral	\mathbf{E}	V/m
2-form	surface integral	\mathbf{B}	(Vs)/m ²
3-form	volume integral	ρ	C/m ³

- ▶ Exactness: $\text{Im}(\text{grad}) = \text{Ker}(\text{curl})$, $\text{Im}(\text{curl}) = \text{Ker}(\text{div})$.

Structure preserving discretization

Finite Element Exterior Calculus (FEEC): Mathematical theory for finite element discretization of differential forms.²

Discrete de Rham complex: Projections Π_k commute with exterior derivatives.

$$\begin{array}{ccccccc}
 H^1(\Omega) & \xrightarrow{\text{grad}} & H(\text{curl}, \Omega) & \xrightarrow{\text{curl}} & H(\text{div}, \Omega) & \xrightarrow{\text{div}} & L^2(\Omega) \\
 \Pi_0 \downarrow & & \Pi_1 \downarrow & & \Pi_2 \downarrow & & \Pi_3 \downarrow \\
 V_0 & \xrightarrow{\text{grad}} & V_1 & \xrightarrow{\text{curl}} & V_2 & \xrightarrow{\text{div}} & V_3
 \end{array}$$

Exact sequence property on matrix level:

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

with $\text{Im } \mathbb{G} = \text{Ker } \mathbb{C}$, $\text{Im } \mathbb{C} = \text{Ker } \mathbb{D}$.

² Arnold, Falk, Winther, Acta Numerica, 2006.

Finite Element Exterior Calculus (FEEC)

- Function spaces, for configuration space $\Omega \subset \mathbb{R}^3$

1. $H(\text{grad}, \Omega) = \{\phi \in L^2(\Omega) | \nabla \phi \in \mathbf{L}^2(\Omega)\} = H^1(\Omega)$

2. $H(\text{curl}, \Omega) = \{A \in \mathbf{L}^2(\Omega) | \text{curl } A \in \mathbf{L}^2(\Omega)\}$

3. $H(\text{div}, \Omega) = \{E \in \mathbf{L}^2(\Omega) | \text{div } E \in L^2(\Omega)\}$

where L^2 denotes square integrable functions and \mathbf{L}^2 denotes square integrable vectors, e.g., $\int_{\Omega} d^3x |E|^2$.

- Properties

1. $\nabla(H(\text{grad}, \Omega)) \subset H(\text{curl}, \Omega)$

2. $\nabla \times (H(\text{curl}, \Omega)) \subset H(\text{div}, \Omega)$

3. $\nabla \cdot (H(\text{div}, \Omega)) \subset L^2(\Omega)$

FEEC (cont)

- Finite-Dimensional (Discrete) Subspaces

1. $V_0 \subset H(\text{grad}, \Omega)$

2. $V_1 \subset H(\text{curl}, \Omega)$

3. $V_2 \subset H(\text{div}, \Omega)$

4. $V_3 \subset L^2(\Omega)$

- Discrete Subspace Properties

1. $\mathbb{G}V_0 \subset V_1 \iff \text{Im}(\mathbb{G}) \subseteq \text{Ker}(\mathbb{C})$

2. $\mathbb{C}V_1 \subset V_2 \iff \text{Im}(\mathbb{C}) \subseteq \text{Ker}(\mathbb{D})$

3. $\mathbb{D}V_2 \subset V_3 \quad \mathbb{D}\mathbb{C} = 0 \text{ and } \mathbb{C}\mathbb{G} = 0$

where the discrete grad, \mathbb{G} , curl, \mathbb{C} , and div, \mathbb{D} , are matrices defined by restriction to the subspaces.

FEEC (cont)

$$\begin{array}{ccccccc}
 H^1(\Omega) & \xrightarrow{\text{grad}} & H(\text{curl}, \Omega) & \xrightarrow{\text{curl}} & H(\text{div}, \Omega) & \xrightarrow{\text{div}} & L^2(\Omega) \\
 \pi^0 \downarrow & & \pi^1 \downarrow & & \pi^2 \downarrow & & \pi^3 \downarrow \\
 V_0 & \xrightarrow{\mathbb{G}} & V_1 & \xrightarrow{\mathbb{C}} & V_2 & \xrightarrow{\mathbb{D}} & V_3
 \end{array}$$

\exists Compatibility or “Conforming” finite element spaces.

On tetrahedra H^1 conforming \mathbb{P}_k Lagrange finite elements for V_0 , the $H(\text{curl})$ conforming Nédéc elements for V_1 , the $H(\text{div})$ conforming Raviart-Thomas elements for V_2 and discontinuous Galerkin elements for V_3 . A similar sequence can be defined on hexahedra based on the H^1 conforming \mathbb{Q}_k Lagrange finite elements for V_0 .

Spline de Rham complex^a

^aBuffa, Rivas, Sangalli, Vásquez, SIAM J. Numer. Anal., 2011

- ▶ 0-form basis: $V_0 = \text{span}\{\mathcal{S}^p(x_1)\mathcal{S}^p(x_2)\mathcal{S}^p(x_3)\}$
- ▶ 1-form basis:

$$V_1 = \text{span} \left\{ \begin{pmatrix} \mathcal{S}^{p-1}\mathcal{S}^p\mathcal{S}^p \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \mathcal{S}^p\mathcal{S}^{p-1}\mathcal{S}^p \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \mathcal{S}^p\mathcal{S}^p\mathcal{S}^{p-1} \end{pmatrix} \right\}$$

- ▶ 2-form basis:

$$V_2 = \text{span} \left\{ \begin{pmatrix} \mathcal{S}^p\mathcal{S}^{p-1}\mathcal{S}^{p-1} \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \mathcal{S}^{p-1}\mathcal{S}^p\mathcal{S}^{p-1} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \mathcal{S}^{p-1}\mathcal{S}^{p-1}\mathcal{S}^p \end{pmatrix} \right\}$$

- ▶ 3-form basis: $V_3 = \text{span}\{\mathcal{S}^{p-1}(x_1)\mathcal{S}^{p-1}(x_2)\mathcal{S}^{p-1}(x_3)\}$

Relation between splines of degree p and $p-1$:

$$\frac{d}{dx} \mathcal{S}_i^p(x) = \frac{p}{x_{i+p}-x_i} \mathcal{S}_i^{p-1}(x) - \frac{p}{x_{i+1+p}-x_{i+1}} \mathcal{S}_{i+1}^{p-1}(x).$$

Discretization of the electromagnetic fields

- ▶ Semi-discrete electric field: $\mathbf{E}_h(\mathbf{x}) = \sum_i^{N_1} e_i(t) \boldsymbol{\Lambda}_i^1(\mathbf{x})$.
- ▶ Semi-discrete magnetic field: $\mathbf{B}_h(\mathbf{x}) = \sum_i^{N_2} b_i(t) \boldsymbol{\Lambda}_i^2(\mathbf{x})$.
- ▶ Functionals restricted to the semi-discrete fields can be considered as functions of the finite element coefficients: $F[\mathbf{E}_h] = \hat{F}[\mathbf{e}]$ and $F[\mathbf{B}_h] = \hat{F}[\mathbf{b}]$.
- ▶ Replace functional derivatives of $F[\mathbf{E}_h]$, $F[\mathbf{B}_h]$ by partial derivatives of $\hat{F}[\mathbf{e}]$ and $\hat{F}[\mathbf{b}]$:

$$\frac{\delta F[\mathbf{E}_h]}{\delta \mathbf{E}} = \sum_{i,j=1}^{N_1} \frac{\partial \hat{F}(\mathbf{e})}{\partial e_i} (M_1^{-1})_{ij} \boldsymbol{\Lambda}_j^1(\mathbf{x}),$$

$$\frac{\delta F[\mathbf{B}_h]}{\delta \mathbf{B}} = \sum_{i,j=1}^{N_2} \frac{\partial \hat{F}(\mathbf{b})}{\partial b_i} (M_2^{-1})_{ij} \boldsymbol{\Lambda}_j^2(\mathbf{x}),$$

where $(M_{1,2})_{i,j} = \int \boldsymbol{\Lambda}_i^{1,2}(\mathbf{x}) \boldsymbol{\Lambda}_j^{1,2}(\mathbf{x}) d\mathbf{x}$ denotes the mass matrix.

Discretization of the distribution function

- ▶ Particle distribution function

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

- ▶ Functionals restricted to the particle distribution function can be considered as functions of the particle phasespace trajectories:
 $F[f_h] = \hat{F}[\mathbf{X}, \mathbf{V}]$.
- ▶ Replace functional derivative of $F[f_h]$ by particle derivatives with respect to $(\mathbf{x}_a, \mathbf{v}_a)$:

$$\frac{\partial \hat{F}}{\partial \mathbf{x}_a} = w_a \nabla_{\mathbf{x}} \frac{\delta F}{\delta f} \Big|_{(\mathbf{x}_a, \mathbf{v}_a)} \quad \text{and} \quad \frac{\partial \hat{F}}{\partial \mathbf{v}_a} = w_a \nabla_{\mathbf{v}} \frac{\delta F}{\delta f} \Big|_{(\mathbf{x}_a, \mathbf{v}_a)}.$$

Semi-discrete equations

- ▶ Dynamical variables: $\mathbf{u} = (\mathbf{X}, \mathbf{V}, \mathbf{e}, \mathbf{b})^\top$.

- ▶ Discrete Hamiltonian:

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

- ▶ Semi-discrete equations of motion:

$$\dot{\mathbf{X}} = \{\mathbf{X}, \hat{\mathcal{H}}\}, \quad \dot{\mathbf{V}} = \{\mathbf{V}, \hat{\mathcal{H}}\}, \quad \dot{\mathbf{e}} = \{\mathbf{e}, \hat{\mathcal{H}}\}, \quad \dot{\mathbf{b}} = \{\mathbf{b}, \hat{\mathcal{H}}\}.$$

- ▶ Replace functional derivatives by particle derivatives w.r.t. \mathbf{u} .
- ▶ Semi-discrete equations of motion

$$\dot{\mathbf{X}} = \mathbf{V}$$

$$\dot{\mathbf{x}} = \mathbf{v},$$

$$\dot{\mathbf{V}} = \mathbb{M}_p^{-1} \mathbb{M}_q (\mathbb{A}^1(\mathbf{X}) \mathbf{e} + \mathbb{B}(\mathbf{X}, \mathbf{b}) \mathbf{V})$$

$$\dot{\mathbf{v}} = \frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}),$$

$$\dot{\mathbf{e}} = M_1^{-1} (\mathbb{C}^\top M_2 \mathbf{b}(t) - \mathbb{A}^1(\mathbf{X})^\top \mathbb{M}_q \mathbf{V})$$

$$\begin{aligned} \frac{\partial \mathbf{E}}{\partial t} &= \operatorname{curl} \mathbf{B} - \mathbf{J}, \\ \frac{\partial \mathbf{B}}{\partial t} &= -\operatorname{curl} \mathbf{E}. \end{aligned}$$

$$\dot{\mathbf{b}} = -\mathbb{C}\mathbf{e}(t)$$

Semi-discrete equations

- ▶ Dynamical variables: $\mathbf{u} = (\mathbf{X}, \mathbf{V}, \mathbf{e}, \mathbf{b})^\top$.

- ▶ Discrete Hamiltonian:

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

- ▶ Semi-discrete equations of motion:

$$\dot{\mathbf{X}} = \{\mathbf{X}, \hat{\mathcal{H}}\}, \quad \dot{\mathbf{V}} = \{\mathbf{V}, \hat{\mathcal{H}}\}, \quad \dot{\mathbf{e}} = \{\mathbf{e}, \hat{\mathcal{H}}\}, \quad \dot{\mathbf{b}} = \{\mathbf{b}, \hat{\mathcal{H}}\}.$$

- ▶ Replace functional derivatives by particle derivatives w.r.t. \mathbf{u} .
- ▶ Semi-discrete equations of motion

$$\dot{\mathbf{X}} = \mathbf{V}$$

$$\dot{\mathbf{x}} = \mathbf{v},$$

$$\dot{\mathbf{V}} = \mathbb{M}_p^{-1} \mathbb{M}_q (\mathbb{A}^1(\mathbf{X}) \mathbf{e} + \mathbb{B}(\mathbf{X}, \mathbf{b}) \mathbf{V})$$

$$\dot{\mathbf{v}} = \frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}),$$

$$\dot{\mathbf{e}} = M_1^{-1} (\mathbb{C}^\top M_2 \mathbf{b}(t) - \mathbb{A}^1(\mathbf{X})^\top \mathbb{M}_q \mathbf{V})$$

$$\begin{aligned} \frac{\partial \mathbf{E}}{\partial t} &= \operatorname{curl} \mathbf{B} - \mathbf{J}, \\ \frac{\partial \mathbf{B}}{\partial t} &= -\operatorname{curl} \mathbf{E}. \end{aligned}$$

$$\dot{\mathbf{b}} = -\mathbb{C}\mathbf{e}(t)$$

Semi-discrete Poisson system

- ▶ Semi-discrete equations of motion expressed with Poisson matrix:

$$\dot{\mathbf{u}} = \mathcal{J}(\mathbf{u}) D_{\mathbf{u}} \hat{\mathcal{H}}(\mathbf{u}).$$

- ▶ Poisson matrix:

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

- ▶ Some properties:

- ▶ Semi-discrete Poisson bracket satisfies Jacobi identity.
- ▶ $\mathbb{C}\mathbb{G} = 0$.
- ▶ Discrete Gauss' law: $\mathbb{G}^\top M_1 \mathbf{e} = -\mathbb{A}^0(\mathbf{X})^\top \mathbb{M}_q \mathbb{1}_{N_p}$.

Hamiltonian splitting

- ▶ Split Hamiltonian and solve equations for each part separately.
- ▶ Combine the various substep using splitting methods of different order (Lie-Trotter, Strang, composition methods).
- ▶ Our splitting:

$$\hat{\mathcal{H}}_{p_\mu} = \frac{1}{2} \mathbf{V}_\mu^\top \mathbb{M}_p \mathbf{V}_\mu, \quad \hat{\mathcal{H}}_E = \frac{1}{2} \mathbf{e}^\top M_1 \mathbf{e}, \quad \hat{\mathcal{H}}_B = \frac{1}{2} \mathbf{b}^\top M_2 \mathbf{b}.$$

- ▶ Subsystems $\dot{\mathbf{u}} = \{\mathbf{u}, \hat{\mathcal{H}}_{p_\mu, E, B}\}$ can all be integrated over time analytically yielding explicit equations (except for mass matrix inversion).

Examples

Nonlinear Landau Damping

Integrate Vlasov-Poisson

Initial condition:

$$f(x, v, t = 0) = f_M(v)(1 + A \cos(kx)) \quad \text{with} \quad A, k = .5$$

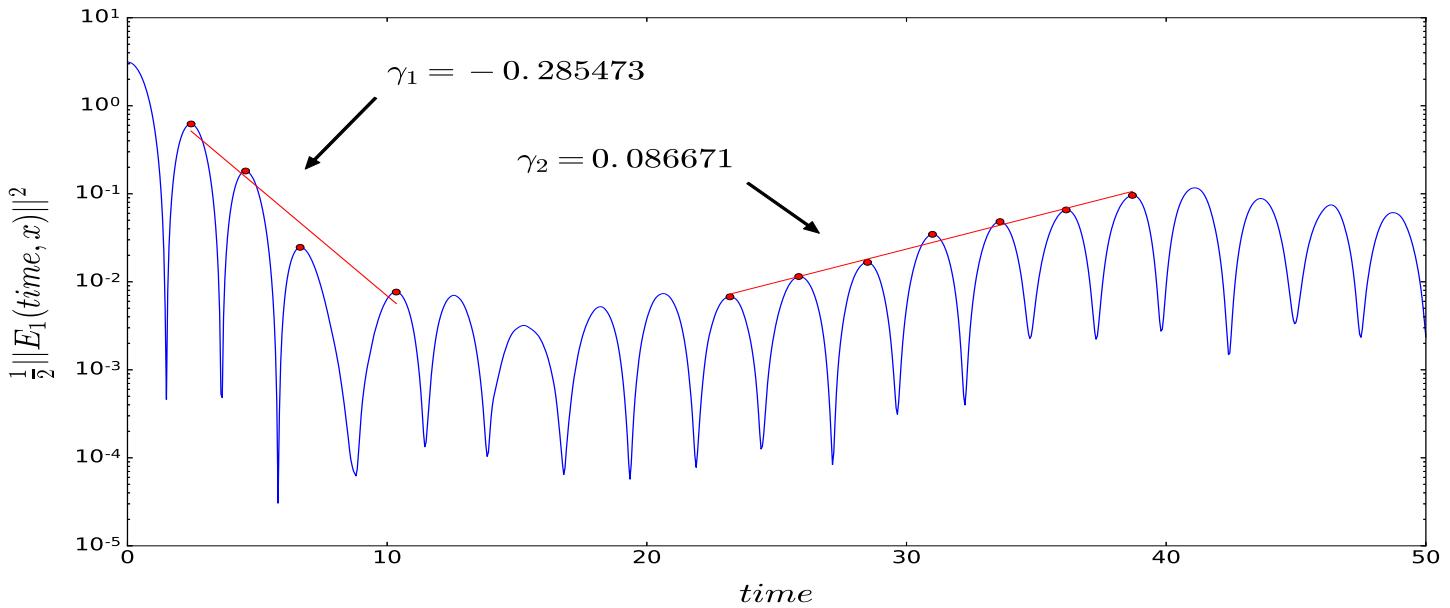


Figure 5: Landau damping: Electric energy with fitted damping and growth rates.

Integrator	γ_1	γ_2
GEMPIC	-0.286	+0.087
viVlasov1D [48]	-0.286	+0.085
Cheng & Knorr [22]	-0.281	+0.084
Nakamura & Yabe [74]	-0.280	+0.085
Ayuso & Hajian [31]	-0.292	+0.086
Heath, Gamba, Morrison, Michler [43]	-0.287	+0.075
Cheng, Gamba, Morrison [23]	-0.291	+0.086

Table 3: Damping and growth rates for strong Landau damping.

Example: Streaming Weibel

Single electron species, $\mathbf{x} = (x, 0, 0)$, $\mathbf{v} = (v_1, v_2, 0)$,
 $\mathbf{E}(x, t) = (E_1, E_2, 0)$, $\mathbf{B}(x, t) = (0, 0, B_3)$, $f(\mathbf{x}, \mathbf{v}, t) = f(x, v_1, v_2, t)$,

Vlasov:

$$\frac{\partial f(x, \mathbf{v}, t)}{\partial t} + v_1 \frac{\partial f(x, \mathbf{v}, t)}{\partial x} + \frac{q}{m} \left[\mathbf{E}(x, t) + \mathbf{B}_3(x, t) \begin{pmatrix} v_2 \\ -v_1 \end{pmatrix} \right] \cdot \frac{\partial f(x, \mathbf{v}, t)}{\partial \mathbf{v}} = 0,$$

Maxwell:

$$\begin{aligned} \frac{\partial E_1(x, t)}{\partial t} &= -J_1(x), \\ \frac{\partial E_2(x, t)}{\partial t} &= -\frac{\partial B(x, t)}{\partial x} - J_2(x), \\ \frac{\partial B(x, t)}{\partial t} &= -\frac{\partial E_2(x, t)}{\partial x}, \quad \frac{\partial E_1(x, t)}{\partial x} = \rho, \end{aligned}$$

Sources

$$\rho = q \int d\mathbf{v} f, \quad J_1 = q \int d\mathbf{v} f v_1, \quad J_2 = q \int \mathbf{v} f v_2.$$

Note that $\nabla \cdot \mathbf{B} = 0$ is manifest.

Initial distribution:

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

$$B_3(x, t = 0) = \beta \sin(kx), \quad E_2(x, t = 0) = 0,$$

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

Parameters:

$$\sigma = 0.1/\sqrt{2}, k = 0.2, \beta = -10^{-3}, v_{0,1} = 0.5, v_{0,2} = -0.1, \delta = 1/6.$$

Details:

Domain $x \in [0, 2\pi/k]$, 2,000,000 particles, 128 grid points, splines of degree 3 and 2, and $\Delta t = 0.01$.

Same as Califano (1997), Cheng et al. (2014)

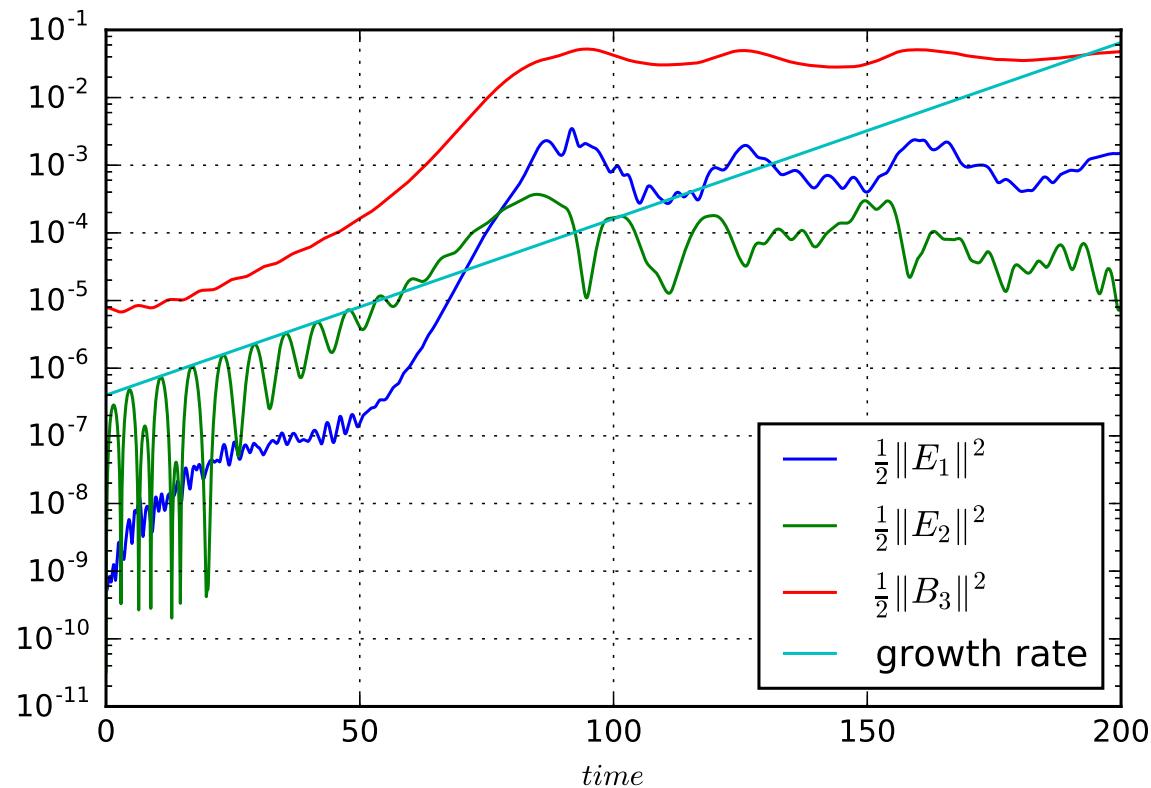


Figure 3: Streaming Weibel instability: The two electric and the magnetic energies together with the analytic growth rate.

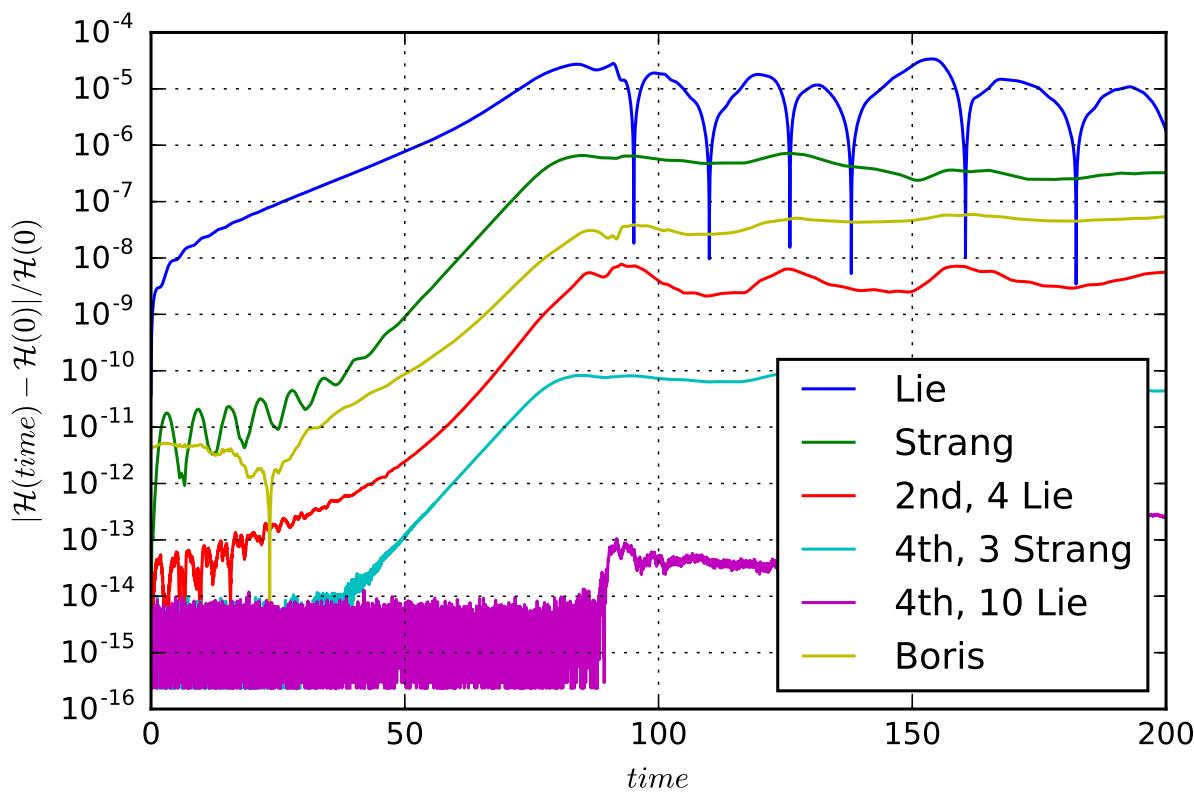


Figure 4: Streaming Weibel instability: Difference of total energy and its initial value as a function of time for various integrators.

Underview

- Hamiltonian Structure. Background material.
- Extended MHD. Aesthetically pleasing.
- Vlasov Computation. Pleasing and practical.