Geometric electromagnetic PIC models

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Structure preserving semi-discretisation of Vlasov–Maxwell

Time discretization

Energy conserving time discretization

Numerical results

Conclusions

Vlasov–Maxwell equations

The non-relativistic Vlasov equation:

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_s = 0.$$

Maxwell equations:

$$\frac{\partial \mathbf{E}}{\partial t} - \operatorname{curl} \mathbf{B} = -\mathbf{J}, \qquad \frac{\partial \mathbf{B}}{\partial t} + \operatorname{curl} \mathbf{E} = 0,$$

$$\operatorname{div} \mathbf{E} = \rho, \qquad \operatorname{div} \mathbf{B} = 0.$$

Charge density: $\rho = \sum_s q_s \int f_s \mathrm{d}\mathbf{v}$.
Current density: $\mathbf{J} = \sum_s q_s \int f_s \mathbf{v} \mathrm{d}\mathbf{v}$.

Characteristic equations:

$$\frac{\mathrm{d}\mathbf{X}}{\mathrm{d}t} = \mathbf{V}, \quad \frac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} = \mathbf{E} + \mathbf{V} \times \mathbf{B}.$$

Conservation properties of Vlasov–Maxwell

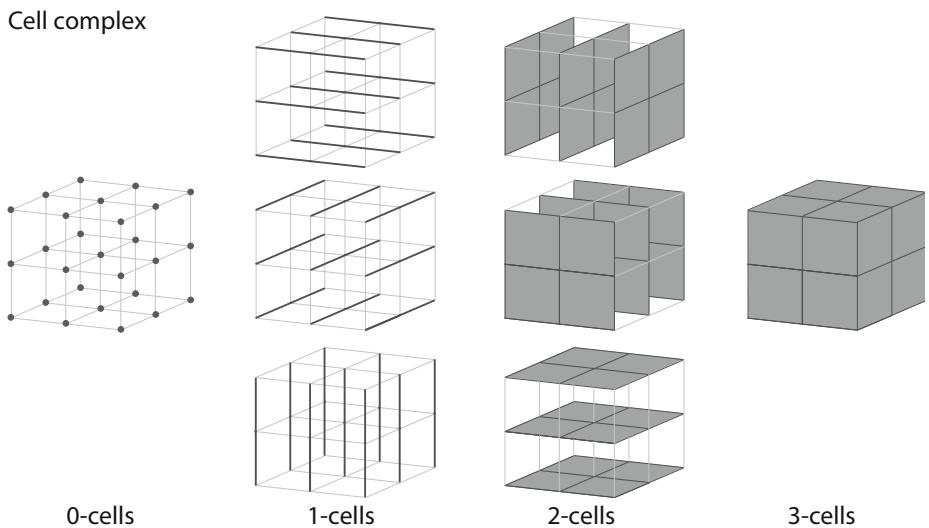
- Energy, momentum, and charge conservation.
- Only dynamical equations need to be time advanced: $\operatorname{div} \mathbf{B} = 0$, $\operatorname{div} \mathbf{E} = \rho$ automatically remain satisfied over time, provided they are initially.
- The Vlasov-Maxwell equations conserve a Poisson structure: Formulation with Poisson bracket and Hamiltonian (Morrison-Marsden-Weinstein)

Importance of structure preservation in simulations

- For ODEs preservation of symplectic structure well known. Exact preservation of approximate energy enables efficient integrators over very long times.
- In many cases keeping structure of continuous equations at discrete level more important than order of accuracy.
  - Avoid spurious eigenmodes in Maxwell's equations.
  - Avoid spurious perpendicular diffusion in parallel transport.
  - Stability issues when not preserving $\nabla \cdot \mathbf{B} = 0$ or $\nabla \cdot \mathbf{E} = \rho$ in Maxwell or MHD
- Big success of structure preserving methods
  - L-shaped domain for Maxwell's equations
  - Non simply connected domains, *i.e.* annulus, torus. Non trivial space of harmonic functions.

Geometric description of physics

- Geometric objects provide a more accurate description of physics and also a natural path for discretisation.
  1. Potentials are naturally evaluated at points
  2. The action of a force is measured through its circulation along a path
  3. Current is the flux through a surface of current density
  4. Charge is integral over volume of charge density
- Should be discretized accordingly



- Related to discretization of differential 0-,1-,2- and 3-forms.

Integral form of Maxwell's equations

Integral equations	Differential equations
$\oint_{\partial \mathbf{S}} \mathbf{H} \cdot \mathrm{d}\ell = \int_{\mathbf{S}} \left(\mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \right) \cdot \mathrm{d}\mathbf{S}$	$\operatorname{curl} \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$
$\oint_{\partial \mathbf{S}} \mathbf{E} \cdot \mathrm{d}\ell = \int_{\mathbf{S}} \left(-\frac{\partial \mathbf{B}}{\partial t} \right) \cdot \mathrm{d}\mathbf{S}$	$\operatorname{curl} \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$
$\oint_{\partial \mathbf{V}} \mathbf{D} \cdot \mathrm{d}\mathbf{S} = \int_{\mathbf{V}} \rho \mathrm{d}\mathbf{V}$	$\operatorname{div} \mathbf{D} = \rho$
$\oint_{\partial \mathbf{V}} \mathbf{B} \cdot \mathrm{d}\mathbf{S} = 0$	$\operatorname{div} \mathbf{B} = 0$

- **D** and **E** as well as **H** and **B** are related by constitutive equations dependent on material properties.
- Exact discrete version of integral form can be obtained provided degrees of freedom for **H** and **E** are edge integrals and degrees of freedom for **D** and **B** (and **J**) are face integrals.

Exact relations between degrees of freedom

- Denote by respectively $\mathcal{V}_i$, $\mathcal{F}_i$, $\mathcal{E}_i$, $\mathbf{x}_i$, the volumes (cells), faces, edges and points of the mesh.
- Degrees of freedom are (*e.g.* for $\mathbf{B}$ and $\mathbf{E}$)

$$\mathcal{F}_i(\mathbf{B}) = \int_{\mathcal{F}_i} \mathbf{B} \cdot \mathrm{d}\mathbf{S}, \quad \mathcal{E}_i(\mathbf{E}) = \int_{\mathcal{E}_i} \mathbf{E} \cdot \mathrm{d}\ell, \quad \ldots$$

- Then integral form of Maxwell yields exact relations involving each face and its 4 boundary edges

$$\mathcal{F}_i(\mathbf{J}) + \frac{\partial \mathcal{F}_i(\mathbf{D})}{\partial t} = \mathcal{E}_{i,1}(\mathbf{H}) + \mathcal{E}_{i,2}(\mathbf{H}) - \mathcal{E}_{i,3}(\mathbf{H}) - \mathcal{E}_{i,4}(\mathbf{H}) \qquad (1)$$

$$\frac{\partial \mathcal{F}_i(\mathbf{B})}{\partial t} = -\mathcal{E}_{i,1}(\mathbf{E}) - \mathcal{E}_{i,2}(\mathbf{E}) + \mathcal{E}_{i,3}(\mathbf{E}) + \mathcal{E}_{i,4}(\mathbf{E}) \qquad (2)$$

- Similar exact relations for divergence constraints.
- This depends only on mesh connectivity and remains true if mesh is smoothly deformed (without tearing).

Reconstruction of fields from degrees of freedom

- Discrete constitutive equations still needed to couple Ampere and Faraday.
- Need to evaluate fields at arbitrary particle positions.
- The fields associated to different degrees of freedom (point values, edge integrals, face integrals, volume integrals) need to be reconstructed in a compatible manner.
- Related to geometric discretisation of various PDEs:
  - Dual meshes: Mimetic Finite Differences, Compatible Operator Discretisation, Discrete Duality Finite Volumes. Intuitive metric association between primal and dual mesh.
  - Dual operators: Finite Element formulation, mathematically more elaborate: Primal operators (strong form) on primal complex, dual operators (weak form) on dual complex.
- Charge conserving PIC algorithms (Villasenor-Bunemann, Esirkepov,..) can also be understood in this framework.

Finite Element Exterior Calculus (FEEC)

- Mathematical framework for Finite Element Maxwell solvers is provided by Finite Element Exterior Calculus (FEEC) introduced by Arnold, Falk and Winther.
- Continuous and discrete complexes for splines are the following

$$
\begin{array}{ccccccc}
 & \xrightarrow{\mathbf{grad}} & & \xrightarrow{\mathbf{curl}} & & \xrightarrow{\mathrm{div}} & \\
H^1(\Omega) & \longrightarrow & H(\mathbf{curl},\Omega) & \longrightarrow & H(\mathrm{div},\Omega) & \longrightarrow & L^2(\Omega) \\
\downarrow \Pi_0 & & \downarrow \Pi_1 & & \downarrow \Pi_2 & & \downarrow \Pi_3 \\
 & \xrightarrow{\mathbf{grad}} & & \xrightarrow{\mathbf{curl}} & & \xrightarrow{\mathrm{div}} & \\
V_0 & \longrightarrow & V_1 & \longrightarrow & V_2 & \longrightarrow & V_3 \\
= & & = & & = & & \\
\mathcal{S}^{p,p,p} & \longrightarrow & \begin{pmatrix} \mathcal{S}^{p-1,p,p} \\ \mathcal{S}^{p,p-1,p} \\ \mathcal{S}^{p,p,p-1} \end{pmatrix} & \longrightarrow & \begin{pmatrix} \mathcal{S}^{p,p-1,p-1} \\ \mathcal{S}^{p-1,p,p-1} \\ \mathcal{S}^{p-1,p-1,p} \end{pmatrix} & \longrightarrow & \mathcal{S}^{p-1,p-1,p-1}
\end{array}
$$

- Commuting diagram is an essential piece

$$\Pi_1 \mathbf{grad}\psi = \mathbf{grad}\Pi_0\psi, \quad \Pi_2 \mathbf{curl}\mathbf{A} = \mathbf{curl}\Pi_1\mathbf{A}, \quad \Pi_3 \mathrm{div}\mathbf{A} = \mathrm{div}\Pi_2\mathbf{A}.$$

The commuting projection operators

- Commuting diagram by interpolating right degrees of freedom:
  - Elements of V_0 are characterized by point values
  - Elements of V_1 are characterized by edge integrals
  - Elements of V_2 are characterized by surface integrals
  - Elements of V_3 are characterized by volume integrals
- $\Pi_0\psi = \psi_h \in V_0$ defined by $\psi_h(\mathbf{x}) = \sum_i c_i^0 \Lambda_i^0(\mathbf{x})$, with c_i^0 solution of the interpolation problem $\psi_h(\mathbf{x}_j) = \psi(\mathbf{x}_j)\ \forall j$
- $\Pi_1\mathbf{A} = \mathbf{A}_h \in V_1$ defined by $\mathbf{A}_h(\mathbf{x}) = \sum_i c_i^1 \mathbf{\Lambda}_i^1(\mathbf{x})$, with c_i^1 solution of

$$\int_{\mathcal{E}_j} \mathbf{A}_h(\mathbf{x}) \cdot \mathrm{d}\ell = \int_{\mathcal{E}_j} \mathbf{A}(\mathbf{x}) \cdot \mathrm{d}\ell \quad \forall j$$

- $\Pi_2\mathbf{B} = \mathbf{B}_h \in V_2$ defined by $\mathbf{B}_h(\mathbf{x}) = \sum_i c_i^2 \mathbf{\Lambda}_i^2(\mathbf{x})$, with c_i^2 solution of

$$\int_{\mathcal{F}_j} \mathbf{B}_h(\mathbf{x}) \cdot \mathrm{d}\mathbf{S} = \int_{\mathcal{F}_j} \mathbf{B}(\mathbf{x}) \cdot \mathrm{d}\mathbf{S} \quad \forall j$$

- $\Pi_3\varphi = \varphi_h \in V_3$ defined by $\varphi_h(\mathbf{x}) = \sum_i c_i^3 \mathbf{\Lambda}_i^3(\mathbf{x})$, with c_i^3 solution of $\int_{\mathcal{V}_j} \varphi_h(\mathbf{x})\mathrm{d}\mathbf{x} = \int_{\mathcal{V}_j} \varphi(\mathbf{x})\mathrm{d}\mathbf{x}\ \forall j$

Particle mesh coupling

- Charge and current computed on mesh using smoothed particles. For some given smoothing function S, typically a B-spline (at least quadratic to reduce aliasing and variance)

$$f_N(t, \mathbf{x}, \mathbf{v}) = \sum_k w_k S(\mathbf{x} - \mathbf{x}_k(t))\delta(\mathbf{v} - \mathbf{v}_k(t)).$$

- From this expression, we can compute the charge and current densities

$$\rho_N = \sum_k w_k q_k S(\mathbf{x} - \mathbf{x}_k(t)),$$

$$\mathbf{J}_N = \sum_k w_k q_k \mathbf{v}_k S(\mathbf{x} - \mathbf{x}_k(t)).$$

- Discrete values defined by projecting associated charge and current

$$\mathbf{J}_h = \Pi_2(\mathbf{J}_N), \qquad \rho_h = \Pi_3(\rho_N).$$

Semi-discrete continuity equation

- A direct calculation shows that

$$\frac{\partial \rho_N}{\partial t} = -\sum_k w_k q_k \mathbf{v}_k \cdot \nabla S(\mathbf{x} - \mathbf{x}_k(t)) = -\operatorname{div} \mathbf{J}_N.$$

- Applying Π_3 we get

$$\Pi_3 \frac{\partial \rho_N}{\partial t} = \frac{\partial \rho_h}{\partial t} = -\Pi_3 \operatorname{div} \mathbf{J}_N = -\operatorname{div} \Pi_2 \mathbf{J}_N = -\operatorname{div} \mathbf{J}_h,$$

- using the commutation property. Hence

$$\frac{\partial \rho_h}{\partial t} + \operatorname{div} \mathbf{J}_h = 0.$$

- Then also

$$\frac{\partial \operatorname{div} \mathbf{E}_h}{\partial t} = -\frac{1}{\varepsilon_0} \operatorname{div} \mathbf{J}_h = \frac{1}{\varepsilon_0} \frac{\partial \rho_h}{\partial t},$$

- Gauss is a consequence of Ampere and initial value as in continuous case.

Finite Element discretisation

- One equation Faraday or Ampere discretized strongly, with no approximation. The other weakly with integration by parts:
  - Strong Ampere - Weak Faraday. Smooth J_N needed

$$-\frac{\partial \mathbf{E}_h}{\partial t} + c^2 \operatorname{curl} \mathbf{B}_h = \frac{1}{\varepsilon_0} \sum_p q_p \Pi_2 [\mathbf{v}_p S(\mathbf{x} - \mathbf{x}_k(t))] = \frac{1}{\varepsilon_0} \mathbf{J}_h,$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \mathbf{B}_h \cdot \mathbf{C}_h \mathrm{d}\mathbf{x} + \int_\Omega \mathbf{E}_h \cdot \operatorname{curl} \mathbf{C}_h \mathrm{d}\mathbf{x} = 0 \quad \forall \mathbf{C}_h \in V_1.$$

  - Weak Ampere - Strong Faraday

$$-\int_\Omega \frac{\partial \mathbf{E}_h}{\partial t} \cdot \mathbf{F}_h \mathrm{d}\mathbf{x} + c^2 \int_\Omega \mathbf{B}_h \cdot \operatorname{curl} \mathbf{F}_h \mathrm{d}\mathbf{x} = \frac{1}{\varepsilon_0} \int \mathbf{J}_h \cdot \mathbf{F}_h \mathrm{d}\mathbf{x}, \quad \forall \mathbf{F}_h \in V_1,$$

$$\frac{\partial \mathbf{B}_h}{\partial t} + \operatorname{curl} \mathbf{E}_h = 0$$

No smoothing needed because of integral on $\mathbf{J}_h$, but smoothing or filtering can be added.

GEMPIC framework

- Discretization of fields: Compatible spline finite elements (discrete deRham complex):
  - Strong Faraday **E** edge elements (1-form), **B** face elements (2-form)
  - Strong Ampere **B** edge elements (1-form), **E** face elements (2-form)
- Discretization of f with (smoothed) particles
  $f(t,x,v) = \sum w_p S(x - x_p(t))\delta(v - v_p(t))$,
  S can be δ for strong Faraday.
- Plug discretizations for f, E and B into Lagrangian to get formulation of equations based on a semi-discrete Hamiltonian and Poisson bracket.
- Time discretizations: Hamiltonian splitting or Discrete Gradient

Paper on strong Faraday without smoothing:
M. Kraus, K. Kormann, P.J. Morrison, E. Sonnendrücker - JPP 17

Semi-discrete equations

- Discretization obtained by plugging expressions for $f_h, \phi_h, \mathbf{A}_h$ into Lagrangian: $\mathbf{E}_h = \partial_t \mathbf{A}_h - \nabla \phi_h$, $\mathbf{B}_h = \operatorname{curl} \mathbf{A}_h$.
- Dynamical variables: particles positions and velocities, spline coefficients of $\mathbf{E}_h$ and $\mathbf{B}_h$: $\mathbf{u} = (\mathbf{X}, \mathbf{V}, \mathbf{e}, \mathbf{b})^\top$.
- 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 expressed with discrete unknowns

$$\dot{\mathbf{X}} = \mathbf{V} \qquad \dot{\mathbf{x}} = \mathbf{v},$$

$$\dot{\mathbf{V}} = \mathbb{M}_p^{-1} \mathbb{M}_q \left(\mathbb{\Lambda}^1(\mathbf{X}) \mathbf{e} + \mathbb{B}(\mathbf{X}, \mathbf{b}) \mathbf{V} \right) \qquad \dot{\mathbf{v}} = \frac{q_s}{m_s} \left(\mathbf{E} + \mathbf{v} \times \mathbf{B} \right),$$

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

$$\dot{\mathbf{b}} = -\mathbb{C} \mathbf{e}(t) \qquad \frac{\partial \mathbf{B}}{\partial t} = -\operatorname{curl} \mathbf{E}.$$

Semi-discrete Poisson system

- Semi-discrete equations of motion have following structure:

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

- Poisson matrix:

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

- Defines semi-discrete Poisson bracket:

$$\{F,G\} = \nabla F^\top \mathcal{J}(\mathbf{u})\nabla G \Rightarrow \frac{\mathrm{d}(F(\mathbf{u}))}{\mathrm{d}t} = \nabla F^\top \dot{\mathbf{u}} = \{F(\mathbf{u}),\mathcal{H}(\mathbf{u})\}.$$

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

Strong Faraday: relativistic

- Same action principle with relativistic particle Lagrangian

$$L_s(\mathbf{x}, \mathbf{p}, \dot{\mathbf{x}}, t) = (\mathbf{p} + q_s\mathbf{A}) \cdot \dot{\mathbf{x}} - \left((\gamma - 1)m_s c^2 + q_s\phi\right),$$

- Denoting by $U = \gamma(V)V$ evolution equations become

$$\begin{aligned}
\frac{\mathrm{d}\mathbf{X}}{\mathrm{d}t} &= \mathbf{V} \\
M_m \frac{\mathrm{d}\mathbf{U}}{\mathrm{d}t} &= M_q(\mathbb{\Lambda}^1(\mathbf{X})\mathbf{e} + \hat{\mathbf{B}}_h(\mathbf{X}, \mathbf{b})\mathbf{V}) \\
M_1 \frac{\mathrm{d}\mathbf{e}}{\mathrm{d}t} &= \mathbb{C}^\top M_2 \mathbf{b} - \mathbf{\Lambda}^1(\mathbf{X})^\top M_q \mathbf{V}, \\
\frac{\mathrm{d}\mathbf{b}}{\mathrm{d}t} &= -\mathbb{C}\mathbf{e}
\end{aligned}$$

- Discrete Poisson structure with same Poisson matrix $\mathcal{J}(\mathbf{u})$ as non relativistic but

$$\mathcal{H} = \mathbf{c}_2^\top M_m \boldsymbol{\gamma} + \frac{1}{2}\mathbf{e}^\top M_1 \mathbf{e} + \frac{1}{2}\mathbf{b}^\top M_2 \mathbf{b}.$$

Strong Ampere

- Use action principle (denoting by $S_k = S(\mathbf{x} - \mathbf{x}_k(t))$

$$\mathcal{A} = \sum_k \int_{t_1}^{t_2} (m_k \mathbf{v}_k \cdot \dot{\mathbf{x}}_k - \frac{1}{2} m_k \mathbf{v}_k^2) \mathrm{d}t + q_k \int_{t_1}^{t_2} \int_\Omega (\mathbf{A}_h \cdot \Pi_2[\dot{\mathbf{x}}_k S_k] - \phi_h \Pi_3 S_k) \, \mathrm{d}\mathbf{x} \mathrm{d}t$$

$$- \int_{t_1}^{t_2} \left(\frac{\varepsilon_0}{2} \int_\Omega |\mathbf{E}_h|^2 \mathrm{d}\mathbf{x} + \frac{1}{2\mu_0} \int_\Omega |\mathbf{B}_h|^2 \mathrm{d}\mathbf{x} \right.$$

$$\left. -\varepsilon_0 \int_\Omega \left(\frac{\partial \mathbf{A}_h}{\partial t} \cdot \mathbf{E}_h - \phi_h \operatorname{div} \mathbf{E}_h \right) \mathrm{d}\mathbf{x} - \frac{1}{\mu_0} \int_\Omega \mathbf{A}_h \cdot \operatorname{curl} \mathbf{B}_h \mathrm{d}\mathbf{x} \right) \mathrm{d}t.$$

- Evolution equations

$$\frac{\mathrm{d}X}{\mathrm{d}t} = V$$

$$\frac{\mathrm{d}V}{\mathrm{d}t} = (M_m)^{-1} M_q (\underline{\sigma}^2 (S(X))^\top M_2 \mathbf{e} + \mathcal{R}(b, X) V)$$

$$\frac{\mathrm{d}\mathbf{e}}{\mathrm{d}t} = \mathbb{C}\mathbf{b} - M_q \underline{\sigma}^2 (S(X)) V$$

$$\frac{\mathrm{d}\mathbf{b}}{\mathrm{d}t} = -M_1^{-1} \mathbb{C}^\top M_2 \mathbf{e}$$

Strong-Ampere, Poisson structure

- Denoting by $U = (X, V, \mathbf{e}, \mathbf{b})^\top$, this can be cast in the Poisson structure

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \mathcal{J}(U)\nabla_U H$$

with the Poisson matrix

$$\mathcal{J}(U) = \begin{pmatrix} 0 & (M_m)^{-1} & 0 & 0 \\ -(M_m)^{-1} & (M_m)^{-1} M_q \mathcal{R}(X, \mathbf{b}))(M_m)^{-1} & (M_m)^{-1} M_q \underline{\sigma}^2 (S(X))^\top & 0 \\ 0 & -(M_m)^{-1} M_q \underline{\sigma}^2 (S(X)) & 0 & \mathbb{C} M_1^{-1} \\ 0 & 0 & -M_1^{-1} \mathbb{C}^\top & 0 \end{pmatrix}.$$

- Smoothing function S appears in current assignment and Force term.

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Time-discretization of Poisson structure

- Poisson form $\frac{\mathrm{d}U}{\mathrm{d}t} = \mathcal{J}(U)\nabla_U H$ generalizes symplectic structure
- Thm(Ge, Marsden) Only exact flow preserves both symplectic structure and energy. $\Rightarrow$ need to choose.
- 2 options:
  1. Hamiltonian splitting preserves Poisson structure including Casimirs ($\mathrm{div}\,\mathbf{B} = 0$, weak Gauss), but only modified energy.
  2. Energy conserving discretisations can be derived based on Discrete Gradient or Average Vector Field methods.

Time advance via Hamiltonian splitting

- Following the prescription of Crouseilles-Einkemmer-Faou (JCP 15) a Hamiltonian splitting can be performed, treating the three terms of the Hamiltonian separately

$$H = \frac{1}{2}\mathbf{v}^\top M_p \mathbf{v} + \frac{1}{2}\mathbf{e}^\top M_1 \mathbf{e} + \frac{1}{2}\mathbf{b}^\top M_2 \mathbf{b} = H_p + H_e + H_b.$$

- Split and solve successively

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \Omega(u)\nabla H_i, \quad i = p, e, b$$

- Lie-Trotter splitting (first order), Strang splitting (second order) or even higher order.
- Exact solution possible for H_e and H_b.
- For H_p split further between the three components. Other possibility: use variational integrator

Discrete solution of H_e

- The equations read

$$\begin{aligned}
\dot{x}_p &= 0, \\
\dot{v}_p &= \left(\Lambda^1(x_p(t))\right)^\top e(t), \\
\dot{e} &= 0, \\
\dot{b} &= -Re(t).
\end{aligned}$$

- and its exact solution on one time step

$$\begin{aligned}
x_p(h) &= x_p(0), \\
v_p(h) &= v_p(0) + \left(\Lambda^1(x_p(0))\right)^T e(0), \\
e(h) &= e(0), \\
b(h) &= b(0) - Re(0).
\end{aligned}$$

Discrete solution of H_b

- The equations read

$$\begin{aligned}
\dot{x}_p &= 0, \\
\dot{v}_p &= 0, \\
M_1 \dot{e} &= R^T M_2 b(t), \\
\dot{b} &= 0.
\end{aligned}$$

- and its exact solution on one time step

$$\begin{aligned}
x_p(h) &= x_p(0), \\
v_p(h) &= v_p(0), \\
M_1 e(h) &= M_1 e(0) + R^T M_2 b(0), \\
b(h) &= b(0).
\end{aligned}$$

Discrete solution of H_p

- The equations read

$$\begin{aligned} \dot{x}_p &= v_p, \\ \dot{v}_p &= v_p \times b(t)\,\Lambda^2(x_p), \\ M_1 \dot{e} &= -\Lambda^1(x_p) \cdot M_p v_p, \\ \dot{b} &= 0, \end{aligned}$$

- For general magnetic field coefficients b, this system cannot be exactly integrated
- As each component of the equation for $\dot{v}_p$ does not depend on v_p, we can split this system once more into

$$H_p = H_{p,1} + H_{p,2} + H_{p,3} \qquad \text{for} \qquad i \in \{1, 2, 3\},$$

with

$$H_{p,i} = \tfrac{1}{2} \left(v_p^i\right)^T M_p v_p^i.$$

Then an exact solution can be obtained.

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The Discrete gradient method

(Mc Lachland, Quispel, Robidoux 1999)

- For a skew-symmetric matrix $\mathcal{J}(\mathbf{u})$, consider an ODE of the form

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathcal{J}(\mathbf{u})\nabla H$$

- Discrete gradient methods conserve exactly a discrete Hamiltonian. They are based on a discrete gradient such that

$$(\mathbf{u}^{n+1} - \mathbf{u}^n)^\top \bar{\nabla} H(\mathbf{u}^n, \mathbf{u}^{n+1}) = H(\mathbf{u}^{n+1}) - H(\mathbf{u}^n),$$

- Then the scheme $\frac{\mathbf{u}^{n+1}-\mathbf{u}^n}{\Delta t} = \bar{\mathcal{J}}\bar{\nabla} H(\mathbf{u}^n, \mathbf{u}^{n+1})$ conserves H, indeed

$$H(\mathbf{u}^{n+1}) - H(\mathbf{u}^n) = (\mathbf{u}^{n+1} - \mathbf{u}^n)^\top \bar{\nabla} H(\mathbf{u}^n, \mathbf{u}^{n+1}) = \Delta t \bar{\nabla} H^\top \bar{\mathcal{J}}^\top \bar{\nabla} H = 0$$

provided $\bar{\mathcal{J}}$ is a skew-symmetric approximation of $\mathcal{J}(\mathbf{u})$.

Examples of discrete gradient schemes

- Straightforward discrete gradients for quadratic hamiltonians,

$$\bar{\nabla} H(\mathbf{u}^n, \mathbf{u}^{n+1}) = (\mathbb{M}_m \frac{\mathbf{V}^n + \mathbf{V}^{n+1}}{2}, M_1 \frac{\mathbf{e}^n + \mathbf{e}^{n+1}}{2}, M_2 \frac{\mathbf{b}^n + \mathbf{b}^{n+1}}{2})$$

- General method: Average-vector-field[1]:

$$\bar{\nabla} H(U^n, U^{n+1}) = \int_0^1 \nabla H((1-\xi)U^n + \xi U^{n+1}) \mathrm{d}\xi$$

- $\mathcal{J}(\mathbf{u})$ can also be averaged or approximated differently
- Yields implicit energy conserving time discretization
- Since the Poisson matrix is antisymmetric, we can apply this method to our semi-discrete equations: fully nonlinear coupled system.
- Our solution: apply Discrete Gradient method to antisymmetric splitting of the Poisson matrix.

[1] Celledoni et al., J. Comput. Phys. 231, 2012

Splitting Poisson matrix, keeping antisymmetry

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

- Split $\mathcal{J}(\mathbf{u})$ keeping antisymmetric matrices. Keep full Hamiltonian
- The split steps become

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathcal{J}_1(\mathbf{u})\nabla\mathcal{H}, \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathcal{J}_2(\mathbf{u})\nabla\mathcal{H}, \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathcal{J}_3(\mathbf{u})\nabla\mathcal{H}, \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathcal{J}_4(\mathbf{u})\nabla\mathcal{H}$$

- Successive application = Lie splitting of order 1, symmetric application = Strang-splitting of order 2.
- Higher order also possible by appropriate combination.

The reduced systems

- Split $\mathcal{J}(\mathbf{u})$ keeping antisymmetric matrices. Keep full Hamiltonian
  1. $\dot{\mathbf{X}} = \mathbf{V}, \quad (\dot{\mathbf{V}} = 0, \dot{\mathbf{e}} = 0, \dot{\mathbf{b}} = 0\ )$,
  2. $\dot{\mathbf{V}} = \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{B}(\mathbf{X},\mathbf{b})\mathbf{V}, \quad (\dot{\mathbf{X}} = 0, \dot{\mathbf{e}} = 0, \dot{\mathbf{b}} = 0\ )$.
  3. $\dot{\mathbf{V}} = \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{\Lambda}^1(\mathbf{X})\mathbf{e}$, $\dot{\mathbf{e}} = -M_1^{-1}\mathbb{\Lambda}^1(\mathbf{X})^\top\mathbb{M}_q\mathbf{V}, \quad (\dot{\mathbf{X}} = 0, \dot{\mathbf{b}} = 0\ )$.
  4. $\dot{\mathbf{e}} = M_1^{-1}\mathbb{C}^\top M_2\mathbf{b}$, $\dot{\mathbf{b}} = -\mathbb{C}\mathbf{e}, \quad (\dot{\mathbf{X}} = 0, \dot{\mathbf{V}} = 0)$.
- Steps 1 and 2 can be solved explicitly.
- Steps 3 and 4 linearly implicit. Use Schur complement in 3 to reduce implicit parts to the field equations.
- Summary: implicit in field coefficients only, conserves energy but not discrete Gauss.
- Splitting in only 3 parts (2 and 3 are kept together) one recovers the ECSIM time discretisation proposed by Lapenta and can define a higher-order version.

Modification to conserve Gauss' law

- Observation: Current part of Ampere's law

$$M_1 \mathbf{e}^{m+1} = M_1 \mathbf{e}^m - \int_{t_m}^{t_{m+1}} \mathbb{\Lambda}^1(\mathbf{X}(\tau))^\top \mathbb{M}_q \mathbf{V}(\tau)\, \mathrm{d}\tau,$$

  needs to be solved *exactly*, i.e. satisfying $\frac{\mathrm{d}\mathbf{X}}{\mathrm{d}t} = V$.
- Modify the splitting: Keep together 1 (**X** push) and 3 (**V**+**e** push).
- New discrete gradient scheme for 1+3:

Energy and Gauss conserving scheme:

$$\begin{aligned}
\frac{\mathbf{X}^{m+1} - \mathbf{X}^m}{\Delta t} &= \frac{\mathbf{V}^m + \mathbf{V}^{m+1}}{2} \\
\frac{\mathbf{V}^{m+1} - \mathbf{V}^m}{\Delta t} &= \mathbb{M}_p^{-1} \mathbb{M}_q \frac{1}{\Delta t} \int_{t_m}^{t_{m+1}} \mathbb{\Lambda}_i^1(\mathbf{X}(\tau))\, \mathrm{d}\tau \left(\frac{\mathbf{e}^m + \mathbf{e}^{m+1}}{2} \right) \\
\frac{\mathbf{e}^{m+1} - \mathbf{e}^m}{\Delta t} &= -M_1^{-1} \frac{1}{\Delta t} \int_{t_m}^{t_{m+1}} \mathbb{\Lambda}_i^1(\mathbf{X}(\tau))^\top\, \mathrm{d}\tau \mathbb{M}_q \left(\frac{\mathbf{V}^m + \mathbf{V}^{m+1}}{2} \right)
\end{aligned}$$

Subcycling

- New splitting conserving energy and Gauss law is nonlinearly implicit on fields. Picard iterations are used. Anderson acceleration reduces number of iterations.
- Time discretisation similar to method proposed by Chen, Chacon and Barnes (JCP 2011) and more recent Vlasov-Darwin versions by Chen, Chacon (CPC 2016)
- Subcycling of particle push can be introduced, taking care to conserved symmetry between push and current deposition for exact energy conservation.

Subcycling: new update

- Keeping the electric field constant over all the substeps, push the particles according to $\mathbf{X}_m^0 = \mathbf{X}^m$, $\mathbf{V}_m^0 = \mathbf{V}^m$ and then for $\nu = 0$ to $N_\nu - 1$

$$\begin{aligned}
\frac{\mathbf{X}_m^{\nu+1} - \mathbf{X}_m^{\nu}}{\Delta\tau_\nu} &= \frac{\mathbf{V}_m^{\nu} + \mathbf{V}_m^{\nu+1}}{2} \\
\frac{\mathbf{V}_m^{\nu+1} - \mathbf{V}_m^{\nu}}{\Delta\tau_\nu} &= \mathbb{M}_p^{-1}\mathbb{M}_q \frac{1}{\Delta\tau_\nu} \int_{\tau_\nu}^{\tau_{\nu+1}} \mathbb{\Lambda}_i^1(\mathbf{X}_m(\tau))\,\mathrm{d}\tau \left(\frac{\mathbf{e}^m + \mathbf{e}^{m+1}}{2}\right)
\end{aligned}$$

  with $\mathbf{X}_m(\tau) = ((\tau_{\nu+1} - \tau)\mathbf{X}_m^{\nu} + (\tau - \tau_\nu)\mathbf{X}_m^{\nu+1})/\Delta\tau_\nu$.

- Corresponding electric field updated over the full time step:

$$\frac{\mathbf{e}^{m+1} - \mathbf{e}^m}{\Delta t} = -M_1^{-1}\frac{1}{\Delta t}\sum_{\nu=0}^{N_\nu-1}\left(\int_{\tau_\nu}^{\tau_{\nu+1}} \mathbb{\Lambda}_i^1(\mathbf{X}_m(\tau))^\top\,\mathrm{d}\tau\right)\mathbb{M}_q\left(\frac{\mathbf{V}_m^{\nu} + \mathbf{V}_m^{\nu+1}}{2}\right)$$

Structure preserving semi-discretisation of Vlasov–Maxwell

Time discretization

Energy conserving time discretization

Numerical results

Conclusions

Test case 1: Weibel instability 1d2v

Electron distribution (neutralizing ion background):

$$f(x, \mathbf{v}, t = 0) = \frac{1}{\pi\sigma_1\sigma_2} \exp\left(-\frac{1}{2}\left(\frac{v_1^2}{\sigma_1^2} + \frac{v_2^2}{\sigma_2^2}\right)\right), \; x \in [0, \frac{2\pi}{k}),$$
$$B_3(x, t = 0) = \beta \cos(kx),$$
$$E_2(x, t = 0) = 0,$$

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

Parameters: $\sigma_1 = 0.02/\sqrt{2}$, $\sigma_2 = \sqrt{12}\sigma_1$, $k = 1.25$, $\alpha = 0$, and $\beta = -10^{-4}$.

Test case from Crouseilles, Einkemmer, Faou, J. Comput. Phys. 283, 2015.

Weibel instability: Potential energies and analytic growth rate.

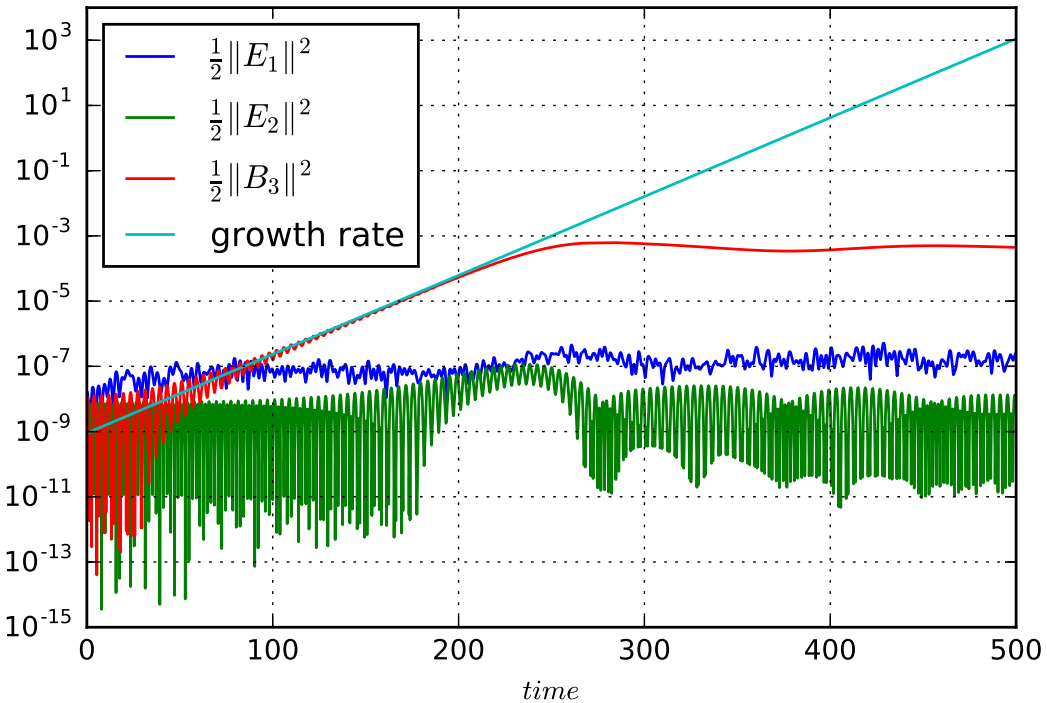

Figure: Weibel instablity: The two electric and the magnetic energies together with the analytic growth rate.

Numerical parameters: 100,000 particles, 32 grid points.

Weibel instability: Conservation properties.

Table: Weibel instability: Maximum error in the total energy, Gauss' law, and total momentum until time 500 for simulation with various integrators (Strang splitting $\Delta t = 0.05$).

Propagator	total energy	Gauss law
Hamiltonian	6.9E-7	2.1E-13
Boris	1.3E-9	4.8E-4
AVF	2.1E-16	1.1E-6
DiscGrad	5.9E-11	2.2E-15

Weibel instability: Error in magnetic energy $\|\mathbf{B}\|^2$.

Δt	Hamiltonian	Boris	AVF	DiscGrad
0.025	5.13E-06	4.48E-06	3.73E-06	3.90E-06 (4.9)
0.05	1.29E-05	1.41E-05	1.83E-05	1.85E-05 (5.9)
0.1	–	–	4.05E-05	3.98E-05 (6.8)
0.2	–	–	1.20E-04	1.13E-04 (8.6)
0.4	–	–	1.60E-04	1.60E-04 (12.0)
0.8	–	–	1.81E-04	1.80E-04 (21.6)
5	–	–	4.41E-04	–

Reference: Solution with 4th, 10 Lie and $\Delta t = 0.025$.
Conclusions: Error about 1st order for $\|\mathbf{B}\|^2$ (i.e. 2nd order for $\mathbf{B}$).
Time step restrictions for explicit methods.

Test case 2: Ion acoustic wave

Electron and ion distribution:

$$f_e(x, \mathbf{v}, t = 0) = \frac{m_e}{\pi T_e} \exp\left(-\frac{v_1^2 + v_2^2}{2 T_e / m_e}\right),$$

$$f_i(x, \mathbf{v}, t = 0) = \frac{m_i}{\pi T_i} \exp\left(-\frac{v_2^2 + v_3^2}{2 T_i / m_i}\right) \left(1 + \alpha \cos(\frac{2\pi}{L} x)\right).$$

Electrostatic test case (without magnetic field).

Parameters: $\frac{T_i}{T_e} = 10^4$, $\frac{m_i}{m_e} = 200$, $\alpha = 0.2$, $L = 10$.

Numerical parameters: $N_x = 32$, $N_p = 128,000$ per species.

Comparison between Hamiltonian splitting and discrete gradient method

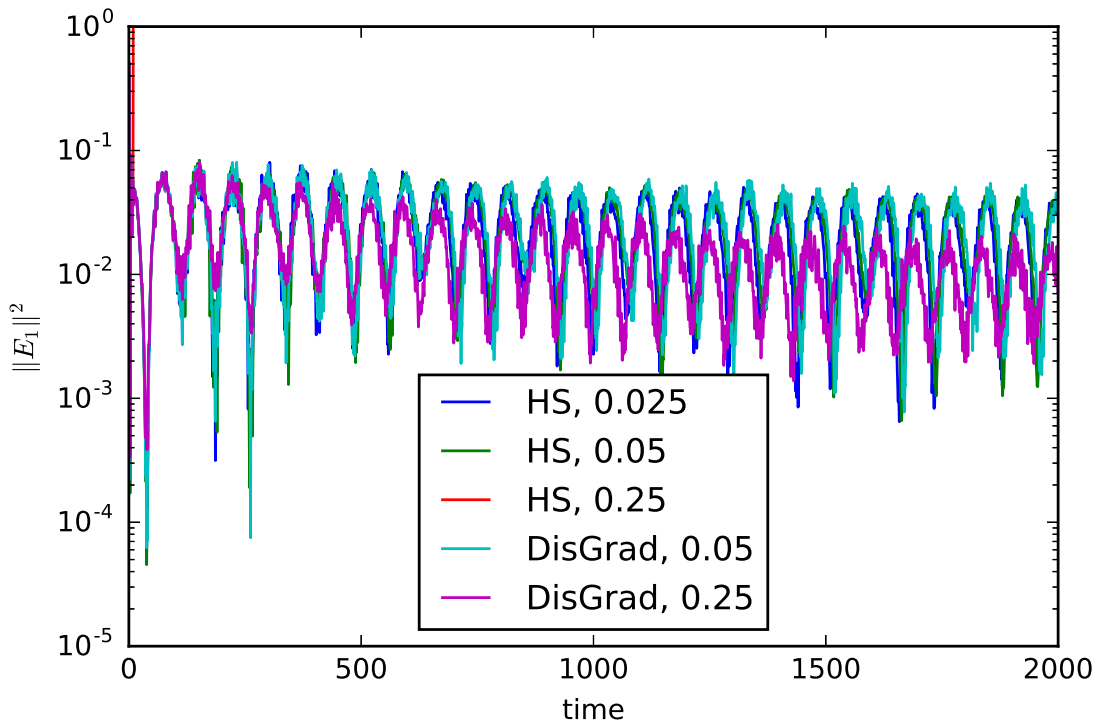

Figure: Ion acoustic wave: Comparison of Hamiltonian splitting (HS) and discrete gradient method (DisGrad).

Discrete gradient method with substepping

Improvement of discrete gradient method: Introduce substepping in (X, V) to capture electron dynamics.[2]

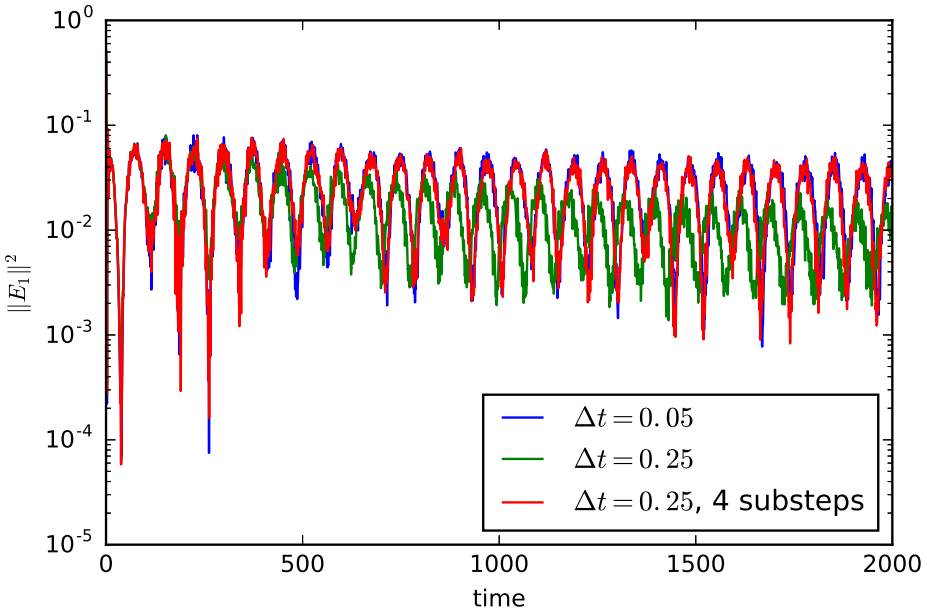

Figure: Ion acoustic wave: Discrete gradient method with and without substepping.

[2] Chen, Chacon, Barnes: An energy- and charge-conserving, implicit, electrostatic particle-in-cell algorithm, J. Comput. Phys. 230, 2014.

Summary and Outlook

Summary

- GEMPIC framework based on discrete Poisson bracket and FEEC.
- Semi-discrete Poisson structure, with conservation of energy and Gauss law.
- AVF-based time splitting conserves energy, not Gauss' law.
- Nonlinear discrete gradient method that conserves energy and Gauss' law. Can easily acomodate particle subcycling, keeping these conservation properties

Outlook

- Version on curvilinear mesh under development.
- Optimize implementation of 2d3v and 3d3v codes.
- Solve low frequency problems in tokamaks. Numerical gyrokinetics!