Méthodes numériques pour des modèles hybrides fluide-cinétique de plasmas

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Outline

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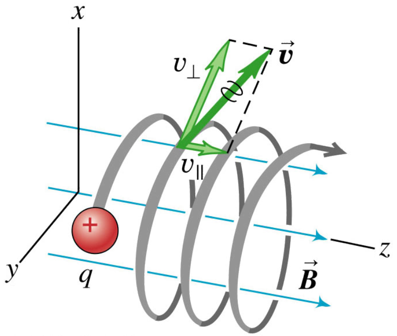
Vlasov-Maxwell $1dz - 3dv$ model

Transport of electron density distribution $f = f(t, z, \boldsymbol{v})$,
$\boldsymbol{B}(t,z) = (B_x, B_y, 0)(t,z)$, $\boldsymbol{E}(t,z) = (E_x, E_y, 0)(t,z) \in \mathbb{R}^2$,
$z \in [0, L]$ (periodic), $\boldsymbol{B}_0 = (0,0,B_0)^\top$, $\boldsymbol{v} \in \mathbb{R}^3$, $v_\perp = (v_x, v_y, 0)^\top \in \mathbb{R}^2$:

$$\begin{cases} \partial_t f + v_z \partial_z f - (\boldsymbol{E} + \boldsymbol{v} \times (\boldsymbol{B} + \boldsymbol{B}_0)) \cdot \nabla_{\boldsymbol{v}} f = 0 \\ \partial_t \boldsymbol{B} = J \partial_z \boldsymbol{E} \\ \partial_t \boldsymbol{E} = -J \partial_z \boldsymbol{B} + \int_{\mathbb{R}^3} v_\perp f \, \mathrm{d}\boldsymbol{v} \end{cases}$$

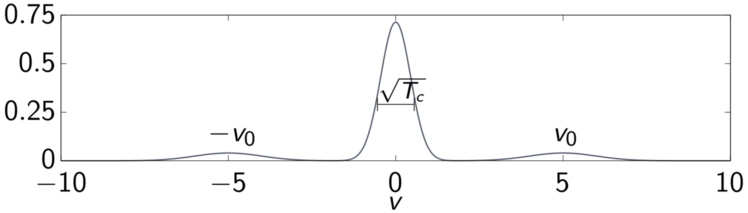
$$J = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



Vlasov-Maxwell $1dz - 3dv$ model

Motivation:

- We want high order methods in $(z, \boldsymbol{v})$
  - FFT in z + WENO in $\boldsymbol{v}$
- We want high order methods in time t
  - splitting method vs exponential integrator



- We consider an initial condition of the form $f = f_c + f_h$ with: $f_c(t=0, z, \boldsymbol{v}) = \rho_c(t, z)\delta_{\boldsymbol{v}=\boldsymbol{u}_c(t,z)}(\boldsymbol{v})$

The idea

Grid methods can't have an initial condition like:

$$f_0(z, \boldsymbol{v}) = \underbrace{\rho_{c,0}(z)\delta_{\boldsymbol{v}-\boldsymbol{u}_{c,0}}(\boldsymbol{v})}_{f_{c,0}} + f_{h,0}(z, \boldsymbol{v})$$

The main idea is to derive a **linearized hybrid fluid/kinetic model**:

- Split $f = f_c + f_h$ (2 Vlasov equations)
- Compute momentum of f_c
  - *Cold plasma approximation*: $\frac{T_c}{T_h} \ll 1 \rightarrow \cancel{f_c(t, z, \boldsymbol{v})} \rightarrow \boldsymbol{j}_c(t, z)$
  - Fluid dynamic for cold particles (no velocity grid) ✔
  - Linearized fluid equations
- Hypothesis on hot particles: $\int_{\mathbb{R}^3} f_h(t, z, \boldsymbol{v})\,\mathrm{d}\boldsymbol{v} \ll \rho_c(t, z)$
  - Kinetic dynamic for hot particles

Tronci et al. 2014, *Plasma Physics and Controlled Fusion*

Holderied et al. 2020, *Journal of Computational Physics*

Linearized hybrid Vlasov-Maxwell $1dz - 3dv$ model

The new model: a nonlinear transport in $(z, v_x, v_y, v_z) \in \Omega \times \mathbb{R}^3$ of:

- a cold (fluid) electron density distribution, reconstruction from current variable $\boldsymbol{j}_c(t,z) = q_e \rho_c(t,z) \boldsymbol{u}_c(t,z) = (j_{c,x}, j_{c,y}, 0)(t,z)$
- a hot (kinetic) electron density distribution $f_h(t, z, \boldsymbol{v})$

$$\begin{cases} \partial_t \boldsymbol{j}_c = \Omega_{pe}^2 \boldsymbol{E} - J \boldsymbol{j}_c B_0 \\ \partial_t \boldsymbol{B} = J \partial_z \boldsymbol{E} \\ \partial_t \boldsymbol{E} = -J \partial_z \boldsymbol{B} - \boldsymbol{j}_c + \int_{\mathbb{R}^3} v_\perp f_h \, \mathrm{d}\boldsymbol{v} \\ \partial_t f_h + v_z \partial_z f_h - (\boldsymbol{E} + \boldsymbol{v} \times (\boldsymbol{B} + \boldsymbol{B}_0)) \cdot \nabla_{\boldsymbol{v}} f_h = 0 \end{cases}$$

with:

$$J = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Convergence when $T_c \to 0$ for 1dx-1dv model

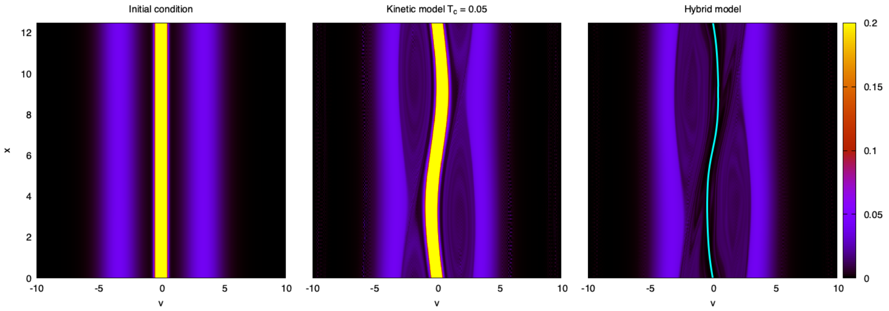


Figure: Initial condition (left), solution at $t = 200$ of the full kinetic model with $T_c = 0.05$ (middle) and the hybrid model (right).

✔ Good agreement between kinetic (f) model and hybrid model ($f_h + u_c$)

Outline

Numerical methods

Semi-discretization in space-velocity:

- In space z: we use a Fourier transform (FFT).
- In velocity $\boldsymbol{v}$: we use WENO5 or Lagrange 5.

Two time integrators to compute a numerical solution of abstract model:

$$\dot{u} = L(t, u) + N(t, u), \quad u(0) = u_0$$

$u \in \mathbb{R}^d$, L and N functions $(t, u) \in \mathbb{R}_+ \times \mathbb{R}^d \mapsto \mathbb{R}^d$, $d \in \mathbb{N}$.

- Splitting method (Lie, Strang, Suzuki)
- Lawson method (LRK(4,4), LDP4(3))

Splitting method

Successive resolution of:

$$\begin{aligned} \dot{u} &= L(t,u) & \to \tilde{u}_t &= \varphi_t^{[L]}(u_0) \\ \dot{u} &= N(t,u) & \to \tilde{u}_t &= \varphi_t^{[N]}(u_0) \end{aligned}$$

Solution at time t:

Lie: order 1 method, composition of sub-steps: $\varphi_t(u_0) \approx \varphi_t^{[L]} \circ \varphi_t^{[N]}(u_0)$

Strang: order 2 method: $\varphi_t(u_0) \approx \mathcal{S}_t(u_0) = \varphi_{t/2}^{[L]} \circ \varphi_t^{[N]} \circ \varphi_{t/2}^{[L]}(u_0)$

Strang 1968, *SIAM Journal on Numerical Analysis*

Suzuki: order 4 method, composition of 5 Strang methods:

$$\varphi_t(u_0) \approx \mathcal{S}_{\alpha_1 t} \circ \mathcal{S}_{\alpha_2 t} \circ \mathcal{S}_{\alpha_3 t} \circ \mathcal{S}_{\alpha_2 t} \circ \mathcal{S}_{\alpha_1 t}(u_0)$$

with: $\alpha_1 = \alpha_2 = \frac{1}{4-\sqrt[3]{4}}$ and $\alpha_3 = \frac{1}{1-4^{\frac{2}{3}}}$

Suzuki 1990, *Physics Letters A*

Splitting method

Pros & Cons

- ✔ Good splitting leads to good long time behavior
- ✔ Error in time only depends on splitting method
- ✔ Split a difficult problem into small easier sub-problems
- ✗ Numerical cost for high order method

Lawson method

$$\dot{u} = Lu + N(t,u)$$

Change of variable: $v = e^{-tL}u$, we obtain:

$$\begin{aligned}\dot{v}(t) &= -Le^{-tL}u(t) + e^{-tL}\underbrace{(Lu(t) + N(t,u))}_{\dot{u}(t)} \\ &= e^{-tL}N(t, e^{tL}v)\end{aligned}$$

which can be solved with a **Runge-Kutta method** in v, that can be rewritten in u. For example with Euler method:

$$v(t^n + \Delta t) \approx v^{n+1} = v^n + \Delta t e^{-t^n L}N(t^n, e^{t^n L}v^n)$$

which can be rewritten, in terms of u:

$$u^{n+1} = e^{\Delta t L}u^n + \Delta t e^{\Delta t L}N(t^n, u^n)$$

Lawson 1967, *SIAM Journal on Numerical Analysis*
Hochbruck and Ostermann 2010, *Acta Numerica*
Hochbruck, Leibold, and Ostermann 2020, *Numerische Mathematik*

Lawson method
Pros & Cons

- ✔ Numerically efficient (order increases linearly-ish with the number of stages)
- ✔ Literature on Runge-Kutta method (embedded-RK, low storage methods, IMEX methods, DIRK methods. . .)
- ✔ Linear part is solved exactly
- ✗ Stability constraint (not from the linear part ✔)
- ✗ Long time behavior
- $\sim$ Needs to compute (efficiently) $e^{\tau L}$ for any $\tau = c_j \Delta t$ and L

Main idea of adaptive time step methods (error estimate)

For a generic ODE $\dot{u} = f(t,u)$, adaptive time step method needs 2 numerical approximations of $u(t^{n+1})$ of different order, p and $p+1$:

$$u^{n+1}_{[p]} = u(t^{n+1}) + \mathcal{O}\left(\Delta t^{p+1}\right), \qquad u^{n+1}_{[p+1]} = u(t^{n+1}) + \mathcal{O}\left(\Delta t^{p+2}\right)$$

Estimate of local error: $$L^{n+1}_{[p]} = \left| u^{n+1}_{[p+1]} - u^{n+1}_{[p]} \right|$$

If $L^{n+1}_{[p]} > tol$: we reject the step and start again from time t^n. **Else** we accept the step. **In both cases**, the optimal new time step is:

$$\Delta t_{\text{opt}} = \sqrt[p]{\frac{tol}{L^{n+1}_{[p]}}}\Delta t^n$$

In practice $u^{n+1}_{[p]}$ is computed from sub-steps of $u^{n+1}_{[p+1]}$.

Dormand and Prince 1978, *Celestial mechanics* (for RK method)

Blanes, Casas, and Thalhammer 2019, *Applied Numerical Mathematics* (for splitting method)

Outline

Linearized hybrid Vlasov-Maxwell model

$U = (\boldsymbol{j_c}, \boldsymbol{B}, \boldsymbol{E}, f_h)^\top$, $\boldsymbol{j_c}(t,z)$,$\boldsymbol{B}(t,z)$,$\boldsymbol{E}(t,z) \in \mathbb{R}^2$,$f_h(t,z,\boldsymbol{v}) \in \mathbb{R}$

$$\begin{cases} \partial_t \boldsymbol{j_c} = \Omega_{pe}^2 \boldsymbol{E} - J \boldsymbol{j_c} B_0 \\ \partial_t \boldsymbol{B} = J \partial_z \boldsymbol{E} \\ \partial_t \boldsymbol{E} = -J \partial_z \boldsymbol{B} - \boldsymbol{j_c} + \int v_\perp f_h \, \mathrm{d}v_\perp \\ \partial_t f_h + v_z \partial_z f_h - (\boldsymbol{E} + \boldsymbol{v} \times (\boldsymbol{B} + \boldsymbol{B}_0)) \cdot \nabla_{\boldsymbol{v}} f_h = 0 \end{cases}$$

we define the Hamiltonian as :

$$\mathcal{H} = \underbrace{\frac{1}{2} \int \|\boldsymbol{E}\|^2 \, \mathrm{d}z}_{\mathcal{H}_E} + \underbrace{\frac{1}{2} \int \|\boldsymbol{B}\|^2 \, \mathrm{d}z}_{\mathcal{H}_B} + \underbrace{\frac{1}{2} \int \frac{1}{\Omega_{pe}^2} \|\boldsymbol{j_c}\|^2 \, \mathrm{d}z}_{\mathcal{H}_{j_c}}$$
$$+ \underbrace{\frac{1}{2} \int \int \|\boldsymbol{v}\|^2 f_h \, \mathrm{d}\boldsymbol{v} \, \mathrm{d}z}_{\mathcal{H}_{f_h}}$$

This Hamiltonian is the basis of a splitting.

Splitting method

4 subsystems $\varphi^{[E]}$, $\varphi^{[B]}$, $\varphi^{[j_c]}$, $\varphi^{[f_h]}$

- Solution with Lie splitting method:

$$U^{n+1} = \varphi^{[E]}_{\Delta t} \circ \varphi^{[B]}_{\Delta t} \circ \varphi^{[j_c]}_{\Delta t} \circ \varphi^{[f_h]}_{\Delta t}(U^n)$$

- or Strang method:

$$U^{n+1} = \varphi^{[E]}_{\Delta t/2} \circ \varphi^{[B]}_{\Delta t/2} \circ \varphi^{[j_c]}_{\Delta t/2} \circ \varphi^{[f_h]}_{\Delta t} \circ \varphi^{[j_c]}_{\Delta t/2} \circ \varphi^{[B]}_{\Delta t/2} \circ \varphi^{[E]}_{\Delta t/2}(U^n)$$

Numerical cost:

- $\varphi^{[B]}$ and $\varphi^{[j_c]}$: almost free ($\mathcal{O}(N_z)$)
- $\varphi^{[E]}$: moderately expensive ($\mathcal{O}(N_z)$ + loop on phase space)
- $\varphi^{[f_h]}$: extremely expensive (multiple loops on phase space)

Splitting method

Example with: $\varphi^{[E]}$

One of sub-steps of Hamiltonian splitting:

$$\varphi^{[E]}(U) = \begin{cases} \partial_t \boldsymbol{j}_c = \Omega_{pe}^2 \boldsymbol{E} \\ \partial_t \boldsymbol{B} = J\partial_z \boldsymbol{E} \\ \partial_t \boldsymbol{E} = 0 \\ \partial_t f_h = \boldsymbol{E} \cdot \nabla_{v_\perp} f_h \end{cases} \quad \rightarrow \varphi_t^{[E]}(U^0) = \begin{pmatrix} \boldsymbol{j}_c(0) + t\Omega_{pe}^2 \boldsymbol{E}(0) \\ \boldsymbol{B}(0) + tJ\partial_z \boldsymbol{E}(0) \\ \boldsymbol{E}(0) \\ f_h(0, z, v_\perp + t\boldsymbol{E}(0), v_z) \end{pmatrix}$$

Numerical tools:

- 2D interpolation using two 5th-Lagrange interpolations to approximate $f_h(0, z, v_\perp + t\boldsymbol{E}(0), v_z)$

Lawson method

$U = (\boldsymbol{j}_c, \boldsymbol{B}, \boldsymbol{E}, f_h)^\top$

$$\dot{U} = LU + N(t, U)$$

with:

$$L = \begin{pmatrix} 0 & -B_0 & 0 & 0 & \Omega_{pe}^2 & 0 & 0 \\ B_0 & 0 & 0 & 0 & 0 & \Omega_{pe}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & \partial_z & 0 \\ 0 & 0 & 0 & 0 & -\partial_z & 0 & 0 \\ -1 & 0 & 0 & -\partial_z & 0 & 0 & 0 \\ 0 & -1 & \partial_z & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -v_z\partial_z \end{pmatrix}, \ N:(t, U) \mapsto \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \int v_x f_h \,\mathrm{d}\boldsymbol{v} \\ \int v_y f_h \,\mathrm{d}\boldsymbol{v} \\ (\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \cdot \nabla_{\boldsymbol{v}} f_h \end{pmatrix}$$

But $e^{\tau L}$ can't be computed even with symbolic computation software.

How to compute $e^{\tau L}$?

2 solutions are proposed:

1. Remove some terms of the linear part L and put them in nonlinear part N.
   - ✓ symbolic computation to write efficient code
   - ✗ add CFL stability condition
2. Approximate $e^{\tau L}$ with Taylor series or Padé approximant.
   - ✓ no CFL stability from all (local) linear terms
   - ✗ add error of approximation

Remove terms

Remove Maxwell equations from linear part L, and add them in nonlinear term N:

$$L = \begin{pmatrix} 0 & -B_0 & 0 & 0 & \Omega_{pe}^2 & 0 & 0 \\ B_0 & 0 & 0 & 0 & 0 & \Omega_{pe}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -v_z\partial_z \end{pmatrix}, \; N(t,U) = \begin{pmatrix} 0 \\ 0 \\ \partial_z E_y \\ -\partial_z E_x \\ -\partial_z B_y + \int v_x f_h \,\mathrm{d}\boldsymbol{v} \\ \partial_z B_x + \int v_y f_h \,\mathrm{d}\boldsymbol{v} \\ (\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \cdot \nabla_{\boldsymbol{v}} f_h \end{pmatrix}$$

- ✔ $e^{\tau L}$ is exactly computed with symbolic computation
- ✗ Add a CFL stability condition in z (coming from explicit resolution of Maxwell equations) which can be estimated.

Approximation of $e^{\tau L}$

Complete linear part L, after Fourier transform in z: $\partial_z \mapsto i\kappa$

$$L = \begin{pmatrix} 0 & -B_0 & 0 & 0 & \Omega_{pe}^2 & 0 & 0 \\ B_0 & 0 & 0 & 0 & 0 & \Omega_{pe}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & i\kappa & 0 \\ 0 & 0 & 0 & 0 & -i\kappa & 0 & 0 \\ -1 & 0 & 0 & -i\kappa & 0 & 0 & 0 \\ 0 & -1 & i\kappa & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -i\kappa v_z \end{pmatrix}$$

We have:

$$\forall \kappa, \sigma(L(\kappa)) \subset i\,\mathbb{R}$$

So that : $\mathrm{sp}(e^{\tau L(\kappa)}) \subset \mathcal{C}(0,1)$ IMPORTANT for numerical stability !

Taylor series

Simplest approximation:

$$T_p(\tau L) = \sum_{k=0}^{p} \frac{\tau^k}{k!} L^k = e^{\tau L} + \mathcal{O}\left(\tau^{p+1}\right)$$

Proposition

Bad behavior of eigenvalues of Taylor series

Proof: compute Taylor series outside of its convergence radius

Conclusion:

- ✗ Bad behavior of eigenvalues
- ✗ Numerical instability in scheme

Padé approximant

Best rational approximation of exponential function.
Defined (for order (p, q)) as:

$$h_{p,q}(M) = \sum_{i=0}^{p} \frac{\frac{p!}{(p-i)!}}{\frac{(p+q)!}{(p+q-i)!}} \frac{M^i}{i!} \quad , \quad k_{p,q}(M) = \sum_{j=0}^{q} (-1)^j \frac{\frac{q!}{(q-j)!}}{\frac{(p+q)!}{(p+q-j)!}} \frac{M^j}{j!}$$

Finally Padé approximant is:

$$P_{p,q}(\tau L) = h_{p,q}(\tau L)\left(k_{p,q}(\tau L)\right)^{-1} = e^{\tau L} + \mathcal{O}\left(\tau^{p+q+1}\right)$$

Theorem

$$sp(L) \subset i\mathbb{R} \implies sp(P_{p,p}(tL)) \subset \mathcal{C}(0,1)$$

Conclusion:

- ✗ Needs matrix inversion, or some tricks:
  - Li, Zhu, and Gu 2011, *Applied Mathematics*
- ✔ Best approximation for this numerical cost
- ✔ Preserves eigenvalues

Proof

L diagonalizable ➜ study only on diagonal terms (iy, $y \in \mathbb{R}$)

$$P_{p,p}(iy) = \left(\sum_{k=0}^{p} \frac{1}{k!}(iy)^k \right) \cdot \left(\sum_{\ell=0}^{p} (-1)^\ell \frac{1}{\ell!}(iy)^\ell \right)^{-1}$$

$$\sum_{k=0}^{p} \frac{1}{k!}(iy)^k = \sum_{k=0}^{\lfloor \frac{p}{2} \rfloor} (-1)^k \frac{y^{2k}}{(2k)!} + i \sum_{k=0}^{\lfloor \frac{p}{2} \rfloor - 1} (-1)^k \frac{y^{2k+1}}{(2k+1)!}$$

$$\sum_{\ell=0}^{p} (-1)^\ell \frac{1}{\ell!}(iy)^\ell = \sum_{\ell=0}^{\lfloor \frac{p}{2} \rfloor} (-1)^\ell \frac{y^{2\ell}}{(2\ell)!} - i \sum_{\ell=0}^{\lfloor \frac{p}{2} \rfloor - 1} (-1)^\ell \frac{y^{2\ell+1}}{(2\ell+1)!}$$

$\lambda^- = \overline{\lambda^+}$ so $\left| \frac{\lambda^+}{\lambda^-} \right| = 1.$

Eigenvalues of symmetric Padé approximants

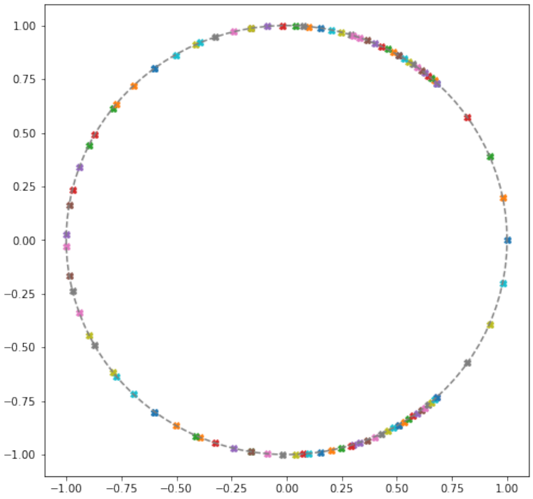


Figure: $P_{2,2}(iy)$ $y \in [-5, 5]$

Eigenvalues of asymmetric Padé approximants

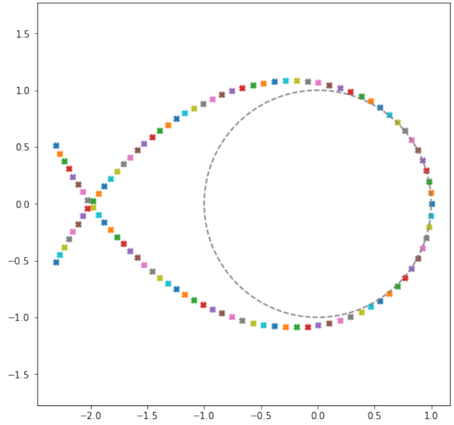


Figure: $P_{2,1}(iy)$ $y \in [-5, 5]$

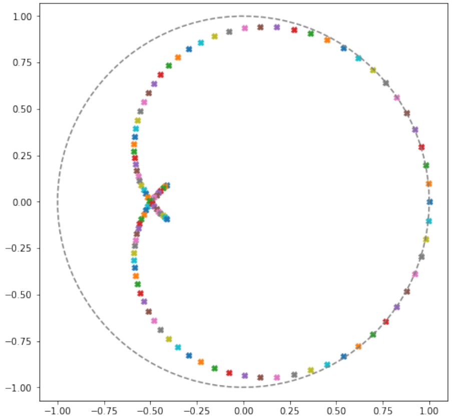


Figure: $P_{1,2}(iy)$ $y \in [-5, 5]$

WIP Splitting method

Breaking news!

We can also approximate $e^{\tau L}$ with truncated BCH formula (or splitting method):

$$L = \underbrace{\begin{pmatrix} 0 & -B_0 & 0 & 0 & \Omega_{pe}^2 & 0 & 0 \\ B_0 & 0 & 0 & 0 & 0 & \Omega_{pe}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -iv_z\kappa \end{pmatrix}}_{L_1} + \underbrace{\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & i\kappa & 0 \\ 0 & 0 & 0 & 0 & -i\kappa & 0 & 0 \\ 0 & 0 & 0 & -i\kappa & 0 & 0 & 0 \\ 0 & 0 & i\kappa & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}}_{L_2}$$

$$S_\tau(L) = e^{\frac{\tau}{2}L_1} e^{\tau L_2} e^{\frac{\tau}{2}L_1} = e^{\tau L} + \mathcal{O}(\tau^3)$$

Error on approximate Lawson method

We note $P_{p,q}(z) = \epsilon^{z}$. We recall:

$$\epsilon^{\tau L} = e^{\tau L} + \mathcal{O}(\tau^{r+1}), \quad \text{with } r = p + q$$

After some calculations, Lawson RK(3,3) rewrites:

$$\begin{aligned}
u^{(1)} &= \epsilon^{\Delta t L} u^n + \Delta t \epsilon^{\Delta t L} N(t^n, u^n) \\
u^{(2)} &= \frac{3}{4} \epsilon^{\frac{\Delta t}{2} L} u^n + \frac{1}{4} \epsilon^{-\frac{\Delta t}{2} L} u^{(1)} + \frac{\Delta t}{4} \epsilon^{-\frac{\Delta t}{2} L} N(t^n + \Delta t, u^{(1)}) \\
u^{n+1} &= \frac{1}{3} \epsilon^{\Delta t L} u^n + \frac{2}{3} \epsilon^{\frac{\Delta t}{2} L} u^{(2)} + \frac{2}{3} \Delta t \epsilon^{\frac{\Delta t}{2} L} N(t^n + \frac{\Delta t}{2}, u^{(2)})
\end{aligned}$$

If L and N commute: $u^{n+1} = \epsilon^{\Delta t L} \left(I + N + \frac{N^2}{2} + \frac{N^3}{6} \right) u^n$, stability is same as RK(3,3).

Crouseilles, Einkemmer, and Massot 2020, *Journal of Computational Physics*
study of Lawson stability in scalar case

Else. . .

Error on approximate Lawson method

If L and N don't commute:

$$u^{n+1} = \Big[e^{\Delta t L} + \Delta t\left(\frac{2}{3}e^{\frac{\Delta t}{2}L}Ne^{\frac{\Delta t}{2}L} + \frac{1}{6}e^{\Delta t L}N + \frac{1}{6}Ne^{\Delta t L}\right)$$

$$\rightsquigarrow e^{\Delta L}\Delta t N + \mathcal{O}(\Delta t^{r+1})$$

$$+ \frac{\Delta t^2}{2}\left(\frac{1}{3}Ne^{\Delta t L}N + \frac{1}{3}e^{\frac{\Delta t}{2}L}Ne^{\frac{\Delta t}{2}L}N + \frac{1}{3}e^{\frac{\Delta t}{2}L}Ne^{-\frac{\Delta t}{2}L}Ne^{\Delta t L}\right)$$

$$\rightsquigarrow e^{\Delta L}\frac{(\Delta t N)^2}{2} + \mathcal{O}(\Delta t^{r+1})$$

$$+ \frac{\Delta t^3}{6}e^{\frac{\Delta t}{2}L}Ne^{-\frac{\Delta t}{2}L}Ne^{\Delta t L}N\Big]u^n \rightsquigarrow e^{\Delta L}\frac{(\Delta t N)^3}{6} + \mathcal{O}(\Delta t^{r+1})$$

Lemma

Truncature error of modified Lawson RK(s,m) is $\mathcal{O}(\Delta t^{\min(r,m)})$

Test 1: measure of order

Simulation of $\partial_t u + a\partial_x u + b\partial_y u = 0$ (2D translation test case).

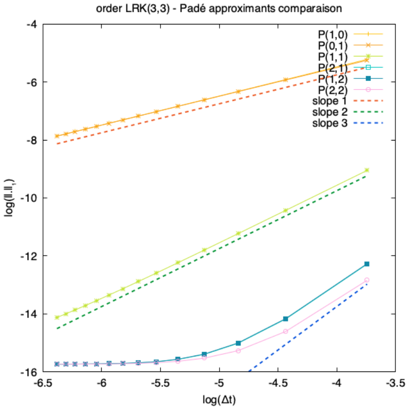


Figure: Convergence order of modified Lawson RK(3,3) methods with Padé approximant ($p, q = 0, 1, 2$)

Test 2: illustration of instability or stability

Simulation of $\partial_t u - y\partial_x u + x\partial_y u = 0$ (2D rotation)

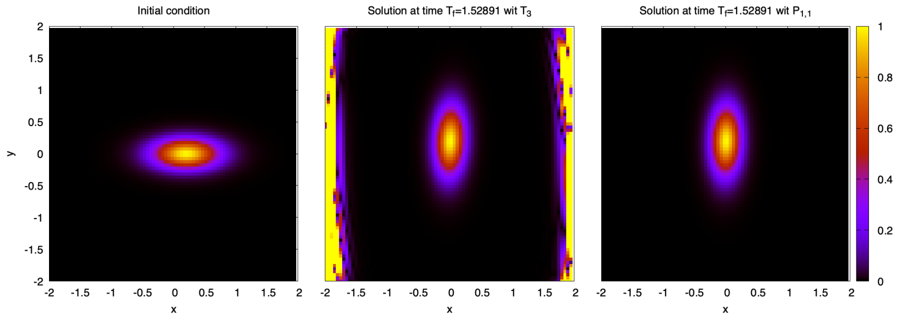


Figure: Solution of the modified Lawson RK(3,3) methods with Taylor T_3 (middle) and Padé $P_{1,1}$ (right).

Outline

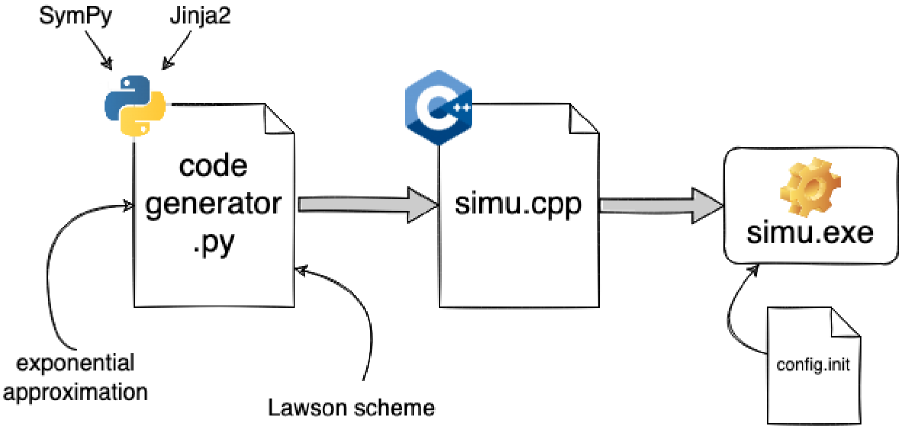
Numerical results

We compare:

- Splitting method:
  - Strang (order 2)
  - Suzuki (order 4)
- Lawson method:
  - LRK(4,4) (order 4)
  - LDP4(3) (adaptive time step method)
- Modified Lawson method with Padé:
  - LRK(4,4) with Padé $(2,2)$ (order 4 + approximation of order $2+2=4$)
  - LDP4(3) with Padé $(2,2)$ (adaptive time step method)

But Padé approximant implies a huge rational function (with invert of matrix), high order Lawson methods have a lot of coefficients, with 7 variables problem. . . ➜ bug source !!!

Code generator



Numerical test

Anisotropic equilibrium, Weibel instability:

$$\begin{cases} \boldsymbol{j}_c(t=0,z) = 0 \\ \boldsymbol{B}(t=0,z) = (\epsilon \sin(Kz), 0, 0) \\ \boldsymbol{E}(t=0,z) = 0 \\ f_h(t=0,z,\boldsymbol{v}) = \dfrac{\rho_h}{(2\pi)^{3/2}\bar{v}_\perp^2 \bar{v}_\parallel} \exp\left(-\dfrac{v_z^2}{2\bar{v}_\parallel^2} - \dfrac{(v_x^2+v_y^2)}{2\bar{v}_\perp^2} \right) \end{cases}$$

with $z \in [0, \frac{2\pi}{K}]$, $\boldsymbol{v} \in [-3.6, 3.6] \times [-3.6, 3.6] \times [-2.4, 2.4]$, $K = 2$, $\bar{v}_\parallel = 0.2$, $\bar{v}_\perp = 0.6$, $\rho_h = 0.2$ and $\epsilon = 10^{-5}$.

Compare energies:

$$\mathcal{H}_E(t) = \frac{1}{2} \int \|\boldsymbol{E}(t,z)\|^2 \,\mathrm{d}z \qquad \mathcal{H}_B(t) = \frac{1}{2} \int \|\boldsymbol{B}(t,z)\|^2 \,\mathrm{d}z$$

$$\mathcal{H}_c(t) = \frac{1}{2\Omega_{pe}^2} \int \|\boldsymbol{j}_c(t,z)\|^2 \,\mathrm{d}z$$

Numerical results: splitting vs Lawson

$N_z \times N_{v_x} \times N_{v_y} \times N_{v_z} = 27 \times 32 \times 32 \times 41$

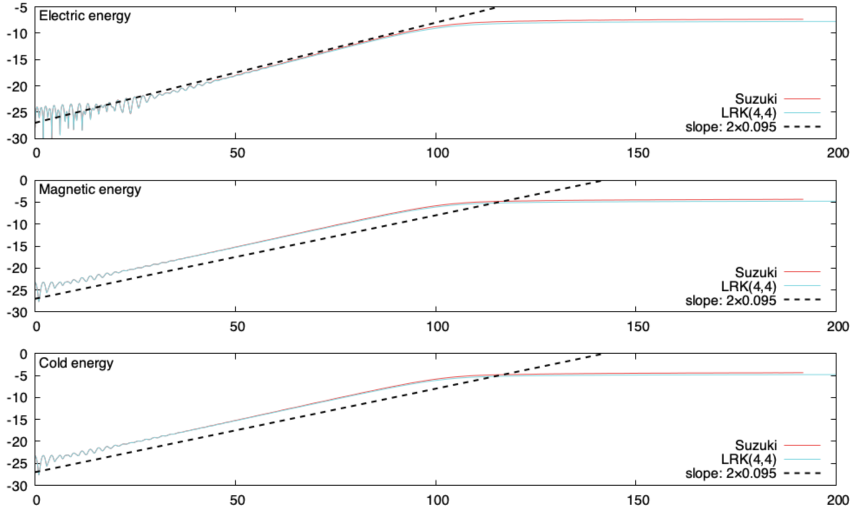


Figure: Energies evolution, $\Delta t = 0.05$

Numerical results: splitting vs Lawson

$N_z \times N_{v_x} \times N_{v_y} \times N_{v_z} = 27 \times 32 \times 32 \times 41$

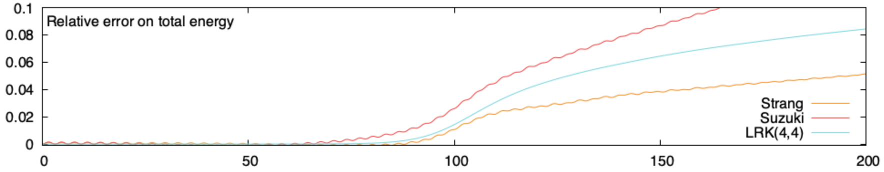


Figure: Relative error on total energy, $\Delta t = 0.05$

Numerical results: splitting vs Lawson

$N_z \times N_{v_x} \times N_{v_y} \times N_{v_z} = 27 \times 32 \times 32 \times 41$

time integrator	simulation time
Lie splitting	13 h 25 min 10 s
Strang splitting	17 h 09 min 54 s
Suzuki splitting	3 j 03 h 05 min 24 s
LRK(3,3)	11 h 29 min 09 s
LRK(4,4)	14 h 06 min 15 s

Table: Computational time for the different methods, on mesh $N_z \times N_{v_x} \times N_{v_y} \times N_{v_z} = 27 \times 32 \times 32 \times 41$ and time step $\Delta t = 0.05$.

Numerical results: Padé-Lawson

$N_z \times N_{v_x} \times N_{v_y} \times N_{v_z} = 27 \times 32 \times 32 \times 41$

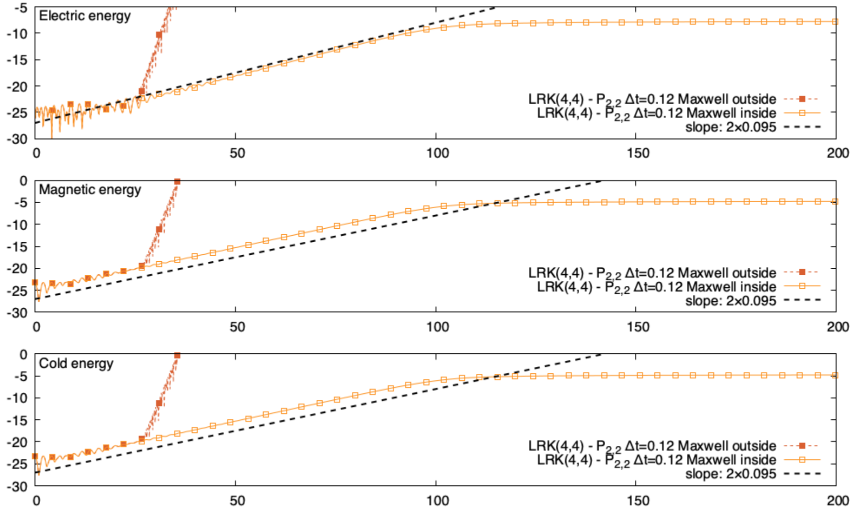


Figure: Energies evolution, Lawson with Padé approximation, $\Delta t = 0.12$

Numerical results: Padé-Lawson adaptive time step

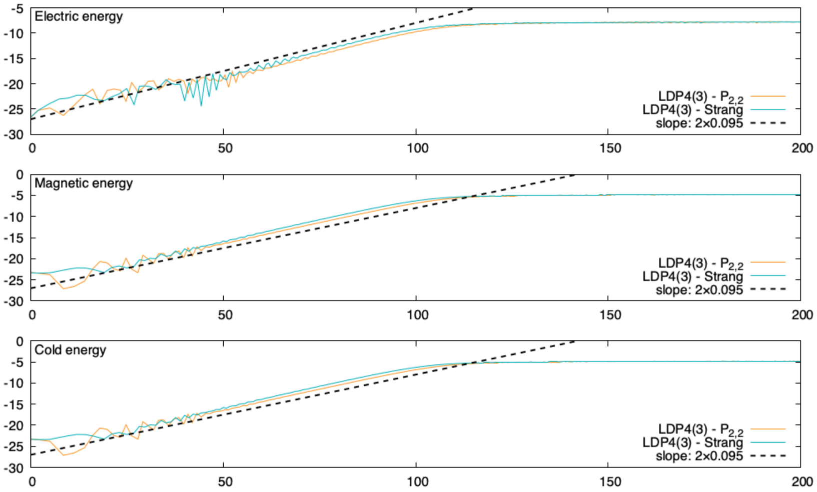


Figure: Energies evolution, Lawson with Padé approximation, Δt^n

Numerical results: Padé-Lawson adaptive time step

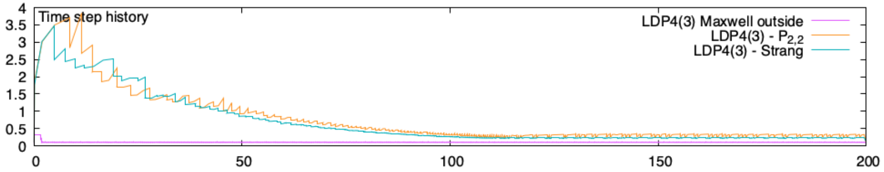


Figure: Time step evolution, classic Lawson (Maxwell outside) and approximate Lawson with Padé or Strang approximation, Δt_n

method	# of iterations	# of succeeded	ratio
LDP4(3) (Maxwell outside)	2794	1970	0.705
LDP4(3)-$P_{2,2}$	919	464	0.504
LDP4(3)-Strang	1131	583	0.515

Computational time

time integrator	simulation time
LRK(3,3)	11 h 29 min 09 s
LRK(3,3) - $P_{1,1}$	10 h 54 min 11 s
LRK(3,3) - $P_{2,2}$	10 h 55 min 26 s
LRK(4,4)	14 h 06 min 15 s
LRK(4,4) - $P_{2,2}$	13 h 59 min 59 s
LDP4(3)	11 h 44 min 04 s
LDP4(3) - $P_{2,2}$	04 h 09 min 44 s
LDP4(3) - Strang	04 h 42 min 25 s

Table: Computational time for the different methods, on mesh $N_z \times N_{v_x} \times N_{v_y} \times N_{v_z} = 27 \times 32 \times 32 \times 41$ and time step $\Delta t = 0.05$ (initial time step for adaptive time step strategy).

Outline

Conclusion

- ✔ Numerical estimation of CFL with Python package: Ponio[1]
- ✔ Comparison between kinetic model and hybrid model thanks dispersion relation and simulations
- ✗ Numerical cost of splitting methods (not bad in $1dz - 1dv$ but very bad in $1dz - 3dv$, must be very very very bad in $3dx - 3dv$)
- ✔ Numerical cost of Lawson methods
- ∼ Behavior of total energy of Lawson method (but we can use high order method easily)
- ✔ Error of approximation with Padé approximant can be lower than time integrator
- ✔ Adaptive time step method with any linear part thanks to approximation of exponential function

[1] `http://jmassot.perso.math.cnrs.fr/ponio.html`

Future works

- Add $\int \boldsymbol{v} f_h \,\mathrm{d}\boldsymbol{v}$ in linear part (for $1dx - 1dv$ model) **WIP**
- Improve code generator (easy to use for other problem) **WIP**
- Parallelized with OpenMP or OpenACC (GPU)
- Combining Lawson integrator to semi-Lagrangian methods
- Comparison with PIC simulation (code developed in IPP Max Planck, Garching)
- Construction of energy preserving Lawson method

Thank you for your attention

Backup

Adaptive time step method for splitting method

Blanes, Casas, and Thalhammer 2019, *Applied Numerical Mathematics* for Suzuki splitting method

$$u_{[4]}^{n+1} = \mathcal{S}_{\Delta t}(u^n) = S_{\alpha_1\Delta t} \circ \underbrace{S_{\alpha_2\Delta t} \circ \underbrace{S_{\alpha_3\Delta t} \circ \underbrace{S_{\alpha_2\Delta t} \circ \underbrace{S_{\alpha_1\Delta t}(u^n)}_{u^{(1)}}}_{u^{(2)}}}_{u^{(3)}}}_{u^{(4)}}.$$

We compute an order 3 approximation from U^n and $U^{(s)}$, $s = 1, 2, 3, 4$:

$$u_{[3]}^{n+1} = -u^n + w_1(u^{(1)} + u^{(4)}) + w_2(u^{(2)} + u^{(3)})$$

with:

$$w_1 = \frac{g_2(1-g_2)}{g_1(g_1-1) - g_2(g_2-1)}, \quad w_2 = 1 - w_1, \quad \begin{array}{l} g_1 = \alpha_1 \\ g_2 = \alpha_1 + \alpha_2 \end{array}$$

and $L_{[3]}^n = \left\| u_{[4]}^{n+1} - u_{[3]}^{n+1} \right\|_2$

backup Adaptive time step method for Lawson method

Lawson methods are built on Runge-Kutta method, embedded Lawson method are written with an underlying embedded Runge-Kutta method.

Dormand and Prince 1978, *Celestial mechanics*

With DP4(3) (Dormand-Prince method of order 4, with embedded 3 method):

$$\left.\begin{array}{c|ccccc}
0 & & & & & \\
\frac{1}{2} & \frac{1}{2} & & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & & \\
1 & 0 & 0 & 1 & & \\
\hline
1 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} & \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{2}{30} & \frac{1}{10}
\end{array}\right\}\text{Classical RK(4,4)}$$

We compute a 3rd order approximation from u^n, $u^{(s)}$, $s = 1, 2, 3, 4$ done by the last line of Butcher tableau.

And $L^n_{[3]} = \left\| u^{n+1}_{[4]} - u^{n+1}_{[3]} \right\|_2$

Poisson bracket

For two given functionals $\mathcal{F}$, $\mathcal{G}$ of $\boldsymbol{j}_c$, $\boldsymbol{B}$, $\boldsymbol{E}$, f_h, the Poisson bracket is given by

$$
\begin{aligned}
\{\mathcal{F},\mathcal{G}\}[\boldsymbol{j}_c,\boldsymbol{B},\boldsymbol{E},f_h] &= \frac{1}{m_e}\int_\Omega\int_{\mathbb{R}^3} f_h\left[\frac{\delta\mathcal{F}}{\delta f_h},\frac{\delta\mathcal{G}}{\delta f_h}\right]_{\boldsymbol{xv}}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{x} \\
&+ \frac{q_e}{m_e\varepsilon_0}\int_\Omega\int_{\mathbb{R}^3} f_h\left(\nabla_{\boldsymbol{v}}\frac{\delta\mathcal{F}}{\delta f_h}\cdot\frac{\delta\mathcal{G}}{\delta\boldsymbol{E}} - \nabla_{\boldsymbol{v}}\frac{\delta\mathcal{G}}{\delta f_h}\cdot\frac{\delta\mathcal{F}}{\delta\boldsymbol{E}}\right)\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{x} \\
&+ \frac{q_e}{m_e^2}\int_\Omega\int_{\mathbb{R}^3} f_h(\boldsymbol{B}+\boldsymbol{B}_0)\cdot\left(\nabla_{\boldsymbol{v}}\frac{\delta\mathcal{F}}{\delta f_h}\times\nabla_{\boldsymbol{v}}\frac{\delta\mathcal{G}}{\delta f_h}\right)\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{x} \\
&+ \frac{1}{\varepsilon_0}\int_\Omega\left(\nabla\times\frac{\delta\mathcal{F}}{\delta\boldsymbol{E}}\cdot\frac{\delta\mathcal{G}}{\delta\boldsymbol{B}} - \nabla\times\frac{\delta\mathcal{G}}{\delta\boldsymbol{E}}\cdot\frac{\delta\mathcal{F}}{\delta\boldsymbol{B}}\right)\mathrm{d}\boldsymbol{x} \\
&+ \int_\Omega \Omega_{pe}^2\left(\frac{\delta\mathcal{F}}{\delta\boldsymbol{j}_c}\cdot\frac{\delta\mathcal{G}}{\delta\boldsymbol{E}} - \frac{\delta\mathcal{G}}{\delta\boldsymbol{j}_c}\cdot\frac{\delta\mathcal{F}}{\delta\boldsymbol{E}}\right)\mathrm{d}\boldsymbol{x} \\
&+ \frac{q_e\varepsilon_0}{m_e}\int_\Omega \Omega_{pe}^2\boldsymbol{B}_0\cdot\left(\frac{\delta\mathcal{F}}{\delta\boldsymbol{j}_c}\times\frac{\delta\mathcal{G}}{\delta\boldsymbol{j}_c}\right)\mathrm{d}\boldsymbol{x}\,.
\end{aligned}
$$

Splitting method $\varphi^{[j_c]}$

$$\varphi^{[j_c]}(U) = \begin{cases} \partial_t \boldsymbol{j}_c = -J\boldsymbol{j}B_0 \\ \partial_t \boldsymbol{B} = 0 \\ \partial_t \boldsymbol{E} = -\boldsymbol{j}_c \\ \partial_t f_h = 0 \end{cases} \quad \rightarrow \varphi_t^{[j_c]}(U^0) = \begin{pmatrix} e^{-tJ}\boldsymbol{j}_c(0)B_0 \\ \boldsymbol{B}(0) \\ \boldsymbol{E}(0) - J(e^{-tJ} - I)\boldsymbol{j}_c(0) \\ f_h(0) \end{pmatrix}$$

Obtain because: $\int_0^t \exp(-sJ)\boldsymbol{j}_c(0)\,\mathrm{d}s = J(\exp(-tJ) - I)\boldsymbol{j}_c(0)$, with:

$$\exp(-tJ) = \begin{pmatrix} \cos(t) & -\sin(t) \\ \sin(t) & \cos(t) \end{pmatrix}$$

Splitting method $\varphi^{[B]}$

$$\varphi^{[B]}(U) = \begin{cases} \partial_t \boldsymbol{j}_c = 0 \\ \partial_t \boldsymbol{B} = 0 \\ \partial_t \boldsymbol{E} = -J\partial_z \boldsymbol{B} \\ \partial_t f_h = 0 \end{cases} \rightarrow \varphi_t^{[B]}(U^0) = \begin{pmatrix} \boldsymbol{j}_c(0) \\ \boldsymbol{B}(0) \\ \boldsymbol{E}(0) - tJ\partial_z \boldsymbol{B}(0) \\ f_h(0) \end{pmatrix}$$

Numerical tools:

- Solve in Fourier space

Splitting method $\varphi^{[E]}$

$$\varphi^{[E]}(U) = \begin{cases} \partial_t \boldsymbol{j}_c = \Omega_{pe}^2 \boldsymbol{E} \\ \partial_t \boldsymbol{B} = J\partial_z \boldsymbol{E} \\ \partial_t \boldsymbol{E} = 0 \\ \partial_t f_h = \boldsymbol{E} \cdot \nabla_{\boldsymbol{v}} f_h \end{cases} \to \varphi_t^{[E]}(U^0) = \begin{pmatrix} \boldsymbol{j}_c(0) + t\Omega_{pe}^2 \boldsymbol{E}(0) \\ \boldsymbol{B}(0) + tJ\partial_z \boldsymbol{E}(0) \\ \boldsymbol{E}(0) \\ f_h(0, z, \boldsymbol{v} + t\boldsymbol{E}(0), v_z) \end{pmatrix}$$

Numerical tools:

- 2D interpolation with 2 Lagrange 5 interpolations to approximate $f_h(0, z, \boldsymbol{v} + t\boldsymbol{E}(0), v_z)$

Splitting method $\varphi^{[f_h]}$

$$\varphi^{[f_h]}(U) = \begin{cases} \partial_t \boldsymbol{j}_c = 0 \\ \partial_t \boldsymbol{B} = 0 \\ \partial_t \boldsymbol{E} = \int \boldsymbol{v} f_h \,\mathrm{d}\boldsymbol{v} \\ \partial_t f_h = -v_z \partial_z f_h + (\boldsymbol{v} \times (\boldsymbol{B} + \boldsymbol{B}_0)) \cdot \nabla_{\boldsymbol{v}} f_h \end{cases}$$

This step is split again onto 3 parts.

backup Splitting method $\varphi^{[f_h]}$, $f_{h,\star}$, $\star \in \{x, y\}$

$$\varphi^{[f_{h,x}]}(U)=\begin{cases} \partial_t \boldsymbol{j}_c = 0 \\ \partial_t \boldsymbol{B} = 0 \\ \partial_t E_x = \int v_x f_h \,\mathrm{d}\boldsymbol{v} \\ \partial_t E_y = 0 \\ \partial_t f_h = -v_x B_0 \partial_{v_y} f_h + v_x B_y \partial_{v_z} f_h \end{cases} \to \varphi_t^{[f_{h,x}]}(U^0)=\begin{pmatrix} \boldsymbol{j}_c(0) \\ \boldsymbol{B}(0) \\ E_x(0) + t\int v_x f_h(0)\,\mathrm{d}\boldsymbol{v} \\ E_y(0) \\ f_h(0,z,v_x,v_y - tv_xB_0, v_z + tB_yv_x) \end{pmatrix}$$

Numerical tools:

- 2D interpolation with Lagrange 5 interpolation to approximate $f_h(0, z, v_x, v_y - tv_x B_0, v_z + tB_y v_x)$

Same thing for $\varphi^{[f_{h,y}]}$ in v_y direction.

Splitting method $\varphi^{[f_h]}$, $f_{h,z}$

$$\varphi^{[f_{h,z}]}(U) = \begin{cases} \partial_t \boldsymbol{j}_c = 0 \\ \partial_t \boldsymbol{B} = 0 \\ \partial_t \boldsymbol{E} = 0 \\ \partial_t f_h = -v_z \partial_z f_h + (-v_z B_y \partial_{v_x} f_h + v_z B_x \partial_{v_y} f_h) \end{cases}$$

Numerical tools:

- Split **again** onto 3 parts, with change of variable $g(t, z, \boldsymbol{v}) := f(t, z + tv_z, \boldsymbol{v})$
- 2D interpolation with Lagrange 5 interpolation to approximate $g(0, z, v_x - \sum_k \hat{B}_y(0,k)\frac{1}{ik}e^{ikz}(e^{iktv_z} - 1), v_y + \sum_k \hat{B}_x(0,k)\frac{1}{ik}e^{ikz}(e^{iktv_z} - 1), v_z)$
- Revert change of variable with Fourier transform

Splitting method

For Lie method:

$$U^{n+1} = \varphi_{\Delta t}^{[j_c]} \circ \varphi_{\Delta t}^{[B]} \circ \varphi_{\Delta t}^{[E_{v_x}]} \circ \varphi_{\Delta t}^{[E_{v_y}]} \circ \varphi_{\Delta t}^{[f_{h,x,v_x}]} \circ \varphi_{\Delta t}^{[f_{h,x,v_z}]} \circ \varphi_{\Delta t}^{[f_{h,y,v_y}]} \circ \varphi_{\Delta t}^{[f_{h,y,v_z}]} \circ \varphi_{\Delta t}^{[f_{h,z,1}]} \circ \varphi_{\Delta t}^{[f_{h,z,2}]} \circ \varphi_{\Delta t}^{[f_{h,z,3}]}(U^n)$$

Suzuki vs Lawson (adaptive time step)

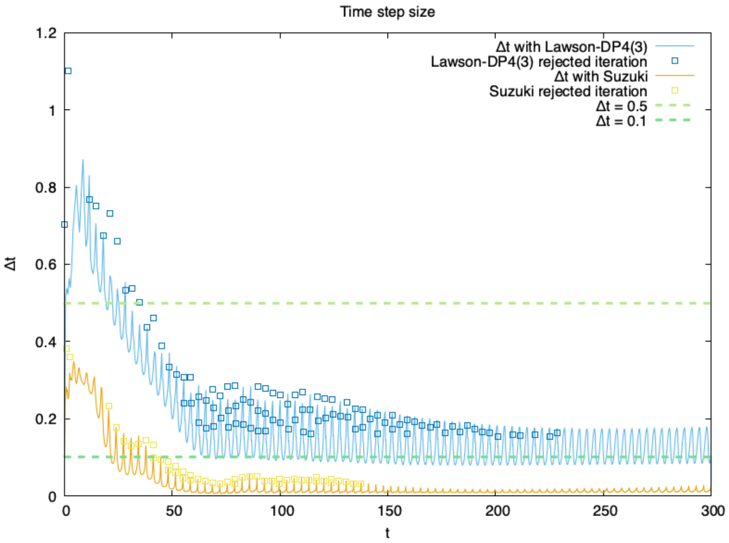
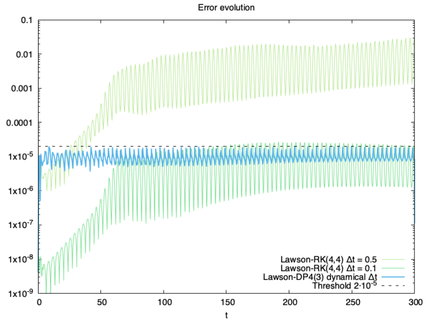


Figure: Time step size in 1dx-1dv

backup Suzuki vs Lawson (adaptive time step)



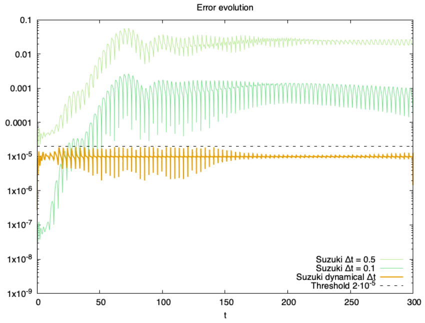


Figure: Local error estimate Lawson (left) and Suzuki (right)

Time comparaison

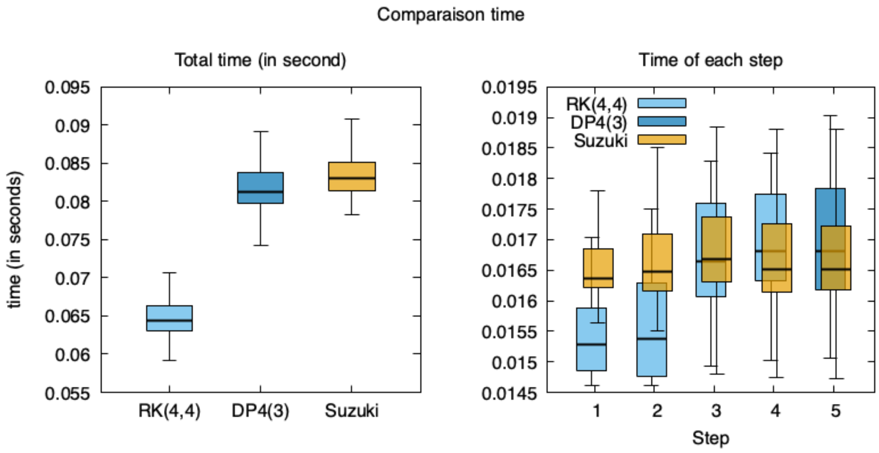


Figure: Simulation time of each step

Number of lines

Language	Files	Lines	Code	Comments	Blanks
C header	16	6010	4352	870	788
C++	67	39837	28463	5428	5946
Makefile	1	120	84	9	27
Python	13	2747	2149	221	377
Shell	1	35	21	8	6
Total	98	48749	35069	6536	7144