Implicit Time Integration for Particle Treatment within a Particle-in-Cell Solver

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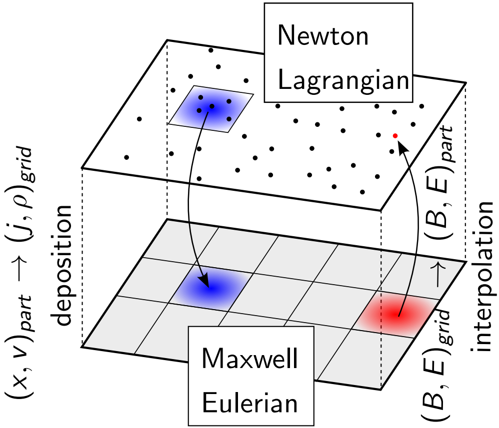
IAG

Is There a Good Reason for Implicit Time Integration?



Explicit Solver

- Highly efficient
- Easy programming
- Easy to optimize

Implicit Solver

- Time scale requirements
- $\Delta t_{\mathrm{P,heavy}} > \Delta t_{\mathrm{P,e}} \gg \Delta t_{\mathrm{Field}}$
- Promise: Significant speed up

Content

Hyperbolic-Parabolic Maxwell's Equations

By the use of Lagrangian multipliers, Maxwell's Equations are modified to include the divergence constraints ($\nabla \cdot \vec{E} = \tilde{\rho}$ and $\nabla \cdot \vec{B} = 0$).[1],[2]

$$\frac{\partial \vec{E}}{\partial t} = c^2 \nabla \times \vec{B} - \chi c^2 \nabla \Psi - \frac{\vec{j}}{\varepsilon_0}$$

$$\frac{\partial \vec{B}}{\partial t} = - \nabla \times \vec{E} - \chi \nabla \Phi$$

$$\frac{\partial \Phi}{\partial t} = - \chi c^2 \nabla \cdot \vec{B} - \kappa \Phi$$

$$\frac{\partial \Psi}{\partial t} = - \chi \nabla \cdot \vec{E} + \chi \frac{\varrho}{\varepsilon_0} - \kappa \Psi$$

- Scalar multipliers: Φ - Magnetic field and Ψ - Electric field

[1] C.-D. Munz et al. "Divergence Correction Techniques for Maxwell Solvers Based on a Hyperbolic Model". In: *J. of Comp. Phys.* 161.2 (2000), pp. 484–511.

[2] A. Dedner et al. "Hyperbolic Divergence Cleaning for the MHD Equations". In: *J. of Comp. Phys.* 175.2 (2002), pp. 645–673.

Equation of Motion

Approximation of the distribution function by a certain number of particles

$$f(\vec{x}, \vec{v}, t) = \sum_{k=1}^{N} w_k \delta(\vec{x} - \vec{x}_k(t)) \delta(\vec{v} - \vec{v}_k(t)).$$

For each particle the equation of motion is

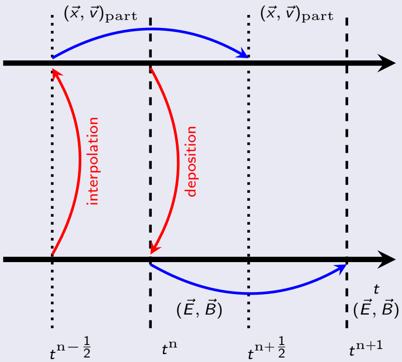
$$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \vec{v}$$
$$\frac{\mathrm{d}\gamma\vec{v}}{\mathrm{d}t} = \frac{q}{m_0}\left[\vec{E} + \vec{v} \times \vec{B}\right]$$

with

$$\gamma = \frac{1}{\sqrt{1 - |\vec{v}|^2/c^2}}$$

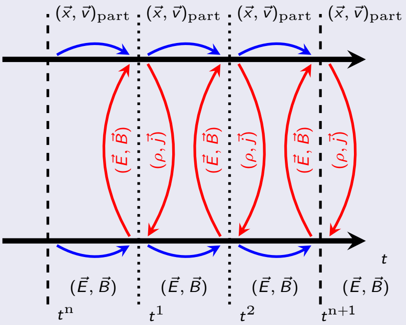
Approach to Time Integration

Typical Explicit PIC



- energy-bounded

Implicit Runge-Kutta



- high-order
- implicit-explicit[3]

[3] C. A. Kennedy and M. H. Carpenter. "Additive Runge–Kutta schemes for convection–diffusion–reaction equations". In: *Appl. Num. Math.* 44.1–2 (2003), pp. 139–181.

Implicit Particle Treatment

- Implicit equation of motion

$$\vec{x}^{s+1} - \vec{x}^{s} + \alpha \Delta t \, \vec{v}^{s+1} = 0$$
$$\vec{v}^{s+1} - \vec{v}^{s} + \alpha \Delta t \, \frac{q}{m_0} \left[\vec{E}^{s+1} + \vec{v}^{s+1} \times \vec{B}^{s+1} \right] = 0$$

  - Particles only interact via Lorentz force
  - Solved by Jacobian-Free Newton-GMRES (6x6) per particle[4]
- Decoupling of implicit Maxwell solver and implicit particle solver[5]
  - Field and particles are solved separately
  - Linear field equation is solved by a Krylov-subspace method[6]

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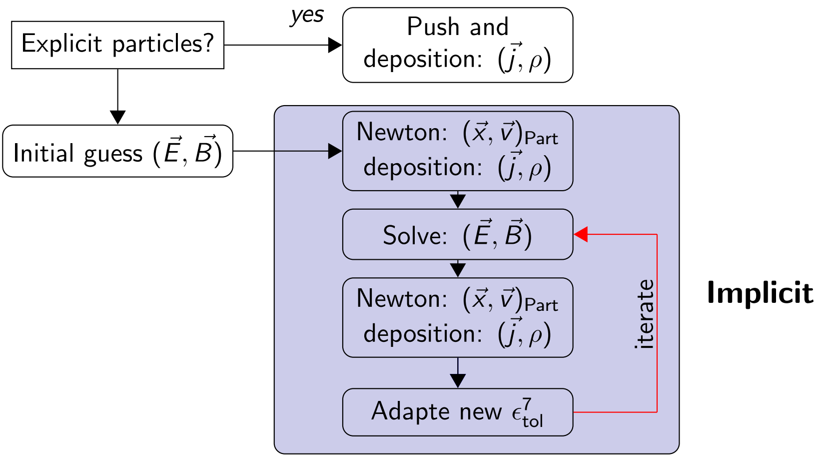
[4] C. T. Kelley. *Iterative methods for linear and nonlinear equations*. SIAM, 1995.

[5] G. Lapenta. "Particle simulations of space weather ". In: *J. of Comp. Phys.* 231.3 (2012), pp. 795–821.

[6] Youcef Saad. *Iterative Methods for Sparse Linear Systems*. 2. ed. SIAM, 2003.

Solving the Complete System



[7] S. C. Eisenstat and H. F. Walker. "Choosing the Forcing Terms in an Inexact Newton Method". In: *SIAM J. Sci. Comp.* 17.1 (1996), pp. 16–32.

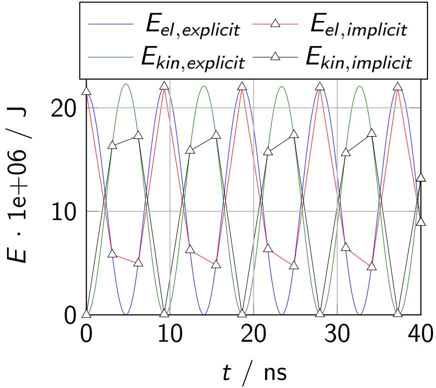
Plasma Wave

Setup

- $N_{\text{Part}} = 1.6 \times 10^3$ electrons & positrons
- Domain: $2\pi x 0.2 x 0.2$
- $1D$ shape-function

Time Integration

- ERK-ESDIRK $O4$



Conclusion

- Proof of concept: explicit, implicit-explicit or fully implicit particles

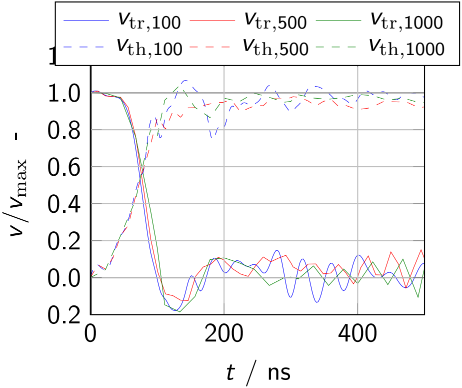
Two-Stream Instability

Setup

- $N_{\text{Beam}} = 900$ electrons
- $3D$ shape-function

Time Integration

- EXRK-ESDIRK $O4$
- CFL$= 100, 500, 1000$



Conclusion

- Conversion from translational into thermal velocity.

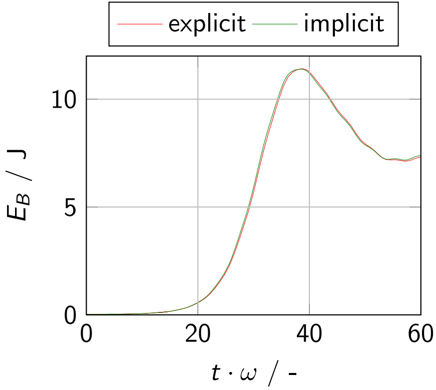
Weibel Instability

Setup

- $(15 \times 15 \times 1)\frac{c}{\omega}$
- $N_{\mathrm{p,i}} = 9 \times 10^5$
- $N_{\mathrm{DG}} = 5$
- $3D$ shape-function

Time Integration

- Low-storage ERK $O4$
- ESDIRK $O4$



Conclusion

- Increase in $|\vec{B}|$ is observed.

Conclusion

Summary

- Fully implicit and implicit-explicit particle treatment
- Splitting of implicit step
  - Particles by Jacobian-free Newton-GMRES
  - Field by BiCGStab
- Speed-up compared to pure Maxwell solver
- In contrast to pure explicit scheme: memory limitation

Outlook

- Limitation: each MPI process requires whole domain
- Investigate different optimized purely implicit schemes
- Automatic selection of implicit-explicit particle treatment

Thank you for your attention!

Numerics Research Group (IAG)

New numerical methods, analysis, efficient implementations, multi-scale problems, high performance computing

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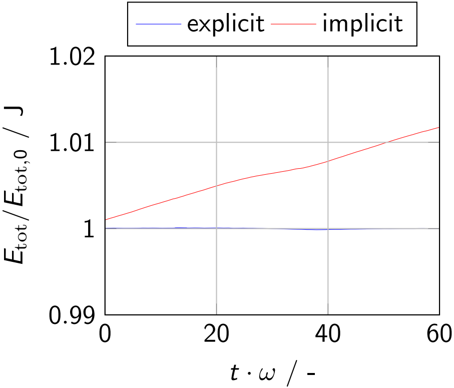
Weibel Instability - Total Energy

Setup

- $15 \times 15 \times 1 \frac{c}{\omega}$
- $N_{\mathrm{p,i}} = 9 \times 10^5$
- $N_{\mathrm{DG}} = 5$
- $3D$ shape-function

Time Integration

- Low-storage ERK *O4*
- ESDIRK *O4*



Conclusion

- Implicit scheme: Δt, dissipative, ϵ,..?

Approximation of Matrix-Vector

Newton: $F(x) = 0$
A Matrix-vector multiplication

$$A\vec{v} = F'(x)\vec{v}$$

requires to construct the Jacobian matrix A. However, this could be approximated by

$$A\vec{v} \approx \frac{F(x + hv) - F(x)}{h} \quad \text{with}$$

$$h = \sqrt{\epsilon_{\mathrm{mach}}}||x||/||v||$$

8

[8] C. T. Kelley. *Iterative methods for linear and nonlinear equations.* SIAM, 1995.

Computational Time

- Physics of interest remains captured

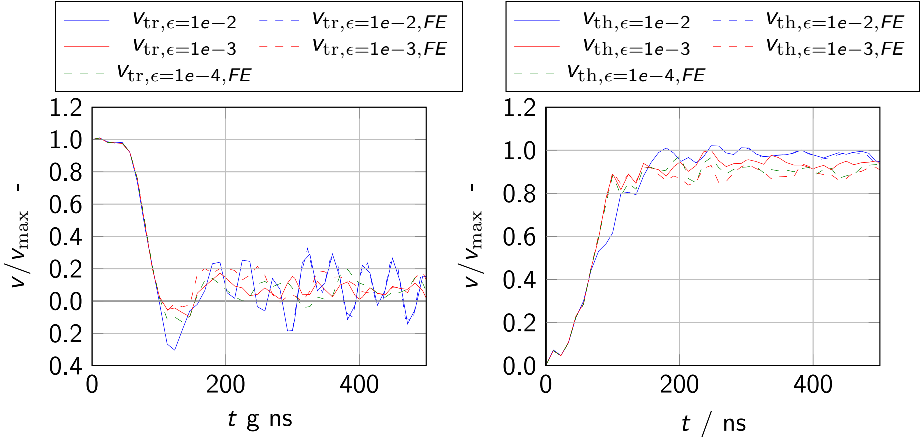
Table: computational time

$\Delta t/\Delta t_{\text{ex}}$	explicit 1.0	imex 95	190	470	950
$t_{\text{sim}}/t_{\text{sim,ex}}$	1.0	7.5	3.6	5.2	9.2

Table: impact of tolerance for $\Delta t/\Delta t = 470$

rel. tolarance Eisenstat-Walker	1×10^{-4} 1/1/1	1×10^{-3} 1/1/0&1	1×10^{-2} 1/1/0	1×10^{-2} 1/1/1	1×10^{-1} 1/1/0&1
$t_{\text{sim}}/t_{\text{sim,ex}}$	1.3	1.0	0.7	0.3	-

Twostream Tolerance Issue



- Huge impact of abort tolerance

Comparision with explicit Boris-Leapfrog

Superposition of gyration and $\nabla \vec{B}$ drift[9] compared with RK[10]

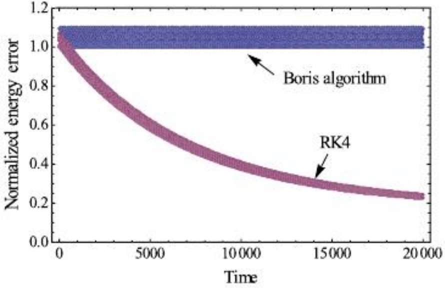


Figure: Results copied from Qin et al.

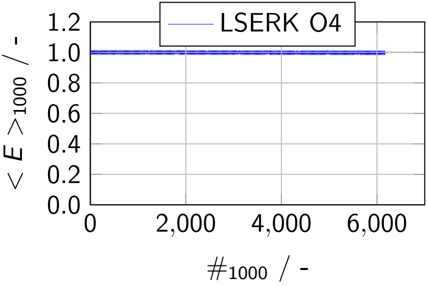


Figure: Similar setup, optimized low storage RK

[9] H. Qin et al. "Why is Boris algorithm so good?" In: *Phys. of Plasmas* 20.8 (2013), p. 084503.

[10] M. H Carpenter. "Fourth-Order 2N-Storage Runge-Kutta Schemes". In: *NASA Technical Memorandum* 109112 (1994), pp. 1–26.

Modeling the Physics

Most general expression of a collision-free plasma (Vlasov,1945)

$$\frac{\partial f(\vec{x},\vec{v},t)}{\partial t} + \overbrace{\vec{v}\cdot\nabla_{\vec{x}} f(\vec{x},\vec{v},t)}^{\text{convection}} + \overbrace{\frac{\vec{F}}{m}\cdot\nabla_{\vec{v}} f(\vec{x},\vec{v},t)}^{\text{Lorentz force}} = 0$$

The Vlasov equation describes

- The change of microscopic distribution functions $f(\vec{x},\vec{v},t)$ over time

Depending on

- The velocities of particles and their spatial distribution and
- The acceleration of particles due to the Lorentz forces

$$\vec{F} = q\left[\vec{E}(\vec{x},t) + \vec{v}\times\vec{B}(\vec{x},t)\right]$$

Discontinuous Galerkin Spectral Element Formulation

In flux formulation, the Maxwell's equations yield

$$\vec{u}_t + \sum_{\mathrm{d}=1,3} \underline{\underline{F}}_d \vec{u}_{x_\mathrm{d}} = \vec{s}$$

Transformation into a unit reference element, multiplication by a test function ϕ and a spacial integration yield

$$\int_\Omega J \frac{\partial \vec{u}}{\partial t} \phi d\vec{\xi} + \sum_{\mathrm{d}=1,3} \int_\Omega \underline{\underline{\mathcal{K}}}_d \frac{\partial \vec{u}}{\partial \xi_\mathrm{d}} \phi d\xi_\mathrm{d} = \int_\Omega J \vec{s} \phi d\vec{\xi}$$

An integration by part results in

$$\frac{\partial}{\partial t} \int_\Omega J \vec{u} \phi d\vec{\xi} + \int_{\partial\Omega} \underline{\underline{\mathcal{F}_\mathrm{n}}} \vec{u}^* \phi d\partial\xi - \sum_{\mathrm{d}=1,3} \int_\Omega \underline{\underline{\mathcal{K}}}_d \frac{\partial \phi}{\partial \xi_\mathrm{d}} \vec{u} d\xi_\mathrm{d} = \int_\Omega J \vec{s} \phi d\vec{\xi}$$

[11], [12]

[11] D. A. Kopriva. *Implementing Spectral Methods for Partial Differential Equations*. Springer, 2009, p. 401. ISBN: 978-90-481-2260-8.

[12] F. Hindenlang et al. "Explicit discontinuous Galerkin methods for unsteady problems". In: Computers & Fluids 61 (May 2012), pp. 86–93.

Solving the non-linear complete System

Process during each RK stage:

- Push of explicit particles and source $(\vec{j}, \rho)$
- Initial guess for $\vec{E}, \vec{B}$
- Outer iteration:
  1. Particle Newton to update $\vec{x}, \vec{v}$
  2. Recompute implicit source $(\vec{j}, \rho)$
  3. Update $\vec{E}, \vec{B}$ by a linear solver
  4. Adapt tolerance for next step[13].

Iterate steps (1) – (4) until convergence is achieved.

[13] S. C. Eisenstat and H. F. Walker. "Choosing the Forcing Terms in an Inexact Newton Method". In: *SIAM J. Sci. Comp.* 17.1 (1996), pp. 16–32.