(Approximate) Exponential methods for solving hyperbolic problems for electron hybrid model

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October 21, 2021

Outline

Outline

Introduction

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 $\boldsymbol{j}_c$) and a hot (kinetic) electron density distribution f_h:

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

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

with:

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

We want:

- High order time integrator and space integrator (FFT + WENO)
- Efficient adaptive time step method

Outline

Lawson method

We would like to solve

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

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

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

which can be solve 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, Leibold, and Ostermann 2020, *Numerische Mathematik*

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

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

Why this could be complicated ?

✗ We would like a formal form depending on time parameter τ and all hidden parameters of matrix L

Solutions:

Taylor series: simplest and first method studing

Padé approximant: defined as the best rational approximation of a function

. . . : Some other methods don't explor yet

Moler and Van Loan 2003, *SIAM Review*

Simplification:

- Suppose L diagonalizable and all its eigenvalues are pure imaginary $\mathrm{sp}(L) \subset i\mathbb{R} \implies \mathrm{sp}(e^{tL}) \subset \mathcal{C}(0,1)$.

Taylor series

Simplest approximation:

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

Theorem

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

Proof: compute Taylor series outside of its convergence radius

Conclusion:

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

Eigenvalues of Taylor series

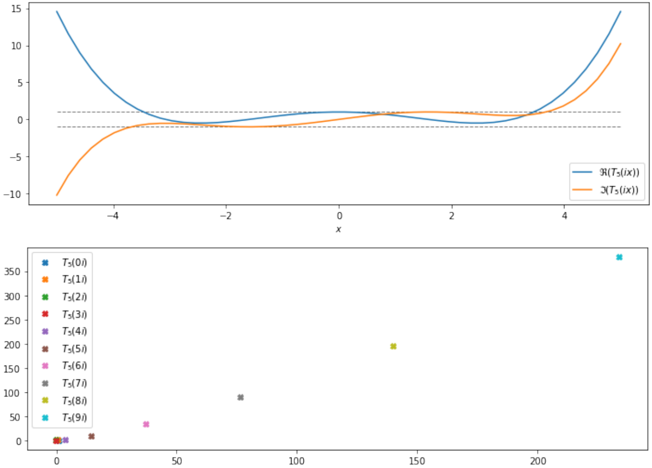

Figure: $T_5(ix)$, $x \in [\![0, 9]\!]$

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
- ✔ Preserve eigenvalues

Proof

L diagonalizable and $\mathrm{sp}(L) \subset i\mathbb{R} \implies L = Q^{-1}DQ$

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

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

with $D = \mathrm{diag}(\{i\alpha_j, j = 1, \dots, d\})$

$$\sum_{k=0}^{p} \frac{1}{k!} D^k = \mathrm{diag}\left(\left\{\sum_{k=0}^{\lfloor \frac{p}{2} \rfloor} (-1)^k \frac{\alpha_j^{2k}}{2k!} + i \sum_{k=0}^{\lfloor \frac{p}{2} \rfloor - 1} (-1)^k \frac{\alpha_j^{2k+1}}{(2k+1)!}, j \in [\![0, d]\!]\right\}\right)$$

$$\sum_{\ell=0}^{p} (-1)^\ell \frac{1}{\ell!} D^\ell = \mathrm{diag}\left(\left\{\sum_{\ell=0}^{\lfloor \frac{p}{2} \rfloor} (-1)^\ell \frac{\alpha_j^{2\ell}}{2\ell!} - i \sum_{\ell=0}^{\lfloor \frac{p}{2} \rfloor - 1} (-1)^\ell \frac{\alpha_j^{2\ell+1}}{(2\ell+1)!}, j \in [\![0, d]\!]\right\}\right)$$

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

Eigenvalues of Padé approximant

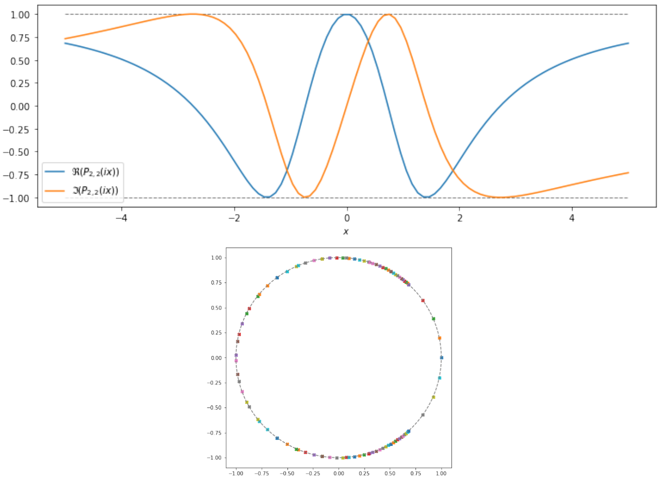

Figure: $P_{2,2}(ix)$, $x \in [-5, 5]$

Eigenvalues of assymetric Padé approximants

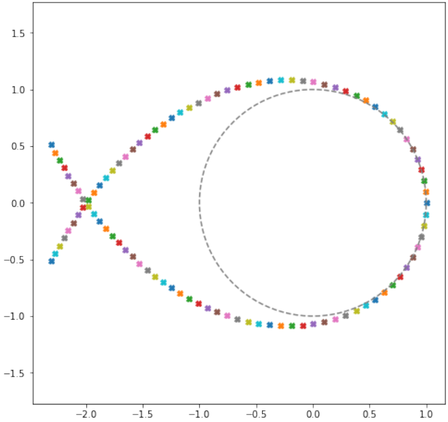

Figure: $P_{2,1}(ix)$ $x \in [-5, 5]$

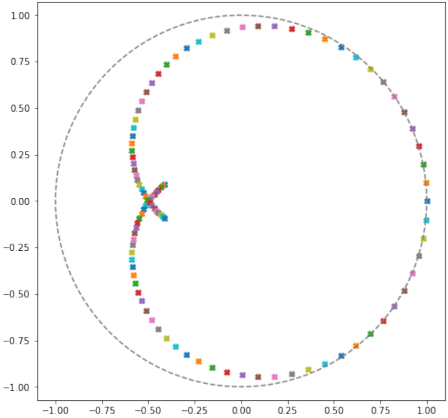

Figure: $P_{1,2}(ix)$ $x \in [-5, 5]$

Eigenvalues of assymetric Padé approximants

✔ If $p = q$, no problem !

➜Good choice !

Error on approximate Lawson method

We note $\mathfrak{exp}(L) = P_{p.q}(L)$ or $T_p(L)$, generic approximation.

$$\mathfrak{exp}(L) = e^L + \mathcal{O}(L^{r+1})$$

Lawson RK(3,3) method:

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

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

Error on approximate Lawson method

If L and N don't commute:

$$
\begin{aligned}
u^{n+1} = \Big[e^{\Delta t L} &+ \Delta t \left(\frac{2}{3} e^{\frac{\Delta t}{2}L} N e^{\frac{\Delta t}{2}L} + \frac{1}{6} e^{\Delta t L} N + \frac{1}{6} N e^{\Delta t L} \right) \rightsquigarrow e^{\Delta L} \Delta t N \\
&+ \frac{\Delta t^2}{2} \left(\frac{1}{3} N e^{\Delta t L} N + \frac{1}{3} e^{\frac{\Delta t}{2}L} N e^{\frac{\Delta t}{2}L} N + \frac{1}{3} e^{\frac{\Delta t}{2}L} N e^{-\frac{\Delta t}{2}L} N e^{\Delta t L} \right) \\
&\qquad \rightsquigarrow e^{\Delta L} \frac{(\Delta t N)^2}{2} \\
&+ \frac{\Delta t^3}{6} e^{\frac{\Delta t}{2}L} N e^{-\frac{\Delta t}{2}L} N e^{\Delta t L} N \Big] u^n \rightsquigarrow e^{\Delta L} \frac{(\Delta t N)^3}{6}
\end{aligned}
$$

Same results if $e^{\Delta t L} \mapsto \mathfrak{exp}(\Delta t L) = e^{\Delta t L} + \mathcal{O}(\Delta t^{r+1})$

Lemma

Error for Lawson RK(m,s) is always in $\mathcal{O}(\Delta t^{m+1}) + \mathcal{O}(\Delta t^{r+1})$

Outline

$$\partial_t u + a\partial_x u + b\partial_y u = 0$$

After a Fourier transform in y

$$\partial_t \hat{u} + \underbrace{\imath bk\hat{u}}_{L\hat{u}} + \underbrace{\widehat{a\partial_x u}}_{N(\hat{u})} = 0$$

First test with:

- Lawson RK(3,3) method
- Lawson RK(3,3) method with Taylor series T_p, $p \in [\![1,4]\!]$
- Lawson RK(3,3) method with Padé approximant $P_{p,q}$, $p,q \in [\![1,2]\!]$

Mesure order: $x,y \in [-2,2]$, $N_x = N_y = 243$, $a = 1.0$, $b = 0.75$, $T_f = 0.07111$, $\Delta t \in [0.00158, 0.02370]$.

Test 1

2D translation test case: mesure of order

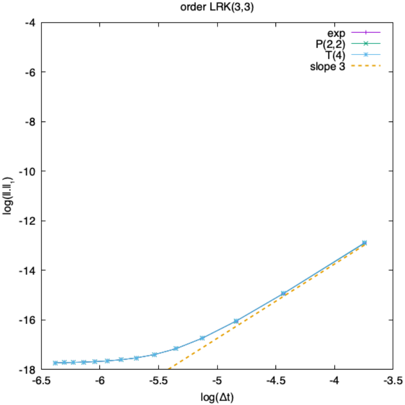

Figure: Order of Lawson RK(3,3) method, and Lawson RK(3,3), $P_{2,2}$ approximant method and Lawson RK(3,3) T_4 series method.

Test 1

2D translation test case: mesure of order

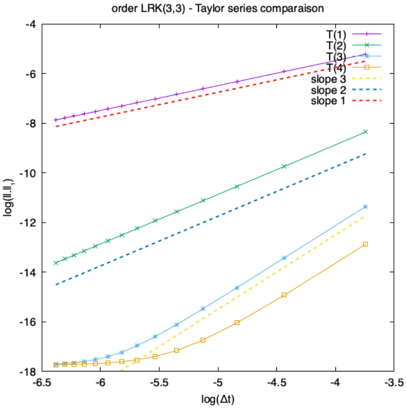

Figure: Order of Lawson RK(3,3) T_p series method, $p = 1, \ldots, 4$.

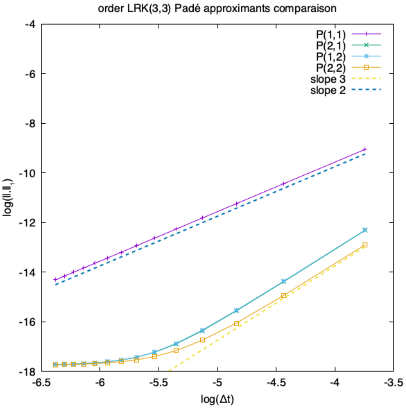

Figure: Order of Lawson RK(3,3) $P_{p,q}$ approximant, $p = 1, 2$, $q = 1, 2$

Test 2

2D rotation test case

$$\partial_t u - y\partial_x u + x\partial_y u = 0$$

After a Fourier transform in y

$$\partial_t \hat{u} + \underbrace{\imath x k \hat{u}}_{L\hat{u}} + \underbrace{\widehat{-y\partial_x u}}_{N(\hat{u})} = 0$$

Second test with same methods:

- Lawson RK(3,3) method
- Lawson RK(3,3) method with Taylor series T_3, $p = 3$
- Lawson RK(3,3) method with Padé approximant $P_{1,1}$, $p = q1$

Test Taylor instability: $x, y \in [-2, 2]$, $N_x = N_y = 81$, $T_f = 1.52891$, $\Delta t = 0.020944$.

Test 2

2D rotation test case: test Taylor series instability

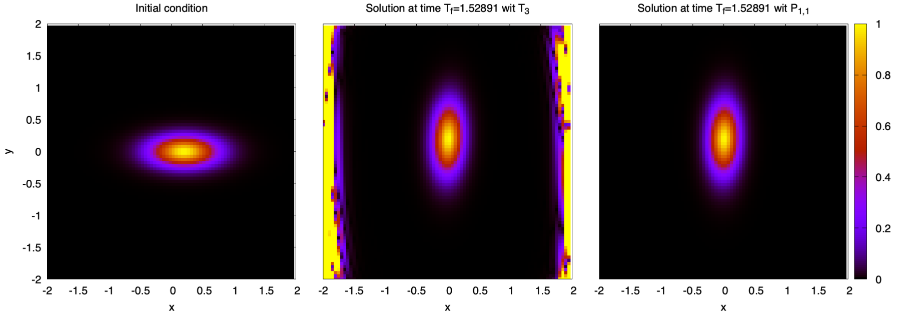

Figure: Initial condition (left), solution with Lawson RK(3,3) T_3 series (middle) and Lawson RK(3,3) $P_{1,1}$ approximant (right)

Outline

4D hybrid fluid-kinetic plasma model

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

- Cold electrons ➜fluid: cold current $(j_{c,x}(t,z), j_{c,y}(t,z))$
- Hot electrons ➜kinetic: density in phase space $f_h(z, v_x, v_y, v_z)$

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

with $U = (j_{c,x}, j_{c,y}, B_x, B_y, E_x, E_y, f_h)^\top$ and

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

✗can't compute e^{tL} formally ✔$P_{p,p}(tL)$ Padé approximant!

Simulation code

We compare on this model:

- Strang *classical* method, based on Hamiltonian splitting: order 2
- Lawson RK(4,4) classical (but some terms added in nonlinear term: Maxwell equations): order 4
- Lawson RK(4,4) with Padé $P_{2,2}$ approximant: order 4
- Lawson DP4(3) with Padé $P_{2,2}$ approximant: adaptive time step method

Implementation details:

Problem with 7 variables, Padé approximant implies huge rational functions (with invert of matrix), high order Lawson methods have a lot of coefficients. . . Code generation ✔

Main idea of adaptive time step methods (error estimate)

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

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

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

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)

Numerical results

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

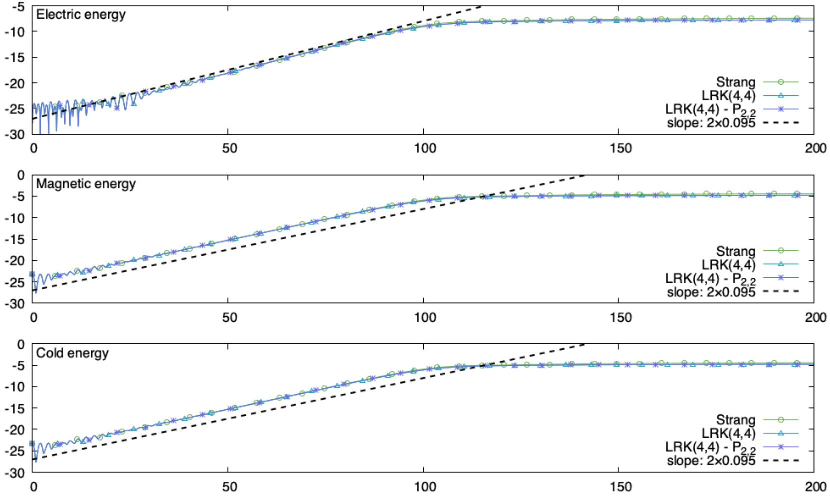

Figure: Energies evolution for Strang, LRK(4,4) and LRK(4,4)-$P_{2,2}$ methods

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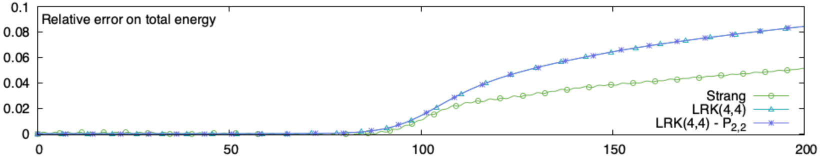

Figure: Relative error on total energy for Strang, LRK(4,4) and LRK(4,4)-$P_{2,2}$ methods

Numerical results

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

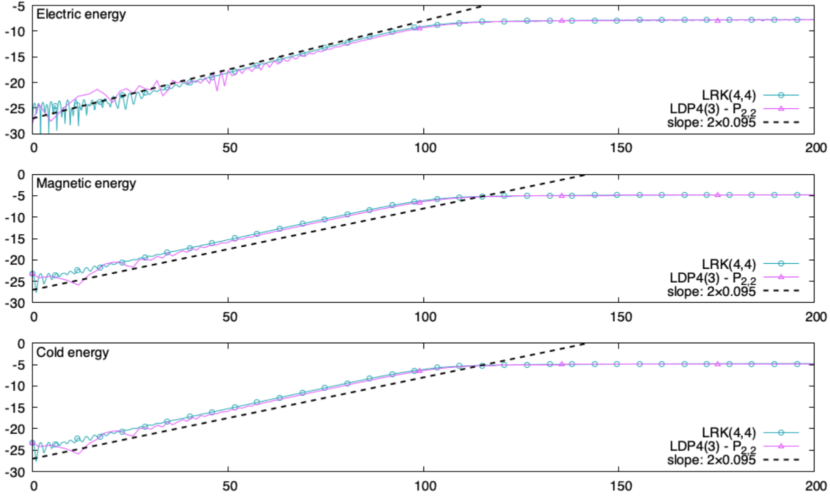

Figure: Energies evolution for LDP4(3)-$P_{2,2}$ method

Numerical results

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

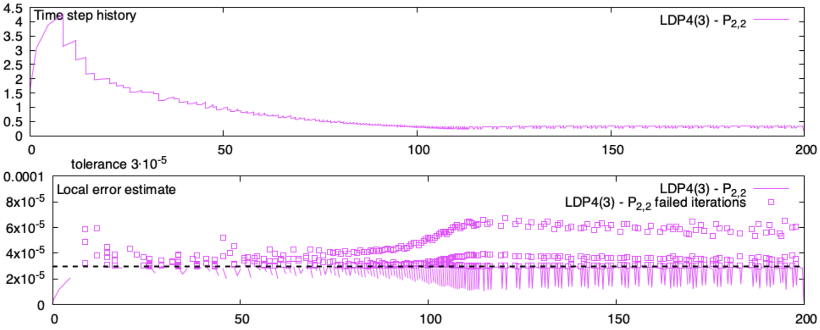

Figure: Time step and estimate of local error evolution for LDP4(3)-$P_{2,2}$ method

Simulation time

time integrator	simulation time
Strang splitting	17 h 09 min 54 s
LRK(4,4)	14 h 06 min 15 s
LRK(4,4) - $P_{2,2}$	13 h 59 min 59 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

Conclusion:

- ✗ Numerical cost of Hamiltonian splitting methods (not bad in $1dx - 1dv$ but very bad in $1dz - 3dv$, must be very very very bad in $3dx - 3dv$ case)
- ✔ Numercial cost of Lawson methods
- $\sim$ 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
- ✔ Very efficient adaptive time step method with computation of $e^{\tau L}$ with Padé approximant (more thinks can be in linear part)

Future works

- Add $\int \boldsymbol{v} f_h \,\mathrm{d}\boldsymbol{v}$ in linear part (for $1dx - 1dv$ Vlasov-Ampère model)

Thank you for your attention

Backup