Semi-Lagrangian Vlasov solvers

Eric Sonnendrücker

IRMA
Université de Strasbourg, France

project-team CALVI
INRIA Nancy Grand Est

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In collaboration with
J.-P. Braeunig, N. Crouseilles, V. Grandgirard, G. Latu, M. Mehrenberger

Outline

1. Numerical methods for kinetic equations
2. Classical semi-Lagrangian method
3. Conservative semi-Lagrangian method
4. Mapped mesh
5. Application of CSL to the drift-kinetic model
6. Forward semi-Lagrangian method

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The model

- An abstract form of a kinetic equation reads

$$\frac{\partial f}{\partial t} + \mathbf{a}(\mathbf{z}, t) \cdot \nabla f = 0,$$

  z are the phase space coordinates, $\mathbf{a}$ depends non linearly and non locally on f, through e.g. the electromagnetic field.
- The velocity field a is divergence free so that the equation can also be written in conservative form

$$\frac{\partial f}{\partial t} + \nabla \cdot (f\mathbf{a}) = 0.$$

- Mathematically for a given $\mathbf{a}$ the non conservative form is a transport equation which can be solved using the characteristics, which are the solution of the ODE

$$\frac{d\mathbf{Z}}{dt} = \mathbf{a}(\mathbf{Z}, t).$$

Applications of semi-Lagrangian codes

Our semi-Lagrangian codes have been used with collaborators (*P. Bertrand, A. Ghizzo, N. Besse, V. Grandgirard, X. Garbet, Y. Sarazin, A. Friedman, J.L. Vay,...*) for several applications

- Laser-plasma interaction.
- Beam physics.
- Magnetic fusion, via the gyrokinetic model (see talk by *V.Grandgirard* later in this session).

History of semi-Lagrangian schemes for Vlasov

- Cheng-Knorr (JCP 1976): splitting method for 1D Vlasov-Poisson. Cubic spline interpolation.
- ES-Roche-Bertrand-Ghizzo (JCP 1998): general semi-Lagrangian framework for Vlasov-type equations.
- Nakamura-Yabe (CPC 1999): semi-Lagrangian CIP method with Hermite interpolation
- Filbet-ES-Bertrand (JCP 2001) : semi-Lagrangian PFC method: positive and conservative
- N. Besse - ES (JCP 2003) : semi-Lagrangian solver on unstructured grids.
- Crouseilles-Respaud-ES (2009): Forward semi-Lagrangian method.
- Crouseilles-Mehrenberger-ES (2010): Equivalence of point based and conservative methods for Vlasov-Poisson + new class of positive filters.
- Qiu-Christlieb (JCP 2010): conservative SL WENO schemes.
- Qiu-Shu (Brown preprint 2010): Semi-Lagrangian DG.

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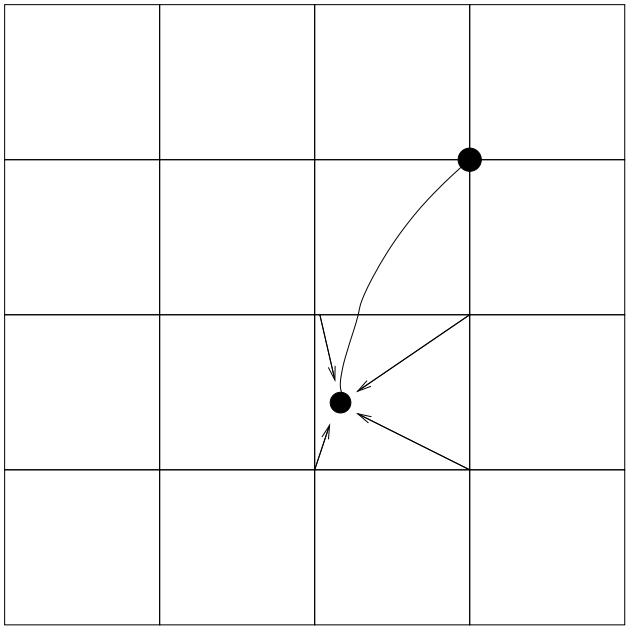
The backward semi-Lagrangian Method



- f conserved along characteristics
- Find the origin of the characteristics ending at the grid points
- Interpolate old value at origin of characteristics from known grid values $\rightarrow$ High order interpolation needed

- Typical interpolation schemes.
  - Cubic spline (Cheng-Knorr)
  - Cubic Hermite with derivative transport (Nakamura-Yabe)

Interpolation

- Cubic spline interpolation originally proposed by Cheng and Knorr is still our method of choice.
- Other methods have been tried: different variants of Lagrange, Hermite, higher order splines. None has proved superior to cubic splines for our applications.
- Features needed by interpolation: accuracy and robustness. Needs to degrade well when distribution is not resolved on the mesh.
- New implementations. Local splines
  - Series approximation of derivative on boundary: Crouseilles, Latu, ES JCP 2007.
  - Fast algorithm by Unser IEEE Trans on Pattern Analysis and Machine Intelligence, vol 13 (3), 1991 for signal processing. Cholesky decomposition with constant coefficients on diagonal and off-diagonal. Iterations started with series using directly f.

Computation of the origin of the characteristics

- Transport equation

$$\frac{\partial f}{\partial t} + \mathbf{a} \cdot \nabla f = 0,$$

- Characteristics

$$\frac{dX}{dt} = \mathbf{a}$$

- Computation of the origin of the characteristics :
  - Explicit solution if $\mathbf{a}$ does not depend on x
  - Else, numerical algorithm needed.

Splitting for exact computation of characteristics

- In many cases splitting can enable to solve a constant coefficient advection at each split step. Ideal case.
- E.g. separable Hamiltonian $H(\mathbf{q},\mathbf{p}) = U(\mathbf{q}) + V(\mathbf{p})$.
  - Vlasov equation in canonical coordinates reads

$$\frac{\partial f}{\partial t} + \nabla_p H \cdot \nabla_q f - \nabla_q H \cdot \nabla_p f = 0.$$

  - Split equations then become

$$\frac{\partial f}{\partial t} + \nabla_p V \cdot \nabla_q f = 0, \qquad \frac{\partial f}{\partial t} - \nabla_q U \cdot \nabla_p f = 0,$$

    where U does not depend on $\mathbf{p}$ and V does not depend on $\mathbf{q}$
    $\Rightarrow$ characteristics can be solved explicitly.
  - Vlasov-Poisson falls into this category with $\mathbf{q} = \mathbf{x}$, $\mathbf{p} = \mathbf{v}$, $H(\mathbf{x},\mathbf{v}) = \frac{1}{2} m \mathbf{v}^2 + q\phi(\mathbf{x},t)$.

Backward computation of characteristics in general case.

- Consider general case. Characteristics defined by

$$\frac{d\mathbf{X}}{dt} = \mathbf{a}(\mathbf{X}, t).$$

- Backward solution: $\mathbf{X}^{n+1}$ is known and $\mathbf{a}^n$ known on the grid. Does not allow standard ODE integrator.
- Numerical method for EDO can be derived using a quadrature formula on RHS of system by integrating on one time step, e.g. left or right rectangle rule for 1st order:

$$\mathbf{X}^{n+1} - \mathbf{X}^n = \Delta t\, \mathbf{a}^n(\mathbf{X}^n) \quad \text{or} \quad \mathbf{X}^{n+1} - \mathbf{X}^n = \Delta t\, \mathbf{a}^{n+1}(\mathbf{X}^{n+1}).$$

- No explicit solution:
  - Fixed point procedure needed in first case (e.g. Newton).
  - Predictor-corrector method on $\mathbf{a}$ needed in second case.

A two step second order method

- Solve characteristics defined by $\frac{d\mathbf{X}}{dt} = \mathbf{a}(\mathbf{X}, t)$.
- Centered quadrature on two time steps:

$$\mathbf{X}^{n+1} - \mathbf{X}^{n-1} = 2\Delta t\, \mathbf{a}^n(\mathbf{X}^n), \quad \mathbf{X}^{n+1} + \mathbf{X}^{n-1} = 2\mathbf{X}^n + O(\Delta t^2).$$

- Use fixed point procedure to compute $\mathbf{X}^{n-1}$ such that

$$\mathbf{X}^{n+1} - \mathbf{X}^{n-1} = \Delta t\, \mathbf{a}^n\left(\frac{\mathbf{X}^{n+1} + \mathbf{X}^{n-1}}{2}\right).$$

- Problem: compute f^{n+1} from f^{n-1}. Even and odd order time approximations become decoupled after some time. Artificial coupling needs to be introduced.

A one step predictor-corrector second order method

- Solve characteristics defined by $\frac{d\mathbf{X}}{dt} = \mathbf{a}(\mathbf{X}, t)$.
- Centered quadrature on one time step:

$$\mathbf{X}^{n+1} - \mathbf{X}^n = \Delta t\, \mathbf{a}^{n+\frac{1}{2}}(\mathbf{X}^{n+\frac{1}{2}}), \qquad \mathbf{X}^{n+1} + \mathbf{X}^n = 2\mathbf{X}^{n+\frac{1}{2}} + O(\Delta t^2).$$

- Now $\mathbf{a}^{n+\frac{1}{2}}$ is unknown. But can be computed with first order scheme (like in Runge-Kutta methods) for global second order accuracy. Requires two updates of distribution function per time step.
- Use fixed point procedure to compute $\mathbf{X}^n$ such that

$$\mathbf{X}^{n+1} - \mathbf{X}^n = \Delta t\, \mathbf{a}^{n+\frac{1}{2}}\left(\frac{\mathbf{X}^{n+1} + \mathbf{X}^n}{2}\right).$$

- In practice use linear interpolation for evaluation of $\mathbf{a}^{n+\frac{1}{2}}(X)$ to get explicit solution for $\mathbf{X}^n$.

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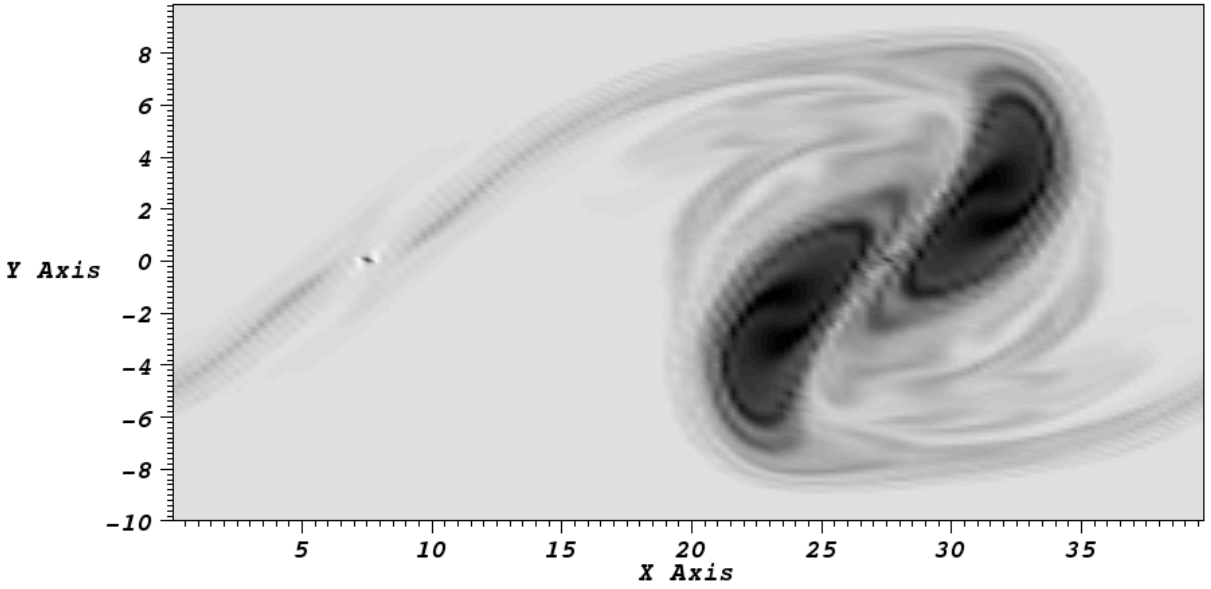
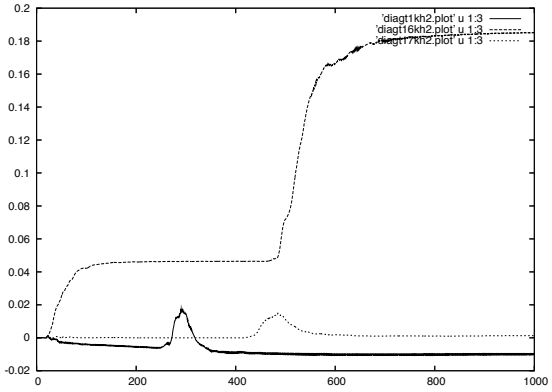
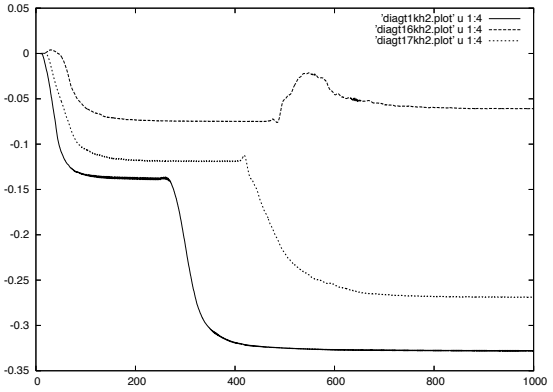
Problem with non conservative Vlasov solver

- When non conservative splitting is used for the numerical solver, the solver is not exactly conservative.
- Does generally not matter when solution is smooth and well resolved by the grid. The solver is still second order and yields good results.
- However: Fine structures develop in non linear simulations and are at some point locally not well resolved by the phase space grid.
- In this case a non conservative solvers can exhibit a large numerical gain or loss of particles which is totally unphysical.
- Lack of robustness.
- Note that by an adequate computation of the electric field from the distribution function, non split classical SL method based on cubic B-splines can be made conservative at lowest order (on displacements).
  very good but not exact conservation observed in actual simulations.

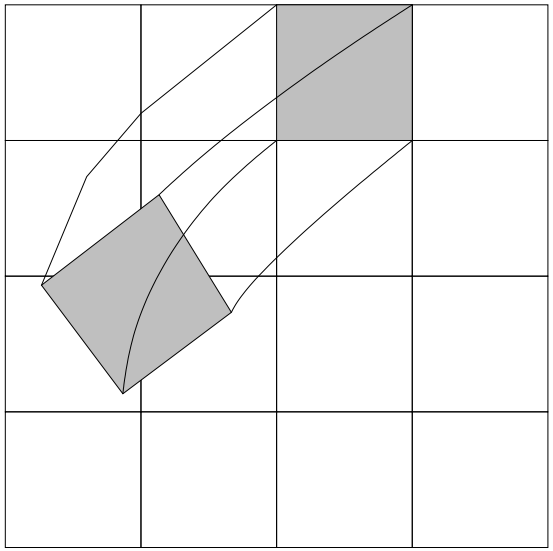
Vortex in Kelvin-Helmholtz instability







Conservative semi-Lagrangian method



- Start from conservative form of Vlasov equation

$$\frac{\partial f}{\partial t} + \nabla \cdot (f\mathbf{a}) = 0.$$

- $\int_V f\, dx\, dv$ conserved along characteristics
- Three steps:
  - High order polynomial reconstruction.
  - Compute origin of cells
  - Project (integrate) on transported cell.

- Efficient with splitting in 1D conservative equations as cells are then defined by their 2 endpoints. A lot more complex for 2D (or more) transport.
- Splitting on conservative form: always conservative.
- Filtering for positivity and damping of oscillations due to high-order interpolation.

Choice of interpolation

- What interpolation should be chosen for primitive?
- Lagrange interpolation with centered stencil (used in PFC: Filbet, ES, Bertrand JCP 2001).
- ENO type interpolation. Lagrange with varying stencil. Not efficient for Vlasov.
- WENO. Recent positive results (Carrillo-Vecil, Qiu-Christlieb).
- Cubic spline interpolation: cubic polynomial on each cell, globally C^2 $\rightarrow$ reconstructed function is then locally a quadratic polynomial and globally C^1. Linked to cubic spline interpolation for classical semi-Lagrangian method.
- Related but different method : SL DG uses a Galerkin formulation and high order polynomials on each cell (Qiu-Shu). Promising recent results.

Origin of cells and projection

- Compute cell origins:
  - In 1D cell and its origin determined by end points. Compute origin of end points like in classical semi-Lagrangian method.
  - Need to make sure end points do not cross $\rightarrow$ restriction on time step.
- Compute average value of f^{n+1} on cells using

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} f^{n+1}(x)\,dx = \int_{X(t_n;x_{i-\frac{1}{2}},t_{n+1})}^{X(t_n;x_{i+\frac{1}{2}},t_{n+1})} f^{n}(x)\,dx,$$

where $f^n(x)$ is the high order polynomial reconstruction.

Link between classical and conservative semi-Lagrangian methods

- For constant coefficient advections we can show that

$$\text{C-Lag(2d)} \Longleftrightarrow \text{SL-Lag(2d+1)}$$
$$\text{PSM} \Longleftrightarrow \text{SPL}$$

- Consequences:
  1. Classical semi-Lagrangian method is conservative for split schemes reducing to constant coefficients advection for each split step.
  2. PFC (Filbet-ES-Bertrand) corresponds to classical semi-Lagrangian method with cubic Lagrange interpolation.
  3. PSM corresponds to classical semi-Lagrangian method with cubic spline interpolation.
- Note that Collella and Woodward PPM Finite Volume scheme is also algebraically equivalent for constant coefficient advections.

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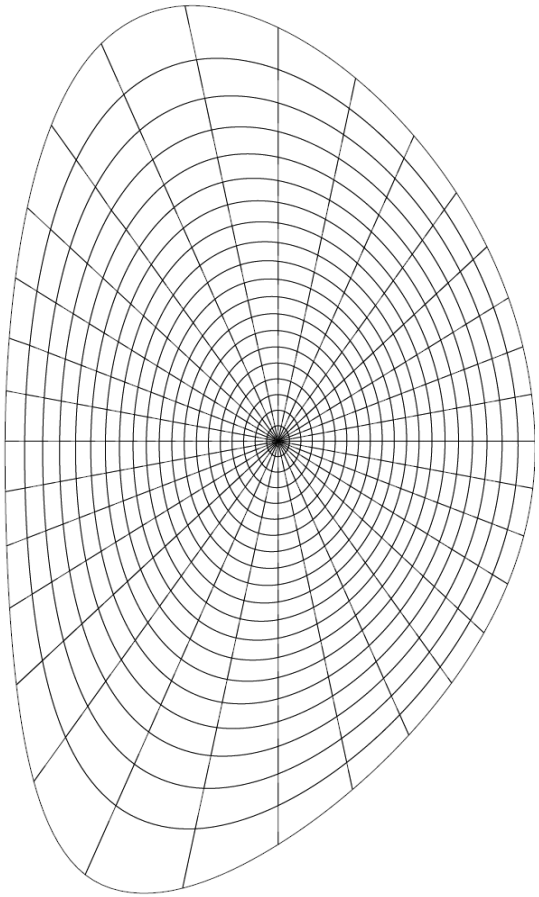
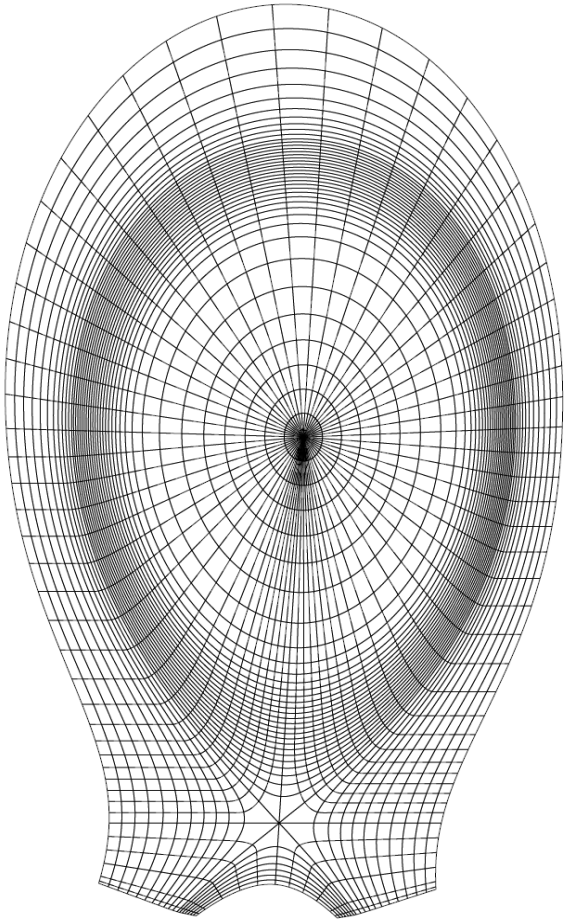
Motivation for curvilinear mesh for gyrokinetic simulations

- Due to confinement by large magnetic field particle travel a lot faster along magnetic field lines than across.
- Look at typical turbulence simulation shows that large scale structures form along field lines and small scale structures across.
- Significant anisotropy of flow
- For optimal resolution anisotropic mesh needed.
- To keep numerical efficiency of structured meshes: use mapped mesh which defines curvilinear coordinates almost aligned with magnetic field lines.

Structured mesh using Bézier splines (JOREK, G. Huysmans)

Mesh aligned on magnetic flux surfaces, without and with X-point.





Splines and NURBS

Splines are smooth piecewise polynomial functions.

Let $T = (t_i)_{1 \leqslant i \leqslant N+k}$ be a non-decreasing sequence of knots.

- The i-th B-Spline of order k is defined by the recurrence relation:

$$N_j^k = w_j^k N_j^{k-1} + (1 - w_{j+1}^k) N_{j+1}^{k-1}$$

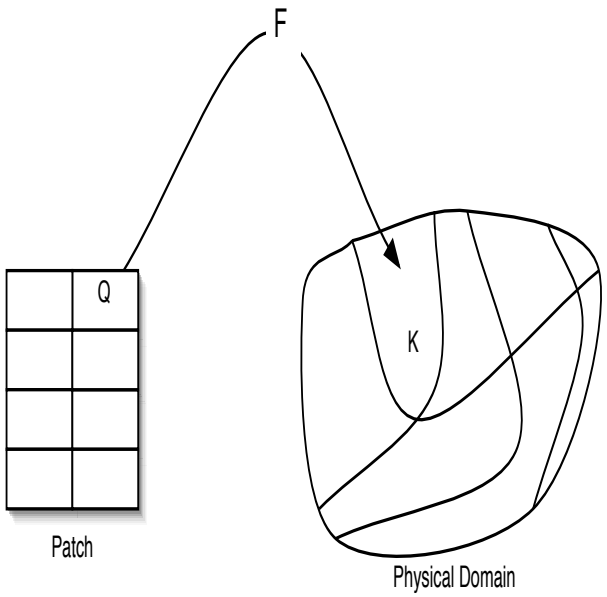
$$\text{where} \qquad w_j^k(x) = \frac{x - t_j}{t_{j+k-1} - t_j}, \quad N_j^1(x) = \chi_{[t_j, t_{j+1}[}(x)$$

- The i-th NURBS of order k associated to the knot vector T and the weights ω, is defined by

$$R_i^k = \frac{\omega_i N_i^k}{\sum_{j=1}^N \omega_j N_j^k}.$$

Mapped mesh

- A mapped mesh is defined by a mapping e.g. $F : \mathbb{R}^2 \to \mathbb{R}^2$ from a structured uniform logical mesh parametrized by (ξ_1, ξ_2) to the physical domain in cartesian coordinates $x_1 = F_1(\xi_1, \xi_2), \quad x_2 = F_2(\xi_1, \xi_2)$.
- Mapping can be analytical coordinate transformation or defined by spline or NURBS curves.



- We then have the contravariant (curvilinear) coordinates A^i: $A^i = A \cdot \nabla_x \xi_i$ with A the velocity vector expressed in cartesian coordinates.
- Vlasov equation in curvilinear coordinates then writes:

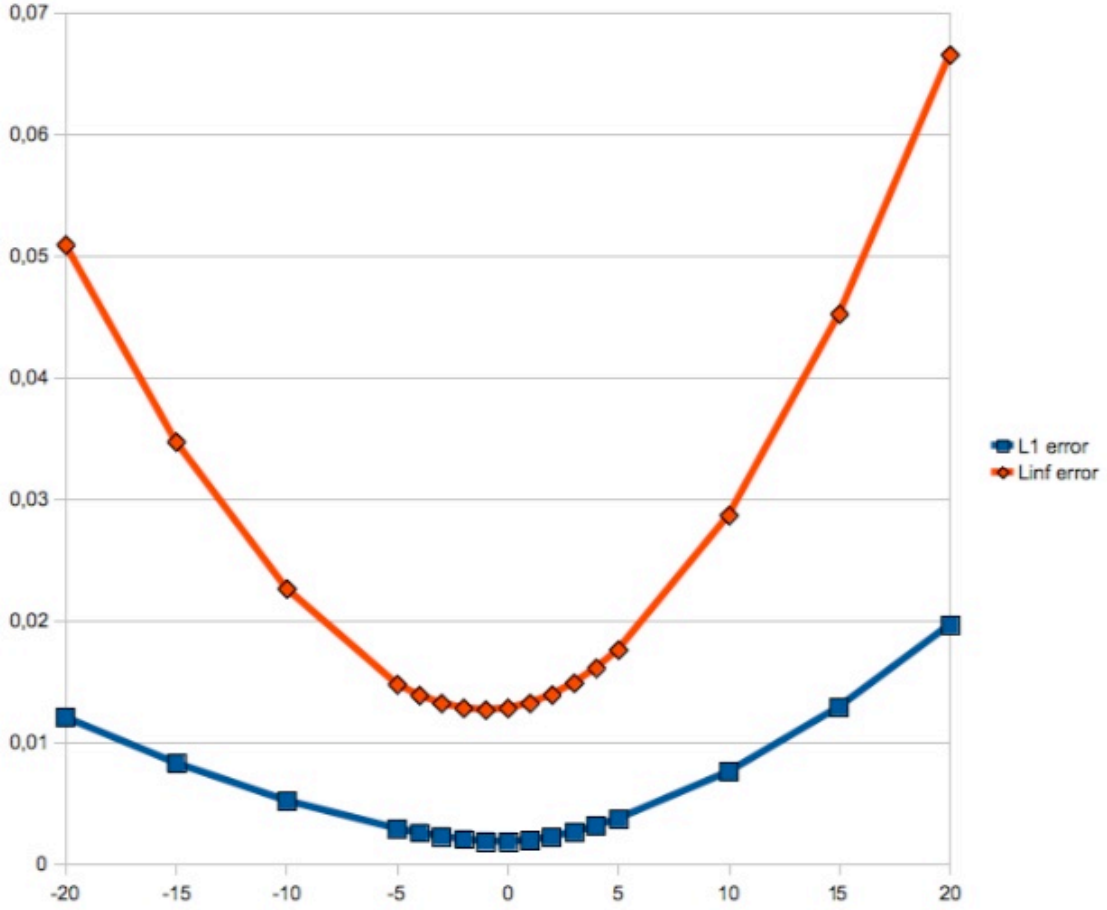
$$\sqrt{g}\frac{\partial f}{\partial t} + \sum_k \frac{\partial}{\partial \xi_k}\left(\sqrt{g}\ f\ A^k\right) = 0,$$

with the transformation matrix jacobian $1/\sqrt{g} = det\left(\frac{d\xi}{dx}\right)$.

Approximate alignment

L^1 and L^∞ norms of relative error for oblic advection (travel 10 times the domain) function of the angle between advection direction and mesh lines

direction:



Guiding-Center model

It is a reduced 2D model:

$$\frac{\partial \rho}{\partial t} + E^{\perp} \cdot \nabla_x \rho = 0$$

$$-\Delta \Phi = \nabla \cdot E = \rho.$$

with $E = -\nabla \Phi = (E_x, E_y)$ and $E^{\perp} = (-E_y, E_x)$.

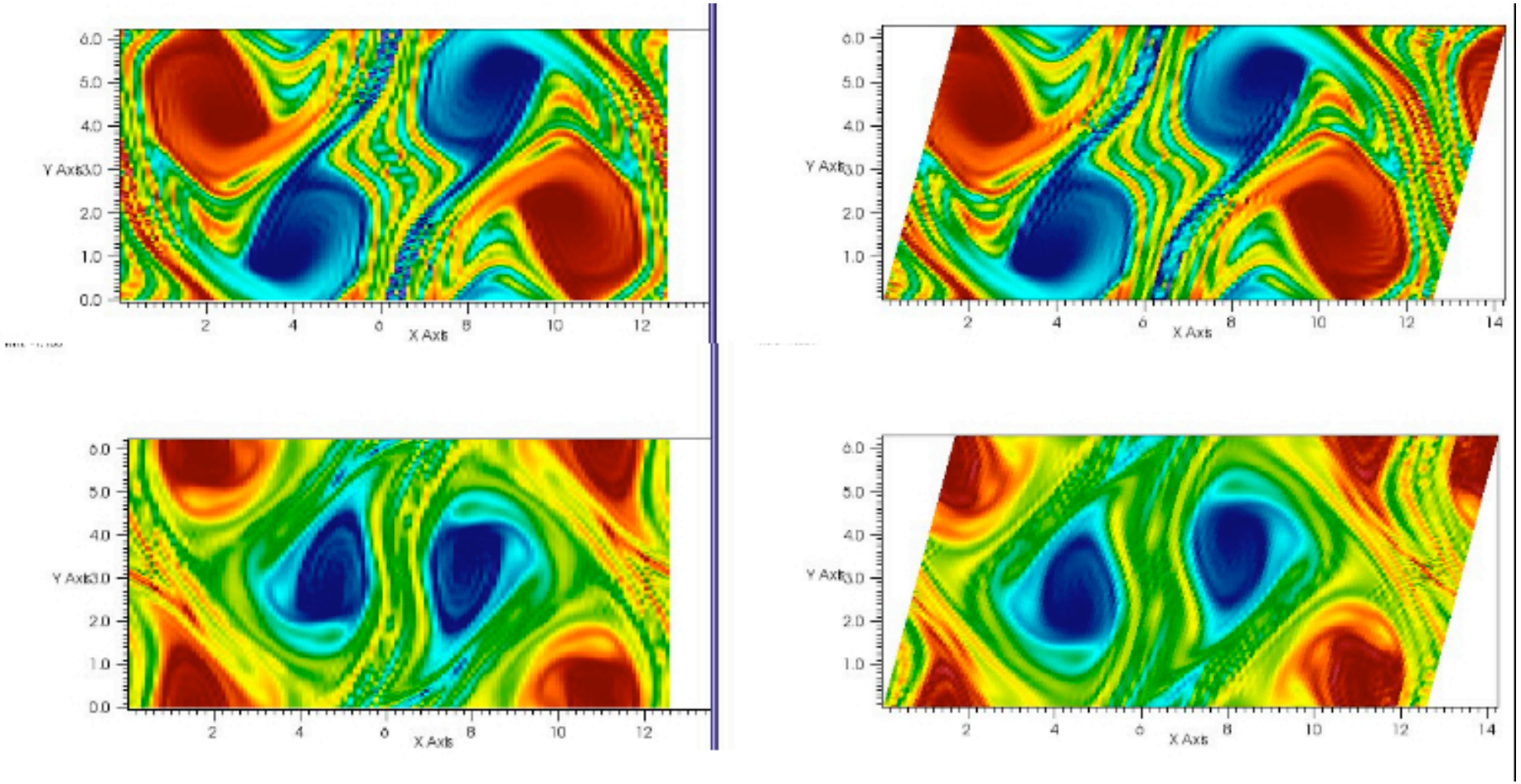
Since $\nabla \cdot E^{\perp} = -\partial_x \partial_y \Phi + \partial_y \partial_x \Phi = 0$,
one can write the Vlasov equation in a conservative formulation:

$$\frac{\partial \rho}{\partial t} + \nabla_X \cdot (\rho E^{\perp}) = 0.$$

Therefore a conservative directional splitting is possible.

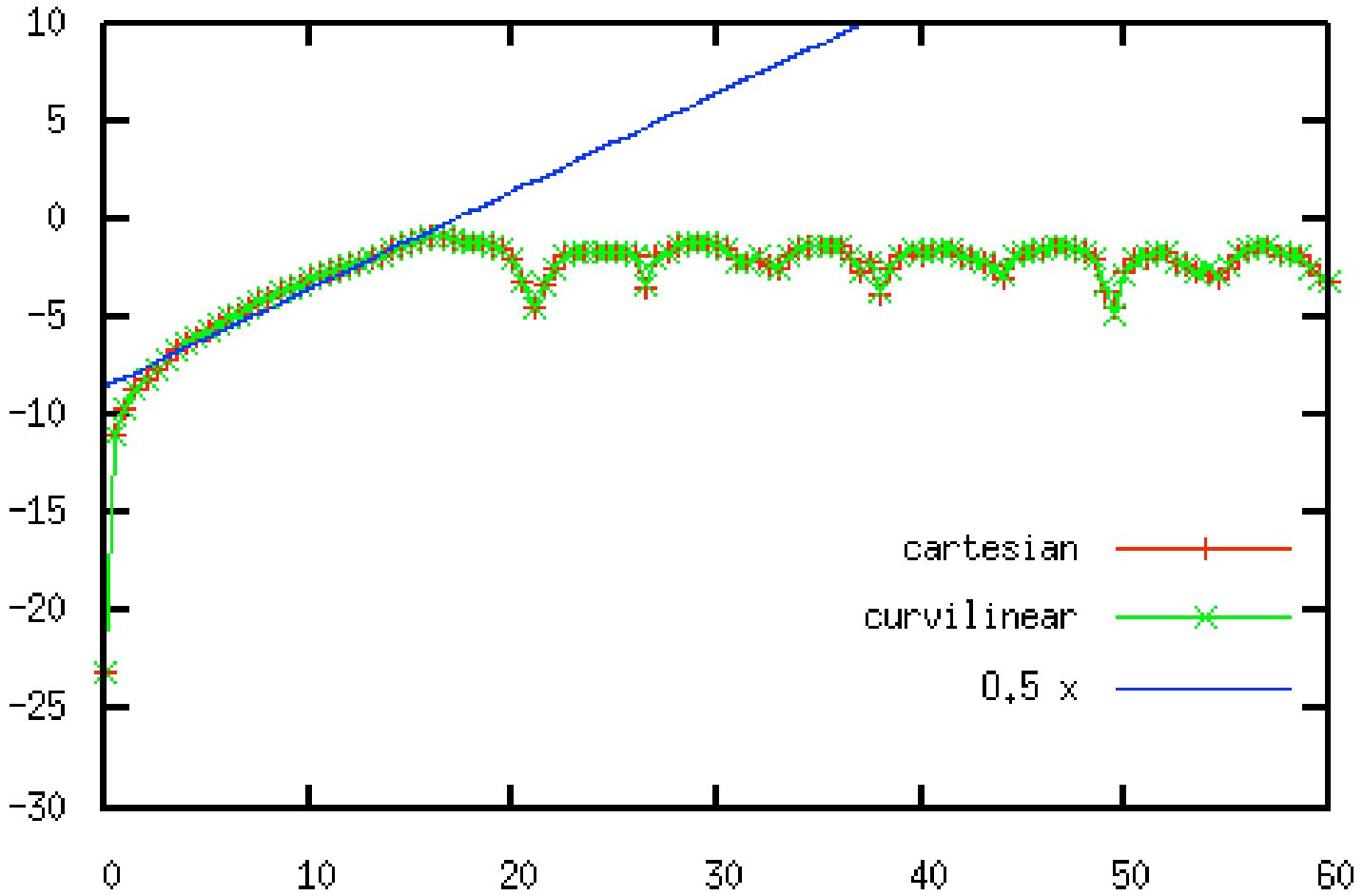
Mapped mesh GC model

Qualitative comparison between PSM computations on cartesian and curvilinear meshes of a periodic-periodic instability for the GC model.



Mapped mesh GC model

Fourier analysis of the solution:
The growth rate of the unstable mode is in good agreement in the linear phase with the expected value $Im(\omega) = 1/2$ for both meshes.



Mapped mesh Vlasov-Poisson for beam simulation

J. Abiteboul, G. Latu, V. Grandgirard, A. Ratnani, E. Sonnendrucker and A. Strugarek ESAIM Proceedings (to appear).

- 2D mapped grid based either on analytical mapping or Bézier mapping.
- Characteristics followed backward in physical space. Inverse mapping is used to bring points back to logical space for interpolation.
- Velocity integral needs interpolation. Sparse matrix can be constructed for this at initialization.
- Performance (1024 time steps, 512x512 mesh)

	Field solve	Spline coeff.	Advection	Total
no mapping	2.3	16.4	78	97
analytical	10.1	18.4	115	143
bézier	9.2	17.3	275	301

A few issues with semi-Lagrangian methods on mapped grids

- In semi-Lagrangian framework, computation of characteristics well split.
- Free stream preservation exact when characteristics are computed in physical space.
- No exact free stream preservation when characteristic computed using logical coordinates. However verified up to the accuracy of computation of characteristics, which can be very good and robust using adequate ODE solver.
- Velocity integral needs inverse mapping, but can be precomputed at initialization for interpolation points.
- Discrete divergence of advection field should exactly vanish.

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4D drift-kinetic model

Similar model as gyrokinetic models with $\mu = 0$ in cylindrical geometry $\Rightarrow$ relevant for numerical tests.

The 4D velocity field $a = (v_{GC_r}, v_{GC_\theta}, v_\parallel, q/m_i\ E_z)^t$ is divergence free:

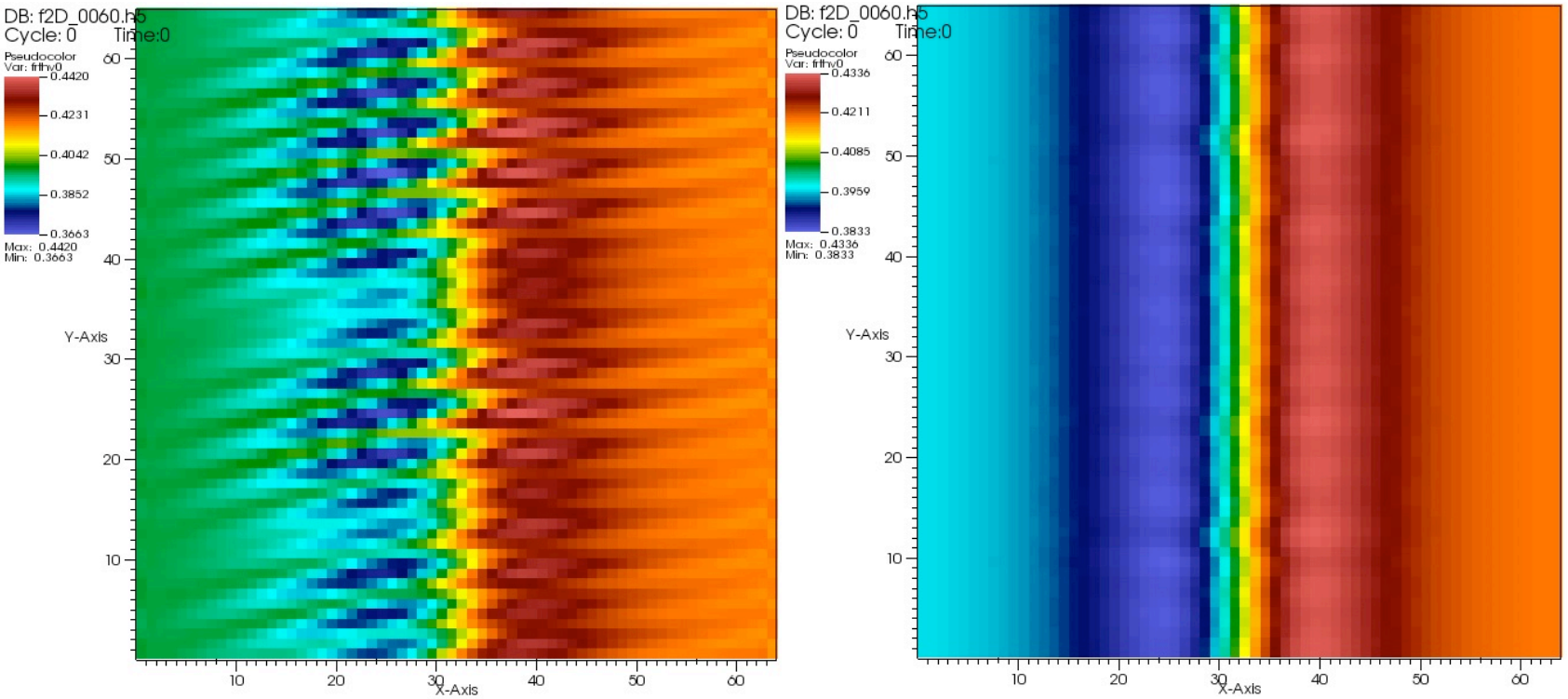
$$\nabla \cdot a = \frac{1}{r}\partial_r(r\ v_{GC_r}) + \frac{1}{r}\partial_\theta(v_{GC_\theta}) + \partial_z v_\parallel + \partial_{v_\parallel}(q_i/m_i\ E_z) = 0$$

with

$$v_{GC_r} = \frac{1}{B_z}\left(-\frac{1}{r}\partial_\theta \Phi\right) \quad \text{and} \quad v_{GC_\theta} = \frac{1}{B_z}\left(\partial_r \Phi\right)$$

This property should be satisfied at discrete level, to conserve cell volumes in the phase space and thus have a maximum principle.

4D drift-kinetic model



Advection field computed with cubic splines (left) and with one that satisfies the discrete divergence free condition (right).
4D simulation of 128x128x64x32 cells, result at time $t = 60$.

4D drift-kinetic model

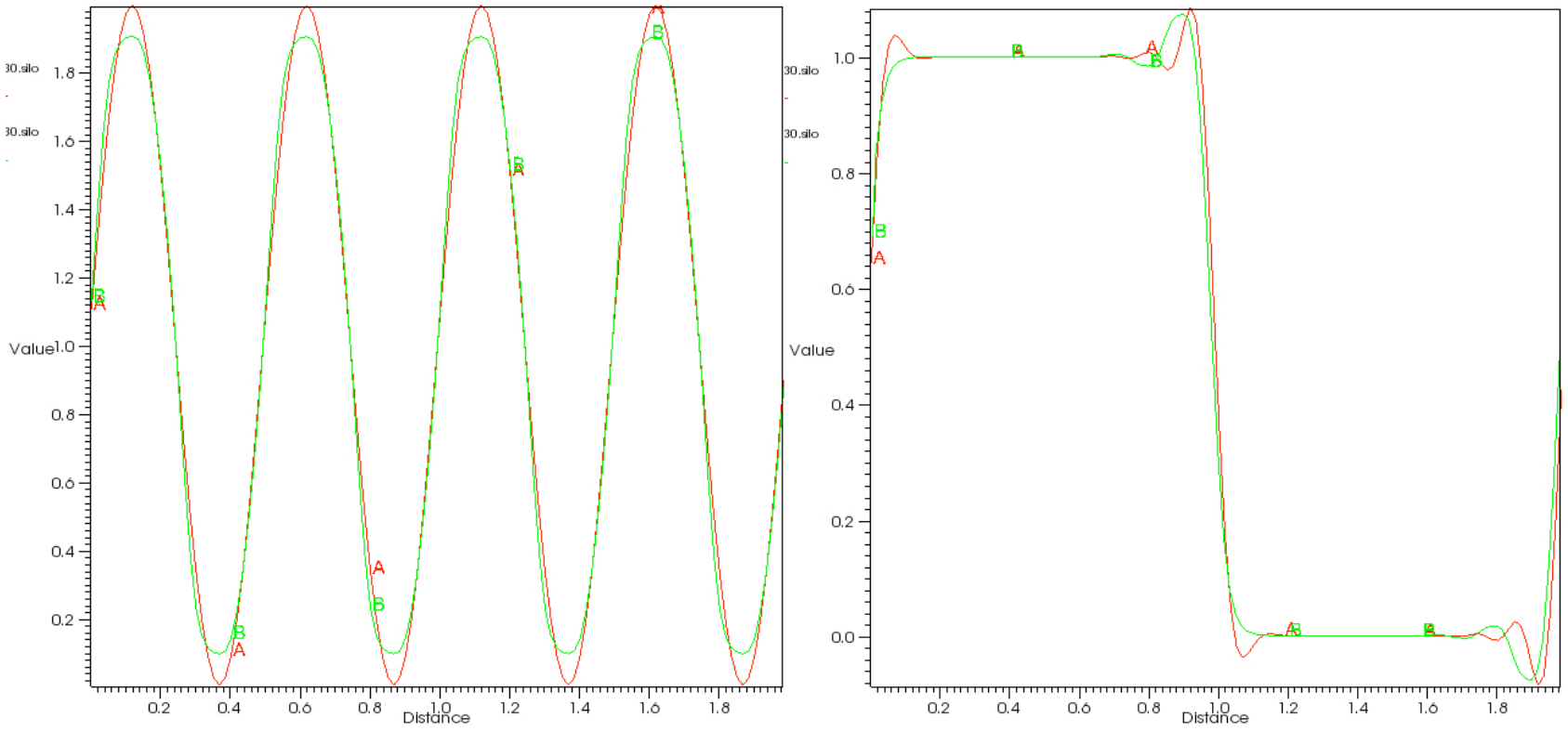
The PSM scheme does not ensure a maximum principle (positivity), which is crucial for a model without physical dissipation.
The following conditions should be satisfied at discrete level:

- cells volumes conservation in the phase space $Vol_i^n = Vol_i^{n+1}$, even when using a directional splitting.
- the average of the reconstructed function on an arbitrary volume satisfies the maximum principle.

$\Rightarrow$ we propose numerical limiters of two kinds:

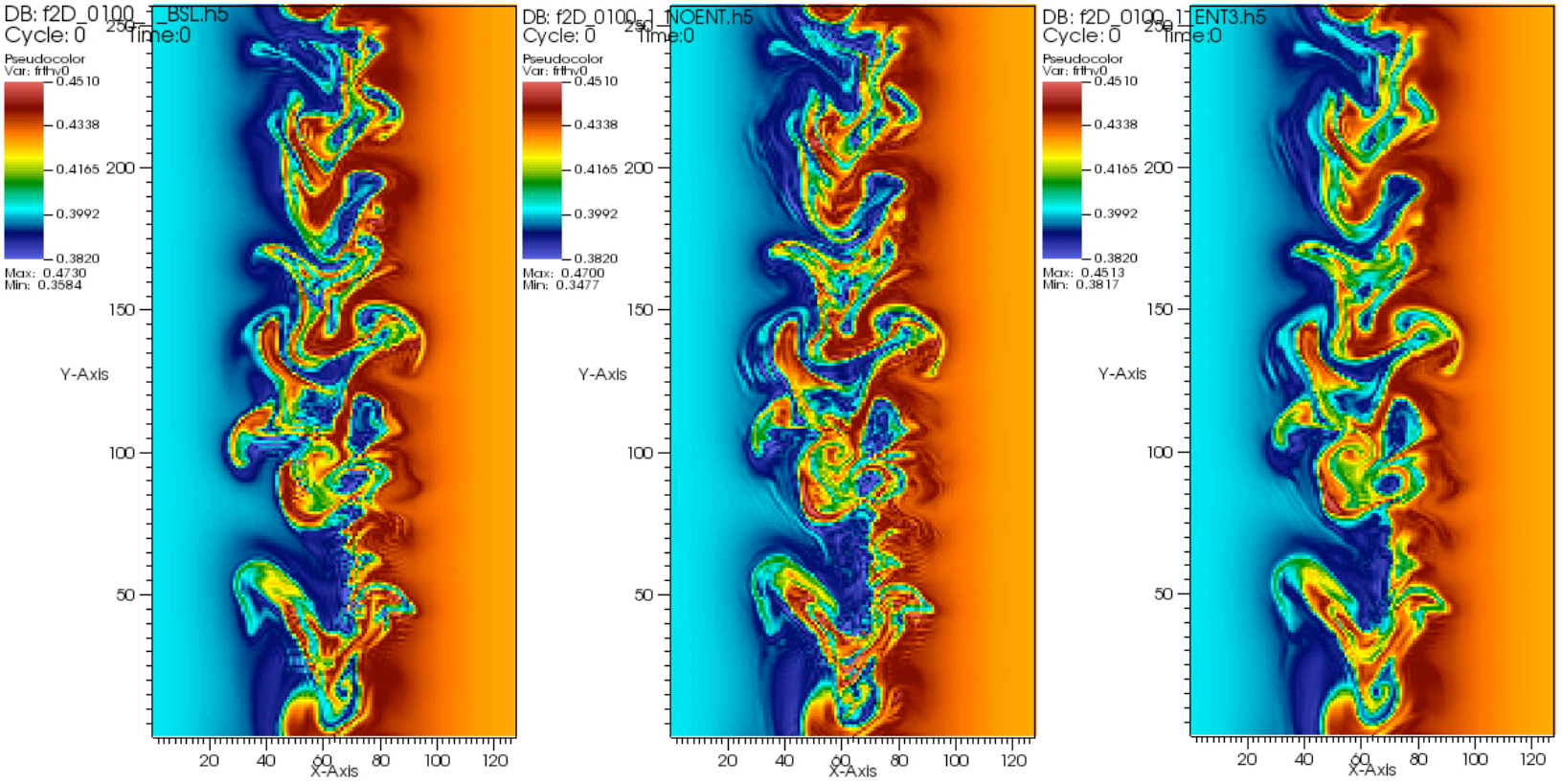
- correction of the cubic spline reconstruction using monotonicity criterions (Crouseilles, Mehrenberger, Sonnendrücker, JCP 2010),
- "Entropic Flux Limiter" that evaluates the sign of the numerical diffusion and cuts off anti-diffusion when occurs (Braeunig et al, INRIA Report 2009).

4D drift-kinetic simulation



The PSM scheme without (red) and with (green) "Entropic Flux Limiter".
The shapes travel 10 times the domain, domain length is 2 with 120 cells.

4D drift-kinetic model



From left to right: BSL, PSM and PSM with entropic flux limiter.
4D simulation of 128x256x128x64 cells, time =2000.

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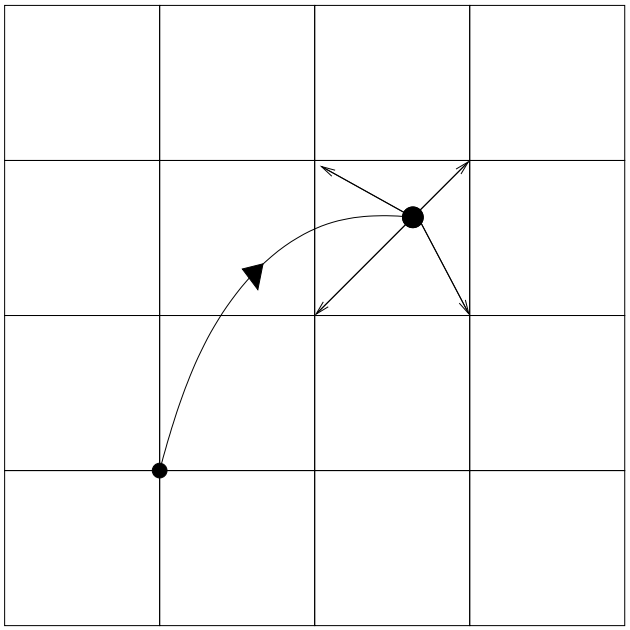


Crouseilles, Respaud, ES: CPC 2009

- f conserved along characteristics
- Characteristics advanced with same time schemes as in PIC method or any classical ODE solver.
- Leap-Frog Vlasov-Poisson
- Runge-Kutta or Cauchy-Kovalevsky for guiding-center or gyrokinetic

- Values of f deposited on grid of phase space using convolution kernel.
- Identical to PIC deposition scheme but in whole phase space instead of configuration space only.
- Similar to PIC method with reconstruction introduced by Denavit (JCP 1972).

Discrete distribution function

- Function projected on partition of unity basis for conservativity.
- Linear B-splines very diffusive. Not useful in practice.
- Good choice is cubic B-splines.
- f is reprojected on mesh at each time step.
- Between t_n and t_{n+1}

$$f_h(x,v,t) = \sum_{i,j} w_{i,j} B(x - X(t; x_i, v_j, t_n)) B(v - X(t; x_i, v_j, t_n)).$$

Weight $w_{i,j}$ associated to the particle starting from grid point (x_i, v_j) at t_n is coefficient of spline satisfying interpolation conditions

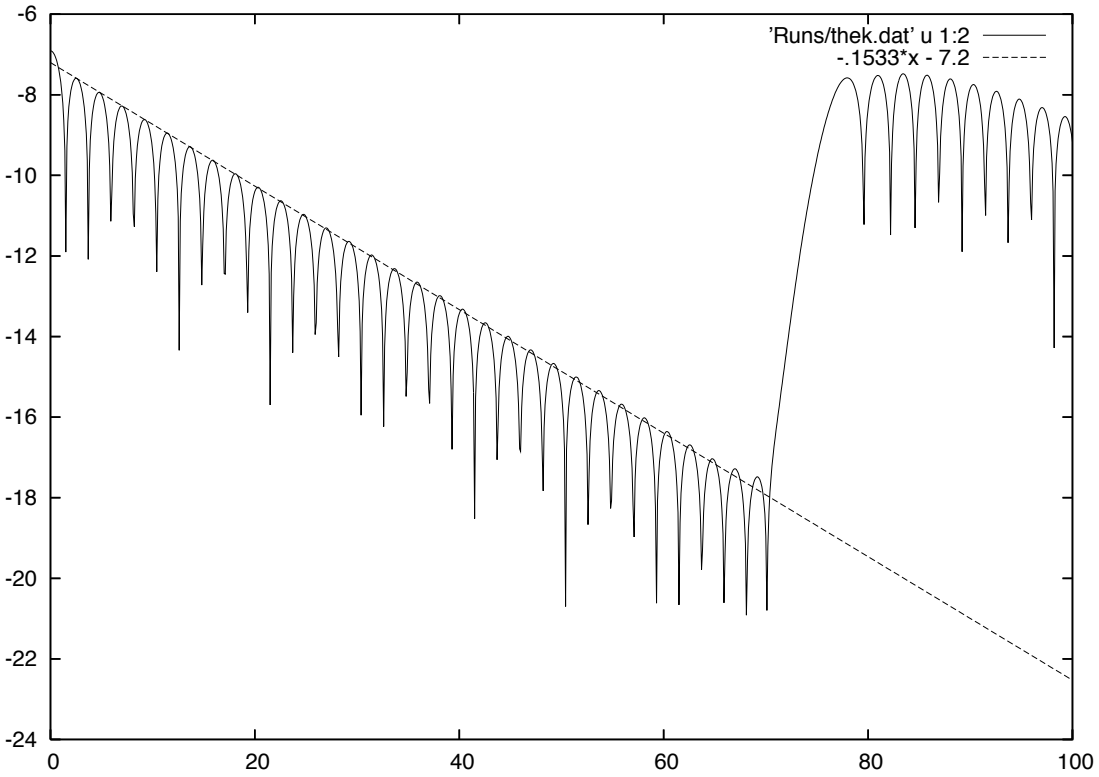
$$f_h(x_k, v_l, t_n) = \sum_{i,j} w_{i,j} B(x_k - x_i) B(v_l - v_j).$$

- Projection on phase space mesh is obtained with formula

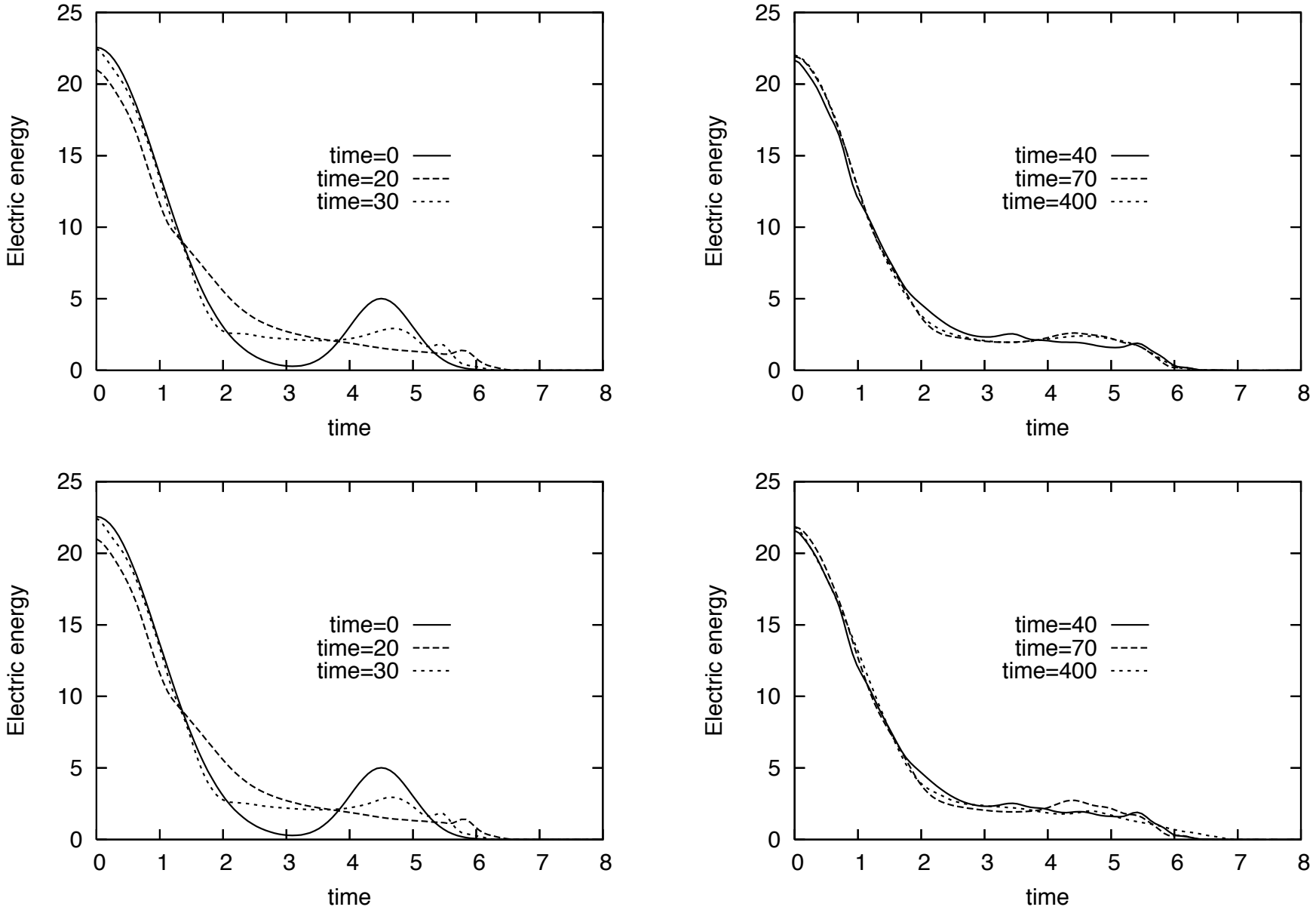
$$f^{n+1}(x_k, v_l) = \sum_{i,j} w_{i,j} B(x_k - X(t_{n+1}, x_i, v_j, t_n)) B(v_l - V(t_{n+1}, x_i, v_j, t_n)).$$

Landau damping

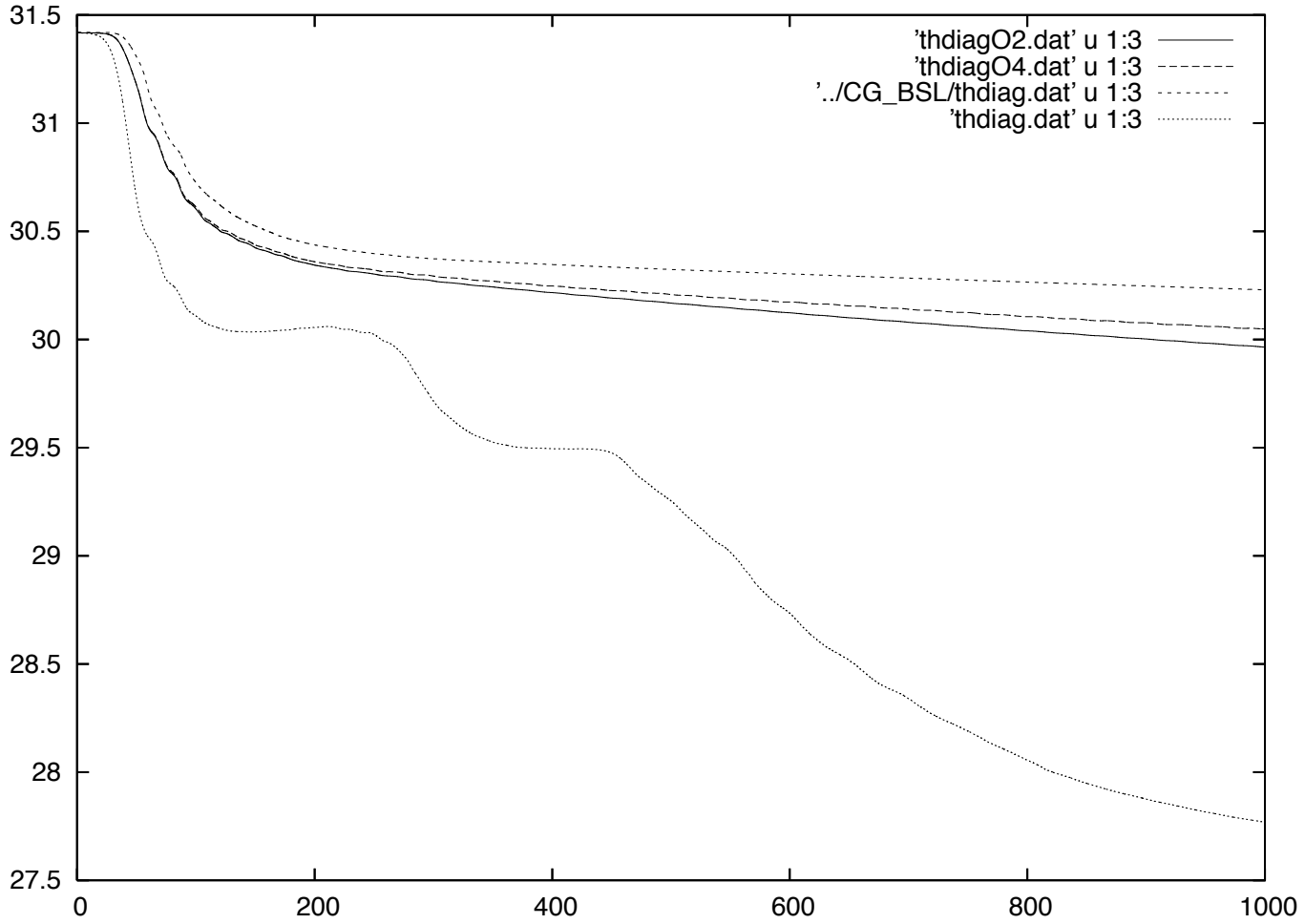
$$f_0(x,v) = (1 + 0.001\cos(kx))\frac{1}{\sqrt{2\pi}}e^{-\frac{v^2}{2}}, \quad L = 4\pi.$$



Bump on tail (BSL (top) vs. FSL (bottom))



Energy conservation for Kelvin-Helmoltz instability



FSL vs. BSL

- Forward semi-Lagrangian method very promising.
- Accurate description of whole phase-space in particular tail of distribution function and small perturbations.
- A little more diffusive than BSL. Better with smaller time steps.
- Some advantages: classical explicit EDO solver can be used, in particular high order if needed. No need for predictor-corrector or fixed point algorithm.
- Can benefit from charge conserving PIC algorithms (Villasenor-Buneman).
- Can be used like a PIC method for several time steps with redeposition when needed (problem dependent).

Conclusions and perspectives

- Semi-Lagrangian idea very fruitful to remove the numerical time step constraint.
- Several flavours: backward, forward, finite volume.
- All flavours identical for constant coefficient advections (used in time-split Vlasov-Poisson simulations).
- Can accomodate easily and efficiently structured meshes based on mapped coordinates.
- For some applications like gyrokinetics different directions play very different roles. Only perpendicular plane features strong nonlinear effects. Consider different methods for different directions.