Enhanced convergence estimates for semi-Lagrangian schemes with application to the Vlasov-Poisson system

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Recent Advances on Theory and Applications
of Semi-Lagrangian Methods
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Collaboration : Bruno Després, Frédérique Charles, HAL report 2011

- Semi-Lagrangian estimates with Strang splitting

$$O(\Delta t^2 + \frac{\Delta x^{p+1}}{\Delta t})$$

- Optimality of the estimate often raised, not much documented
- more likely $O(\Delta t^2 + \Delta x^p)$ for small time step ($CFL << 1$)
- cf Tutorial I, Ferretti
- see also Bermejo talk, Morton, Süli, 1995 for similar results

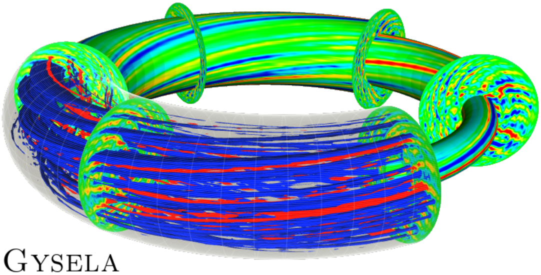
$\Rightarrow$ Here such enhanced estimate for the Vlasov Poisson system
$\Rightarrow$ Also refined estimate for the linear advection
$\Rightarrow$ Completed with some overview and other results of SL schemes for Vlasov Poisson

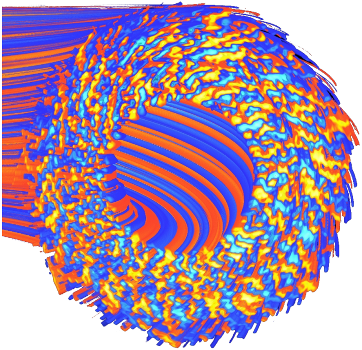
Outline

- Introduction
- Vlasov-Poisson system $1D \times 1D$
- Time discretization for VP
- Space discretization for VP

GYSELA

GYSELA code (GYrokinetic SEmi LAgrangian), CEA Cadarache





(Courtesy V. Grandgirard)
$5D$ mesh of $272 \cdot 10^9$ points. 31 days on 8192 processors

SeLaLib

SEmi LAgrangian LIbrary

Goal

modular library for the gyrokinetic simulation model by a semi-Lagrangian method

Support

- Large scale Initiative Fusion of INRIA
- ANR Project GYPSI (2010-2014)
- INRIA CALVI Project
- Collaboration with CEA Cadarache

Vlasov equation

Distribution function $f(t,x,v)$ solution of the Vlasov equation
$f(t,x,v)\mathrm{d}x\mathrm{d}v$ represents the probability of finding particules in a volume element $\mathrm{d}x\mathrm{d}v$ at time t at point (x,v) (position, velocity)

$$\partial_t f + v \cdot \nabla_x f + F(t,x) \cdot \nabla_v f = 0$$

• Transport equation
• Non linearity through the field F which depends on f (Poisson, Maxwell)
• Description of the dynamic of charged particles in a plasma

Vlasov-Poisson (1D $\times$ 1D)

Vlasov-Poisson system

$$\partial_t f(t,x,v) + v\partial_x f(t,x,v) + E(t,x)\partial_v f(t,x,v) = 0,$$

where the field E is solution of the Poisson equation

$$\partial_x E(t,x) = \int_{\mathbb{R}} f(t,x,v)dv - 1$$

with zero mean condition ($\int_0^L E(t,x)dx = 0$)

$\Rightarrow$ Simplified model ; first plasmas test cases
$\Rightarrow$ Smooth solution but development of small scales

Time semi-discretization : Strang Splitting

Transport in x over $\Delta t/2$

$$\partial_t f(t,x,v) + v\partial_x f(t,x,v) = 0$$

Update of E through the Poisson equation
Transport in v over Δt

$$\partial_t f(t,x,v) + E(t,x)\partial_v f(t,x,v) = 0$$

Transport in x over $\Delta t/2$

$$\partial_t f(t,x,v) + v\partial_x f(t,x,v) = 0$$

About time discretizations

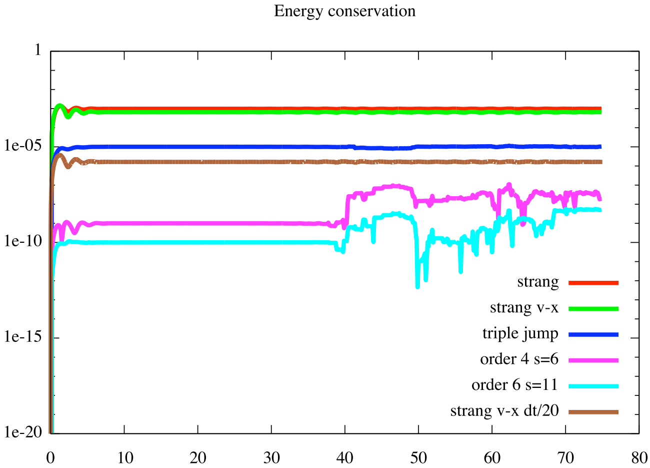
- Strang splitting often used (since Cheng-Knorr [1976]), leads to $O(\Delta t^2)$ error
- Higher order splitting possible (Yoshida[1990], Blanes et al [2000,2008], Schaeffer [2009], Watanabe-Sugama [2004])

$$\text{splitting steps} : a_0, \dots, a_{2s}$$
$$\text{Strang splitting} : s = 1,\ a_0 = 1/2, a_1 = 1, a_2 = 1/2$$

- An alternative : Integral Deferred Corrections (Qiu-Christlieb-Morton[2011])

Benefit of high order time discretizations

Strong Landau damping testcase



Order conditions

Theorem (N. Crouseilles, E. Faou, M. M.)

For the Vlasov-Poisson system, with splitting steps $a_0, \dots, a_{2s}$*, we get the same order conditions as RKN conditions derived for ODE up to the fourth order :*

$$p_{2s+1} = 0,\ B_1 = 1,\ B_2 = 0,\ B_{3a} = B_{3b} = 0,\ B_{4a} = -4B_{4b} = 4B_{4c},$$

as soon as we assume that the following functions inside the brackets are independent : $\{vI_0(x) - 1, I_1(x) - \bar{I}_1\}$*,*
$\{\partial_x I_2(x) + v^2 \partial_x I_0(x) - 2v\partial_x I_1(x), E(0,x)\}$ *and*

$$\{-\partial_x^2 I_3(x) + 3\partial_x^2 I_2(x)v - 3v^2\partial_x^2 I_1(x) + v^3\partial_x^2 I_0(x),$$
$$(I_0(x) - 1)(I_1(x) - vI_0(x)), (I_0(x) - 1)((I_0(x) - 1)v - \bar{I}_1)\}.$$

Order conditions

We have set

$$p_0 = 0,\ p_{j+1} = a_j - p_j,\ j = 0, \dots, 2s,$$

together with $B_1 = \sum_{j=1}^{2s} p_j,\ B_2 = \sum_{j=1}^{2s} (-1)^j p_j^2$

$$B_{4a} = \sum_{j=1}^{2s} (-1)^j p_j^4, B_{4b} = \sum_{j=1}^{s} (p_{2j}^3 + p_{2j-1}^3) \sum_{k=1}^{2j-1} p_k,$$

$$B_{4c} = \sum_{j=1}^{s} (p_{2j}^2 - p_{2j-1}^2) \left(\sum_{k=1}^{j-1} p_{2k} \sum_{\ell=1}^{2k-1} p_\ell + \sum_{k=1}^{j} p_{2k-1} \sum_{\ell=1}^{2k-1} p_\ell \right).$$

$$I_k(x) = \int_{\mathbb{R}} v^k f_0(x,v)dv,\ k = 0, 1, 2,\ \bar{I}_1 = \frac{1}{L} \int_0^L I_1(y)dy$$

Some remarks

- Long but elementary computations : backward characteristics at each substep $\to$ electric field $\to$ forward
- Arbitrary number of steps
- negative coefficients automatically for degree ≥ 3
- Minimal number of stages not always the best
- problem of time data representation for too large time steps
- No good order for intermediate electric fields ; CK procedure possible for having it (cf Rossmanith, Seal, 2011)
- link with Poisson structure

$$\{\{T, U\}_f, U\}_f = 2U,$$

which implies the RKN type relation

$$\{\{\{T, U\}_f, U\}_f, U\}_f = 0$$

$\Rightarrow$ hope to have larger choice of coefficients for degree ≥ 5.

Linear transport equations

$$\partial_t f(t,x,v) + v\partial_x f(t,x,v) = 0,\ \partial_t f(t,x,v) + E(t,x)\partial_v f(t,x,v) = 0$$

Some schemes and history

- SL with cubic splines (Cheng-Knorr, 1976)
  - good compromise between cost and accuracy
  - general framework (Sonnendrücker et al., 1998), used in GYSELA
- Fourier-Hermite (see e.g. Schumer, Holloway, 1998)
- SL with Hermite interpolation (Nakamura, Yabe, 1999)
- SL PFC method : positive and conservative (Filbet et al., 2001)
- SL on unstructured grids (Besse, Sonnendrücker, 2003)
- Forward SL (Crouseilles, Respaud, Sonnendrücker, 2009)
- Conservative SL WENO schemes (Qiu, Christlieb, Shu, 2011)
- Discontinuous Galerkin SL (Qiu, Shu ; Rossmanith, Seal, 2011 ; CEMRACS 2010, vladg project)

Conservative formulation

Linear advection $\partial_t f(t,x) + a\partial_x f(t,x) = 0$
From $f_j^n \simeq f(t_n, x_j),\ j = 0, \ldots, N-1$, reconstruct f_h^n such that

$$\frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} f_h^n(x)dx = f_j^n$$

and update through

$$f_j^{n+1} = \frac{1}{\Delta x}\int_{x_{(j-1/2)^*}}^{x_{(j+1/2)^*}} f_h^n(x)dx,\ x_{(j-1/2)^*} = x_{j-1/2} - a\Delta t/\Delta x.$$

Framework of **uniform grid and periodic conditions**
Equivalence with classical SL point based methods and possibility to add filters (Crouseilles, M., Sonnendrücker, 2010)
Adaptation for the WENO context (Qiu-Shu, 2011)

Lagrange reconstructions : LAG-2d+1

Cell based formulation
Search f_h^n of degree $\leq 2d$ on $]x_{j-1/2}, x_{j+1/2}[$ such that

$$\frac{1}{\Delta x}\int_{x_{k-1/2}}^{x_{k+1/2}} f_h^n(x)dx = f_k^n,\ k = j-d, \dots, j+d.$$

Point based formulation $f_j^{n+1} = P_h^n(x_j - a\Delta t/\Delta x)$, where P_h^n is of degree $\leq 2d+1$ on $[x_{j^*}, x_{j^*+1}]$, with

$$P_h^n(x_k) = f_k^n,\ k = j^* - d, \dots, j^* + d + 1$$

- For $d = 0$, upwind scheme (under $CFL \leq 1$)
- $d = 1$, PFC no limiter (Laprise, Plante, 1995 ; Filbet et al, 2001)
- Strang schemes of odd order (see Després, 2008, 2009) $CFL \leq 1$
- **Shifted odd Strang schemes** (compact, explicit)

SPL-d

Spline interpolation Use of *B*-splines

$$B_d(x) = \int_{\mathbb{R}} B_{d-1}(t)B_0(x-t)dt,\ B_0(x) = 1_{[-1/2,1/2]}(x).$$

$\Rightarrow$ spline interpolation on primitive function
$\Rightarrow$ take $f_j - \frac{1}{N}\sum f_k$ for keeping periodic boundary conditions
$\Rightarrow$ FFT like implementation possible

- $d = 3$ generally used
- Classical cubic spline interpolation (point based formulation)
- Also PSM scheme (cell based formulation) Zerroukat et al, 2006
- Possible use of local splines, Crouseilles, Latu, Sonnendr., 2007

Hermite formulation

We consider on the cell $[x_{j-1/2}, x_{j+1/2}]$, f_h^n of degree ≤ 2 satisfying

$$\frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} f_h^n(x)dx = f_j^n,\; f_h^n(x_{j-1/2}^+) = f_{(j-1/2)^+}^n,\; f_h^n(x_{j+1/2}^-) = f_{(j+1/2)^-}^n$$

Centered reconstructions

- stencil $j-1-d,\ldots,j+d$ for $f_{(j-1/2)}^n = f_{(j-1/2)^+}^n = f_{(j-1/2)^-}^n$
  - $d=0$ PPM0 : $f_{(j-1/2)}^n = \frac{f_{j-1}^n + f_n^j}{2}$
  - $d=1$ PPM1 : Colella, Woodward, 1984
  - $d=2$ PPM2 : Colella, Sekora, 2008
- PSM with Simpson approximation of $\int_{x_{j-3/2}}^{x_{j+1/2}} f(x)dx$

Upwind reconstructions

- stencil $j-d,\ldots,j+d$ for $f_{(j-1/2)^+}$
- $d=1$: LAG-3
- similar to LAG-2d+1 for small Δt ; finite volume limit (FOV project, CEMRACS 2011)

New convergence estimates

Theorem (Charles, Després, M.)

For Vlasov Poisson, with time splitting and LAG-2d+1 reconstruction, we have the convergence estimate

$$||f^n - f(t_n)||_2 \leq C\left(\min\left(\frac{\Delta x}{\Delta t}, 1\right)\Delta x^{2d+1} + \Delta t^2\right).$$

Error minimisation ($d \geq 1$) for $\Delta t \simeq \Delta x^{(2d+1)/2}$ and thus $\min\left(\frac{\Delta x}{\Delta t}, 1\right) = 1$

$\Rightarrow$ displacement smaller than a cell, for a semi-lagrangian scheme !

Former result (Besse, M. 2008) : $\Delta x^{2d+2}/\Delta t + \Delta t^2$

Stability of the scheme in L^2 norm

- known since Strang, 1962 ; Strang-Iserles, 1983
- new proofs : Undsdorfer-Verwer, 2003, Besse, M., 2008, Després 2009...
- Després shows also stability on $L^p,\ p \geq 1$ norm for odd Lagrange schemes of the linear advection
- see also work of Falcone-Ferretti, 1998, Ferretti, 2010

Lemma (Strang, 1962)

Let $d \in \mathbb{N}^*$, $\theta \in \mathbb{R}$.
Let P polynomial of degree $\leq 2d$ satisfying

$$P(k) = \exp(i\theta k),\ k = -d, \ldots, d.$$

Then we have

$$|P(x)| \leq 1,\ -1 \leq x \leq 1.$$

Improved estimates for the linear advection

Lemma (Charles, Després, M.)

Considering the linear advection $\partial_t f(t,x) + a\partial_x f(t,x) = 0$ *and writing*

$$x_j - a\Delta t = x_{j+r} + \alpha \Delta x,\ 0 \leq \alpha < 1,$$

the error for n steps, $n\Delta t \leq T$ *satisfies*

$$\|(f(t_n, x_j) - f_j^n)_j\|_2 \leq C_d T \frac{(1-\alpha)\alpha \Delta x^{2d+2}}{\Delta t} \|u_0^{(2d+2)}\|_{L^2}.$$

with

$$C_d = O\left(\frac{(d+1)!d!}{(2d+2)!(2d+2)^{3/4}}\right) = O\left(\frac{1}{2^{2d} d^{1/4}}\right).$$

Some remarks

- Proof based of fine estimation of the Fourier kernel (Després)
- Other proof thanks to results on B-splines maximum norm (Meinardus et al. 1995)
  - use of kernel representation error with B-splines
  - sharp estimate thanks to uniform grid
- Easy proof when no care of sharp constant against d is searched
- Not valid for all interpolation schemes (see e.g. Lax Friedrichs : no convergence for small Δt !)
- Enables convergence of exponential integrators ; link with finite volume schemes (fov project, CEMRACS2011)
- Adaptation to Vlasov-Poison with electric field via error decomposition (see details in HAL)

L^2 stability for splines

Lemma (De Boor, 1976)

Let $m \in \mathbb{N}^*$, $\theta \in \mathbb{R}$.
LetB_m the B-spline of order m defined by convolution of the characteristic function $1_{[-\frac{1}{2},\frac{1}{2}]}$.
Then the quantity

$$\Phi_m(\alpha) := \left| \sum_{k \in \mathbb{Z}} B_m(k+\alpha) e^{ik\theta} \right|^2$$

admit its maximum on the integers.

Used in Besse, M. 2008
Other stability lemma for other reconstructions ; generally affordable with computer for given degree ; proof more difficult for *arbitrary* degree.

Error estimation for cubic splines

From Hermite representation, the error writes

$$(\Delta x)^4\alpha^2(1-\alpha)^2\frac{\max_\xi |f^{(4)}(\xi)|}{4!}+\Delta x\max|f_j'-f'(x_j)|\alpha(1-\alpha),$$

with cubic splines, we have

$$\max|f_j'-f'(x_j)|\leq C\max_\xi|f^{(5)}(\xi)|(\Delta x)^4,$$

The error then writes

$$error\leq\min\left(1,\frac{\Delta t}{\Delta x}\right)^2 O\left(\frac{\Delta x^4}{\Delta t}\right)+\min\left(1,\frac{\Delta t}{\Delta x}\right)O\left(\frac{\Delta x^5}{\Delta t}\right).$$

For example : $\Delta t=\Delta x^2$ leads to $error\leq O(\Delta x^4)$.

Discontinuous Galerkin method

C. Steiner, Master report ; preliminary results

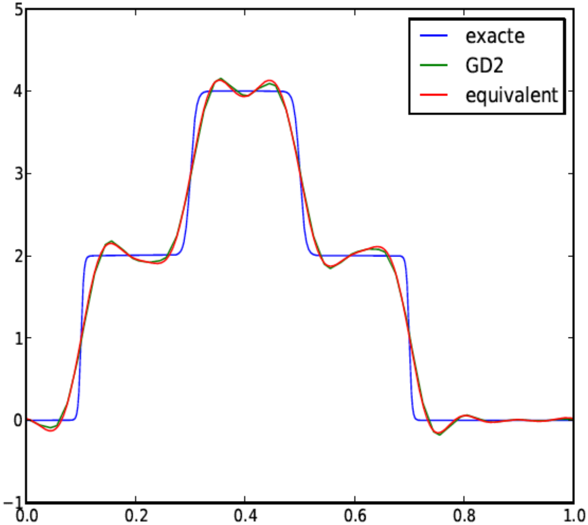
- Characteristic Galerkin like method

$$\int_{x_{j-1/2}}^{x_{j+1/2}} f^{n+1}(x)\phi(x)dx = \int_{x_{j-1/2}-a\Delta t}^{x_{j+1/2}-a\Delta t} f^{n}(x)\phi(x+a\Delta t)dx$$

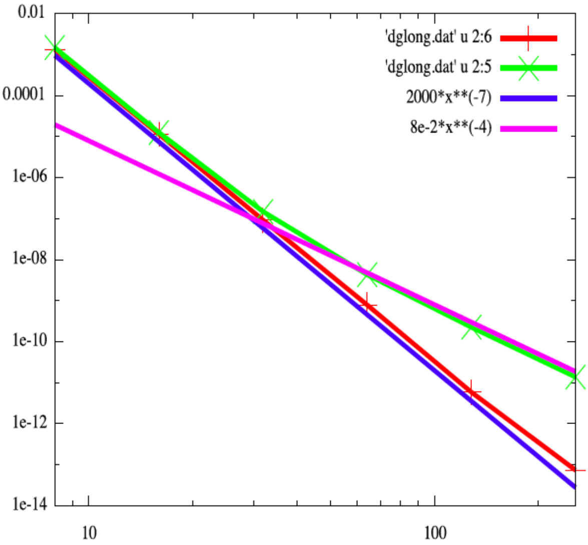
- use of Gauss points
- simplicity of constant advection is helpful
- super convergence : order $2d+1$ for mean value

$$\sum_{j=0}^{d} \omega_j f_{i,j}$$

Equivalent equation $d = 2$ and order 5 and 6 terms



Order for $d = 3$


0.01
0.0001
1e-06
1e-08
1e-10
1e-12
1e-14
10
100
'dglong.dat' u 2:6
'dglong.dat' u 2:5
2000*x**(-7)
8e-2*x**(-4)

Algebraic proof of super convergence

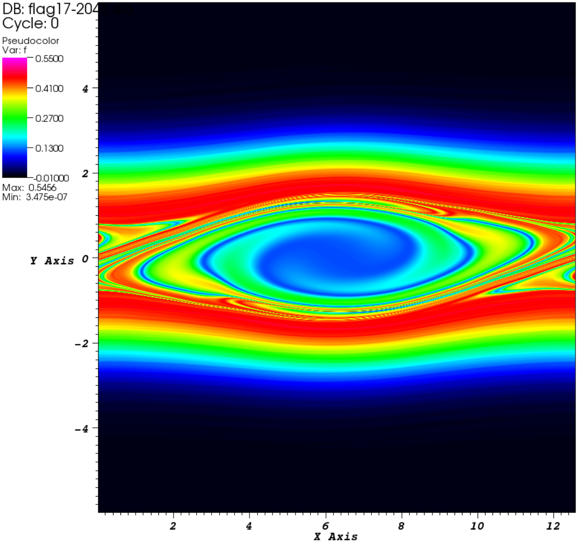
Lemma

We have the relation

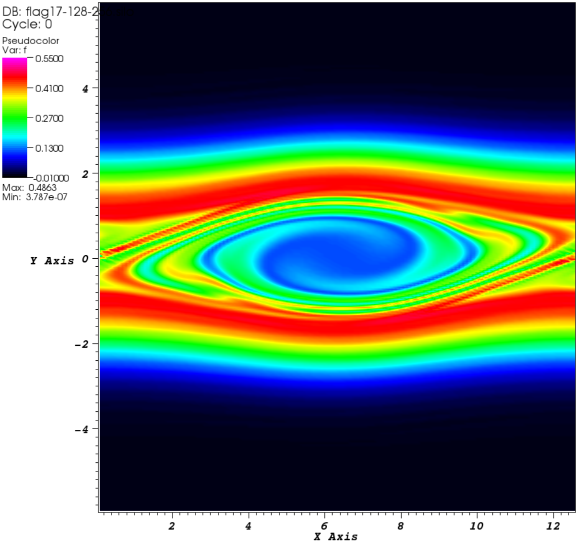
$$\sum_{j,j'=0}^{d} (\alpha_{j'} - \alpha_j - 1)^k \int_\alpha^1 \phi^{j'}(s)\phi^j(s-\alpha)ds$$
$$+ (\alpha_{j'} - \alpha_j)^k \int_0^\alpha \phi^{j'}(s)\phi^j(s+1-\alpha)ds = (\alpha - 1)^k,\ k = 1, \dots, 2d+1$$

- We use $\sum_{j=0}^{d} P(\alpha_j)\phi^j(s) = P(s), \deg P \leq d$ and alternatively $\int_0^1 P(x)dx = \sum_{j=0}^{d} \omega_j P(\alpha_j), \deg P \leq 2d+1$
- Related results Lowrie, 1996 ; Cheng, Shu 2008

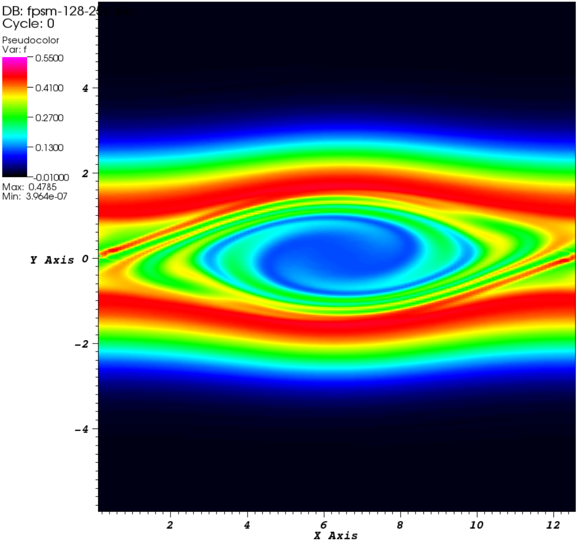
TSI Lagrange 17 Nx=Nv=2048



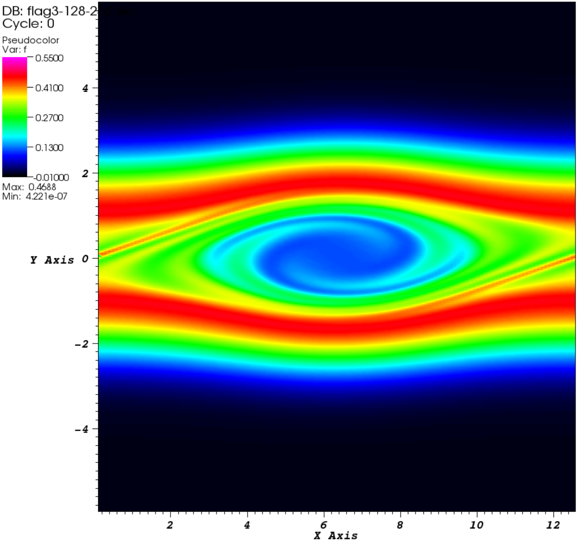
TSI Lagrange 17 Nx=128 Nv=256



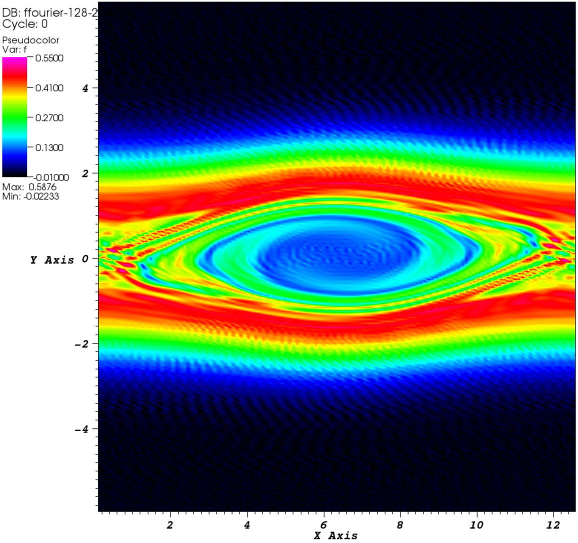
TSI PSM Nx=128 Nv=256



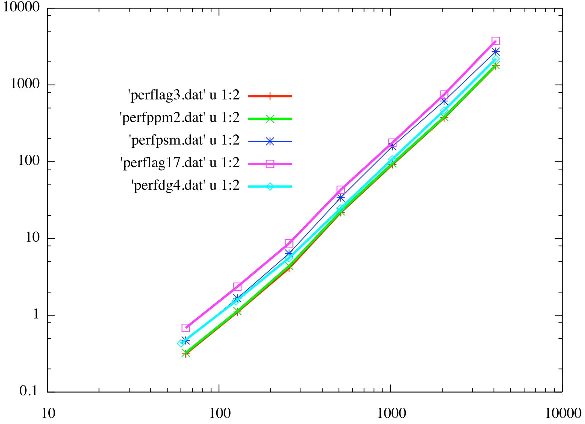
TSI Lagrange 3 Nx=128 Nv=256



Fourier Nx=128 Nv=256



Temps (sec. vs Nx=Nv) SLD dt=0.1 1000 iterations



Conclusion/Perspectives

- Study of the behavior of SL schemes for small Δt
- Improvement of convergence estimates of SL schemes for VP
- Fine estimation of error in Lagrange schemes
- To combine with high order in time
- Quality criteria for choosing "best" interpolation (?)
- Convergence for such high order SL schemes when no splitting is done or when splitting implies non constant advection : widely open ?
- Convergence on non uniform meshes ?
- Study/Convergence on mapped meshes ?
- Mix of SL (for linear fast dynamic) and FV schemes ?

About filters

- Extrema definition : positive, global, local (Umeda, 2006)
- Extrema limitation : adaptation of Hyman, 1983
- Oscillation limitations
  - tests in Vlasov-Poisson
  - adapted in GYSELA code Braeunig et al 2009, other filters
- useful for Vlasov-Poisson ?
- maybe more mandatory for more difficult situations
- loss of symmetry or gain in stability ?
- how to prove some mathematical properties ?
- Other strategies : WENO (Qiu, Shu)...

About conservative update in 2D

- CEMRACS 2011, FOV project
  - exploring quadrature based method for the flux
    - CFL condition
    - $2D$ different from $1D$
  - Banks, Hittinger, 2010 methodology
    - better upwind schemes
    - CFL condition
- $2D$ remapping, as in Lauritzen, 2010 (P. Glanc, PhD thesis)
  - no CFL condition a priori
  - needs mesh intersection
  - simplifications as one mesh is cartesian
  - first straight lines approximations
  - coupling with specific time integrator (Crouch-Grossman...)
- Other strategies...