Structure-preserving particle-in-cell simulations with an outlook on the relativistic Vlasov-Maxwell equations

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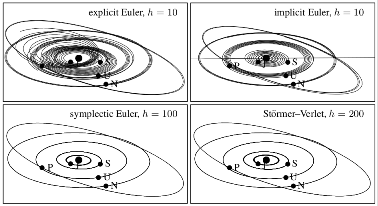
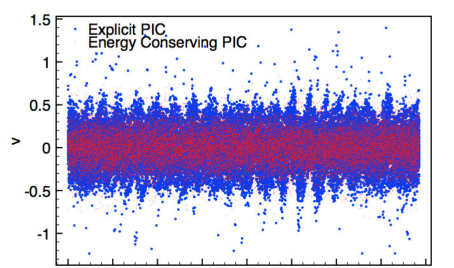
Structure-preserving numerics: What and why?

- Simulations in physics are extremely complex and closed solutions are unknown. Physics cross multiple scales that cannot all be resolved at the same time.
- How do we know that our solution is reliable? $\mapsto$ We can check certain known physical properties, like conservation laws.
- Structure-preserving numerics: Design numerical methods that mimic the conservation properties of the physical system.
- **Gain**: Robust and reliable numerical methods.

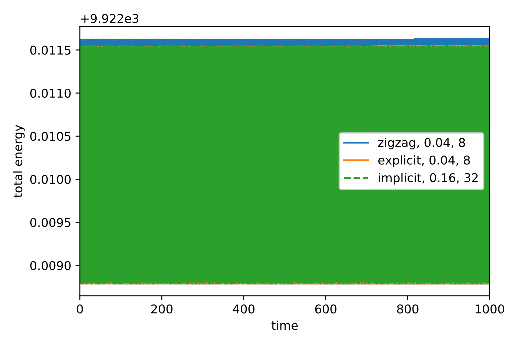
Why structure preserving?

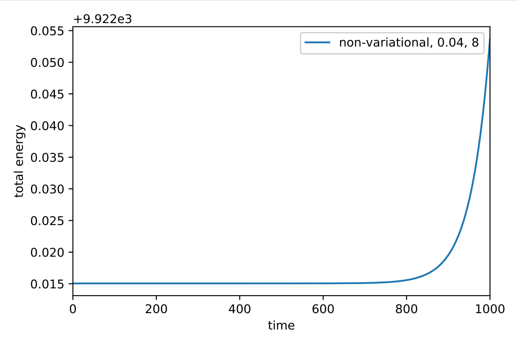
- A classical example: N-body problem of motion of five planets around the sun [from Haier, Lubich, Wanner, Springer 2005]
- Grid heating as example for instability in plasma simulations: Tendency of non-energy conserving codes to heat or cool. Heating creates extra free energy that can cause numerical instabilities. [Visulation from Markidis & Lapenta, J. Compt. Phys., 2011]





Long-time simulations





Relativistic Vlasov–Maxwell system

Vlasov equation for a species with charge q_s and mass m_s:

$$\partial_t f_s(t,\boldsymbol{x},\boldsymbol{p}) + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_s(t,\boldsymbol{x},\boldsymbol{p}) + q_s\big(\boldsymbol{E}(t,\boldsymbol{x}) + \boldsymbol{v}\times\boldsymbol{B}(t,\boldsymbol{x})\big)\cdot\nabla_{\boldsymbol{p}} f_s(t,\boldsymbol{x},\boldsymbol{p}) = 0$$

$\boldsymbol{p} = \gamma m_s \boldsymbol{v}$ with Lorentz factor $\gamma = \sqrt{1 + \frac{|\boldsymbol{p}|^2}{m_s^2 c^2}}$

Maxwell equations:

$$\frac{1}{c^2}\partial_t \boldsymbol{E}(t,\boldsymbol{x}) = \operatorname{curl} \boldsymbol{B}(t,\boldsymbol{x}) - \mu_0 \boldsymbol{J}(t,\boldsymbol{x})$$

$$\partial_t \boldsymbol{B}(t,\boldsymbol{x}) = -\operatorname{curl} \boldsymbol{E}(t,\boldsymbol{x})$$

$$\operatorname{div} \boldsymbol{E}(t,\boldsymbol{x}) = \rho(t,\boldsymbol{x})/\varepsilon_0$$

$$\operatorname{div} \boldsymbol{B}(t,\boldsymbol{x}) = 0$$

$$\rho(t,\boldsymbol{x}) = \sum_s q_s \int_{\mathbb{R}^3} f_s(t,\boldsymbol{x},\boldsymbol{v})\,\mathrm{d}\boldsymbol{p}, \qquad \boldsymbol{J}(t,\boldsymbol{x}) = \sum_s q_s \int_{\mathbb{R}^3} \boldsymbol{v} f_s(t,\boldsymbol{x},\boldsymbol{v})\,\mathrm{d}\boldsymbol{p}.$$

Structure of the Vlasov–Maxwell system

- Energy, momentum, and charge **conservation**.
- Ampère's equation and Faraday's law have a unique solution by themselves (provided adequate initial and boundary conditions). The **divergence constraints** remain satisfied over time.
- Equations of motion can be derived from a action or an Hamiltonian principle.

Structure of the Maxwell's equation

- Electromagnetic quantities

quantity	symbol	unit	differential form
scalar electric potential	ϕ	V	0-form
electric field intensity	$\boldsymbol{E}$	$\frac{V}{m}$	1-form
magnetic flux density	$\boldsymbol{B}$	$\frac{Vs}{m^2}$	2-form
charge density	ρ	$\frac{As}{m^3}$	3-form

- 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 $\phi \in H^1(\Omega)$, $\boldsymbol{E}, \boldsymbol{A} \in H(\text{curl}, \Omega)$, $\boldsymbol{B}, \mathrm{J} \in H(\text{div}, \Omega)$, and $\rho \in L^2(\Omega)$.
- Complex property: div curl $= 0$, curl grad $= 0$.

Compatible finite elements for Maxwell's equation

- computing diagram operators: $\operatorname{grad}\Pi^0 = \Pi^1 \operatorname{grad}$, $\operatorname{curl}\Pi^1 = \Pi^2 \operatorname{curl}$, $\operatorname{div}\Pi^2 = \Pi^3 \operatorname{div}$.
- continuous field: $\boldsymbol{B} \in V^1$, $\boldsymbol{E}, \boldsymbol{J} \in V^2$
- discrete Maxwell's equations:

$$\frac{1}{c^2}\frac{\partial \boldsymbol{E}_h}{\partial t} - \operatorname{curl} \boldsymbol{B}_h = -\mu_0 \Pi^2(\boldsymbol{J}),$$

$$\frac{\partial \boldsymbol{B}_h}{\partial t} + \operatorname{curl}_w \boldsymbol{E} = 0,$$

$$\operatorname{div} \boldsymbol{E}_h = \frac{\Pi^3(\rho)}{\varepsilon_0},$$

$$\operatorname{div}_w \boldsymbol{B}_h = 0.$$

functional de Rham structure

$$\begin{array}{ccccccc}
V^0 & \xrightarrow{\text{grad}} & V^1 & \xrightarrow{\text{curl}} & V^2 & \xrightarrow{\text{div}} & V^3 \\
\Pi^0 \downarrow & & \Pi^1 \downarrow & & \Pi^2 \downarrow & & \Pi^3 \downarrow \\
V_h^0 & \xrightarrow{\text{grad}} & V_h^1 & \xrightarrow{\text{curl}} & V_h^2 & \xrightarrow{\text{div}} & V_h^3
\end{array}$$

GEMPIC framework

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- **Discretisation**: Conforming finite elements for fields (discrete deRham complex), Particle–In–Cell for distribution functions.
  - Semi-discrete electric field: $\boldsymbol{E}_h(\boldsymbol{x},t) = \sum_i^{N_1} e_i(t)\boldsymbol{\Lambda}_i^2(\boldsymbol{x})$.
  - Semi-discrete magnetic field: $\boldsymbol{B}_h(\boldsymbol{x},t) = \sum_i^{N_2} b_i(t)\boldsymbol{\Lambda}_i^1(\boldsymbol{x})$.
  - Particle distribution function

$$f_h(\boldsymbol{x},\boldsymbol{v},t) = \sum_{a=1}^{N_p} w_a\, S\big(\boldsymbol{x}-\boldsymbol{X}(t)\big)\,\delta\big(\boldsymbol{u}-\boldsymbol{U}(t)\big), \quad \boldsymbol{u} = \boldsymbol{p}/m$$

- **Derivation** of the semi-discrete equations based on discrete Poisson bracket or discrete action principle.
- **Temporal discretisations**: Hamiltonian splitting and (semi)-implicit methods based on discrete gradient methods.

Variational principle

Principle of least action: The path taken by a system is the one for which the action is stationary to the first order.
Equations of motion can be derived from the Euler–Lagrange equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial \mathcal{L}}{\partial q}$$

Lagrangian of the Vlasov–Maxwell system

$$\mathcal{L}(\boldsymbol{X}, \dot{\boldsymbol{X}}, \boldsymbol{P}, \boldsymbol{A}, \dot{\boldsymbol{A}}, \phi) = \sum_s \int f_s(t_0, \boldsymbol{x}_0, \boldsymbol{p}_0) \Big((\boldsymbol{P} + q_s \boldsymbol{A}(t, \boldsymbol{X})) \cdot \dot{\boldsymbol{X}} - \big((\gamma - 1) m_s c^2 + q_s \phi(t, \boldsymbol{X}) \big) \Big) \, \mathrm{d}\boldsymbol{x}_0 \, \mathrm{d}\boldsymbol{v}_0 + \frac{\varepsilon_0}{2} \int_\Omega |\operatorname{grad} \phi(t, \boldsymbol{x}) + \dot{\boldsymbol{A}}(t, \boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} - \frac{1}{2\mu_0} \int_\Omega |\operatorname{curl} \boldsymbol{A}(t, \boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x}.$$

where $\boldsymbol{E} = -\partial_t \boldsymbol{A} - \operatorname{grad} \phi$ and $\boldsymbol{B} = \operatorname{curl} \boldsymbol{A}$.

Semi-discrete Lagrangian

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$$\mathcal{L}_h = \sum_{p=1}^{N} w_p \left(\left(\boldsymbol{P}_p + q_s \boldsymbol{A}^S(\boldsymbol{X}_p) \right) \cdot \dot{\boldsymbol{X}}_p - \left((\gamma - 1) m_s c^2 + q_s \phi^S(\boldsymbol{X}_p) \right) \right)$$
$$+ \frac{1}{2} \int_\Omega |\operatorname{grad}_w \phi_h(\boldsymbol{x}) + \dot{\boldsymbol{A}}_h(\boldsymbol{x})|^2 \mathrm{d}\boldsymbol{x} - \frac{1}{2} \int_\Omega |\operatorname{curl}_w \boldsymbol{A}_h(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x}.$$

$\boldsymbol{A}_h \in V_h^2$, $\phi_h \in V_h^3$ and $\boldsymbol{X}_p(t), \boldsymbol{V}_p(t), w_p$ the particle trajectories and weights

$$\begin{cases} \boldsymbol{A}^S(\boldsymbol{X}_p) := \sum_{\alpha=1}^{3} \mathrm{e}_\alpha \int_\Omega \left(\boldsymbol{A}_h \cdot \Pi^2(\mathrm{e}_\alpha S_{\boldsymbol{X}_p}) \right) \mathrm{d}\boldsymbol{x}, \\ \phi^S(\boldsymbol{X}_p) := \int_\Omega \left(\phi_h \Pi^3(S_{\boldsymbol{X}_p}) \right) \mathrm{d}\boldsymbol{x} \end{cases}$$

where $S_{\boldsymbol{X}_p}(\boldsymbol{x}) = S(\boldsymbol{x} - \boldsymbol{X}_p)$ denotes the shape function centered on a particle.

Variational equations of motion

Faraday and Ampère

$$\begin{cases} -\frac{1}{c^2}\partial_t \boldsymbol{E}_h + \operatorname{curl} \boldsymbol{B}_h = \mu_0 \Pi^2 \boldsymbol{J}_N^S \\ \partial_t \boldsymbol{B}_h + \operatorname{curl}_w \boldsymbol{E}_h = 0 \end{cases} \quad \text{with} \quad \Pi^2 \boldsymbol{J}_N^S = \sum_{p=1\cdots N} q_p \Pi^2 (\boldsymbol{V}_p S_{\boldsymbol{X}_p})$$

Particle equations

$$\begin{cases} \frac{\mathrm{d}\boldsymbol{X}_p}{\mathrm{d}t} = \boldsymbol{V}_p \\ \frac{\mathrm{d}\boldsymbol{U}_p}{\mathrm{d}t} = \frac{q_p}{m_p}(\boldsymbol{E}^S(\boldsymbol{X}_p) + \boldsymbol{V}_p \times \boldsymbol{B}^S(\boldsymbol{X}_p)) \end{cases} \quad \text{for } p = 1, \ldots, N$$

where $\boldsymbol{U} = \boldsymbol{P}/m_s$ with coupling fields defined by

$$\boldsymbol{E}^S(\boldsymbol{X}_p) = \sum_{\alpha=1}^{3} \boldsymbol{e}_\alpha \int_\Omega \boldsymbol{E}_h \cdot \Pi^2(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p}), \qquad \boldsymbol{B}^S(\boldsymbol{X}_p) = \sum_{\alpha=1}^{3} \boldsymbol{e}_\alpha \int_\Omega \boldsymbol{B}_h \cdot \Pi^1(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p}).$$

Gauss' laws

$$\begin{cases} \operatorname{div} \boldsymbol{E}_h = \Pi^3 \rho_N^S / \varepsilon_0 \\ \operatorname{div}_w \boldsymbol{B}_h = 0 \end{cases} \quad \text{with} \quad \rho_N^S = \sum_{p=1}^{N} q_p S_{\boldsymbol{X}_p}.$$

Conservation properties

- conservation of Gauss law:

$$\partial_t \left(\operatorname{div} \boldsymbol{E}_h\right) = -\mu_0 \operatorname{div} \Pi^2 \boldsymbol{J} = -\Pi^3 \operatorname{div} \boldsymbol{J} = \partial_t \left(\Pi^3 \rho\right)$$

$$\partial_t \left(\operatorname{div} \boldsymbol{B}_h\right) = -\operatorname{div}(\operatorname{curl} \boldsymbol{E}_h) = 0$$

- conservation of energy:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\int |\boldsymbol{E}_h|^2 + |\boldsymbol{B}_h|^2\right) = \int \boldsymbol{E}_h \cdot \left(\operatorname{curl} \boldsymbol{B}_h - \Pi^2 \boldsymbol{J}\right) - \boldsymbol{B}_h \cdot \operatorname{curl} \boldsymbol{E}_h = -\int \boldsymbol{E}_h \cdot \Pi^2 \boldsymbol{J}$$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\sum_p w_p m_p \gamma_p c^2 = \sum_p w_p \boldsymbol{v}_p \cdot \left(\boldsymbol{v}_p \times \boldsymbol{B}_h^S(\boldsymbol{x}_p) + \boldsymbol{E}_h^S(\boldsymbol{x}_p)\right) = \sum_p w_p \int \Pi^2 \left(\boldsymbol{v}_p S(\boldsymbol{x} - \boldsymbol{x}_p)\right) \cdot \boldsymbol{E}_h(\boldsymbol{x})$$

Semi-discrete Poisson system

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- Dynamic variables: $\boldsymbol{Z} = (\boldsymbol{X}, \boldsymbol{U}, \boldsymbol{e}, \boldsymbol{b})^\top$
- Discrete Hamiltonian: $\mathcal{H}(\boldsymbol{U}, \boldsymbol{e}, \boldsymbol{b}) = \sum_{p=1}^{N} m_p w_p c^2 \gamma_p + \boldsymbol{e}^\top \mathbb{M}^2 \boldsymbol{e} + \boldsymbol{b}^\top \mathbb{M}^1 \boldsymbol{b}$
- Poisson matrix:

$$\mathcal{J}(\boldsymbol{X}, \boldsymbol{b}) = \begin{pmatrix} 0 & \mathbb{W}_{1/m} & 0 & 0 \\ -\mathbb{W}_{1/m} & \mathbb{W}_{q/m}\mathbb{B}(\boldsymbol{X}, \mathrm{b})\mathbb{W}_{1/m} & \mathbb{W}_{q/m}\mathbb{S}^2(\boldsymbol{X}) & 0 \\ 0 & -\mathbb{S}^2(\boldsymbol{X})^\top \mathbb{W}_{q/m} & 0 & \mathbb{C}\left(\mathbb{M}^1\right)^{-1} \\ 0 & 0 & -\left(\mathbb{M}^1\right)^{-1}\mathbb{C}^\top & 0 \end{pmatrix}$$

  - $\mathbb{S}^2_{p,k}$: Π^2 coupling of pth particle with DoF k
  - $\mathrm{B}(\boldsymbol{X}, \boldsymbol{B})_{p,p}$: magnetic rotation of pth trajectory with Π^1 coupling
- Semi-discrete equations of motion: $\frac{\mathrm{d}\boldsymbol{Z}}{\mathrm{d}t} = \mathcal{J}\mathbb{D}_{\boldsymbol{Z}}\mathcal{H}$ with $\mathbb{D}_{\boldsymbol{Z}} = (0, \mathbb{W}_m \boldsymbol{V}, \mathbb{M}^1 \boldsymbol{e}, \mathbb{M}^2 \boldsymbol{b})^\top$

Derivation of structure-preserving propagators

RUB

System of the form $\dot{\boldsymbol{Z}} = \mathcal{J}(\boldsymbol{Z})\,\mathbb{D}_{\boldsymbol{Z}}\hat{\mathcal{H}}(\boldsymbol{Z})$ with $\mathcal{J}^\top = -\mathcal{J}$ and $\mathbb{D}_{\boldsymbol{Z}}\hat{\mathcal{H}}(\boldsymbol{Z})$ linear.

- **Variational integrator**: Splitting of the Hamiltonian and explicit solution of the subsystems (or symplectic integration).
- **Energy conserving** discrete gradient methods (for quadratic Hamiltonian):

$$\frac{\boldsymbol{Z}^{n+1} - \boldsymbol{Z}^n}{\Delta t} = \bar{\mathcal{J}}(\boldsymbol{Z}^{n+1}, \boldsymbol{Z}^n) D_{\boldsymbol{Z}} \mathcal{H}\left(\frac{\boldsymbol{Z}^{n+1} + \boldsymbol{Z}^n}{2}\right)$$

with antisymmetric $\bar{\mathcal{J}}(\boldsymbol{Z}^{n+1}, \boldsymbol{Z}^n)$.
Nonlinearity can be reduced by antisymmetric splitting of $\bar{\mathcal{J}}(\boldsymbol{Z}^{n+1}, \boldsymbol{Z}^n)$.

Semi-implicit scheme

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Antisymmetric splitting of the Poisson matrix

$$\mathcal{J}(\boldsymbol{X}, \mathrm{b}) = \begin{pmatrix} 0 & \mathbb{W}_{\mathbf{1}/m} & 0 & 0 \\ -\mathbb{W}_{\mathbf{1}/m} & \mathbb{W}_{q/m}\mathbb{B}^{\mathbf{1}}(\boldsymbol{X}, \mathrm{b})\mathbb{W}_{\mathbf{1}/m} & \mathbb{W}_{q/m}\mathbb{S}^{\mathbf{2}}(\boldsymbol{X}) & 0 \\ 0 & -\mathbb{S}^{\mathbf{2}}(\boldsymbol{X})^\top \mathbb{W}_{q/m} & 0 & \mathbb{C}(\mathbb{M}^{\mathbf{1}})^{-\mathbf{1}} \\ 0 & 0 & -(\mathbb{M}^{\mathbf{1}})^{-\mathbf{1}}\mathbb{C}^\top & 0 \end{pmatrix}$$

Resulting subsystems:

1. $\dot{\boldsymbol{X}} = \boldsymbol{V}$.
2. $\dot{\boldsymbol{U}} = \mathbb{W}_{q/m}\boldsymbol{B}(\boldsymbol{X}, \boldsymbol{b})\boldsymbol{V}$.
3. $\dot{\boldsymbol{U}} = \mathbb{W}_{q/m}\mathbb{S}^2(\boldsymbol{X})\boldsymbol{e}$, $\dot{\mathbf{e}} = -\mathbb{S}^2(\boldsymbol{X})^\top \mathbb{W}_q \boldsymbol{V}$.
4. $\dot{\mathbf{e}} = \mathbb{C}\boldsymbol{b}$, $\dot{\boldsymbol{b}} = -(\mathbb{M}^1)^{-1}\mathbb{C}^\top\mathbb{M}^2\boldsymbol{e}$.

Implicit steps: 3. and 4.

Step 3: Implicit part could be confined to the field part in the absence of γ. Now there is a nonlinear dependence on the velocity but violation of the energy conservation might be tolerable for weakly relativistic plasmas.

Implicit scheme

Antisymmetric splitting of the Poisson matrix

$$\mathcal{J}(\boldsymbol{X}, \mathrm{b}) = \begin{pmatrix} 0 & \mathbb{W}_{\mathbf{1}/m} & 0 & 0 \\ -\mathbb{W}_{\mathbf{1}/m} & \mathbb{W}_{q/m}\mathbb{B}^{\mathbf{1}}(\boldsymbol{X}, \mathrm{b})\mathbb{W}_{\mathbf{1}/m} & \mathbb{W}_{q/m}\mathbb{S}^{\mathbf{2}}(\boldsymbol{X}) & 0 \\ 0 & -\mathbb{S}^{\mathbf{2}}(\boldsymbol{X})^\top \mathbb{W}_{q/m} & 0 & \mathbb{C}(\mathbb{M}^{\mathbf{1}})^{-\mathbf{1}} \\ 0 & 0 & -(\mathbb{M}^{\mathbf{1}})^{-\mathbf{1}}\mathbb{C}^\top & 0 \end{pmatrix}$$

Resulting subsystems:

1. $\dot{\boldsymbol{U}} = \mathbb{W}_{q/m}\boldsymbol{B}(\boldsymbol{X}, \boldsymbol{b})\boldsymbol{V}$.
2. $\dot{\boldsymbol{X}} = \boldsymbol{V}$, $\dot{\boldsymbol{U}} = \mathbb{W}_{q/m}\mathbb{S}^2(\boldsymbol{X})\boldsymbol{e}$, $\dot{\boldsymbol{e}} = -\mathbb{S}^2(\boldsymbol{X})^\top \mathbb{W}_q \boldsymbol{V}$.
3. $\dot{\boldsymbol{e}} = \mathbb{C}\boldsymbol{b}$, $\dot{\boldsymbol{b}} = -(\mathbb{M}^1)^{-1}\mathbb{C}^\top\mathbb{M}^2\boldsymbol{e}$.

Step 2: Exact integration of the current can be implemented. Picard iteration to resolve the implicit character in $\boldsymbol{X}$, $\boldsymbol{U}$ and $\boldsymbol{e}$.

Some very first results with the relativistic version

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Test case: Landau damping type problem from Crouseilles et al., Computer Physics Communications 209, 2016.

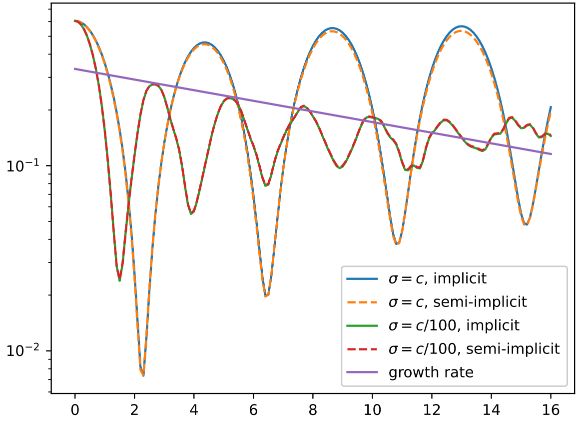
- Initial conditions:

$$f(\boldsymbol{x}, \boldsymbol{u}, t = 0) = \frac{1}{(2\pi\sigma)^{3/2}} \exp\left(-\frac{|\boldsymbol{u}|^2}{2\sigma^2}\right)(1 + \alpha \cos(kx_1))$$

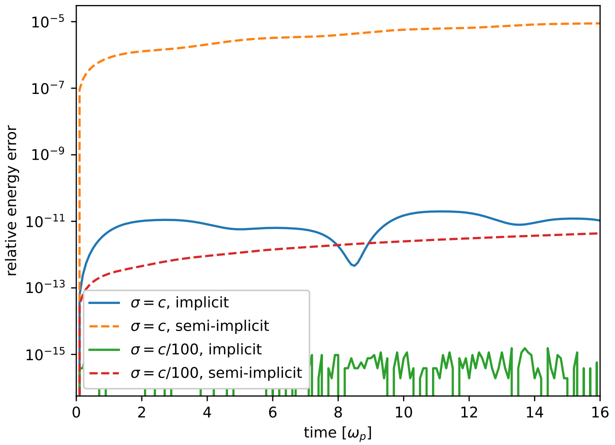
$$B_3(\boldsymbol{x}, t = 0) = \frac{\alpha}{k\sigma/c} \sin(kx_1)$$

- Resolution: grid points $16 \times 8 \times 8$, particles $2,000,000$, $\Delta t = 0.1\omega_p$
- Parameters: $\alpha = 0.01$, $k = 0.4$, $\sigma = c$ or $\sigma = \frac{c}{100}$

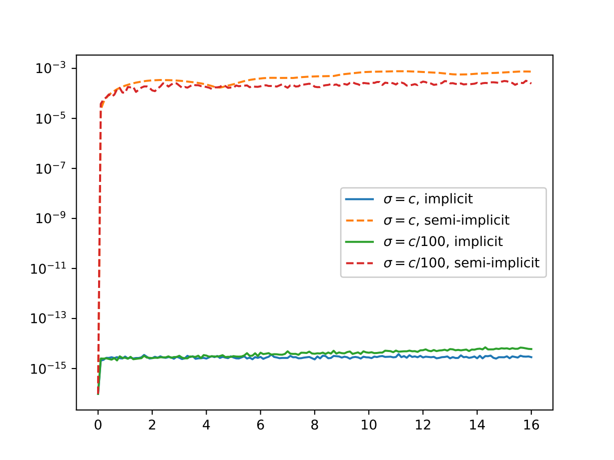
Evolution of the electric energy



Conservation properties



Conservation properties



Costs of Picard iterations: 9 for $\sigma = \frac{c}{100}$ and 8 for $\sigma = c$.

What more to do—HPC

- Implementation of the method based on AMReX.
- AMReX provides data structures for parallelization of particle and field routines, portable to various systems.
- Weak scaling on Cobra@MaxPlanckComputing (INTEL Skylake, 20 cores 2.4 GHz, connected through 100 Gb/s OmniPath interconnect) for 1000 particles per cell starting with a grid of $10 \times 10 \times 10$ cells:

cores	wall time [s]	efficiency
1	55.6	1.00
8	58.0	1.04
64	58.6	1.05
1000	60.8	1.09
8000	61.9	1.11
24389	63.1	1.13

What more to do—Subcycling

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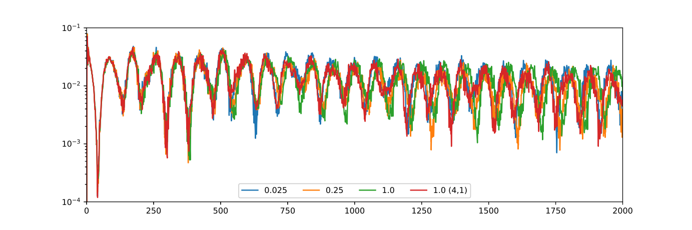
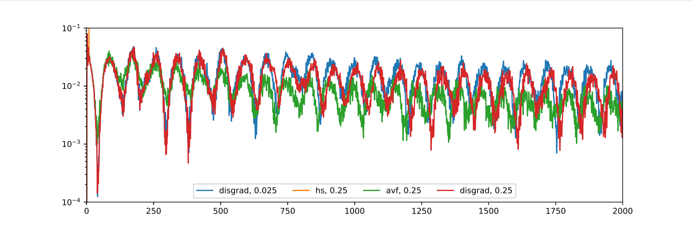
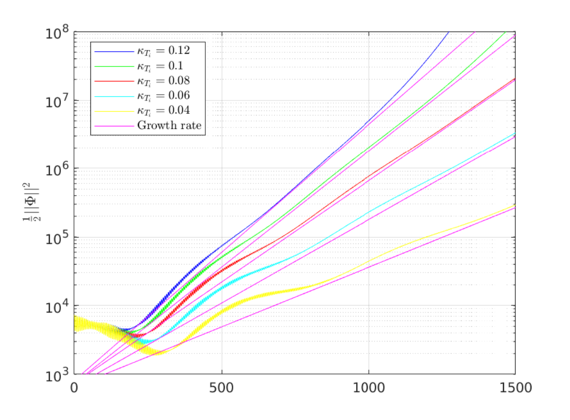
Tackle fast frequencies by implicit method and/or partial subcycling





What more to do—Physics

Example from fusion: Ion-temperature gradient instability



Next: CIM use cases?