An implicit particle code with *exact* energy and charge conservation for electromagnetic studies of dense plasmas

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Abstract

A collisional particle code based on implicit energy- and charge-conserving methods is presented. The *particle-suppressed* Jacobian-Free Newton-Krylov (PS-JFNK) method is implemented as a fixed-point iteration method for the particle positions. The model can *exactly* conserve global energy and local charge density and can efficiently use time steps larger than the plasma period. The algorithm's ability to simulate dense plasmas accurately and efficiently is quantified by simulating the dynamic compression of a plasma slab via a magnetic piston in 1D planar geometry. Analogous results from a cylindrical implementation of the code are presented.

The θ-implicit PIC method[1,2,4,5]

Particles & fields advanced using:

- time-centered velocity/current
- time-biased fields

$$\mathbf{h}^{n+\theta} = (1-\theta)\,\mathbf{h}^{n} + \theta\mathbf{h}^{n+1}$$

$$1/2 \le \theta \le 1$$

$$\bar{\mathbf{h}} \equiv \left(\mathbf{h}^{n} + \mathbf{h}^{n+1}\right)/2$$

Ensemble of macro particles for f(x,v)

$$\frac{\mathbf{x}_p^{n+1} - \mathbf{x}_p^{n}}{\Delta t} = \bar{\mathbf{v}}_p,$$

$$\frac{\mathbf{v}_p^{n+1} - \mathbf{v}_p^{n}}{\Delta t} = \frac{q_p}{m_p}\left(\mathbf{E}_p^{n+\theta} + \bar{\mathbf{v}}_p \times \mathbf{B}_p^{n+\theta}\right)$$

$$\bar{\mathbf{J}}_g = \sum_s \sum_{p\in s} \frac{q_p \bar{\mathbf{v}}_p}{\Delta V_g} S_{gp}^{\mathbf{J}}$$

$$\mathbf{E}_p^{n+\theta} = \sum_g \mathbf{E}_g^{n+\theta} S_{gp}^{\mathbf{E}},$$

$$\mathbf{B}_p^{n+\theta} = \sum_g \mathbf{B}_g^{n+\theta} S_{gp}^{\mathbf{B}},$$

Finite difference for fields

$$\frac{\mathbf{E}_g^{n+1} - \mathbf{E}_g^{n}}{c^2\Delta t} = \nabla \times \mathbf{B}_g^{n+\theta} - \mu_0 \bar{\mathbf{J}}_g,$$

$$\frac{\mathbf{B}_g^{n+1} - \mathbf{B}_g^{n}}{\Delta t} = -\nabla \times \mathbf{E}_g^{n+\theta},$$

- Monte-Carlo scattering method for Coulomb collisions[3]
- Charge-conserving shape factor used for $\mathbf{J}_g$ (i.e., S_{gp}^{J})[1,7,8]
- Fully implicit ➔ can use large grid cells (e.g., wrt Debye length) and large time steps (e.g., wrt plasma period), but need to solve large nonlinear system

Discrete law for global energy

$$W_E^n + W_B^n = \frac{\epsilon_0}{2}\sum_g |\mathbf{E}_g^n|^2 \Delta V_g + \frac{1}{2\mu_0}\sum_g |\mathbf{B}_g^n|^2 \Delta V_g, \quad W_{parts}^n = \sum_s \sum_{p\in s} \frac{m_p}{2}|\mathbf{v}_p^n|^2$$

$$W_{tot}^{n+1} - W_{tot}^{n} + \sum_{g\in\mathbf{A}} \mathcal{S}_g^{n+\theta}\cdot\Delta\mathbf{A}\Delta t = -\phi \sum_g \left[\epsilon_0 |\mathbf{E}_g^{n+1} - \mathbf{E}_g^{n}|^2 + \frac{1}{\mu_0}|\mathbf{B}_g^{n+1} - \mathbf{B}_g^{n}|^2\right]\Delta V_g$$

$$W_{tot} \equiv W_E + W_B + W_{parts}$$

adjustable numerical damping ($0 \le \phi = \theta - 1/2 \le 1/2$)

- Global energy law requires $S_{gp}^{E} = S_{gp}^{J}$
- $\theta > ½$ ➔ $\phi > 0$ ➔ implicit-biased scheme with inherent damping of high-frequency modes
- $\theta = ½$ ➔ $\phi = 0$ ➔ time-centered scheme where global energy is *exactly* conserved

Implicit solver implementation

Predictor stage (nonlinear iteration $nl = 0$):

1: Initial half time step advance of particle positions: $\bar{\mathbf{x}}_p^{(0)} = \mathbf{x}_p^n + \mathbf{v}_p^n \Delta t/2$.
2: Compute mass matrices, $\mathbb{M}_{gg'}$, using $\bar{\mathbf{x}}_p^{(0)}$ and $\mathbf{B}_g^{(0)} = \mathbf{B}_g^n$.
3: With $\partial\bar{\mathbf{J}}_g/\partial\mathbf{E}_{g'} = \mathbb{M}_{gg'}$, use GMRES to solve Maxwell's Eqs. for $\mathbf{E}_g^{(1)}$ and $\mathbf{B}_g^{(1)}$.

Corrector stage (start with nonlinear iteration $nl = 1$):

4: With $\mathbf{E}_g^{(nl)}$, $\mathbf{B}_g^{(nl)}$, use a Picard method to update the particle quantities, $\bar{\mathbf{x}}_p^{(nl)}$ and $\bar{\mathbf{v}}_p^{(nl)}$.
5: Compute mass matrices, $\mathbb{M}_{gg'}$, using $\bar{\mathbf{x}}_p^{(nl)}$ and $\mathbf{B}_g^{(nl)}$.
6: With $\partial\bar{\mathbf{J}}_g/\partial\mathbf{E}_{g'} = \mathbb{M}_{gg'}$, use GMRES to solve Maxwell's Eqs. for $\mathbf{E}_g^{(nl+1)}$ and $\mathbf{B}_g^{(nl+1)}$.
Option A: repeat steps 4-6 until convergence of system residual, and then go to step 8.
Option B: proceed to step 7.

Finalization stage:

7: With $\mathbf{E}_g^{n+\theta} = \mathbf{E}_g^{(nl+1)}$, $\mathbf{B}_g^{n+\theta} = \mathbf{B}_g^{(nl)}$, and $\bar{\mathbf{x}}_p^{(nl)}$, compute $\bar{\mathbf{v}}_p$ and then set $\bar{\mathbf{x}}_p = \mathbf{x}_p^n + \bar{\mathbf{v}}_p\Delta t/2$.
8: Transform the system variables from $t_{n+\theta}$ and $t_{n+1/2}$ to t_{n+1}.
9: Update particle velocities via scattering: $\mathbf{v}_p^{n+1} \to \mathbf{v}_p^{n+1}$.

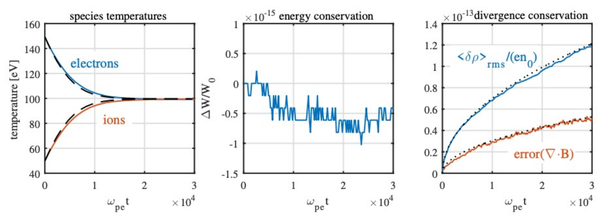
- **Option A** ➔ full nonlinear convergence ➔ exact conservation of global energy and local charge density, but can be computationally expensive (per particle per time step)
- **Option B** ➔ exact conservation of global energy and efficient, but only approximately conserves local charge density.

$$\bar{\mathbf{J}}_g = \hat{\mathbf{J}}_g + \sum_{g'} \mathbb{M}_{gg'}\mathbf{E}_{g'}^{n+\theta} \Rightarrow \partial\bar{\mathbf{J}}_g/\partial\mathbf{E}_{g'}^{n+\theta} = \mathbb{M}_{gg'} \quad \text{(mass matrices[6])}$$

$$\mathbb{M}_{gg'}^{ij} \equiv \sum_s \frac{\Delta t q_s^2}{2m_s}\frac{}{\Delta V_g}\sum_{p\in s} q_p\left[\mathbb{R}_p = \frac{\mathbb{I} - \mathbb{I}\times\mathbf{b}_p + \mathbf{b}_p\mathbf{b}_p}{1+b_p^2}\right] S_{g'p}^{E_j} S_{gp}^{J_i}, \quad \mathbf{b}_p = \frac{\Delta t q_s}{2m_s}\mathbf{B}_p^{n+\theta}$$

Mass matrices are used in place of a direct calculation from the particles (cost ~ num particles) when computing the Jacobian during GMRES iterations (cost ~ num grid points)

2D simulations of thermalization



- Electron-proton plasma: $n_0 = 10^{30}/m^3$, $N_{ppc} = 256$, $\omega_{pe}\Delta t = 0.1$, $\Delta X = \Delta Y = \delta_e/4$, $N_x = N_Y = 40$
- Dashed curves are from 0D Spitzer thermalization model
- Global energy conserved to machine precision
- Root-mean-square of errors in Gauss's law and $\nabla\cdot\mathbf{B}$ on the grid are small and obey random walk statistical behavior

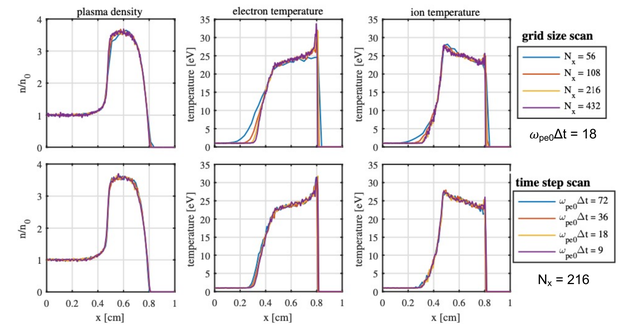
1D Dynamic pinch simulations

Simulating the dynamic compression of a collisional deuterium plasma slab via a magnetic piston (i.e., dynamic pinch)[10] is used to quantify the algorithm's ability to model dense plasmas

- Initial conditions: $R_0 = 1.5$ cm, $T_0 = 1$ eV, $n_0 = 10^{17}/cm^3$
- Magnetic piston is that corresponding to 200 kA of current
- Characteristic implosion time is in the 100-200 ns range

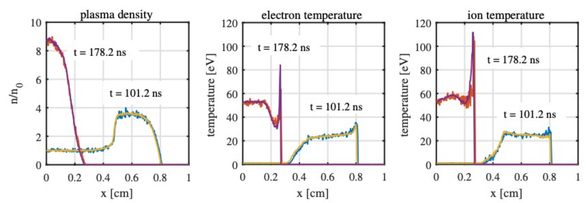
Parameter estimates for different stages of the dynamic pinch simulations

	physical parameters: n [1/cm^3]	T [eV]	B_y [T]	spatial scales [μm]: λ_{De}	δ_e	λ_e	time scales [ps]: $1/\omega_{pe}$	τ_e	$1/\Omega_{ce}$
initial	1.0×10^{17}	1.0	0.0	2.4×10^{-2}	17	0.14	5.6×10^{-2}	0.34	0.0
compresssion	3.8×10^{17}	23.0	2.67	5.8×10^{-2}	8.6	20.0	2.9×10^{-2}	9.9	2.1
stagnation (CAR)	1.0×10^{18}	53.0	2.67	5.4×10^{-2}	5.3	40.5	1.8×10^{-2}	13.3	2.1
stagnation (CYL)	4.5×10^{18}	200	13.4	5.0×10^{-2}	2.5	128	8.4×10^{-3}	21.6	0.43



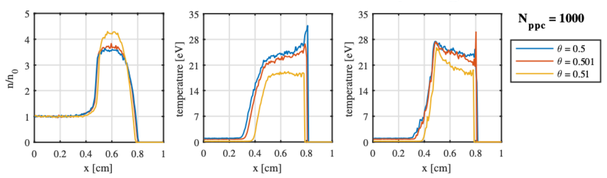
Planar simulation results during compression (t = 101 ns).
➔ Can under resolve Debye length (by factors order 1000 here) and plasma frequency (factors order 100 here) while maintaining physical accuracy

Low vs high particle resolution



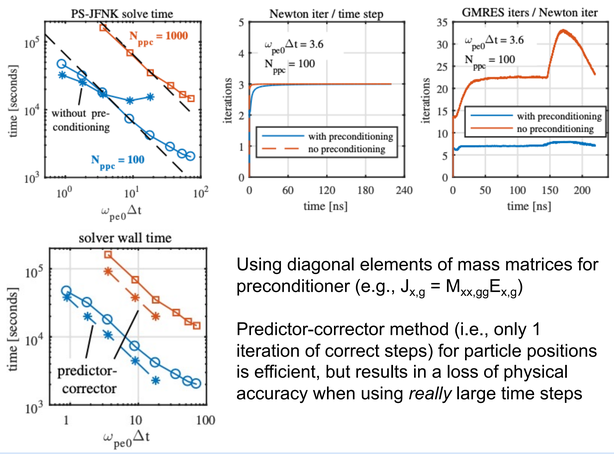
Can use a moderate value for N_{ppc} and maintain accuracy
➔ direct consequence of *exact* energy conservation

Effects of damping



Even a small amount of damping (which is inherent in conventional implicit PIC methods[10]) causes a lack of accuracy due to time-cumulative degradation of energy conservation

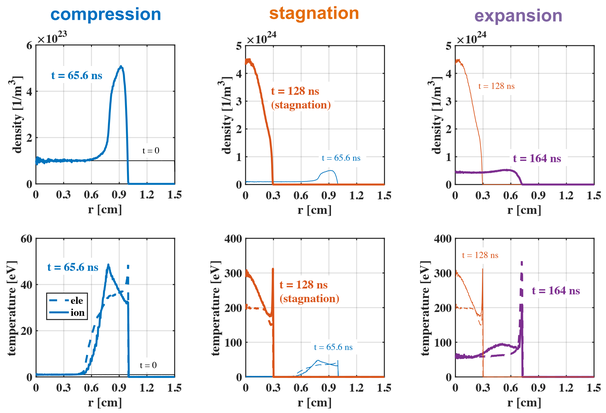
Solver performance with Δt



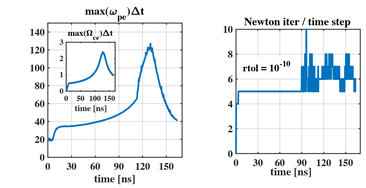
Using diagonal elements of mass matrices for preconditioner (e.g., $J_{x,g} = M_{xx,gg}E_{x,g}$)

Predictor-corrector method (i.e., only 1 iteration of correct steps) for particle positions is efficient, but results in a loss of physical accuracy when using *really* large time steps

Dynamic pinch simulations in cylindrical geometry

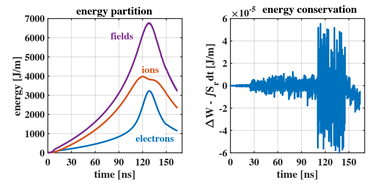


Same physical parameters as before, but in 1D Cylindrical geometry. Tight relative tolerance used for the nonlinear solver (10^{-10}). Nr = 432, Δt = 1ps. Uniform particle weights.



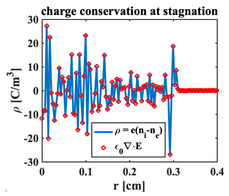
Large time step ✅

More Newton iters needed once hot electrons in shock front reach axis



Global energy conservation ✅

Local charge conservation ✅



Conclusions

Exact global energy conservation + local charge conservation
➔ accurate PIC-MCC simulations of dynamic compression of a plasma with large grid cells, large time steps, and modest number of particles.
Next steps: 2D cylindrical and 1D spherical geometries.

References

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