Advective and conservative semi-Lagrangian schemes on uniform and non-uniform grids

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5 September 2013

Outline

- Presentation of some semi-Lagrangian schemes on uniform grid
    - advective case
    - conservative case
    - limitations
- Adaptation to non-uniform grid
  $\Rightarrow$ application to KEEN waves
- Adaptation to polar/curvilinear grid
  $\Rightarrow$ application to guiding center model

Basics on semi-Lagrangian schemes

We consider a transport equation

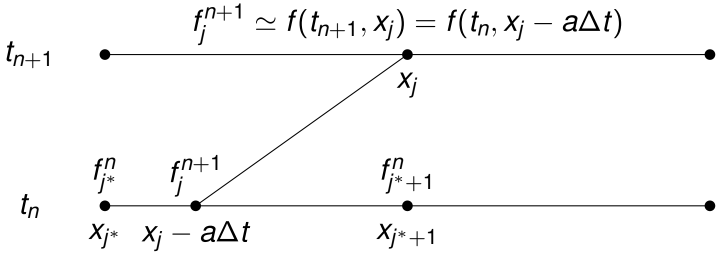
$$\partial_t f + \nabla \cdot (af) = \partial_t f + a \cdot \nabla f = 0,\ \nabla \cdot a = 0$$

which leads to the property "**f is constant along the characteristics**"

$$f(t_{n+1}, x) = f(t_n, X(t_n; t_{n+1}, x)),\ X'(t) = a(t, X(t))$$

- Computation of the characteristics
- Interpolation step

Schematic example for 1D constant advection



A general remark

- Many semi-Lagrangian schemes have been developed
- General framework
- different independent options
- Genericity/modularity

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Advective approach with cubic splines

Unknowns are $f_j^n \simeq f(t_n, x_j)$

Classical cubic splines approach

- Compute spline coefficients from (f_j^n)
  - tridiagonal solver for each direction (non local)
- Interpolation at foot of characteristic for each grid point
  - 4^d coefficient contributions in dimension d

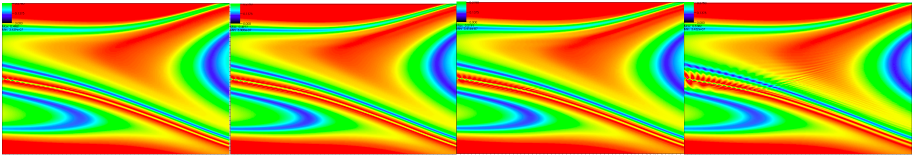
- *good compromise between cost and accuracy*
- *adopted with* $1D$ *(*`Cheng-Knorr, JCP 1976` *) or* $2D$ *splitting (*`Sonnendrücker et al, JCP 1999`*)*
- *still method used in gyrokinetic code GYSELA (with local splines)*

Cubic splines : what else ?

- Other choices are possible
  - Lagrange
  - higher order splines
  - Hermite with or without derivative reconstructions
  - ENO, WENO, limiters...
- How to choose, classify ?
  - Order of accuracy
  - conservation properties
  - cost
  - diffusion vs dispersion
- Looking for a unified framework
  - easy change of method
  - comparison, influence of numerics

Numerical dispersion of cubic splines for small Δt

Two stream instability test case ; zoom of distribution function

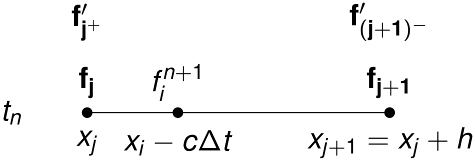


- Cubic splines with standard $\Delta t = 0.1$
- Lagrange interpolation of degree 17 with standard $\Delta t = 0.1$
- Lagrange interpolation of degree 17 with very small $\Delta t = 0.001$
- Cubic splines with very small $\Delta t = 0.001$

`Charles-Després-M, SINUM 2013`

Advective approach with derivative reconstruction

We start from a cubic Hermite formulation



Different possibilities for the reconstruction of the derivatives :

- Simpson formula for getting cubic splines
- compact finite difference of order p, **FD(p)** :

$$f'_{j^+},\ \ f'_{(j+1)^-} \text{obtained from formula with stencil } j - \lfloor \frac{p}{2} \rfloor, j + \lfloor \frac{p+1}{2} \rfloor$$

Advective approach with Hermite formulation

Unknowns are $f_j^n \simeq f(t_n, x_j)$
Hermite formulation approach

- Compute derivatives from (f_j^n)
    - explicit stencil formula for each direction (FD(p) case)
    - tridiagonal solver for each direction (cubic splines case)
    - possibility of using FFT in both cases
- Interpolation at foot of characteristic for each grid point
    - 4^d coefficient contributions in dimension d

- *enables to unify several interpolation schemes*
- *similar structure, as in the case of cubic splines*
- *limitation to third order, as in the case of cubic splines*
- *use of more temporary memory for storing the derivatives*

Remarks and advantages of FD(p)

- Formulae are explicit
  - $\rightarrow$ easy change of parameter p in the code
- Interpolation becomes local and remains third order
  - $\rightarrow$ generalizations not prohibitive w.r.t cost
- For p even, we get a C^1 reconstruction with $f'_{j^+} = f'_{j^-}$
- For p odd, upwinding effect ; better for small Δt
  - $\rightarrow$ no dispersion effect as for p even or cubic splines
  - $\rightarrow$ more temporary storage of derivatives
- FD3 = Lagrange of order 3
- FD(2d+1) $\simeq$ Lagrange of order 2d+1, $d \geq 2$
  - equality for limit $\Delta t \rightarrow 0$
  - schemes remain different, as FD(2d+1) is third order
- FD6 $\simeq$ cubic splines

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Conservative approach : the 1D case

Unknowns are $f_j^n \simeq \frac{1}{x_{j+1/2}-x_{j-1/2}} \int_{x_{j-1/2}}^{x_{j+1/2}} f(t_n, x)dx$

$$f_j^{n+1} \simeq \frac{1}{x_{j+1/2} - x_{j-1/2}} \int_{x_{j-1/2}-a\Delta t}^{x_{j+1/2}-a\Delta t} f(t_n, x)dx$$

- use of advective approach for primitive function $F(x) = \int_{x_{-1/2}}^{x} f$
- adhoc integration constant for dealing with a periodic primitive

- *here equivalent to advective approach for constant advection*
- *possibility of adding limiters for positivity...*
- *Multi-D with splitting see* `talk of Güclü`

Filbet-Sonnendrücker-Bertrand, JCP 2001
Crouseilles-M-Sonnendrücker, JCP 2010
Qiu-Shu, JCP and CCP 2011

Conservative approach : the 2D case

Method is fixed by the way of displacing backward the cells

$$C_{i,j} = [x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}]$$

- translation of $C_{i,j}$ from the center $x_{i,j} \to x^*_{i,j}$
  - $\rightarrow$ not (always) conservative
  - $\rightarrow$ equivalent to previous advective approach

  some similarities with `talk of Yang`
- quadrilateral formed by vertices $x^*_{i\pm1/2,j\pm1/2}$
  - $\rightarrow$ $x^*_{i\pm1/2,j\pm1/2}$ from linear interpolation of $x^*_{i,j}$
    - keep uniformity with advective approach
    - information of field generally better known on $x_{i,j}$
    - sort of stabilization of deformed cell
  - $\rightarrow$ effectively conservative (displaced cells form a mesh)
  - $\rightarrow$ needs mesh intersection

  `Lauritzen-Ramachandran-Ullrich, JCP 2010`

  `Glanc(PhD 2010-2013)-Crouseilles-M`

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Difficulties/questions/other methods

- 4D advection ?
- Conservation of mass AND constant states ?
- Conservation of energy ?
- How to deal with non uniform grid ?

Solutions exist now with CFL condition. Examples :

- DG : see `talk of Ayuso and Restelli`
- finite volume : see `Crouseilles, Filbet, JCP 2004; talk of Hittinger`

Forward strategies/PIC like : see `talk of Campos Pinto`
Mixed approaches are envisaged
`Latu et al., INRIA report 8054`

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KEEN wave simulation on uniform grid

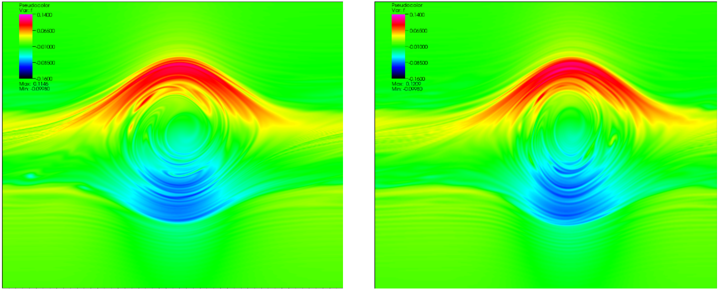


FIGURE: $f(1000, x, v) - f_0(x, v)$, $\Delta t = 0.05$. Cubic splines, with $N_x = N_v = 4096$ on CPU (left) and Lagrange interpolation of degree 17 $N_x = N_v = 2048$ on GPU double precision (right).

Region becomes smaller for some parameters of interest. See `talk of Afeyan`

$\Rightarrow$ **Need of non uniform grid in velocity**

What for non uniform grid ?

Non uniform grid is linked to a continuous mapping $[0,1] \to [0,1]$

$$\frac{i}{N} \to v_i$$

A possible generation of $v_i,\ i = 0, \ldots N$:

- (input 1) definition of 3 zones ; typically $0 < 0.53 < 0.69 < 1$
- (input 2) definition of grid density for each zone $1; 32; 1$
- (output 1) i_1, i_2 such that $v_{i_1} \simeq 0.53,\ v_{i_2} \simeq 0.69$
- (output 2) from (output1) : $v_i,\ i = 0, \ldots, N$

Two grid : a simple non uniform grid

uniform grid with a refined zone

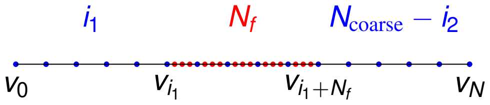
Mesh spacing on coarse/fine grids are

$$\Delta v_{\text{coarse}} = \frac{v_{\max} - v_{\min}}{N_{\text{coarse}}}, \; \Delta v_{\text{fine}} = \frac{v_{\max} - v_{\min}}{N_{\text{fine}}}$$

and N_{fine} is an integer multiple of N_{coarse}.

The refined zone is chosen with $0 \leq i_1 < i_2 \leq N_{\text{coarse}}$ and the total number of cells is

$$N = i_1 + N_f + N_{\text{coarse}} - i_2, \; N_f = \frac{N_{\text{fine}}}{N_{\text{coarse}}}(i_2 - i_1)$$



Hermite formulation

Hermite formulation is still valid for general non uniform grid
The question is : how to compute the derivatives ?

- classical non uniform cubic splines
  $\rightarrow$ again tridiagonal solver for derivatives
- FD(p) may *not* be a good alternative on general non uniform grid
  - possible stability issues
  - complication of formulae
- possible design of formulae *specific* to two grid case

Two grid derivatives

Two-grid cubic splines :

- Compute derivatives on coarse grid points to get it at points

$$v_j,\ j \in \{0, \dots, i_1\} \cup \{i_1 + N_f, \dots, N\}.$$

- Compute it on fine grid points

$$v_j,\ j \in \{i_1, \dots, i_1 + N_f\},$$

  using boundary conditions at points $v_{i_1}, v_{i_1+N_f}$

As in the case of uniform grid, we can adapt the reconstruction of derivatives in the FD(p) case.

Two-grid FD(p) :

- Compute derivatives using *FD* formula on coarse grid
- Compute function values on some boundary fine grid points in $[v_0, v_{i_1}] \cup [v_{i_1+N_f}, v_N]$, that are needed for next step, using interpolation on coarse grid
- Compute derivatives using *FD* formula on fine grid

Conservative version

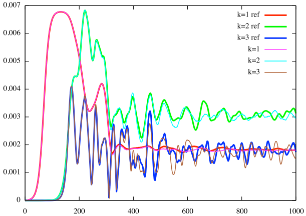
Previous version has to be changed on non uniform grids in order to be mass conservative.

- Unknowns are $u_{j+1/2} = \frac{1}{v_{j+1}-v_j}\int_{v_j}^{v_{j+1}} u(v)dv$
- Use of previous Hermite interpolation on primitive data

$$U(v_j) = \int_{v_0}^{v_j} u(y)dy,\ \ v_j,\ j = 0, \ldots, N$$

- Choose adhoc integration constant for dealing with a primitive that is also periodic

Numerical results



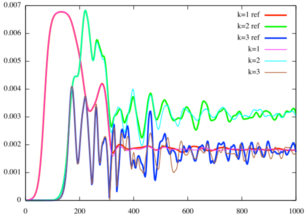


FIGURE: Absolute values of the first three Fourier modes of ρ vs time. Reference solution with LAG17 $N_x = N_v = 2048$ on GPU double precision (red, green and blue) compared to solution on uniform mesh in space (LAG17, $N_x = 256$) and uniform refined mesh in velocity with $N_v = 374$ ($N_{\mathrm{coarse}} = 64$, $N_{\mathrm{fine}} = 2048$, $i_1 = 34$, $i_2 = 44$)
(left) : conservative non uniform cubic splines
(right) : conservative two-grid FD5

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Cartesian case. Results on uniform grid

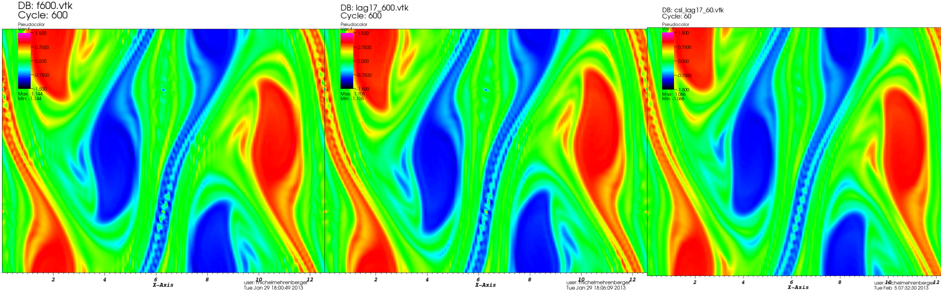


FIGURE: Distribution function at time $T = 60$, $\Delta t = 0.1$, $N = 128$ Advective 2D cubic splines (left), advective 2D FD(17) (middle), conservative 2D FD(17) (right)

Cartesian case. Results on uniform grid

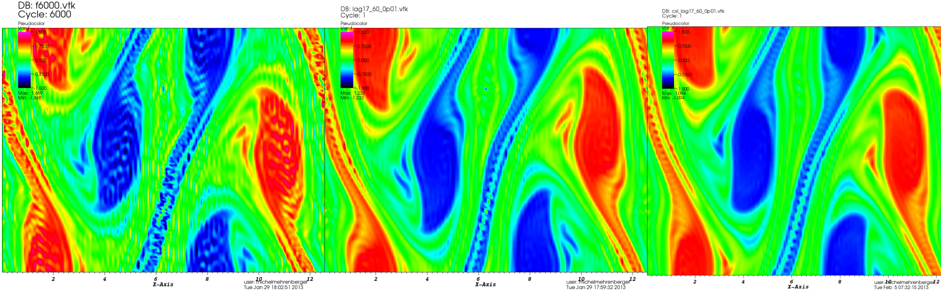


FIGURE: Distribution function at time $T = 60$, $\Delta t = 0.01$, $N = 128$ Classical advective 2D cubic splines (left), advective 2D FD(17) (middle), conservative 2D FD(17) (right)

Cartesian case. Results on curvilinear grid

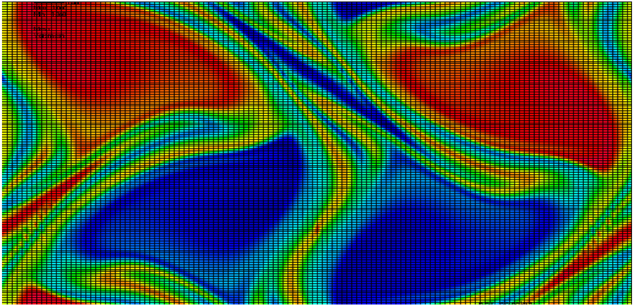
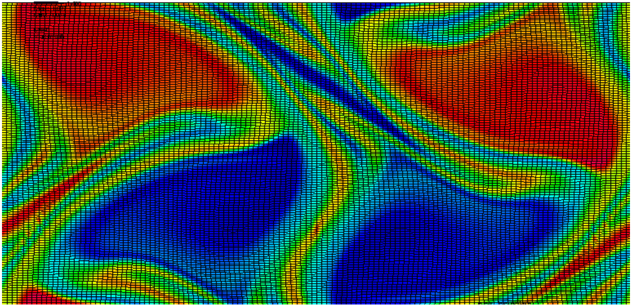


FIGURE: Distribution function and mesh at time $T = 30$, $\Delta t = 0.1$, $N = 128$ classical advective cubic splines, $\alpha = 10^{-6}$

`Hamiaz-M, Back, in preparation`

Cartesian case. Results on curvilinear grid



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Cartesian case. Results on curvilinear grid

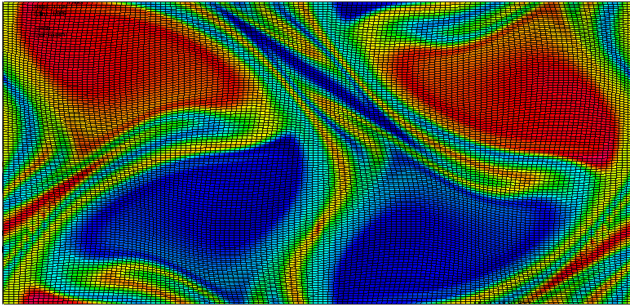
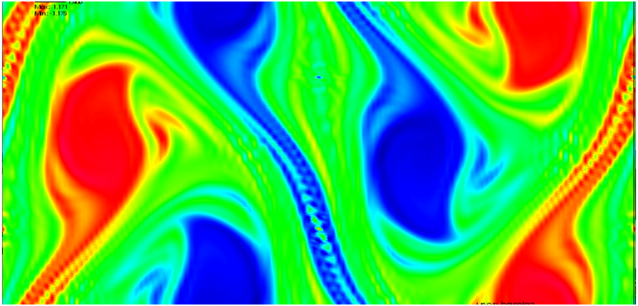


FIGURE: Distribution function and mesh at time $T = 30$, $\Delta t = 0.1$, $N = 128$ classical advective cubic splines, $\alpha = 210^{-1}$

Cartesian case. Results on curvilinear grid



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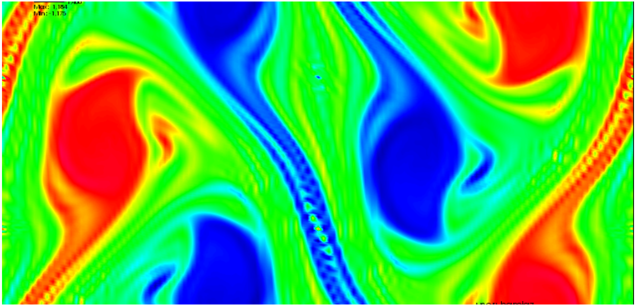
Cartesian case. Results on curvilinear grid



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Cartesian case. Results on curvilinear grid

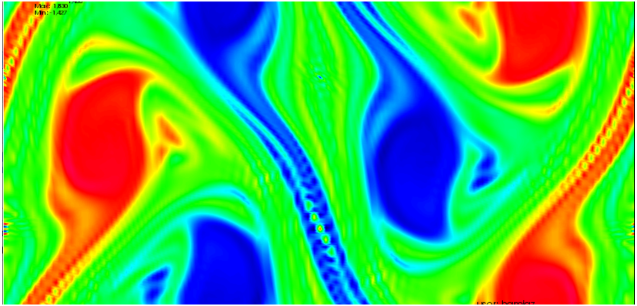

FIGURE: Distribution function at time $T = 60$, $\Delta t = 0.1$, $N = 128$ classical advective cubic splines, $\alpha = 2 \cdot 10^{-1}$

energy and mass conservation

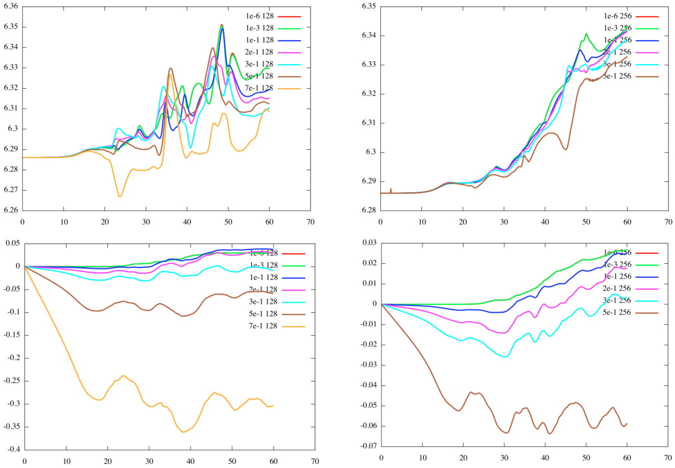

FIGURE: Energy (top) and mass (bottom) conservation $N = 128$ (left), $N = 256$ (right)

energy and mass conservation

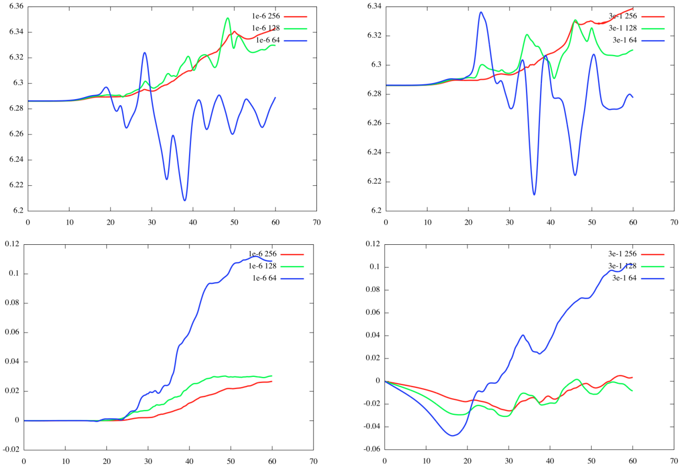

FIGURE: Energy (top) and mass (bottom) conservation $\alpha = 10^{-6}$ (left), $\alpha = 3 \cdot 10^{-1}$ (right)

Polar case. Results in polar geometry

The diocotron instability test case

- Study of energy and mass conservation of the continuous model
- Study of growth rate, following `Davidson, 1990`
- Results *depend* on boundary conditions, here at $r_{\min}$
  - Dirichlet
  - Neumann
  - Neumann for mode 0 and Dirichlet for other modes
- Validation with classical cubic splines method

`Hirstoaga-Madaule-M-Petri, hal-00841504`

Growth rate and density

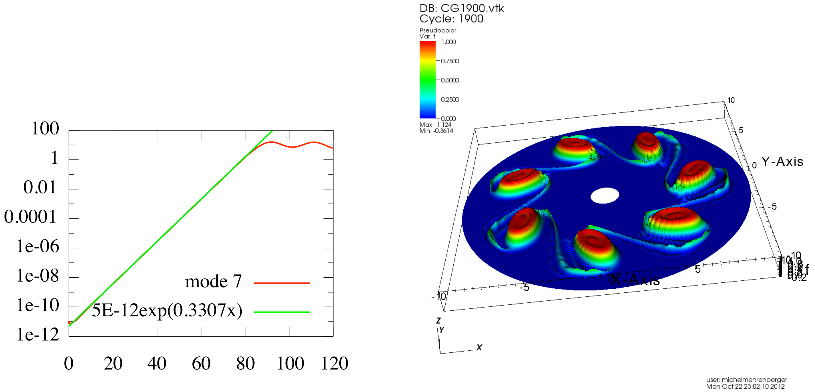

FIGURE: (Left) Square modulus of the 7th Fourier mode of $\int_{r_{\min}}^{r_{\max}} \Phi(t, r, \theta) dr$ vs time t for neumann mode 0 (Right) Density ρ at $t = 95$. Discretization parameters are $N_r = 512$, $N_\theta = 256$ and $\Delta t = 0.05$.

Conservation of energy and mass

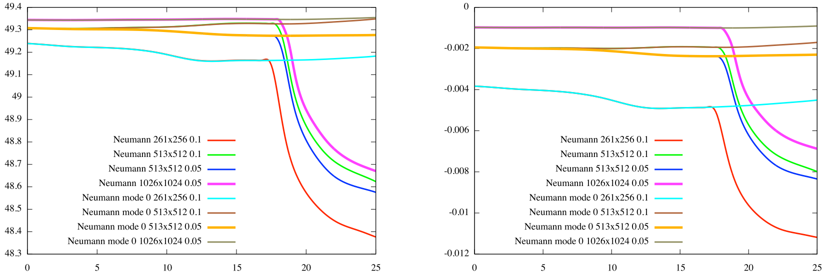

FIGURE: Time evolution of electric energy (left) and relative mass error (right) for Neumann and Neumann mode 0 boundary conditions, with different discretizations ($N_r \times N_\theta$ Δt on legend).

Long time behavior of energy/mass conservation

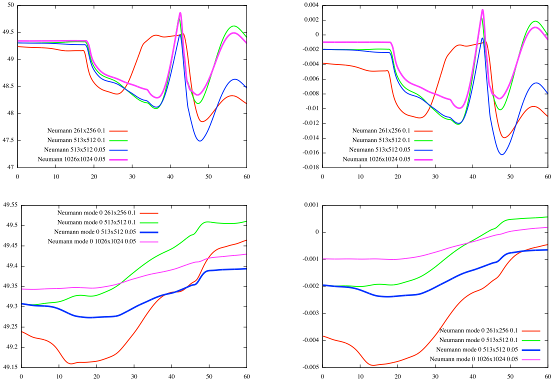

FIGURE: Long time evolution of electric energy (left) and relative mass error (right) for Neumann (top) and Neumann mode 0 (bottom)boundary conditions, with different discretizations ($N_r \times N_\theta$ Δt on legend).

Conclusion/Perspectives

- Description of a class of semi-Lagrangian schemes
- Validation on a hierarchy of simplified test cases

$\Rightarrow$ Continue on Drift kinetic model `Grandgirard et al., JCP 2006, talk of Yang`

$\Rightarrow$ Semi-Lagrangian discontinuous Galerkin [1] on non uniform grid in velocity

$\Rightarrow$ Better or exact conservation study

$\Rightarrow$ Study in HPC context

$\Rightarrow$ Design of intermediate testcases

1. superconvergence property on uniform grid, Steiner-M-Bouche, submitted