Méthodes numériques pour des modèles hybrides fluide-cinétique de plasmas

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Outline

Outline

Vlasov-Maxwell $1dz - 3dv$ model

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

$$\begin{cases} \partial_t f + v_z \partial_z f - (\boldsymbol{E} + \boldsymbol{v} \times (\boldsymbol{B} + \boldsymbol{B}_0)) \cdot \nabla_{\boldsymbol{v}} f = 0 \\ \partial_t \boldsymbol{B} = -\partial_z \boldsymbol{E} \\ \partial_t \boldsymbol{E} = \partial_z \boldsymbol{B} + \int_{\mathbb{R}^3} v_\perp f \, \mathrm{d}\boldsymbol{v} \end{cases}$$
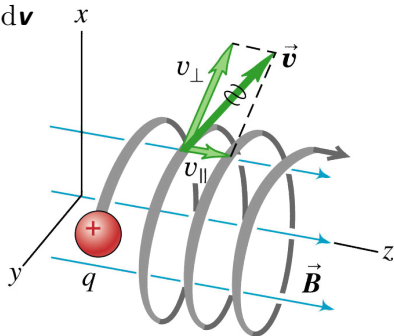
Vlasov-Maxwell $1dz - 3dv$ model

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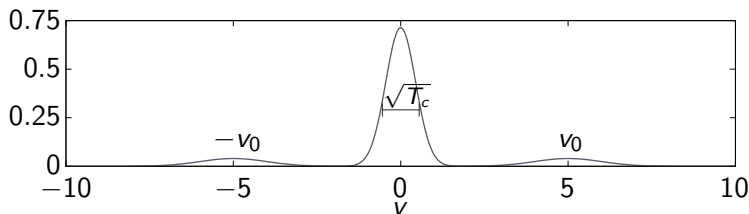
- We consider an initial condition of the form $f = f_c + f_h$ with:
  $f_c(t = 0, z, \boldsymbol{v}) = \rho_c(t, z)\delta_{\boldsymbol{v}=\boldsymbol{u}_c(t,z)}(\boldsymbol{v})$

The idea

Grid methods can't have an initial condition like:

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

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

- Split $f = f_c + f_h$ (2 Vlasov equations)
- Compute momentum of f_c
  - *Cold plasma approximation*: $\frac{T_c}{T_h} \ll 1 \rightarrow f_c(t,z,\boldsymbol{v}) \rightarrow \boldsymbol{j}_c(t,z)$
  - 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*

The new model: a nonlinear transport in $(z, v_x, v_y, v_z) \in \Omega \times \mathbb{R}^3$ of:
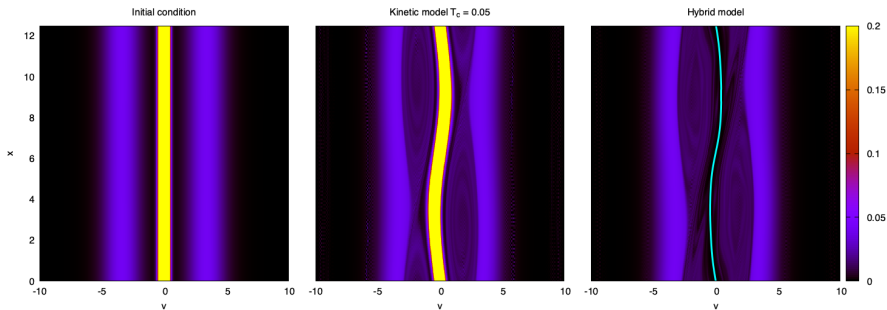
- a cold (fluid) electron density distribution, reconstruction from current variable $\boldsymbol{j}_c(t, z) = q_e \rho_c(t, z) \boldsymbol{u}_c(t, z) = (j_{c,x}, j_{c,y}, 0)(t, z)$
- a hot (kinetic) electron density distribution $f_h(t, z, \boldsymbol{v})$

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

with:

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

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

Figure: Simulation of initial condition (left) with kinetic model with $T_c = 0.05$ (middle) and hybrid model (right) to the time $T_f = 200$

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

Outline

Numerical methods

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))

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

Splitting method

Successive resolution of:

$$\dot{u} = Lu \qquad \rightarrow \tilde{u}_t = \varphi_t^{[L]}(u_0)$$

$$\dot{u} = N(t, u) \quad \rightarrow \tilde{u}_t = \varphi_t^{[N]}(u_0)$$

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*

✔ 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

$$\partial_t u = Lu + N(t, u)$$

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

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

$$= e^{-tL}N(t, e^{tL}v)$$

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

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

or as an expression 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*

- ✔ 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 ✔)
- ✗ Behavior in long time
- ∼ 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 estimations of solution $u(t^{n+1})$ of different order, p and $p+1$:

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

Estimate of local error: $\qquad L_{[p]}^{n+1} = \left| u_{[p+1]}^{n+1} - u_{[p]}^{n+1} \right|$

If $L_{[p]}^{n+1} > tol$: 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:

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

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

📄 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 :

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

$$+ \underbrace{\frac{1}{2} \int \int \|\boldsymbol{v}\|^2 f_h \,\mathrm{d}\boldsymbol{v} \,\mathrm{d}z}_{\mathcal{H}_{f_h}}$$

Following the Hamiltonian we built a Hamiltonian splitting.

Splitting method

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

- Solution with Lie splitting method:

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

- or Strang method:

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

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

One of sub-steps of Hamiltonian splitting:

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

Numerical tools:

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

Lawson method

$$\partial_t U = LU + N(t, U)$$

with:

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

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:

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

- ✔ $e^{\tau L}$ 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 : $\sigma(e^{\tau L(\kappa)}) \subset \mathcal{C}(0,1)$ IMPORTANT for numerical stability !

Taylor series

Simplest approximation:

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

Proposition

$\mathrm{sp}(L) \subset i\mathbb{R} \smallsetminus i[-1, 1]$ implies eigenvalues diverge

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 $\left|\frac{\lambda^+}{\lambda^-}\right| = 1$.
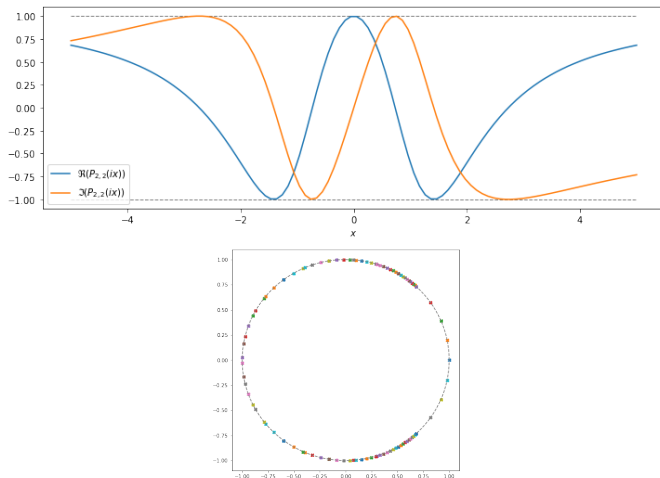
Eigenvalues of Padé approximant

Figure: $P_{2,2}(ix)$, $x \in [-5, 5]$
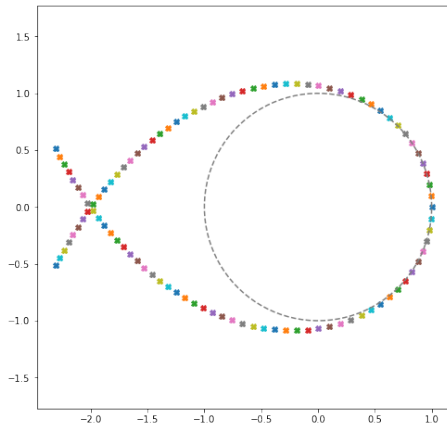
Eigenvalues of assymetric Padé approximants
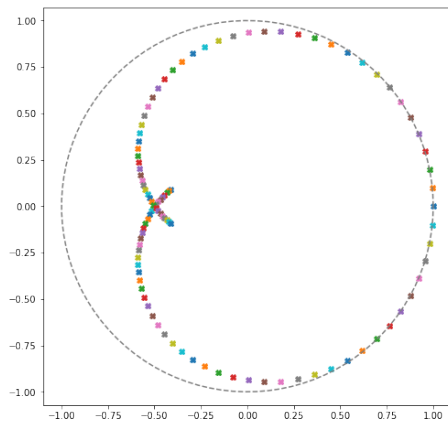

Figure: $P_{2,1}(ix)$ $x \in [-5, 5]$

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

Breaking news!

We can also approximate $e^{\tau L}$ with troncature of BCH formula or splitting method:

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

$$
e^{\tau L} \approx e^{\frac{\tau}{2} L_1} e^{\tau L_2} e^{\frac{\tau}{2} L_1} = S_\tau(L)
$$

Error on approximate Lawson method

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

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

Lawson RK(3,3) method becomes:

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

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

$$u^{n+1} = \frac{1}{3} \epsilon^{\Delta t L} u^n + \frac{2}{3} \epsilon^{\frac{\Delta t}{2} L} u^{(2)} + \frac{2}{3} \Delta t \epsilon^{\frac{\Delta t}{2} L} N(t^n + \frac{\Delta t}{2}, u^{(2)})$$

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:

$$u^{n+1} = \left[\epsilon^{\Delta t L} + \Delta t \left(\frac{2}{3} \epsilon^{\frac{\Delta t}{2} L} N \epsilon^{\frac{\Delta t}{2} L} + \frac{1}{6} \epsilon^{\Delta t L} N + \frac{1}{6} N \epsilon^{\Delta t L} \right) \rightsquigarrow \epsilon^{\Delta L} \Delta t N \right.$$

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

$$\rightsquigarrow \epsilon^{\Delta L} \frac{(\Delta t N)^2}{2}$$

$$\left. + \frac{\Delta t^3}{6} \epsilon^{\frac{\Delta t}{2} L} N \epsilon^{-\frac{\Delta t}{2} L} N \epsilon^{\Delta t L} N \right] u^n \rightsquigarrow \epsilon^{\Delta L} \frac{(\Delta t N)^3}{6}$$

Lemma

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

Test 1: measure of order

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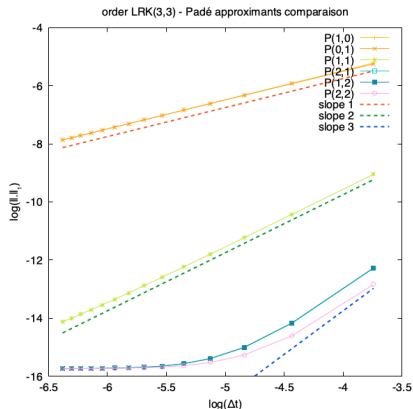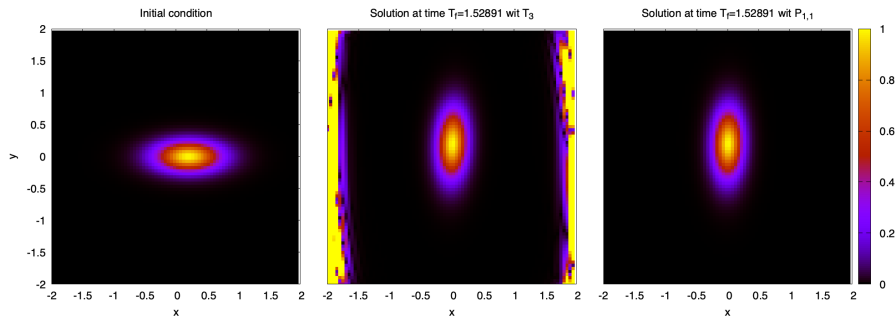

Figure: Order of Lawson RK(3,3) $P(p,q)$ approximant, $p = 1, 2$, $q = 1, 2$

Test 2: illustration of instability or stability

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

Figure: Initial condition (left), solution with Lawson RK(3,3) $T(3)$ series (middle) and Lawson RK(3,3) $P(1,1)$ approximant (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)
- Lawson method with approximation of linear part:
    - 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 !!!
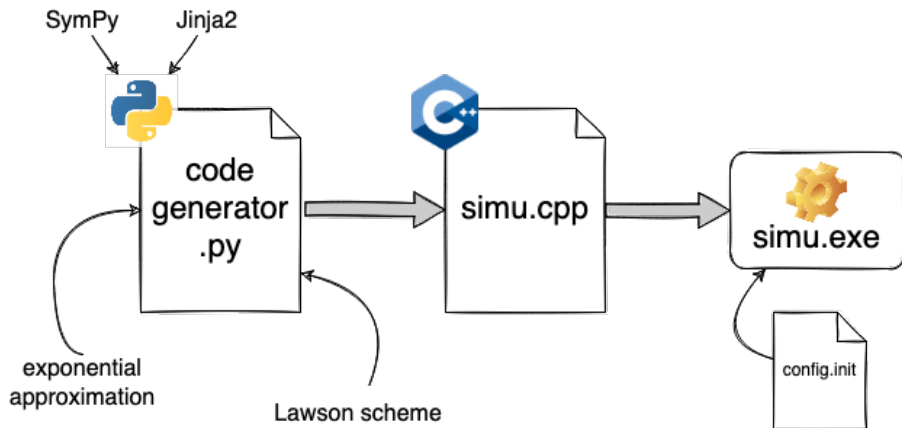
Numerical test

Weibel instability:

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

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:

$$\mathcal{H}_E(t) = \frac{1}{2} \int \|\boldsymbol{E}(t,z)\|_2^2 \, \mathrm{d}z \qquad \mathcal{H}_B(t) = \frac{1}{2} \int \|\boldsymbol{B}(t,z)\|_2^2 \, \mathrm{d}z$$

$$\mathcal{H}_c(t) = \frac{1}{2\Omega_{pe}^2} \int \|\boldsymbol{j}_c(t,z)\|_2^2 \, \mathrm{d}z$$
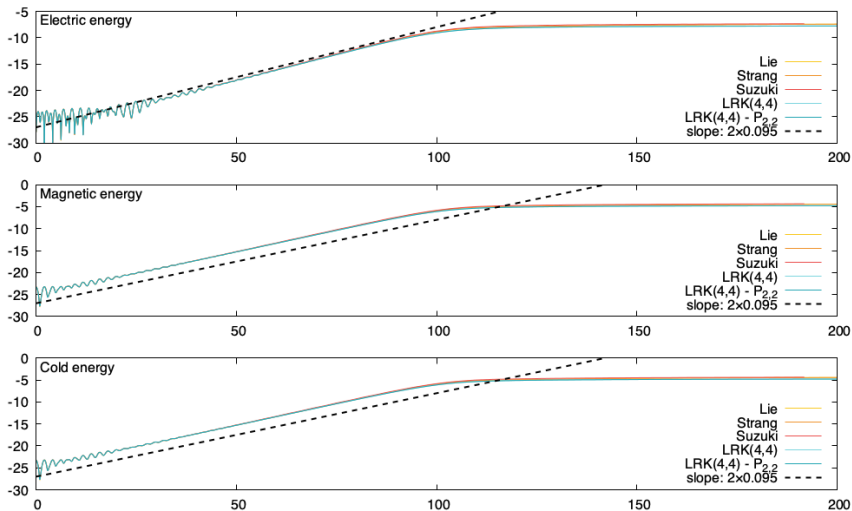
Figure: Energies evolution, $\Delta t = 0.05$
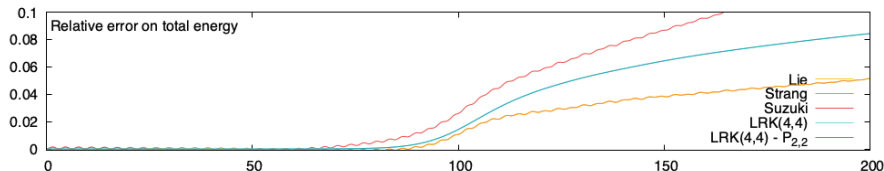
Figure: Relative error on total energy, $\Delta t = 0.05$

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: Simulation time for some simulation, 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 $\Delta t = 0.05$.
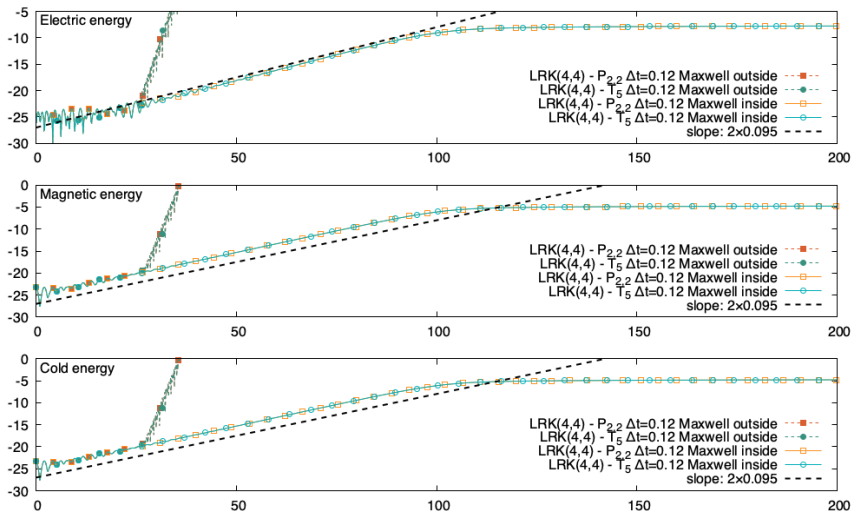
Numerical results: Padé-Lawson

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

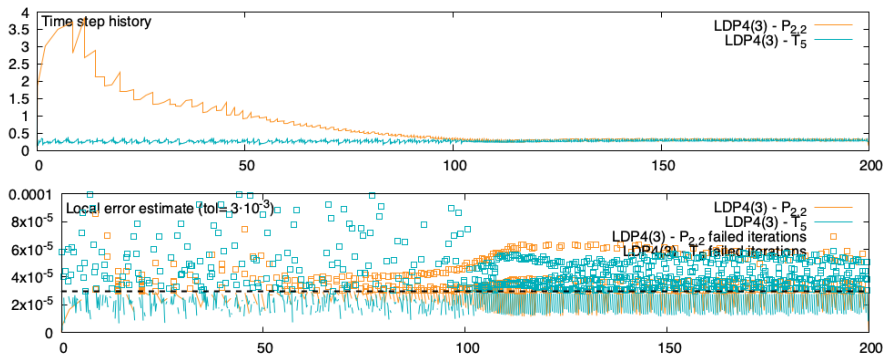Figure: Energies evolution, Lawson with Taylor or Padé approximation, Δt^n

Figure: Time step evolution and estimate of local error, Lawson with Taylor or Padé approximation, Δt^n

Simulation 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

Table: Simulation time for some simulation, 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

- ✔ First simulations of this system using Hamiltonian splitting
- ✘ 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

Future works

- Compare Lawson method with Padé approximant with a PIC simulation
- Add $\int \boldsymbol{v} f_h \, \mathrm{d}\boldsymbol{v}$ in linear part (for $1dx - 1dv$ model)

Thank you for your attention

Backup

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

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

$$\underbrace{\hphantom{S_{\alpha_1 \Delta t}(u^n)}}_{u^{(1)}}$$

$$u^{(2)}$$

$$u^{(3)}$$

$$u^{(4)}$$

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

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):

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

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

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

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

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

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

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

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

Numerical tools:

- Solve in Fourier space

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

Numerical tools:

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

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

This step is split again onto 3 parts.

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

Numerical tools:

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

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

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

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

For Lie method:
$$U^{n+1} = \varphi_{\Delta t}^{[j_c]} \circ \varphi_{\Delta t}^{[B]} \circ \varphi_{\Delta t}^{[E_{v_x}]} \circ \varphi_{\Delta t}^{[E_{v_y}]} \circ \varphi_{\Delta t}^{[f_{h,x,v_x}]} \circ \varphi_{\Delta t}^{[f_{h,x,v_z}]} \circ \varphi_{\Delta t}^{[f_{h,y,v_y}]} \circ \varphi_{\Delta t}^{[f_{h,y,v_z}]} \circ$$
$$\varphi_{\Delta t}^{[f_{h,z,1}]} \circ \varphi_{\Delta t}^{[f_{h,z,2}]} \circ \varphi_{\Delta t}^{[f_{h,z,3}]}(U^n)$$
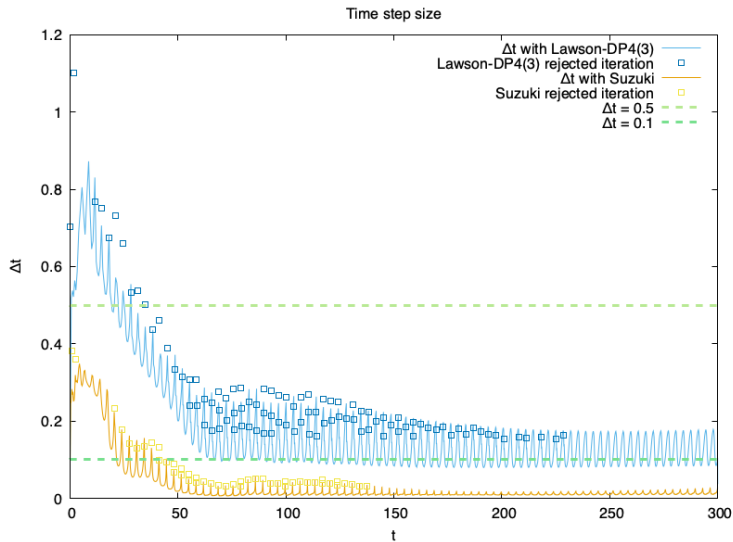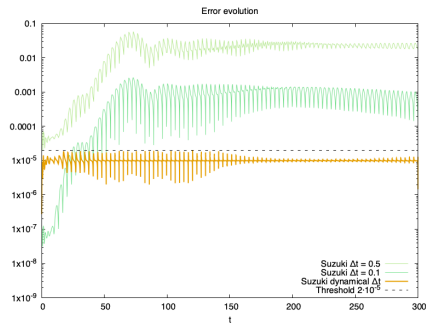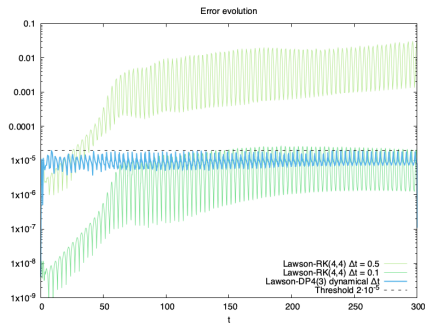
Figure: Time step size in 1dx-1dv
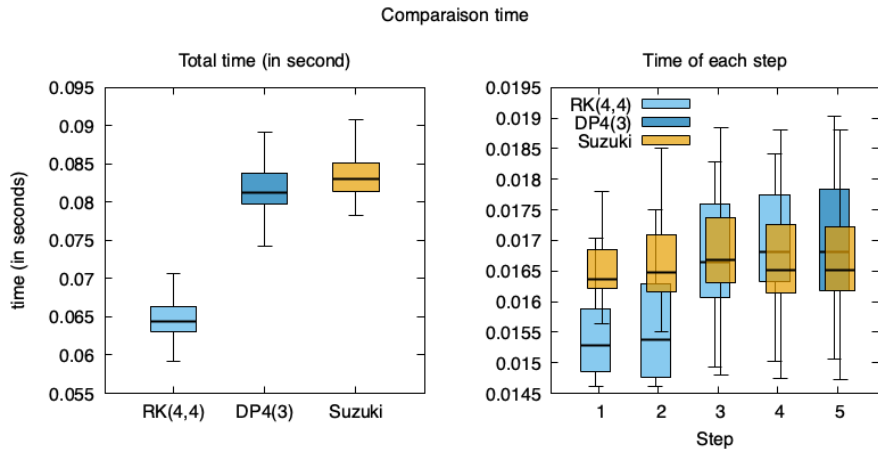
Figure: Local error estimate Lawson (left) and Suzuki (right)

Figure: Simulation time of each step