Gauge Invariance and Conservation Laws in the Variational Formulation of Macro-Particle Plasma Models

B. A. Shadwick

Department of Physics & Astronomy
University of Nebraska-Lincoln

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Background

- Start with the Low Lagrangian
- Macro-particle reduction:

$$f(\boldsymbol{r},\boldsymbol{p},t) = \sum_{\alpha} w_{\alpha}\, S(\boldsymbol{r}-\boldsymbol{\xi}^{\alpha})\, \delta(\boldsymbol{p}-m\gamma_{\alpha}\dot{\boldsymbol{\xi}}^{\alpha})$$

- Continuous space and time.
- Retain energy and momentum conservation and gauge invariance.
- Ultimately would like a canonical Hamiltonian system. Use standard symplectic methods.
- Want a gridded representation of the fields for computational performance.
- Same reduction can be performed in the non-canonical Vlasov–Maxwell bracket.
- A basis expansion of $\boldsymbol{E}$ and $\boldsymbol{B}$ seems necessary.
- For a Fourier representation of the fields, both methods give the same dynamics.

Why Should You Care?

- We want to preserve as much structure of the system consistent with a macro-particle approximation.
- Artifacts can pollute results.
- Identifying and removing unphysical artifacts is time consuming and difficult.
- In a computer almost everything looks like plasma physics.

Background: Low Lagrangian

- Relativistic Low Lagrangian

$$\int d^3\tilde{\boldsymbol{r}}\, d^3\tilde{\boldsymbol{v}}\;\; f_0(\tilde{\boldsymbol{r}}, \tilde{\boldsymbol{v}}) \left(-mc^2\sqrt{1-\frac{v^2}{c^2}} - q\,\varphi + \frac{q}{c}\,\boldsymbol{v}\cdot\boldsymbol{A} \right)$$
$$+ \frac{1}{8\pi}\int d^3\boldsymbol{r}\left[\frac{1}{c^2}\left|\frac{\partial \boldsymbol{A}}{\partial t}\right|^2 + \frac{2}{c}\nabla\varphi\cdot\frac{\partial \boldsymbol{A}}{\partial t} + \boldsymbol{A}\cdot\nabla^2\boldsymbol{A} + (\nabla\cdot\boldsymbol{A})^2 + |\nabla\varphi|^2\right]$$

- $\boldsymbol{r}(t;\tilde{\boldsymbol{r}}, \tilde{\boldsymbol{v}})$ and $\boldsymbol{v}(t;\tilde{\boldsymbol{r}}, \tilde{\boldsymbol{v}})$ are the electron position and velocity, with

$$\boldsymbol{r}(t=0, \tilde{\boldsymbol{r}}, \tilde{\boldsymbol{v}}) = \tilde{\boldsymbol{r}}$$
$$\boldsymbol{v}(t=0, \tilde{\boldsymbol{r}}, \tilde{\boldsymbol{v}}) = \tilde{\boldsymbol{v}}$$

- $f_0(\tilde{\boldsymbol{r}}, \tilde{\boldsymbol{v}})$ is the initial electron phase space distribution.
- Variation of the Lagrangian yields equations for particle orbits (characteristics of the Vlasov equation) and field equations.

Background: Lagrangian Reduction

- Macro-particles:

$$f(\boldsymbol{r},\boldsymbol{p},t) = \sum_\alpha w_\alpha\, S(\boldsymbol{r}-\boldsymbol{\xi}^\alpha)\,\delta(\boldsymbol{v}-\dot{\boldsymbol{\xi}}^\alpha)$$

- Reduced Lagrangian:

$$\mathcal{L} = -\sum_\alpha w_\alpha mc^2\sqrt{1-\frac{|\dot{\boldsymbol{\xi}}^\alpha|^2}{c^2}} + q\sum_\alpha w_\alpha \int d^3\boldsymbol{r}\, S(\boldsymbol{r}-\boldsymbol{\xi}^\alpha)\left(\frac{\dot{\boldsymbol{\xi}}^\alpha}{c}\cdot\boldsymbol{A}-\varphi\right)$$
$$+\frac{1}{8\pi}\int d^3\boldsymbol{r}\left[\frac{1}{c^2}\left|\frac{\partial\boldsymbol{A}}{\partial t}\right|^2 + \frac{2}{c}\nabla\varphi\cdot\frac{\partial\boldsymbol{A}}{\partial t} + \boldsymbol{A}\cdot\nabla^2\boldsymbol{A} + (\nabla\cdot\boldsymbol{A})^2 + |\nabla\varphi|^2\right]$$

Background: Lagrangian Reduction

- Equations of motion

$$-\frac{1}{c}\frac{\partial^2 \boldsymbol{A}}{\partial t^2} - \nabla\frac{\partial \varphi}{\partial t} + c\left[\nabla^2 \boldsymbol{A} - \nabla\left(\nabla\cdot\boldsymbol{A}\right)\right] = 4\pi q \sum_\alpha w_\alpha S(\boldsymbol{r}-\boldsymbol{\xi}^\alpha)\dot{\boldsymbol{\xi}}^\alpha = 4\pi \boldsymbol{J}$$

$$\nabla^2\varphi + \frac{1}{c}\frac{\partial}{\partial t}\nabla\cdot\boldsymbol{A} = -4\pi\, q \sum_a w_\alpha S(r-\boldsymbol{\xi}^\alpha) = -4\pi\rho$$

$$\frac{d\, m\gamma_\alpha\, \dot{\boldsymbol{\xi}}^\alpha}{dt} = q\int d^3\boldsymbol{r}\; S(\boldsymbol{r}-\boldsymbol{\xi}^\alpha)\left(\boldsymbol{E} + \frac{\dot{\boldsymbol{\xi}}^\alpha}{c}\times\boldsymbol{B}\right)$$

- Poisson's equation implies

$$\nabla\cdot\boldsymbol{E} = 4\pi\rho$$

- There is a constraint on the momentum conjugate to $\boldsymbol{A}$:

$$\boldsymbol{\Pi}_A = \frac{\delta\mathcal{L}}{\delta\partial_t\boldsymbol{A}} = \frac{\boldsymbol{E}}{4\pi c^2} \quad \text{giving} \quad \nabla\cdot\boldsymbol{\Pi}_A = \frac{\rho}{c^2}$$

Momentum Conservation

- Variational model will only conserve momentum in an average sense.
- The electrostatic Birdsall & Langdon algorithm conserves total momentum.
- The electromagnetic algorithm exactly conserves charge (with Villasenor & Buneman or Esirkepov).
- Total momentum (particle and field) is not conserved.
- Surprising? Analytically, charge conservation implies momentum conservation.
- Standard PIC discretization breaks this connection.

Momentum Conservation

Example: Non-Relativistic Weibel Instability

- Initial distribution

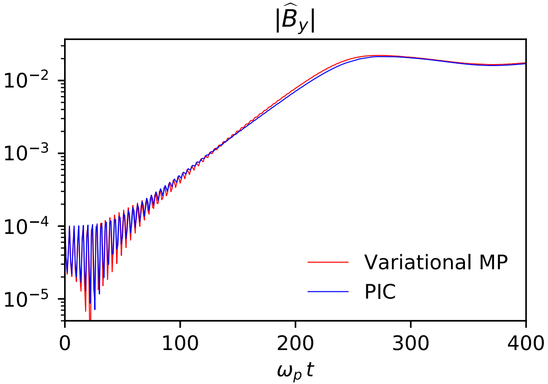
$$f_0(x, v_x, v_z) = \frac{1}{\pi\,\sigma_x\,\sigma_z} \exp\left(-\frac{1}{2}\frac{v_x^2}{\sigma_x^2}\right) \exp\left(-\frac{1}{2}\frac{v_z^2}{\sigma_z^2}\right).$$

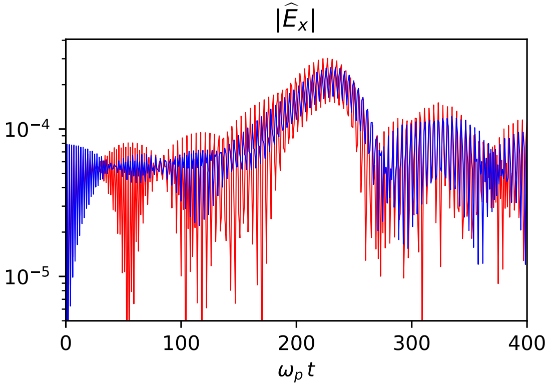
- Initial potential

$$A_x = \frac{\beta}{k}\cos(k\,z).$$

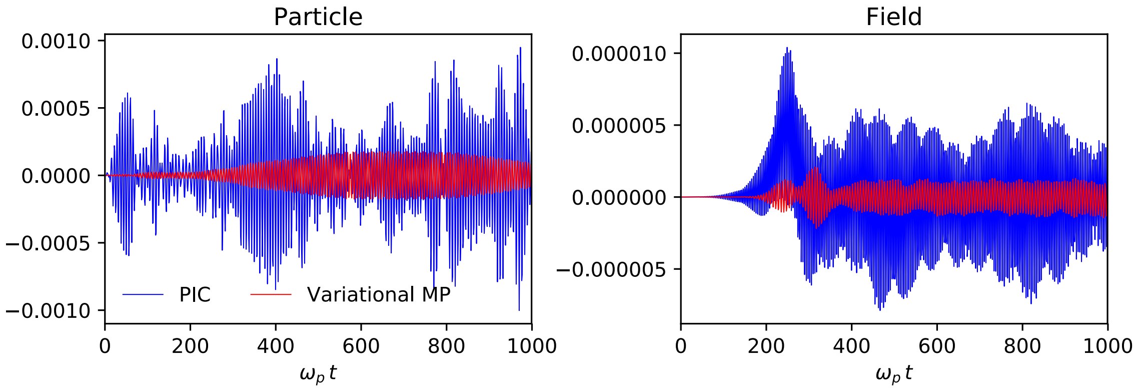
- Parameters: $k = 1.25\,k_p$, $\beta = -10^{-4}$, $\sigma_x = 12\,\sigma_z$, $\sigma_z = c/(50\sqrt{2})$.
- Domain: $0 \leq z < \frac{2\pi}{k}$.

Example: Non-Relativistic Weibel Instability Fields





Example: Non-Relativistic Weibel Instability Momentum



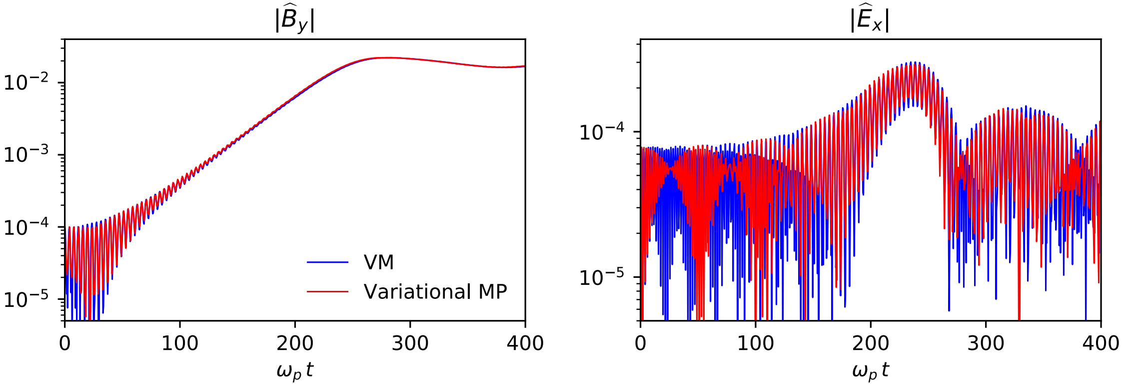
Canonical Hamiltonian

- We can perform a Legendre transformation to obtain a canonical Hamiltonian.
- The momentum conjugate to $\boldsymbol{A}$ is constrained (Gauss' Law).
- Add this constraint to the Hamiltonian with a Lagrange multiplier.
- In continuous space this is the same system as obtained from the noncanonical Hamiltonian.
- Using a grid for the fields, we can obtain a canonical Hamiltonian system (with a constraint).
- Standard symplectic methods can be used on the combined macro-particle and field phase space.

Summary

- The non-canonical and Lagrangian formulations are identical once macro-particles are introduced.
- A truncated Fourier basis representation of the potentials preserves gauge invariance, the continuity equation and momentum conservation. This has significant computational performance limitations but can be used for benchmarking.
- Charge conservation can be restored by imposing a constraint.
- This leads to the same canonical Hamiltonian system as obtained from the noncanonical formulation.

Example: Non-Relativistic Weibel Instability Fields



Example: Non-Relativistic Weibel Instability Momentum