Symplectic and Self-Consistent Algorithms

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TRIUMF

Outline

Symplectic and self-consistent algorithms derived from a:

1. Multi-particle Hamiltonian
2. Lagrangian for collision-less plasma
3. Hamiltonian for collision-less plasma:
   - electromagnetic
   - electrostatic

Multi-Particle Hamiltonian [Qiang, 2017]

$$H(\mathbf{x}^0, \mathbf{P}^0, \ldots, \mathbf{x}^i, \mathbf{P}^i, \ldots; t) = \sum_i \frac{|\mathbf{P}^i|^2}{2m} + \sum_i \sum_j \Lambda(\mathbf{x}^i, \mathbf{x}^j)$$

Symplectic Integrator [Forest and Ruth, 1990], [Qiang, 2017]

$$\left(I - \frac{\Delta t}{2} : \frac{|\mathbf{P}^i|^2}{2m} :\right) \left(I - \Delta t \ : \sum_j \Lambda(\mathbf{x}^i, \mathbf{x}^j) : \right) \left(I - \frac{\Delta t}{2} : \frac{|\mathbf{P}^i|^2}{2m} :\right)$$

Low's Lagrangian – Electrostatic [Low, 1958]

$$L(\mathbf{x}, \dot{\mathbf{x}}, \phi; t) =$$

$$\int f(\mathbf{x}_0, \dot{\mathbf{x}}_0) \left(\frac{m}{2} |\dot{\mathbf{x}}|^2 - q\phi(\mathbf{x}, t) \right) \mathrm{d}\mathbf{x}_0 \mathrm{d}\dot{\mathbf{x}}_0 + \frac{\epsilon_0}{2} \int |\nabla \phi|^2 \mathrm{d}\bar{\mathbf{x}}$$

where $\quad \mathbf{x} = \mathbf{x}(\mathbf{x}_0, \dot{\mathbf{x}}_0, t).$

Low's Lagrangian – Electrostatic [Low, 1958]

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$$\int f(\mathbf{x}_0, \dot{\mathbf{x}}_0) \left(\frac{m}{2} |\dot{\mathbf{x}}|^2 - q\phi(\mathbf{x}, t) \right) \mathrm{d}\mathbf{x}_0 \mathrm{d}\dot{\mathbf{x}}_0 + \frac{\epsilon_0}{2} \int |\nabla \phi|^2 \mathrm{d}\bar{\mathbf{x}}$$

where $\quad \mathbf{x} = \mathbf{x}(\mathbf{x}_0, \dot{\mathbf{x}}_0, t).$

Discretization [Grigoryev et al., 2012], [Shadwick et al., 2014]

$$
\begin{aligned}
f(\mathbf{x}_0, \dot{\mathbf{x}}_0) &= \sum_i w^i \, \delta(\mathbf{x}_0 - \mathbf{x}_0^i)\delta(\dot{\mathbf{x}}_0 - \mathbf{v}_0^i)\,, \\
\phi(\mathbf{x}, t) &= \sum_j \phi^j(t) K(\mathbf{x} - \mathbf{x}^j)
\end{aligned}
$$

Discrete Lagrangian [Shadwick et al., 2014], [Webb, 2016]

$$L_D =$$

$$\frac{m}{2}\sum_i w^i|\dot{\mathbf{x}}^i|^2 - q\sum_{i,j}\phi^j w^i K(\mathbf{x}^i - \mathbf{x}^j) + \frac{\epsilon_0}{2}\int\left(\sum_j \phi^j \nabla K(\bar{\mathbf{x}} - \mathbf{x}^j)\right)^2 \mathrm{d}\bar{\mathbf{x}}$$

Discrete Action [Marsden and West, 2001], [Shadwick et al., 2014], [Webb, 2016]

$$\begin{aligned} S &= \int L_D \, \mathrm{d}t \\ &\approx \Delta t \sum_n L_D(\mathbf{x}_n, \frac{\mathbf{x}_{n+1} - \mathbf{x}_n}{\Delta t}, \phi_n; t) \end{aligned}$$

First-Order Integrator [Marsden and West, 2001], [Webb, 2016]

$$m\frac{\mathbf{x^i_{n+1}} - 2\,\mathbf{x^i_n} + \mathbf{x^i_{n-1}}}{\Delta t} = -q\sum_j \phi_n^j \nabla K(\mathbf{x}_n^i - \mathbf{x}^j)\,,$$

$$\sum_k \phi_n^k \mathcal{M}^{jk} = -\frac{q}{\epsilon_0}\rho_n^j\,,$$

where:

$$\mathcal{M}^{jk} = \int K(\bar{\mathbf{x}} - \mathbf{x}^j)\nabla^2 K(\bar{\mathbf{x}} - \mathbf{x}^k)\,\mathrm{d}\bar{\mathbf{x}}\,,$$

and

$$\rho_n^j = \sum_i w^i K(\mathbf{x}_n^i - \mathbf{x}^j)\,.$$

Electrostatic Hamiltonian?

$$L(\mathbf{x}, \dot{\mathbf{x}}, \phi; t) = \int f(\mathbf{x}_0, \dot{\mathbf{x}}_0) \left(\frac{m}{2} |\dot{\mathbf{x}}|^2 - q\phi(\mathbf{x}, t) \right) \mathrm{d}\mathbf{x}_0 \mathrm{d}\dot{\mathbf{x}}_0 + \frac{\epsilon_0}{2} \int |\nabla \phi|^2 \mathrm{d}\bar{\mathbf{x}}$$

Electromagnetic Hamiltonian [Qin et al., 2016]

$$L(\mathbf{x}, \dot{\mathbf{x}}, \mathbf{A}, \dot{\mathbf{A}}; t) =$$

$$\int f \, \left(\frac{m}{2}|\dot{\mathbf{x}}|^2 + q\,\dot{\mathbf{x}} \cdot \mathbf{A}(\mathbf{x}, t)\right) \, \mathrm{d}\mathbf{x}_0 \mathrm{d}\dot{\mathbf{x}}_0 + \frac{\epsilon_0}{2} \int |\dot{\mathbf{A}}|^2 - |c\nabla \times \mathbf{A}|^2 \, \mathrm{d}\bar{\mathbf{x}}$$

Discretization

$$f(\mathbf{x}_0, \dot{\mathbf{x}}_0) = \sum_i w^i \, \delta(\mathbf{x}_0 - \mathbf{x}_0^i)\delta(\dot{\mathbf{x}}_0 - \mathbf{v}_0^i) \, ,$$

$$\mathbf{A}(\mathbf{x}, t) = \sum_j \mathbf{A}^j(t) K(\mathbf{x} - \mathbf{x}^j)$$

Discrete Lagrangian

$$L_D = \frac{m}{2}\dot{\mathbf{x}}^\intercal\,\mathbf{w}\,\dot{\mathbf{x}} + q\dot{\mathbf{x}}^\intercal\,\mathbf{w}\mathbf{K}\,\mathbf{A} + \frac{\epsilon_0}{2}\dot{\mathbf{A}}^\intercal\,\boldsymbol{\mathcal{K}}\,\dot{\mathbf{A}} - \frac{1}{2\mu_0}\mathbf{A}^\intercal\,\boldsymbol{\mathcal{K}}_\times\,\mathbf{A}$$

where:

$$\begin{aligned}
\mathbf{w} &= \mathrm{diag}(w^i) \\
K^{ij} &= K(\mathbf{x}^i - \mathbf{x}^j) \\
\mathcal{K}^{jk} &= \int K(\bar{\mathbf{x}} - \mathbf{x}^j)K(\bar{\mathbf{x}} - \mathbf{x}^k)\,\mathrm{d}\bar{\mathbf{x}} \\
\mathcal{K}_\times^{jk} &= \int [\nabla K(\bar{\mathbf{x}} - \mathbf{x}^j)]_\times^\intercal\,[\nabla K(\bar{\mathbf{x}} - \mathbf{x}^k)]_\times\,\mathrm{d}\bar{\mathbf{x}}
\end{aligned}$$

Discrete Hamiltonian [Qin et al., 2016]

Canonical momenta are:

$$\mathbf{P} = m\mathbf{w}\dot{\mathbf{x}} + q\mathbf{w}\mathbf{K}\mathbf{A}$$
$$\mathbf{Y} = \epsilon_0 \boldsymbol{\mathcal{K}} \dot{\mathbf{A}} \,.$$

The discrete Hamiltonian becomes $H_D =$

$$\frac{1}{2m}\left(\mathbf{P} - q\mathbf{w}\mathbf{K}\mathbf{A}\right)^{\mathsf{T}} \mathbf{w}^{-1} \left(\mathbf{P} - q\mathbf{w}\mathbf{K}\mathbf{A}\right) + \frac{1}{2\epsilon_0} \mathbf{Y}^{\mathsf{T}} \boldsymbol{\mathcal{K}}^{\mathsf{T}^{-1}} \mathbf{Y} + \frac{1}{2\mu_0} \mathbf{A}^{\mathsf{T}} \boldsymbol{\mathcal{K}}_{\times} \mathbf{A} \,,$$

Electrostatic Hamiltonian

$$L(\mathbf{x}, \dot{\mathbf{x}}, \phi; t) = \int f(\mathbf{x}_0, \dot{\mathbf{x}}_0) \left(\frac{m}{2} |\dot{\mathbf{x}}|^2 - q\phi(\mathbf{x}, t) \right) \mathrm{d}\mathbf{x}_0 \mathrm{d}\dot{\mathbf{x}}_0 + \frac{\epsilon_0}{2} \int |\nabla \phi|^2 \mathrm{d}\bar{\mathbf{x}}$$

Electrostatic Hamiltonian

After integration by substitution:

$$\begin{aligned} S = \int \Bigg[\int f \left(m \frac{x'^2 + y'^2 + 1}{2t'} - q\, t' \phi \right) \mathrm{d}x_0 \mathrm{d}y_0 \mathrm{d}t_0 \mathrm{d}x'_0 \mathrm{d}y'_0 \mathrm{d}t'_0 \\ + \frac{\epsilon_0}{2} \int |\nabla \phi|^2 \, \mathrm{d}\bar{x} \mathrm{d}\bar{y} \mathrm{d}\bar{t} \Bigg] \mathrm{d}z \\ = \int L_z(x, y, t, \phi, x', y', t', \phi'; z) \, \mathrm{d}z \end{aligned}$$

Electrostatic Hamiltonian

Canonical momenta are:

$$\Pi = \epsilon_0 \phi'$$

$$P_x = mf\frac{x'}{t'}$$

$$P_y = mf\frac{y'}{t'}$$

$$-E = -mf\frac{x'^2 + y'^2 + 1}{2t'^2} - qf\phi$$

The Hamiltonian writes

$$H_z = \int \sqrt{2mf(E - qf\phi(\mathbf{r})) - {P_x}^2 - {P_y}^2}\, \mathrm{d}\mathbf{r}_0 \mathrm{d}r'_0 + \frac{1}{2}\int \left(\frac{\Pi^2}{\epsilon_0} - \epsilon_0 |\nabla_\perp \phi|^2\right)\, \mathrm{d}\bar{r}$$

with $\mathbf{r} = (x, y, t)$.

Bibliography

[Forest and Dragt, 1984] Forest, E. and Dragt, A. J. (1984).
Lie algebraic theory of charged particle optics and electron microscopes.
PhD thesis, University of Maryland, College Park, Maryland 20742.

[Forest and Ruth, 1990] Forest, E. and Ruth, R. D. (1990).
Fourth-order symplectic integration.
Physica D: Nonlinear Phenomena, 43(1):105 – 117.

[Grigoryev et al., 2012] Grigoryev, Y. N., Vshivkov, V. A., and Fedoruk, M. P. (2012).
Numerical "Particle-in-Cell" Methods: Theory and Applications.
Walter de Gruyter.

[Low, 1958] Low, F. E. (1958).
A lagrangian formulation of the boltzmann-vlasov equation for plasmas.
Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 248(1253):282–287.

[Marsden and West, 2001] Marsden, J. E. and West, M. (2001).
Discrete mechanics and variational integrators.
Acta Numerica, 10:357514.

[Qiang, 2017] Qiang, J. (2017).
Symplectic multiparticle tracking model for self-consistent space-charge simulation.
Phys. Rev. Accel. Beams, 20:014203.

[Qin et al., 2016] Qin, H., Liu, J., Xiao, J., Zhang, R., He, Y., Wang, Y., Sun, Y., Burby, J. W., Ellison, L., and Zhou, Y. (2016).
Canonical symplectic particle-in-cell method for long-term large-scale simulations of the vlasovmaxwell equations.
Nuclear Fusion, 56(1):014001.

[Shadwick et al., 2014] Shadwick, B. A., Stamm, A. B., and Evstatiev, E. G. (2014).
Variational formulation of macro-particle plasma simulation algorithms.
Physics of Plasmas, 21(5):055708.

[Webb, 2016] Webb, S. D. (2016).
A spectral canonical electrostatic algorithm.
Plasma Physics and Controlled Fusion, 58(3):034007.