An implicit, energy-conserving and asymptotic-preserving time integrator for particle-in-cell simulation of magnetized plasmas

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Outline

Context:

- Kinetic equations for plasmas
- Particle in Cell methods
  - Recent implicit version
- Motion in a strong magnetic field

Implicit, AP time integrator:

- "Effective force" to capture ∇B drift
- Considerable care needed to conserve energy
- Time-step restrictions, FLR effects, and adaptivity

Numerical Examples:

- Single particle motion in magnetic mirror, tokamak equilibrium, etc.

Kinetic Plasma Simulation

We're interested in solving

$$\partial_t f + \mathbf{v} \cdot \nabla_x f + \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_v f = 0 \tag{1}$$

for $f(\mathbf{x}, \mathbf{v}, t)$, particularly in cases for which the magnetic field $\mathbf{B}$ may be "very large".

High-dimensionality motivates particle-based methods: Postulate

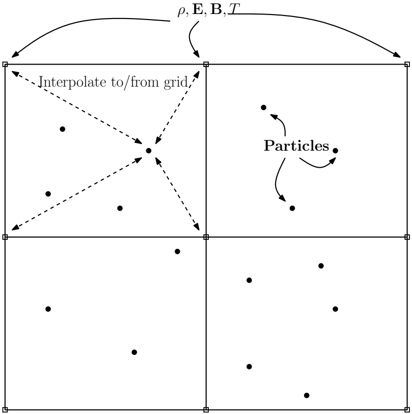
$$f \approx \sum_p S(\mathbf{x} - \mathbf{x}_p)\delta(\mathbf{v} - \mathbf{v}_p), \tag{2}$$

so each "particle" traces characteristics:

$$\dot{\mathbf{x}}_p = \mathbf{v}_p, \qquad \dot{\mathbf{v}}_p = \frac{q}{m} (\mathbf{E} + \mathbf{v}_p \times \mathbf{B}) \tag{3}$$

Computing $\mathbf{E}, \mathbf{B}$ directly via particle-particle interactions is an $O(N_p^2)$ operation (at least, without FMM), so...

PIC Summary



- Interpolate particle properties onto grid
- Compute $\mathbf{E}, \mathbf{B}$ on grid (FEM, FFT, FMM, etc.)
- Interpolate force back onto particle positions
- Update particle $\mathbf{x}$, $\mathbf{v}$ using fields:

$$\mathbf{v}^p_{n+1} = \mathbf{v}^p_n + (\mathbf{E}^p + \mathbf{v}^p \times \mathbf{B}_p)\Delta t$$
$$\mathbf{x}^p_{n+1} = \mathbf{x}^p_n + \mathbf{v}^p_{n+1}\,\Delta t$$

Implicit PIC

Work of Chen, Chacón and others shows that a Crank-Nicolson particle push

$$\begin{aligned} \mathbf{x}^{n+1} &= \mathbf{x}^n + \Delta t \mathbf{v}^{n+1/2}, \\ \mathbf{v}^{n+1} &= \mathbf{v}^n + \Delta t \frac{q}{m}\left[\mathbf{E}^{n+1/2} + \mathbf{v}^{n+1/2} \times \mathbf{B}^{n+1/2}\right] \end{aligned} \tag{4}$$

coupled to a carefully chosen field solve and their novel technique of *particle enslavement* leads to an implicit PIC scheme that is

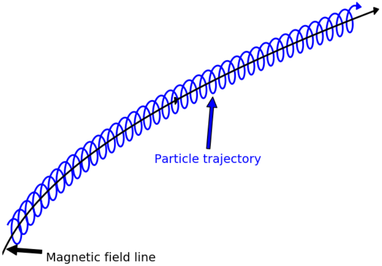
- Computationally feasible
- Exactly energy conserving *for all* Δt, Δx
- Resistant to the finite-grid instability
- Decouples particle and field time-steps
- BUT does not capture guiding center motion for $\Omega_c \Delta t \gg 1$

Fast Gyration

- Aside from high-dimensionality, plasmas suffer from a zoo of disparate time-scales
- We focus on a particular time-scale gap here:
  - In strong magnetic fields, gyration about the field line has frequency

$$\Omega_c = \frac{qB}{m} \tag{5}$$

    that is faster than anything else of interest.



The Traditional Approach: (Drift/Gyro)kinetics

The traditional approach - called (drift/gyro)kinetics - is:

- Analytically remove the fast time-scale from the governing equations by asymptotic expansion
- Numerically solve the new, reduced equations

This has been very successful, but presents two important problems:

- Boundary conditions
- What if $\Omega_c^{-1} \ll \tau_{\text{interesting}}$ is only true in *a portion* of the domain? e.g. tokamak edge

Asymptotic Preserving (AP) Schemes

Asymptotic preserving (AP) schemes take a different approach to confronting the fast scale:

- Numerically simulate the full, original governing equations
- BUT make sure your numerical scheme respects asymptotic limit(s)
- Then, you can take large time-steps compared to fast scale

This avoids both previous issues:

- Boundary conditions are just those for the original equations
- Simple to step over fast scale only when justifiable

Single particle motion

Single particle motion in prescribed electromagnetic fields satisfies

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \mathbf{v}, \\ \frac{d\mathbf{v}}{dt} &= \frac{q}{m}\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right). \end{aligned} \tag{6}$$

When gyroradius $\ll$ length-scales and $\Omega_c^{-1} \ll$ time-scales, asymptotic expansion gives

$$\mathbf{v} \approx \mathbf{u} + v_{\|}\mathbf{b} + \mathbf{v}_E + \mathbf{v}_I + \mathbf{v}_B. \tag{7}$$

- $\mathbf{u}$ = Gyration about field line
- $\mathbf{v}_E = \mathbf{E} \times \mathbf{B}/B^2$.
- $\mathbf{v}_I$ = slow drifts induced by changes in $\mathbf{v}_E$ and $\mathbf{b} = \mathbf{B}/B$.
- $\mathbf{v}_B$ = slow drift induced by spatial variation in B.

Existing integrators

Properties of existing 2nd-order time-stepping schemes for $\Omega_c \Delta t \gg 1$:

	Boris/Leapfrog	Crank-Nicolson	BFV[1]	MI[2]
Energy conserving		$\checkmark$		
Correct gyroradius		$\checkmark$	$\checkmark$	$\checkmark$
$\mathbf{E} \times \mathbf{B}$ drift	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$
Inertial drifts	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$
∇B drift	$\checkmark$		$\checkmark$	$\checkmark$

Our goal: A scheme that checks all the boxes!

1: Brackbill/Forslund '85, Vu/Brackbill '90

2: Genoni et al, '10

Starting point: BFV

- Fundamentally, ∇B drift and mirror force arise from "effective" force acting on the guiding center $\mathbf{F} = -\mu \nabla B$ (where $\mu = mu^2/2B$) that C-N misses for $\Omega_c \Delta t \gg 1$.
- BFV attempts to put that force back in:

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \Delta t \frac{q}{m}\left[\mathbf{E}^{n+1/2} + \mathbf{v}^{n+1/2} \times \mathbf{B}^{n+1/2} + \mathbf{F}_{BFV}\right], \quad (8)$$

where

$$\mathbf{F}_{BFV} = -\frac{m\left\|\mathbf{v}_\perp^{n+1} - \mathbf{v}_\perp^n\right\|^2}{8B^{n+1/2}} \nabla B^{n+1/2} \quad (9)$$

- Satisfies

$$\begin{aligned} \Omega_c \Delta t \ll 1 &\implies \mathbf{F}_{BFV} = O(\Delta t^2), \\ \Omega_c \Delta t \gg 1 &\implies \mathbf{F}_{BFV} \approx -\mu \nabla B. \end{aligned} \quad (10)$$

BUT: $\mathbf{F}_{BFV} \cdot \mathbf{v}^{n+1/2} \neq 0$, breaking energy conservation!

Overconstrained

One would really like an effective force $\mathbf{F}_{\mathit{eff}}$ satisfying

- $\Omega_c \Delta t \ll 1 \implies \mathbf{F}_{\mathit{eff}} = O(\Delta t^2)$
- $\Omega_c \Delta t \gg 1 \implies \mathbf{F}_{\mathit{eff}} \approx -\mu \nabla B$
- $\mathbf{F}_{\mathit{eff}} \cdot \mathbf{v}^{n+1/2} = 0$ for all Δt

Unfortunately, the last two constraints are incompatible:

$$\nabla B \cdot \mathbf{v}^{n+1/2} \neq 0 \tag{11}$$

We can settle for a weaker version of the second constraint:

$$\mathbf{F}_{\mathit{eff}} \approx -\mu \nabla B \longrightarrow \langle \mathbf{F}_{\mathit{eff}} \rangle \approx -\mu \nabla B,$$

where $\langle \cdot \rangle$ denotes average over gyration.

The idea: Time-stepping samples a variety of gyrophases for us, so the average of $\mathbf{F}_{\mathit{eff}}$ over several time-steps approximates the gyroaverage operator for us. We call this "implicit gyroaveraging".

Conservative Effective Force

We postulate an effective force of the form

$$\mathbf{F}_{eff} = \left(\mathbf{b} - \frac{v_\parallel \mathbf{v}_\perp}{v_\perp^2}\right) G_\parallel + \left(\mathbf{I} - \frac{\mathbf{v}_\perp \mathbf{v}_\perp}{v_\perp^2}\right) \cdot \mathbf{G}_\perp \tag{12}$$

- Conserves energy $\forall \mathbf{G}$ and avoids mixing parallel and perpendicular motion

Constraints + algebra $\implies$ form of $\mathbf{G}$:

$$\begin{aligned} \mathbf{G} =& F_{BFV,\parallel}\mathbf{b} + \frac{(\mathbf{I} - \widehat{\mathbf{v}}_E\widehat{\mathbf{v}}_E) \cdot \mathbf{F}_{BFV,\perp}}{1 - \eta^2/2} \\ &+ \frac{2}{\eta^2}\widehat{\mathbf{v}}_E \left(\widehat{\mathbf{v}}_E \cdot \mathbf{F}_{BFV,\perp} + \mathbb{1}_{v_E > u} F_{BFV,\parallel} \frac{v_\parallel}{v_E}\right) \end{aligned} \tag{13}$$

where $\eta = \min\{1, u/v_E\}$, $\widehat{\mathbf{v}}_E = \mathbf{v}_E/v_E$.

Going Further: FLR Effects

Scheme just derived captures *drift*-kinetic limit. To get *gyro*kinetic, need to allow *finite Larmor radius* (FLR) effects:

$$\left(\frac{\|\nabla \mathbf{E}\|}{E}\right)^{-1} \sim \text{gyroradius}. \tag{14}$$

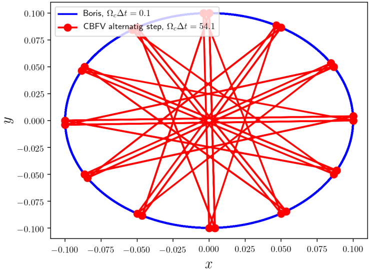
- Changes to asymptotic limit expression: $\mathbf{E} \longrightarrow \langle \mathbf{E} \rangle$
- Challenge for scheme: $\mathbf{E}$ has structure, so can't sample *random* gyrophases, must force time-stepping to sample *equispaced* gyrophases

Going further: FLR effects

Two changes to scheme required:

- Alternate large ($\Omega_c \Delta t \gg 1$) and smaller ($\Omega_c \delta t \sim 1$) time-steps to rig appropriate gyrophase traversal
- Change **E** evaluation from midpoint to trapezoidal so evaluation is on gyro-orbit, not at gyrocenter

$$\mathbf{E}^{n+1/2} = \mathbf{E}\left(\frac{\mathbf{x}^n + \mathbf{x}^{n+1}}{2}\right) \quad \longrightarrow \quad \frac{\mathbf{E}\left(\mathbf{x}^n\right) + \mathbf{E}\left(\mathbf{x}^{n+1}\right)}{2}$$



Time-step Restrictions

Of course, one still cannot take arbitrarily large time-steps. Must resolve spatiotemporal variation in **E**, **B**... but also:

- The time it takes for implicit gyroaverage to be computed accurately must be small
- Anomalous displacement due to inaccuracy in implicit gyroaverage must be small

Time-step Restrictions

Quantitative expressions for the maximum allowable $\Omega_c \Delta t$ are challenging to find in general, but can be done in two important limits:

	Displacement restriction	Avg. restriction
$u^{n+1/2} \gg v_E$	$\min\left\{2(\delta_\perp)^{-1}, \sqrt{2}(\delta_\parallel)^{-1/2}\right\}$	$2\frac{\Omega_c \tau_{res}}{\pi}$
$u^{n+1/2} \ll v_E$	$\sqrt{2}\left(\delta_E + \delta_\parallel\right)^{-1/2}$	$\Omega_c \tau_{res}$

where τ_{res} is the smallest time-scale you wish to resolve,

$$\delta_\perp = \frac{u}{\Omega_c}\frac{\|(\nabla B)_\perp\|}{B}, \quad \delta_\parallel = \frac{v_\parallel}{\Omega_c}\frac{\|(\nabla B)_\parallel\|}{B}, \quad \delta_E = \frac{v_E}{\Omega_c}\frac{\|(\nabla B)_\perp\|}{B}. \tag{15}$$

These restrictions inform adaptive time-stepping procedure.

Numerical Tests

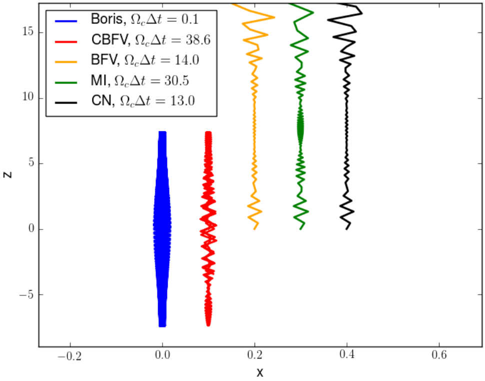
So far, scheme primarily tested on single-particle motion... Several different field configurations:

- Magnetic mirror
- Non-adiabatic jump in μ
- Tokamak equilibrium with electric field

Implementation in self-consistent implicit PIC scheme is in progress with promising initial results.

Configured so that particles with $v_{\|} < v_{crit}$ are confined, others are "passing".

$$\underline{v_{\|} = 0.999 v_{crit}}$$

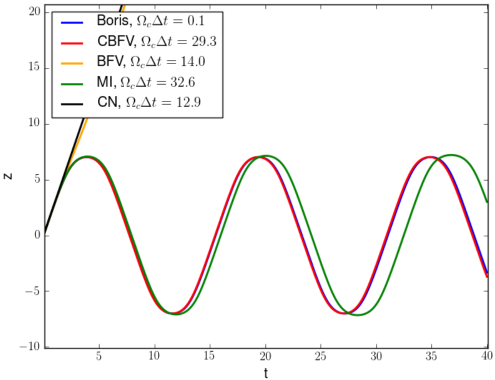


New scheme predicts trapped passing boundary to within 0.05%

Magnetic Mirror

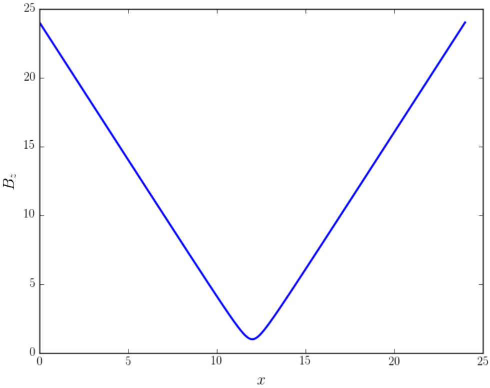
Configured so that particles with $v_{\|} < v_{crit}$ are confined, others are "passing".

$$v_{\|} = 0.98 v_{crit}$$



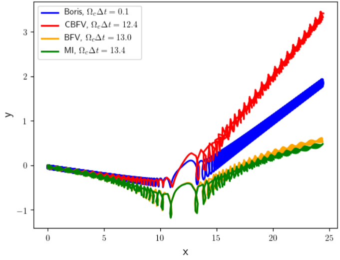
Also get improved prediction of "bounce frequency".

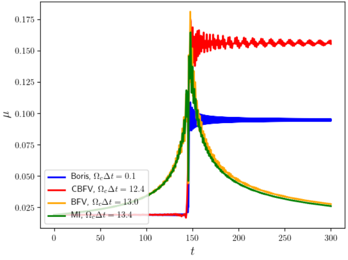
$$\mathbf{E} = 2\widehat{\mathbf{y}}, \qquad \mathbf{B} = \widehat{\mathbf{z}}\sqrt{1 + 4(x-12)^2}$$



$\mathbf{E} \times \mathbf{B}$ drift pushes particle through unmagnetized region...

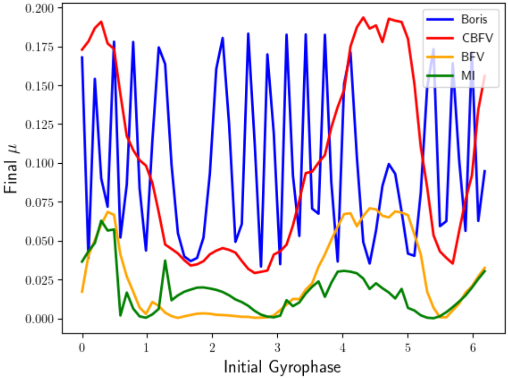
Unmagnetized Region





- Size of jump in μ is *very* sensitive to initial gyrophase
- Can't get jump right for any particular gyrophase b/c $\Omega_c \Delta t > 1$ inherently misses gyrophase information
- BUT can hope to get the jump correct on average

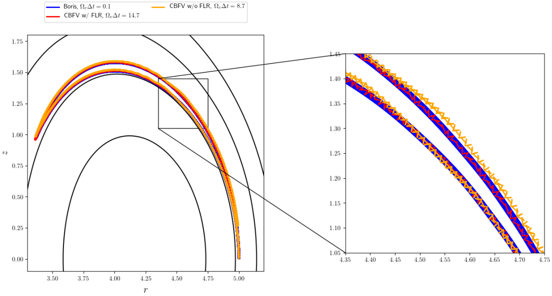
Unmagnetized Region



- Reproduce gyroaveraged μ jump within 0.8%
- Standard deviation within 14%
- (drift/gyro)kinetics would predict no change in μ

Tokamak equilibrium with $\mathbf{E}$ field

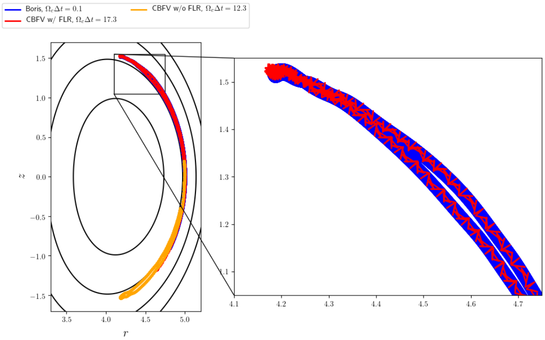
- $\mathbf{B}$ is a Solov'ev equilibrium field + toroidal component $\propto 1/r$
- $\mathbf{E}$ has $k_\perp \rho \approx 1.2$



New version captures small FLR corrections

Tokamak equilibrium with **E** field - Even larger $k_\perp \rho$

- **B** is a Solov'ev equilibrium field + toroidal component $\propto 1/r$
- **E** has $k_\perp \rho \approx 2.4$



FLR corrections still improve accuracy, but working on sensitivity to adaptive time-stepping

Conclusions

- First-of-kind scheme that both preserves asymptotic properties and conserves energy
- An alternative to (drift/gyro)kinetic PIC that can handle arbitrary magnetization
- Energy conservation is not just pedantry, has qualitative consequences on orbits
- Work still to-do:
  - Continue in-progress implementation in implicit PIC schemes
  - Improve preconditioning of implicit solve
  - Further refinement/generalization of adaptive time-stepping

<u>For more detail, see</u>: L.F. Ricketson, L. Chacón, "An energy-conserving and asymptotic-preserving charged-particle orbit implicit time integrator for arbitrary electromagnetic fields." *JCP* (2020): 109639

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