Symplectic Particle-in-Mode Algorithms for Modeling Plasma Accelerators

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Plasmas are Hamiltonian Systems

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{j} + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t}$$

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}$$

$$m\frac{d(\gamma \mathbf{v})}{dt} = q\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right)$$

Update particle coördinates

$$(\mathbf{F}, \mathbf{v}) \mapsto (\mathbf{x}, \mathbf{v})$$

Interpolate forces

$$(\mathbf{E}, \mathbf{B}) \mapsto (\mathbf{F})$$

$$\Delta t$$

Deposit sources

$$(\mathbf{x}, \mathbf{v}) \mapsto (\rho, \mathbf{j})$$

Update electromagnetic fields

$$(\rho, \mathbf{j}) \mapsto (\mathbf{E}, \mathbf{B})$$

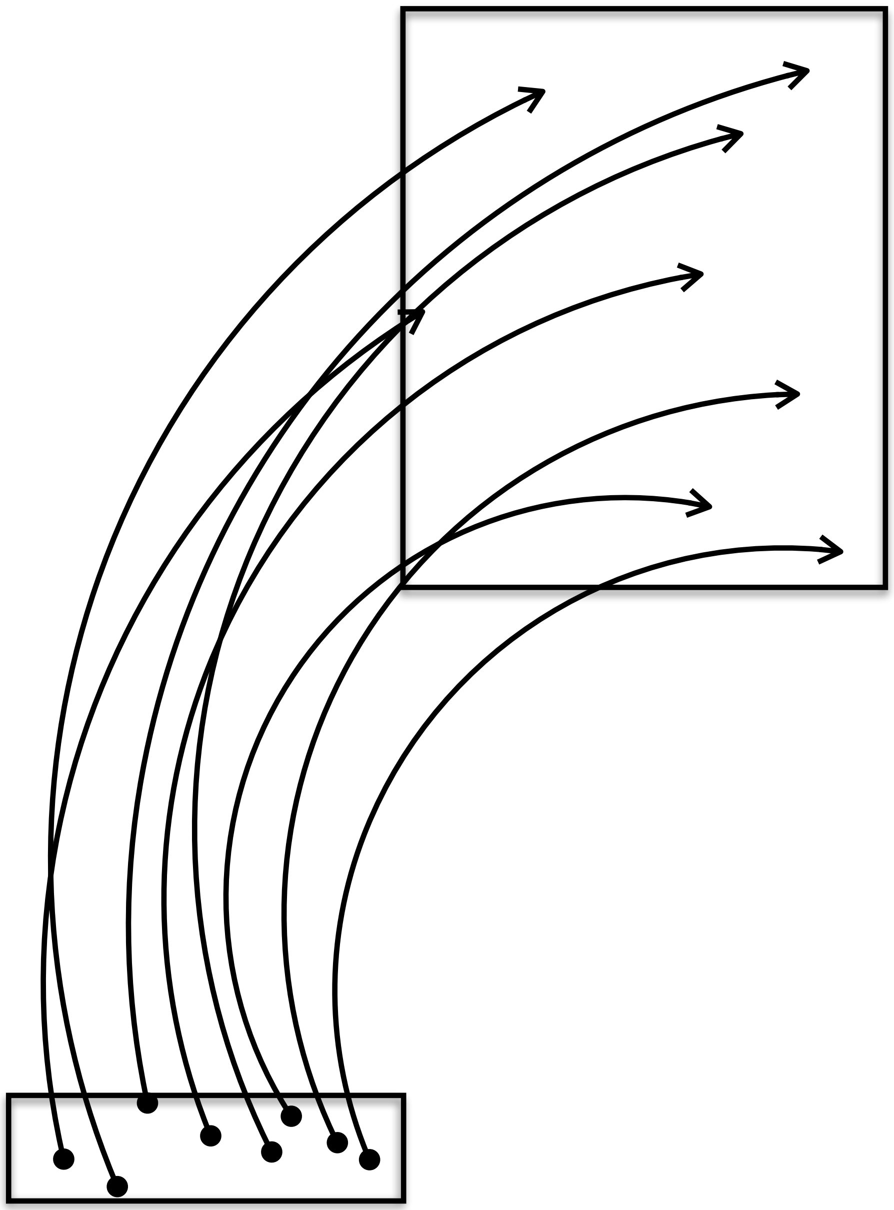
See, e.g., Birdsall & Langdon Plasma Physics via Computer Simulation
or Hockney & Eastwood Computer Simulation Using Particles.

The Vlasov Equation & Hamiltonian Flows

$$D(z,t) = D(\mathscr{M}_{-t} \circ z_0, t=0)$$

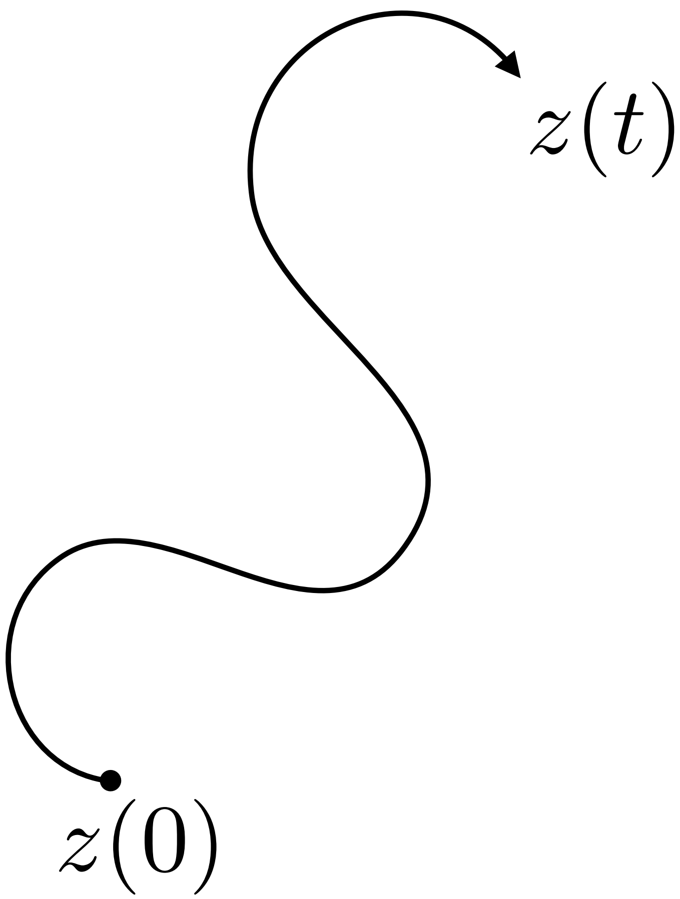
$$\underbrace{\mathbb{M}^t \; J \; \mathbb{M}}_{2D\times 2D} = J \rightarrow \dim_{\mathbb{M}} = 2D^2 + D$$

$D(z,t)$



$D(z_0, t=0)$

Hamiltonian Flows & Symplectic Maps



$$\dot{z} = -\{H, z\}$$

$$z(t) = \mathscr{M}_t \circ z(0)$$

$$\{H, *\} \leftrightarrow :H:$$

$$\dot{\mathscr{M}} = \mathscr{M} :-H:$$

$$H = \frac{1}{2}(p^2 + \omega^2 q^2)$$

$$\mathscr{M} \doteq \begin{pmatrix} \cos\omega t & \omega^{-1}\sin\omega t \\ -\omega\sin\omega t & \cos\omega t \end{pmatrix}$$

$$\mathcal{L} = \int d\mathbf{v}_0 d\mathbf{x}_0 \Bigg\{ -mc^2 \sqrt{1 - \frac{1}{c^2}\left(\frac{\partial \mathbf{x}}{\partial t}\right)^2} + -q\phi(\mathbf{x}) + \frac{q}{c}\frac{\partial \mathbf{x}}{\partial t} \cdot \mathbf{A} \Bigg\} f(\mathbf{v}_0, \mathbf{x}_0) + \frac{1}{8\pi}\int d\mathbf{x} \left(-\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi\right)^2 - (\nabla \times \mathbf{A})^2$$

Relativistic Charged Particle–Electromagnetic Field Lagrangian

B. Shadwick, A. Stamm, & E. Evstatiev, “Variational formulation of macro-particle plasma simulation algorithms”, Phys. Plasmas **21**, 5 (2014).

F. Low, Proc. R. Soc. London Ser. A. Math. Phys. Sci., **248** (1253) pp. 282–287 (1958).

Discretizing the Lagrangian

Macro-particles as Moving Configuration Space Blobs

$$f(\mathbf{x}, \mathbf{v}) = \sum_j w_j \Lambda(\mathbf{x}, \mathbf{x}_j) \delta(\mathbf{v} - \mathbf{v}_j)$$

B. Shadwick, A. Stamm, & E. Evstatiev, “Variational formulation of macro-particle plasma simulation algorithms”, Phys. Plasmas **21**, 5 (2014).

$$\mathcal{L} = \sum_j w_j \Bigg\{ -mc^2 \sqrt{1 - \frac{1}{c^2}\left(\frac{\partial \mathbf{x}_j}{\partial t}\right)^2} +$$

$$-q \int d\mathbf{x}\phi(\mathbf{x})\Lambda(\mathbf{x}, \mathbf{x}_j) + \frac{q}{c}\frac{\partial \mathbf{x}_j}{\partial t} \cdot \int d\mathbf{x}\mathbf{A}(\mathbf{x})\Lambda(\mathbf{x}, \mathbf{x}_j) \Bigg\} +$$

$$\frac{1}{8\pi} \int d\mathbf{x} \left(-\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi \right)^2 - (\nabla \times \mathbf{A})^2$$

Discretizes the phase space bits

So far, assumed 3D Cartesian…

The Relativistic Lagrangian, r-z azimuthal symmetry, Weyl gauge

$$\mathcal{L} = \sum_j w_j \Bigg\{ -mc\sqrt{1 - \dot{r}_j^2 - \dot{z}_j^2 - r_j^2\dot{\theta}_j^2} +$$

$$+\frac{q}{c}\dot{r}\int d\mathbf{x} A_r(\mathbf{x})\Lambda(\mathbf{x},\mathbf{x}_j) + \frac{q}{c}\dot{z}\int d\mathbf{x} A_z(\mathbf{x})\Lambda(\mathbf{x},\mathbf{x}_j)\Bigg\} +$$

$$\frac{1}{8\pi}\int d\mathbf{x}\left(-\frac{\partial\mathbf{A}}{\partial\tau}\right)^2 - (\nabla\times\mathbf{A})^2$$

Conducting boundary modes

$$\mathbf{A} = \sum_{\sigma} \begin{pmatrix} Q_{\sigma}^{(z)} J_0\left(x_m \frac{r}{R}\right) \cos\left(\frac{n\pi}{L} z\right) \\ Q_{\sigma}^{(r)} J_1\left(x_m \frac{r}{R}\right) \sin\left(\frac{n\pi}{L} z\right) \end{pmatrix}$$

Inserted into the Lagrangian…

$$\mathcal{L} = \sum_j w_j \left\{ -mc\sqrt{1 - \dot{r}_j^2 - \dot{z}_j^2 - r_j^2 \dot{\theta}_j^2} + + \frac{q}{c} \dot{r}_j \sum_\sigma I_\sigma^{(r)}(\mathbf{x}_j) + \frac{q}{c} \dot{z}_j I_\sigma^{(z)}(\mathbf{x}_j) \right\} +$$

$$\sum_\sigma \frac{1}{2} \mathcal{M}_\sigma \left(\dot{Q}_\sigma^{(r)\,2} + \dot{Q}_\sigma^{(z)\,2} \right) - \frac{1}{2} \mathcal{M}_\sigma \Omega_\sigma^2 \left(k_r^2 Q_\sigma^{(z)\,2} + 2 k_r k_z Q_\sigma^{(r)} Q_\sigma^{(z)} + k_z^2 Q_\sigma^{(r)\,2} \right)$$

A coördinate transformation to uncouple the harmonic oscillators

$$Q^{(r)} = \frac{k_z Q^{(\omega)} - k_r Q^{(0)}}{\Omega}$$

$$Q^{(z)} = \frac{k_z Q^{(0)} + k_r Q^{(\omega)}}{\Omega}$$

Decouples the Lagrangian and gives space charge and radiative modes

$$\mathcal{L} = \sum_j w_j \left\{ -mc\sqrt{1 - \dot{r}_j^2 - \dot{z}_j^2 - r_j^2\dot{\theta}_j^2} + + \frac{q}{c}\dot{r}_j \sum_\sigma I_\sigma^{(r)}(\mathbf{x}_j) + \frac{q}{c}\dot{z}_j I_\sigma^{(z)}(\mathbf{x}_j) \right\} +$$

$$\sum_\sigma \frac{1}{2}\mathcal{M}_\sigma \left(\dot{Q}_\sigma^{(0)\,2} + \dot{Q}_\sigma^{(\omega)\,2} \right) - \frac{1}{2}\mathcal{M}_\sigma \Omega_\sigma^2 Q_\sigma^{(\omega)\,2}$$

This allows us to compute a Hamiltonian in the usual way

$$
\begin{aligned}
p_j^{(r)} &= \frac{w_j m c \dot{r}_j}{\sqrt{1 - \dot{r}_j^2 - \dot{z}_j^2 - r_j^2 \dot{\theta}_j^2}} + w_j \frac{q}{c} \sum_\sigma I_\sigma^{(r)}(\mathbf{x}_j) \\
p_j^{(z)} &= \frac{w_j m c \dot{z}_j}{\sqrt{1 - \dot{r}_j^2 - \dot{z}_j^2 - r_j^2 \dot{\theta}_j^2}} + w_j \frac{q}{c} \sum_\sigma I_\sigma^{(z)}(\mathbf{x}_j) \\
\mathcal{P}_\sigma^{(0)} &= \mathcal{M}_\sigma \dot{Q}_\sigma^{(0)} \\
\mathcal{P}_\sigma^{(\omega)} &= \mathcal{M}_\sigma \dot{Q}_\sigma^{(\omega)}
\end{aligned}
$$

Hamiltonian for Symplectic Particle-in-Mode Algorithm

$$\mathcal{H} = \underbrace{\sum_j \sqrt{\left(p_j^{(r)} - w_j \frac{q}{c} \sum_\sigma I_\sigma^{(r)}(\mathbf{x}_j)\right)^2 + \left(p_j^{(z)} - w_j \frac{q}{c} \sum_\sigma I_\sigma^{(z)}(\mathbf{x}_j)\right)^2 + \frac{p_j^{(\theta)\,2}}{r_j^2} + w_j^2 m^2 c^2}}_{\mathcal{H}_{p-c}}$$

$$+ \underbrace{\sum_\sigma \frac{\mathcal{P}_\sigma^{(0)\,2}}{2\mathcal{M}_\sigma} + \frac{\mathcal{P}_\sigma^{(\omega)\,2}}{2\mathcal{M}_\sigma} + \frac{1}{2}\mathcal{M}_\sigma \Omega_\sigma^2 Q_\sigma^{(\omega)\,2}}_{\mathcal{H}_{EM}}$$

A Cylindrical Spectral Electromagnetic Algorithm from Symplectic Maps

Requires understanding of symplectic maps…

In order of what you should read:

- A. J. Dragt, "Lectures on nonlinear orbit dynamics", Physics of High Energy Particle Accelerators, pp. 147–313 (1982).
- A. Chao, Lie Algebra Techniques for Nonlinear Dynamics, SLAC-PUB-9574 (2012).
- A. J. Dragt, "A Method of Transfer Maps for Linear and Nonlinear Beam Elements", IEEE Trans. Nucl. Sci. **NS-26** (3) (1979).
- É. Forest, Beam Dynamics: A New Attitude & Framework (1998)
- A. J. Dragt, Lie Methods for Nonlinear Dynamics with Applications to Accelerator Physics (http://www.physics.umd.edu/dsat/, large PDF, ~2500 pages at last count)

Define the Numerical Map w/ 2nd Order Splitting

$$\begin{aligned} \mathscr{N}_{\mathcal{H}}(\Delta\tau) &= e^{-\,:\mathcal{H}_{EM}:\,\Delta\tau/2} e^{-\,:\mathcal{H}_{p-c}:\,\Delta\tau} e^{-\,:\mathcal{H}_{EM}:\,\Delta\tau/2} \\ &= \exp\left\{-\,:\mathcal{H}_{p-c} + \mathcal{H}_{EM}:\Delta\tau + \mathcal{O}\left(\Delta\tau^3\right)\right\} \\ &= \mathscr{M}_{\mathcal{H}}(\Delta\tau) + \mathcal{O}(\Delta\tau^3) \end{aligned}$$

$$\begin{pmatrix} \mathcal{P}_\sigma^{(\omega)} \\ \mathcal{Q}_\sigma^{(\omega)} \end{pmatrix}_{fin} = e^{-:\mathcal{H}_{EM}:\Delta\tau/2} \circ \begin{pmatrix} \mathcal{P}_\sigma^{(\omega)} \\ \mathcal{Q}_\sigma^{(\omega)} \end{pmatrix}_{in}$$

$$\doteq \begin{pmatrix} \cos\Omega_\sigma \frac{\Delta\tau}{2} & -\mathcal{M}_\sigma\Omega_\sigma \sin\Omega_\sigma \frac{\Delta\tau}{2} \\ (\mathcal{M}_\sigma\Omega_\sigma)^{-1} \sin\Omega_\sigma \frac{\Delta\tau}{2} & \cos\Omega_\sigma \frac{\Delta\tau}{2} \end{pmatrix} \begin{pmatrix} \mathcal{P}_\sigma^{(\omega)} \\ \mathcal{Q}_\sigma^{(\omega)} \end{pmatrix}_{in}$$

$$\begin{pmatrix} \mathcal{P}_\sigma^{(0)} \\ \mathcal{Q}_\sigma^{(0)} \end{pmatrix}_{fin} = e^{-:\mathcal{H}_{EM}:\Delta\tau/2} \circ \begin{pmatrix} \mathcal{P}_\sigma^{(0)} \\ \mathcal{Q}_\sigma^{(0)} \end{pmatrix}_{in}$$

$$= \begin{pmatrix} \mathcal{P}_\sigma^{(0)} \\ \mathcal{Q}_\sigma^{(0)} + \frac{\mathcal{P}_\sigma^{(0)}}{\mathcal{M}_\sigma} \frac{\Delta\tau}{2} \end{pmatrix}_{in}$$

Field Map

$$\mathcal{H}_{p-c} = \sum_j \sqrt{\left(p_j^{(r)} - w_j \frac{q}{c} \sum_\sigma I_\sigma^{(r)}(\mathbf{x}_j)\right)^2 + \left(p_j^{(z)} - w_j \frac{q}{c} \sum_\sigma I_\sigma^{(z)}(\mathbf{x}_j)\right)^2 + \frac{p_j^{(\theta)\,2}}{r_j^2} + w_j^2 m^2 c^2}$$

Particle-Coupling Map

Proper Time vs. Lab Time Tracking

$$ds = d\tau/\gamma$$

$$L_s = -\frac{1}{2}mcU^iU_i - \frac{q}{c}U^iA_i \qquad U = (\gamma, \gamma\mathbf{x}')$$

$$K_s = -\frac{(P^i - eA^i)(P_i - eA_i)}{2mc}$$

Y.K. Wu, É. Forest, and D. S. Robin, "Explicit symplectic integrator for s-dependent static magnetic fields", Phys. Rev. E **68**, 046502 (2003).

Proper Time vs. Lab Time Tracking

$$\gamma_j m c = \sqrt{\left(\mathbf{p}_j - w_j \frac{q}{c} \sum_\sigma \mathbf{I}_\sigma(\mathbf{x}_j)\right)^2 + \frac{p_j^{(\theta)\,2}}{r_j^2} + w_j^2 m^2 c^2}$$

$$\overline{\mathcal{H}}_{p-c} = \sum_j \frac{\left(\mathbf{p}_j - w_j \frac{q}{c} \sum_\sigma \mathbf{I}_\sigma^{(r)}(\mathbf{x}_j)\right)^2 + \frac{p_j^{(\theta)\,2}}{r_j^2} + w_j^2 m^2 c^2}{2mc\gamma_j}$$

This Hamiltonian is splittable

$$\mathscr{N}^{(p-c)}(\Delta\tau) = \mathscr{M}^{(\theta)}(\Delta\tau/2)\mathscr{M}^{(z)}(\Delta\tau/2)\mathscr{M}^{(r)}(\Delta\tau)\mathscr{M}^{(z)}(\Delta\tau/2)\mathscr{M}^{(\theta)}(\Delta\tau/2)$$
$$= \mathscr{M}^{(p-c)}(\Delta\tau) + \mathcal{O}(\Delta\tau^3)$$

$$\mathscr{M}^{(\theta)}(\Delta\tau) = \exp\left\{ - : \sum_j \frac{p_j^{(\theta)\,2}}{r_j^2} : \Delta\tau \right\}$$

$$\mathscr{M}^{(z)}(\Delta\tau) = \exp\left\{ - : \sum_j \frac{\left(p_j^{(z)} - w_j \frac{q}{c} I_z(\mathbf{x}_j)\right)^2}{2mc\gamma_j} : \Delta\tau \right\}$$

$$\mathscr{M}^{(r)}(\Delta\tau) = \exp\left\{ - : \sum_j \frac{\left(p_j^{(r)} - w_j \frac{q}{c} I_r(\mathbf{x}_j)\right)^2}{2mc\gamma_j} : \Delta\tau \right\}$$

Similarity Transform on the Magnetic Map

$$e^{-:(p_i - a_i(\mathbf{q}))^2:t} = e^{:-\int a_i(\mathbf{q})dq_i:} e^{-:p_i^2:t} e^{-:-\int a_i(\mathbf{q})dq_i:}$$

$$\begin{aligned}\mathscr{M}^{(r)}(\Delta\tau) &= \exp\left\{-:\sum_j \frac{\left(p_j^{(r)} - w_j \frac{q}{c} I_r(\mathbf{x}_j)\right)^2}{2mc\gamma_j}:\Delta\tau\right\} \\ &= \exp\left\{-:\sum_j w_j \frac{q}{c}\int dr_j I_r(\mathbf{x}_j):\right\} \exp\left\{-:\sum_j \frac{p_j^{(r)\,2}}{2mc\gamma_j}:\Delta\tau\right\} \exp\left\{:\sum_j w_j \frac{q}{c}\int dr_j I_r(\mathbf{x}_j):\right\}\end{aligned}$$

Y.K. Wu, É. Forest, and D. S. Robin, “Explicit symplectic integrator for s-dependent static magnetic fields”, Phys. Rev. E **68**, 046502 (2003).

Action of the Similarity Maps

$$\mathscr{A}^{(r)} = \exp\left\{ - : \sum_j w_j \frac{q}{c} \int dr_j \sum_\sigma Q_\sigma^{(r)} J_1(k_r r_j) \sin(k_z z_j) : \right\}$$

$$\begin{pmatrix} p_j^{(r)} \\ p_j^{(z)} \\ \mathcal{P}_\sigma^{(r)} \\ \mathcal{P}_\sigma^{(z)} \end{pmatrix}_{fin} = \begin{pmatrix} p_j^{(r)} + w_j \frac{q}{c} \sum_\sigma Q_\sigma^{(r)} J_1(k_r r_j) \sin(k_z z_j) \\ p_j^{(z)} - w_j \frac{q}{c} \sum_\sigma Q_\sigma^{(r)} J_0(k_r r_j) \cos(k_z z_j)^{k_z/k_r} \\ \mathcal{P}_\sigma^{(r)} + \sum_j w_j \frac{q}{c} J_1(k_r r_j) \sin(k_z z_j) \\ \mathcal{P}_\sigma^{(z)} \end{pmatrix}_{in}$$

The Full Integrator

$$\mathscr{N} = \mathscr{M}^{(EM)}(\Delta\tau/2)\mathscr{M}^{(\theta)}(\Delta\tau/2)\times$$
$$\mathscr{A}^{(z)}\mathscr{D}^{(z)}(\Delta\tau/2)\left[\mathscr{A}^{(z)}\right]^{-1}\times$$
$$\mathscr{A}^{(r)}\mathscr{D}^{(r)}(\Delta\tau)\left[\mathscr{A}^{(r)}\right]^{-1}\times$$
$$\mathscr{A}^{(z)}\mathscr{D}^{(z)}(\Delta\tau/2)\left[\mathscr{A}^{(z)}\right]^{-1}\times$$
$$\mathscr{M}^{(\theta)}(\Delta\tau/2)\mathscr{M}^{(EM)}(\Delta\tau/2)$$

13 map operations
6 distinct maps

includes angular momentum and self-consistent deposition/interpolation

a few unusual properties…

$$\mathscr{A}\mathscr{D}\mathscr{A}^{-1} \circ \begin{pmatrix} p \\ q \\ \mathcal{P} \\ \mathcal{Q} \end{pmatrix}$$

$$\mathscr{A} = \exp[- : \int dq \mathcal{Q} F(q) :]$$

$$\mathscr{D} = \exp[- : p^2/2 : h]$$

$$z^f = \begin{pmatrix} p^i + \mathcal{Q}^i [F(q^i) - \mathcal{Q}^i F(q^i - p^i h)] \\ q^i - p^i h \\ \mathcal{P}^i + \int dq [F(q^i) - F(q^i - p^i h)] \\ \mathcal{Q}^i \end{pmatrix}$$

Current Deposition/ Force Interpolation

The particles accelerate when the fields update

$$\mathscr{N}^{(\mathscr{H})}(\Delta\tau) = \mathscr{M}^{(EM)}(\Delta\tau/2) \quad \underbrace{\mathscr{M}^{(p-c)}(\Delta\tau)}_{\text{constant magnetic field}} \quad \mathscr{M}^{(EM)}(\Delta\tau/2)$$

$$\gamma_j mc = \sqrt{\left(\mathbf{p}_j - w_j \frac{q}{c} \sum_\sigma \mathbf{I}_\sigma(\mathbf{x}_j)\right)^2 + \frac{p_j^{(\theta)\,2}}{r_j^2} + w_j^2 m^2 c^2}$$

Profoundly constrained dynamics…

$$D = (d) \times (N_{macro.} + N_{modes}) \rightarrow$$

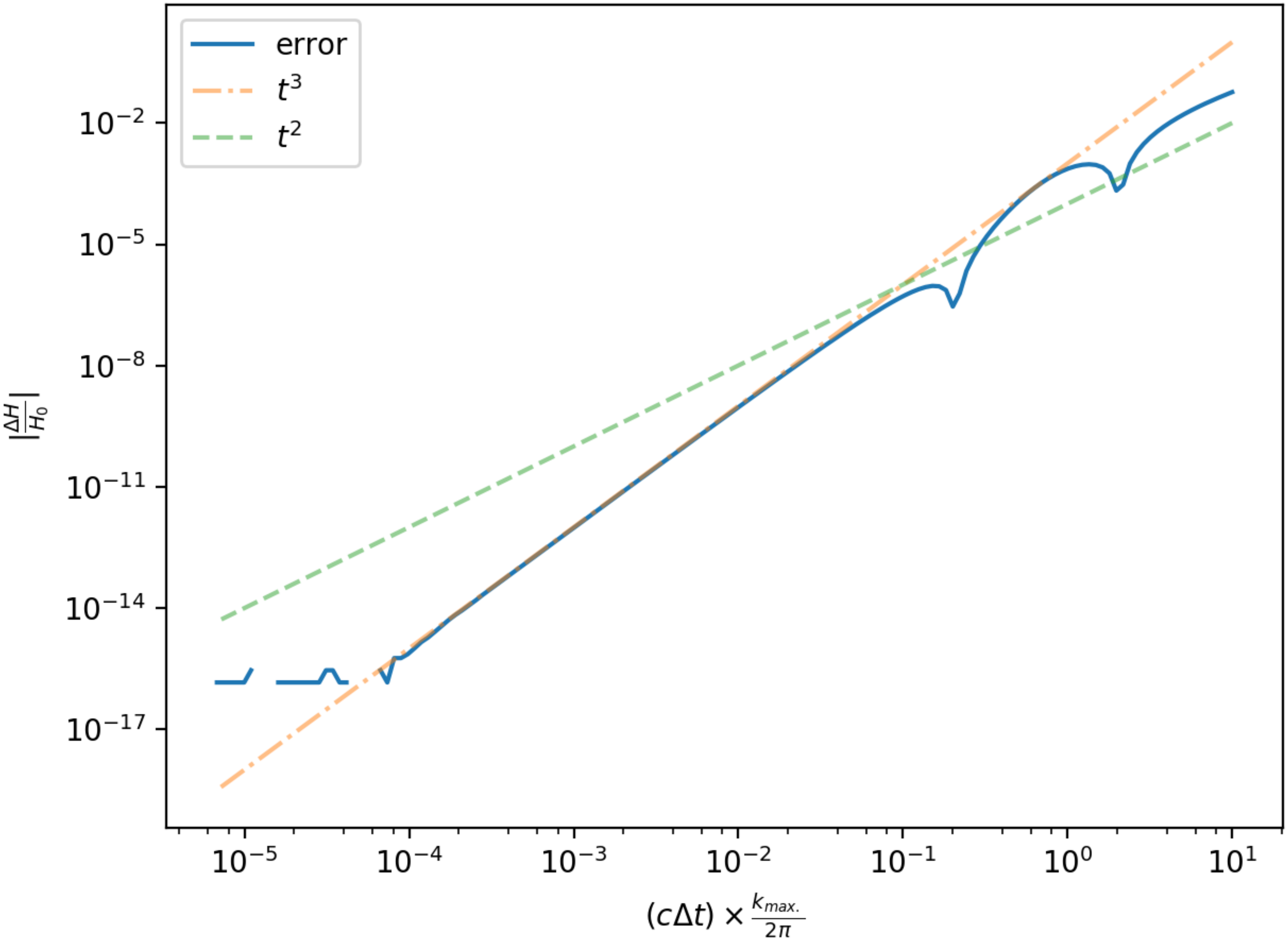
$$2(d) \times (N_{macro.} + N_{modes}) \times [(d)(N_{macro.} + N_{modes}) - 1] \text{ constraints}$$

2nd Order Integrators, Redux

$$\mathscr{N}_{\mathscr{H}} = \exp\left\{ - :\mathscr{H}_{p-c} + \mathscr{H}_{EM}: \Delta\tau + :\mathscr{H}^{(3)}: \Delta\tau^3 + \mathcal{O}(\Delta\tau^5) \right\}$$

from the Baker-Campbell-Hausdorff series

Splitting is Second Order



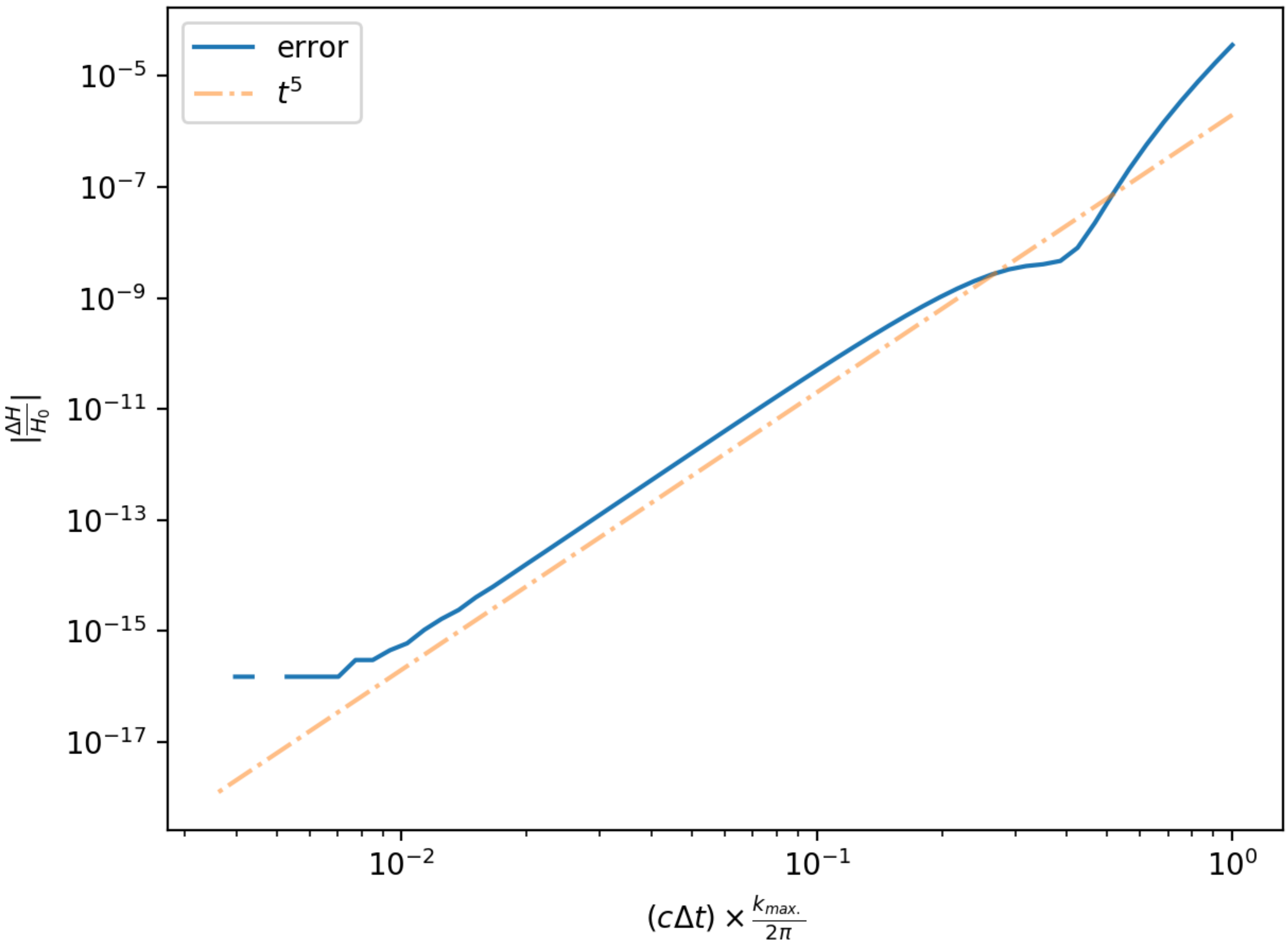
Work by Yoshida shows that three 2nd order integration steps can make a 4th order integrator

$$\mathscr{N}^{(2n+2)}(\Delta\tau) = \mathscr{N}^{(2n)}\left(x_1\Delta\tau\right)\mathscr{N}^{(2n)}\left(x_0\Delta\tau\right)\mathscr{N}^{(2n)}\left(x_1\Delta\tau\right)$$

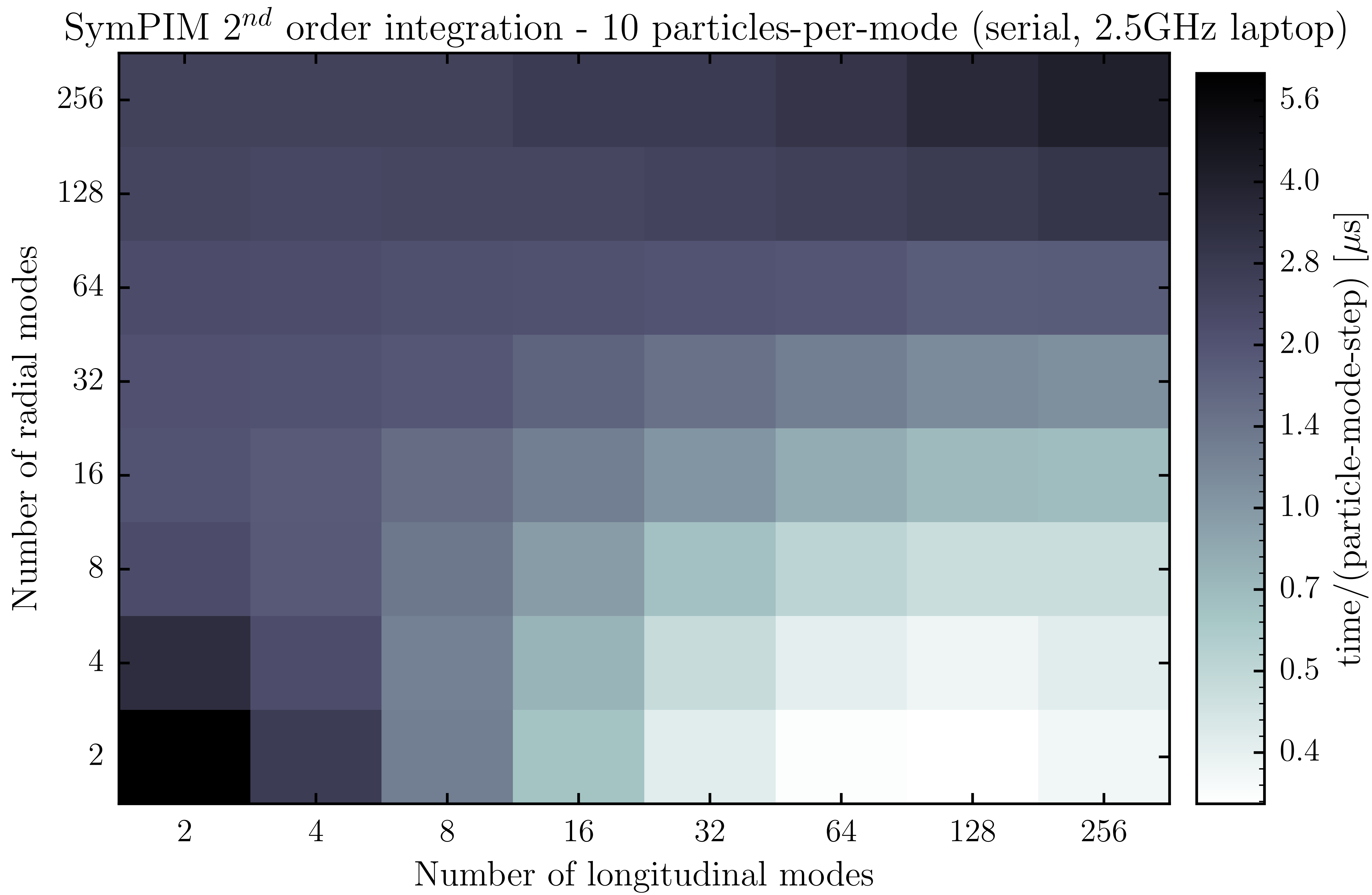
$$x_0 + 2x_1 = 1$$
$$x_0^{2n+1} + 2x_1^{2n+1} = 0$$

H. Yoshida, "Construction of higher order symplectic integrators", Phys. Lett. A **150**, 5–7 (1990)

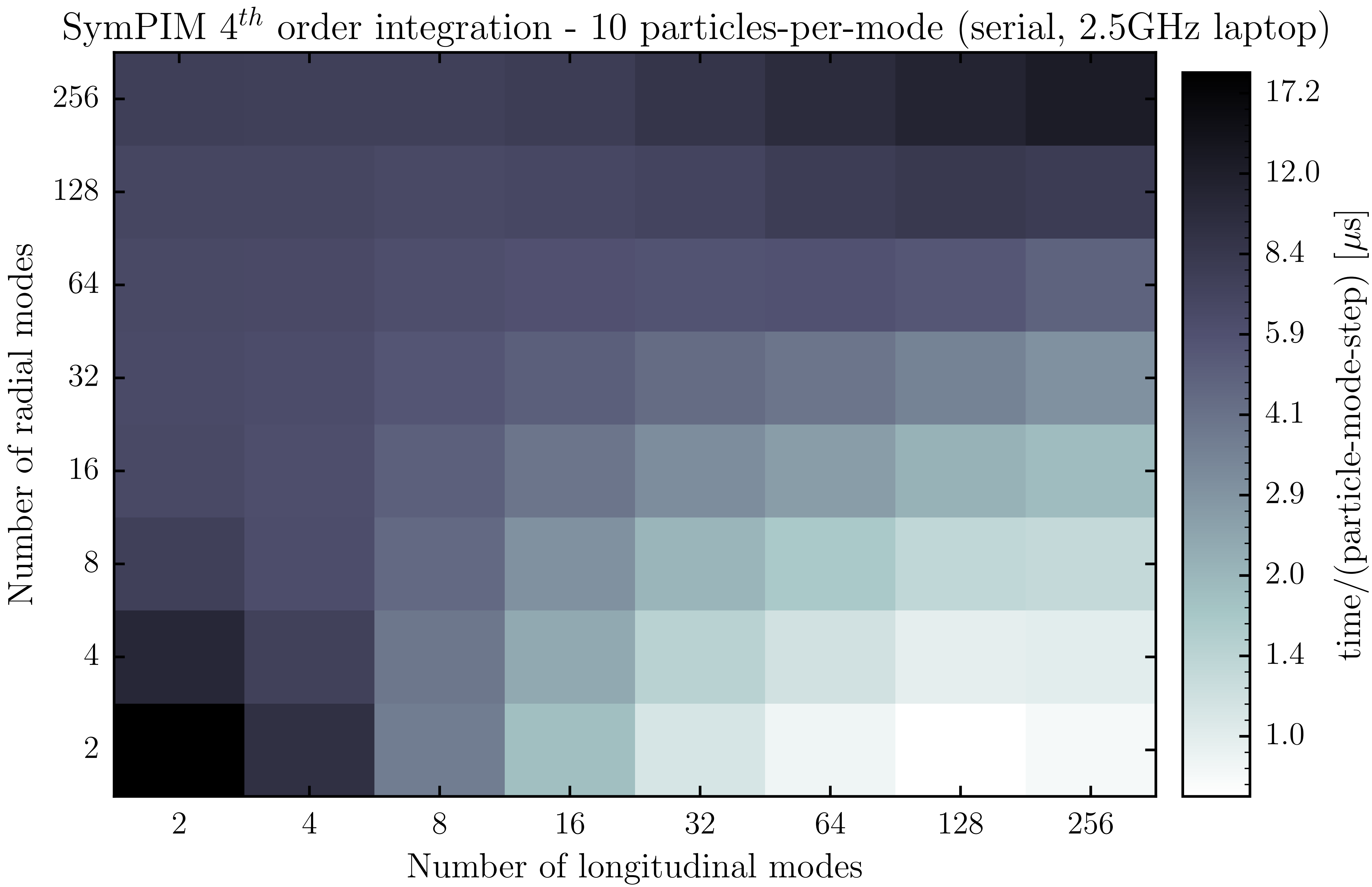
This works for the symplectic particle-in-mode approach



Performance — 2nd Order



Performance — 2nd Order



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