The semi-Lagrangian method using oblic interpolation

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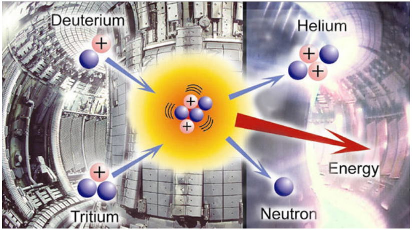
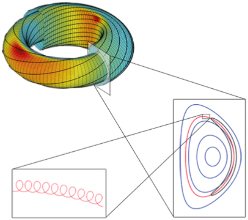
Collaboration with Guillaume Latu & Maurizio Ottaviani (CEA Cadarache, France), Yaman Güclü & Eric Sonnendrücker (IPP Garching, Germany)
Selalib ; Eurofusion ; IPP ; Gysela ; CEA Cadarache

Introduction

Physical context : the ITER project

- Tokamak construction at Cadarache in France
  - Aim : gain of energy by fusion of atoms with magnetic confinement
- Modelisation of plasma by PDE
  - MHD (fluid model)
    - Long time dynamic
    - Instabilities can destroy the machine
  - Multi-species **Vlasov**-Maxwell and **gyrokinetic** approximation
    - Short time dynamic
    - Micro-instabilities can degrade confinement quality
- Interest of numerical **simulations** :
  - Understand how heat flux due to turbulence vary with respect to the size of the plasma





Vlasov equation

$f(t, x, v)$ solution of Vlasov equation
$f(t, x, v)\mathrm{d}x\mathrm{d}v$ represents the probability of finding particules in a volume $\mathrm{d}x\mathrm{d}v$ 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 F that depends on f (Poisson, Maxwell) : $F = E + v \wedge B$
- Description of the dynamic of charged particules in a plasma

$1d \times 1d$	$2d \times 0d$	$3d \times 1d$	$3d \times 1d + \mu$
Vlasov-Poisson	Euler-2d	drift-kinetic	gyrokinetic

Numerical methods : PIC/eulerian/**semi-Lagrangian**

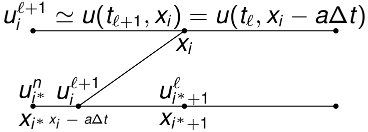
The semi-Lagrangian method

The case of 1d constant advection

$$\partial_t u + a\partial_x u = 0,\ u = u(t,x)$$

$t_{\ell+1} = t_\ell + \Delta t$

t_ℓ

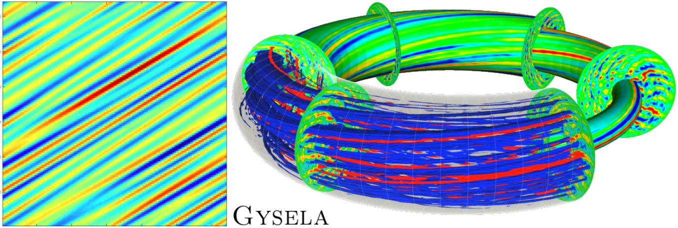


- Characteristics are exact
- Lagrange interpolation :
  - Degree 1 (linear) : x_{i^*}, x_{i^*+1}
  - Degree 3 (cubic) : $x_{i^*-1}, x_{i^*}, x_{i^*+1}, x_{i^*+2}$
- Some known results
  - L^2 stability `Strang, 1962`
  - L^q, $q \geq 1$ stability for odd degree `Després, 2009`
  - The scheme is equivalent to a Lagrange Galerkin scheme (`Pironneau, 1982`) for odd degree ≤ 13 `Ferretti, 2010`
    $\Rightarrow$ other proof of L^2stability

Aligned interpolation for gyrokinetics

Motivation

- Presence of strong magnetic field B
  - $\Rightarrow$ Alignment of the solution along direction of B
- Need to take this into account in the numerics
  - $\Rightarrow$ Design of a numerical method that can avoid to take too much poloidal planes without loosing precision



Numerical tools : PIC/eulerian/**semi-Lagrangian**
New idea (`Hariri-Ottaviani,2013`) : **aligned interpolation**

History of the method

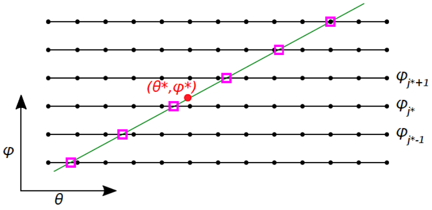
- Aligned mesh in Strasbourg : `Brauenig et al 2012`
  - $1D$ conservative method
  - Curvilinear mesh
  - Question of boundary conditions
- Flux Coordinate Independent method (FCI) `Hariri-Ottaviani 2013, Stegmeier et al 2014`
  - Classical mesh (for example)
  - Aligned interpolation
  - Reduction in the number of poloidal planes
- Our approach (initiated end of 2013)
  - we remain on a flux surface (here $r = cte$)
  - FCISL method on each flux surface

First results of FCISL : `Kwon-Yi-Piao-Kim 2015`

- Lagrange interpolation of degree 3
- no splitting ($4D$ interpolation)
- curvilinear approach for the geometry

Oblic interpolation

Interpolation along a fixed oblic direction



$\Rightarrow$ Reconstruction of the values necessary by interpolation in θ
$\Rightarrow$ Reconstruction in the aligned direction

Constant oblic advection

Convergence result

Constant advection along $\mathbf{b} = (b_\theta, b_\varphi)$

$$\partial_t f + v\mathbf{b}\cdot\nabla f = 0,\ \ f(t=0,\theta,\varphi) = e^{(im\theta+in\varphi)}$$

Lagrange interpolation of odd degree d_θ in θ and

- Standard method : Lagrange of odd degree d_φ in φ

$$\left\|e^{(k)}\right\|_2 \leq C_{d_\theta}\frac{T\left(|m|\Delta\theta\right)^{d_\theta+1}}{\Delta t} + C_{d_\varphi}\frac{T\left(|n|\Delta\varphi\right)^{d_\varphi+1}}{\Delta t}$$

- Aligned method : Lagrange of odd degree d_φ in aligned direction $\mathbf{b}$

$$\left\|e^{(k)}\right\|_2 \leq G_{d_\theta} C_{d_\theta}\frac{T\left(|m|\Delta\theta\right)^{d_\theta+1}}{\Delta t} + C_{d_\varphi}\frac{T\left(\left|n+\frac{b_\theta}{b_\varphi}m\right|\Delta\varphi\right)^{d_\varphi+1}}{\Delta t}$$

- Same accuracy for

$$\Delta\varphi^{\text{aligned}} \simeq \left|\frac{b_\varphi\nabla_\varphi f}{\mathbf{b}\cdot\nabla f}\right|\Delta\varphi^{\text{standard}}.$$

If the error in θ is dominated

FCISL is interesting when f does not much vary along $\mathbf{b}$, while varying a lot along φ :

$$|\nabla f \cdot \mathbf{b}| = |b_\theta m_\theta + b_\varphi n_\varphi||f| << |n_\varphi|||f| = |\nabla_\varphi f|$$

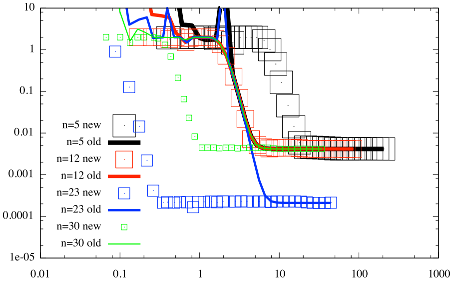
Gain factor is

$$\frac{|n_\varphi|}{|n_\varphi + \frac{b_\theta}{b_\varphi} m_\theta|}.$$

Error versus N_φ/n; $N_\theta = 200$ (or 400 for $n = 23$)

Lagrange interpolation of degree 9

$$n = 5 \qquad n + m\frac{b_\theta}{b_\varphi} = 5 - 34/\sqrt{2} \simeq -19$$
$$n = 12 \qquad n + m\frac{b_\theta}{b_\varphi} = 12 - 34/\sqrt{2} \simeq -12$$
$$n = 23 \qquad n + m\frac{b_\theta}{b_\varphi} = 23 - 34/\sqrt{2} \simeq -1$$
$$n = 30 \qquad n + m\frac{b_\theta}{b_\varphi} = 30 - 34/\sqrt{2} \simeq 6$$



Theoretical overhead for the interpolation in θ

Majoration by the **constant of Landau** (Landau, 1913)

$$G_d = \max_{0 \leq \alpha \leq 1} \sum_{k=-d}^{d+1} |L_k(\alpha)| = \sum_{k=-d}^{d+1} |L_k(\frac{1}{2})|,$$

with $L_k(x) = \prod_{\substack{\ell = -d \\ \ell \neq k}}^{d+1} \frac{x-\ell}{k-\ell}$ elementary Lagrange polynomial

$$G_0 = 1, \; G_1 = 1.25, \; G_2 = 1.390625$$
$$G_3 = 1.48828125, \; G_4 = 1.56304931640625$$
$$G_{18} < 1.999356, \; G_{20} < 2.031608$$

The constant of Landau is smaller than the constant of Lebesgue for polynomial interpolation with Chebychev points : we only consider the middle region for the interpolation

Some references on the constant of Landau

- Landau, 1913

$$G_d \sim \frac{\ln(d)}{\pi}\ ^{1}$$

- Watson, 1930

$$G_d = \frac{1}{\pi}\left(\ln(d+1) + \gamma + 4\ln(2) - \frac{1}{4(d+1)} + \frac{5}{192(d+1)^2} + R_d\right)$$

with $R_d = o(d^{-2})\,; 0 < R_d < \frac{3}{128(d+1)^3}$ Zhao, 2009

- Brutman, 1978

$$1 + \frac{\ln(d+1)}{\pi} \leq G_d < 1.0663 + \frac{\ln(d+1)}{\pi}$$

- Schönhage, 1962

$$G_d < \frac{2}{\pi}\left(\ln(d+2) + \ln(2) + \gamma\right),\ \gamma \simeq 0.577,\ \text{constante d'Euler}$$

- Mills-Smith, 1990 ($d \geq 1$)

$$0.8964675 + \frac{\ln(d+1.5)}{\pi} < G_d < 1.0778 + \frac{\ln(d+1)}{\pi}$$

- Cvijovic-Srivastava, 2009 link between several formulae

1. constant of Lebesgue for Chebychev's points : $2\frac{\ln(d)}{\pi}$ (result of Féjer)

Stability

How to prove that the symbol is smaller than one ?

- Numerical approach (not rigorous)
  - enumeration of intervals where symbol is C^∞ (20 cases for $d_\varphi = 1$; 7872 for $d_\varphi = 8$)
  - use of a maximize function on each interval (systematic and permits to detect unstable cases)
- formal approach (for fixed degree of interest)
  - identification on an equality that gives the inequality
  - prove the identity with computer algebra software
- Mathematical approach (for *arbitrary* degree)

Stability of the aligned method

- We first treat the case of $\lambda = \frac{b_\theta N_\theta}{b_\varphi N_\varphi}$ rational
  - $2d$ symbol writes as a convex combination of $1d$ symbols in aligned direction
    - coefficients are discrete Fourier transform
    - Discrete Fourier transform is real
    - Discrete Fourier transform is **nonnegative**
- Case of λ real by density

More precisely

The symbol can be written as

$$\rho_{\lambda,r_\varphi,\alpha_\varphi}(\omega_\theta,\omega_\varphi) = \sum_{p=0}^{q-1} t_p \exp(ir_\varphi\omega_p) \sum_{k=-d_\varphi}^{d_\varphi+1} L_k^{d_\varphi}(\alpha_\varphi)\exp(ik\omega_p),$$

with $\omega_p = 2\pi p\lambda + \omega_\varphi + \lambda\omega_\theta$, $q\lambda \in \mathbb{Z}$,

$$t_p = \frac{1}{q}\sum_{p_1=0}^{q-1}\sum_{\ell=-d_\theta}^{d_\theta+1} L_\ell^{d_\theta}\left(\frac{p_1}{q}\right)\exp\left(i\left(\ell-\frac{p_1}{q}\right)(\omega_\theta+2\pi p)\right),$$

- t_p is real by symmetry
- difficult part : t_p is **nonnegative**
- t_p is not real for even degree interpolation and we can find unstable situations (for $d_\varphi \geq 1$)
- interpolation along the aligned direction can be changed
- the symbol is in a regular q-polygon

First manipulations

Look at the behavior of

$$t(\omega) = \frac{1}{q} \sum_{p=0}^{q-1} \sum_{\ell=-d}^{d+1} L_\ell^d \left(\frac{p}{q}\right) \exp\left(i\left(\ell - \frac{p}{q}\right)\omega\right)$$

Simple expression of derivative (`Boyer, 2006 and Després, Lecture notes`)

$$t'(\omega) = (-1)^d \frac{2^{2d+1}}{(2d+1)!} \sin^{2d+1}\left(\frac{\omega}{2}\right) \frac{1}{q} \sum_{p=1}^{q-1} \cos\left(\left(\frac{1}{2} - \frac{p}{q}\right)\omega\right) w_d\left(\frac{p}{q}\right).$$

with $w_d(x) = \prod_{\ell=-d}^{d+1}(x-\ell)$; $(-1)^d w_d$ is convex on $(0,1)$.
$t(2n\pi) = 0,\ n = 1, \ldots, q-1.$

Convexity and positive Fourier transform

From Rolle's theorem and degree argument, it is enough to show local convexity around $2n\pi, \ n = 1, \ldots, q-1$, applying (with $f_p = w_d(\frac{p}{q})$)

Lemma (Polyà, 1948; Tuck, 2006)

Let $q \geq 2$ an integer and f_j a sequence of $q+1$ real numbers with $j = 0, \ldots, q$, such that $f_0 = f_q = 0$ and

$$f_{j+1} - 2f_j + f_{j-1} \geq 0, \quad j = 1, \ldots, q-1.$$

We then have

$$\sum_{p=1}^{q-1} \cos\left(2n\pi \frac{p}{q}\right) f_p \geq 0, \quad n = 1, \ldots, q-1.$$

Corollary : proof of SL-LG equivalence

Ferretti, 2010

- SL and LG are equivalent for the $1d$ constant advection, if we can find a function ϕ such that

$$\int_{\mathbb{R}} \phi(\eta + y)\phi(y)dy = \psi(y) \qquad \textbf{auto-correlation integral}$$

- ψ describes the Semi Lagrangian (SL) scheme
- ϕ describes the Lagrange Galerkin (LG) scheme
- In Fourier

$$\hat{\psi}(\omega) = \left|\hat{\phi}(\omega)\right|^2$$

- Example : for degree 3, we have

$$\hat{\psi}(\omega) = \frac{8(6+\omega^2)\sin(\omega/2)^4}{3\omega^4} \in \mathbb{R}^+$$

The result of stability in the oblic context implies the equivalence SL-LG of Ferretti, 2010 *and is valid for an* **arbitrary** *odd degree*

Direct proof of SL-LG equivalence

Ferretti-M, 2016 Algebraic form of the Fourier transform valid for *arbitrary* odd degree (conjectured in Ferretti, 2010)

- Aim : prove that $S(\omega) = \int_0^1 \sum_{\ell=-d}^{d+1} L_\ell(x) \exp\left(i(\ell - x)\omega\right) dx \in \mathbb{R}^+$
- Compact formula for the derivative Boyer/Després's lecture notes

$$S'(\omega) = (-1)^d \frac{2^{2d+1}}{(2d+1)!} \sin^{2d+1}\left(\frac{\omega}{2}\right) \sigma(\omega)$$

- **Integration by parts** for the factor

$$\sigma(\omega) = \int_0^1 \cos\left(\left(x - \frac{1}{2}\right)\omega\right) w(x)\, dx, \;\; w(x) = \prod_{j=-d}^{d+1} (x - j)$$

- Recognize the primitive thanks to relation

$$w^{(2k+1)}(0) = -\frac{d+1}{2k+2} w^{(2k+2)}(0), \;\; k = 0, \dots, d.$$

- Final explicit form

$$S(\omega) = (-1)^d \frac{2^{2d+1}}{(2d+1)!} \sin^{2d+2}\left(\frac{\omega}{2}\right) \sum_{k=0}^{d} \frac{w^{(2k+2)}(0)}{k+1} \frac{(-1)^k}{\omega^{2k+2}}$$

$\Rightarrow$ New proof of L^2 stability of SL scheme for constant advection

Application to gyrokinetics

The gyrokinetic model

$$mB_{\parallel}^* \frac{\partial f}{\partial t} + \left(\frac{\partial H}{\partial v_{\parallel}} \mathbf{B}^* + \frac{m}{e} \mathbf{b} \times \nabla_{\mathbf{x}} H \right) \cdot \nabla_{\mathbf{x}} f - \mathbf{B}^* \cdot \nabla_{\mathbf{x}} H \frac{\partial f}{\partial v_{\parallel}} = 0$$

$$H = \frac{1}{2} m v_{\parallel}^2 + \mu B + e\phi, \text{ with } \mu = m \frac{v_{\perp}^2}{2B}, \; B = |\mathbf{B}|.$$

$$\mathbf{B}^* = \mathbf{B} + \frac{m}{e} v_{\parallel} \nabla \times \mathbf{b}, \; B_{\parallel}^* = \mathbf{b} \cdot \mathbf{B}^*$$

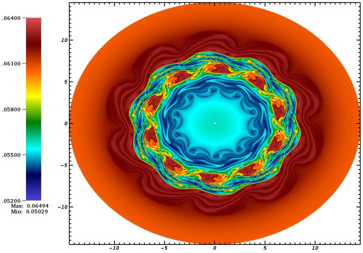
- $f = f(t, \mathbf{x}, v_{\parallel}, \mu)$: distribution function of **ions**
- m : mass of a particule
- e : charge of a particule
- **electrons** are supposed **adiabatic**
- non linear coupling through **Poisson** type equation for ϕ
- gyroaverage operator ommited for presentation

Simplification : drift kinetic model in cylinder geometry

$$\partial_t f - \frac{\partial_\theta \phi}{r B_0} \partial_r f + \frac{\partial_r \Phi}{r B_0} \partial_\theta f + v \nabla_{\parallel} f - \nabla_{\parallel} \Phi \partial_v f = 0, \; \nabla_{\parallel} = \mathbf{b} \cdot \nabla$$

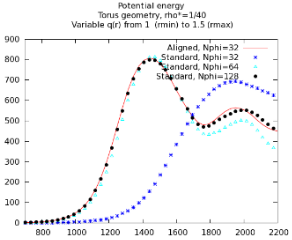
Application : gyrokinetic simulation in Selalib

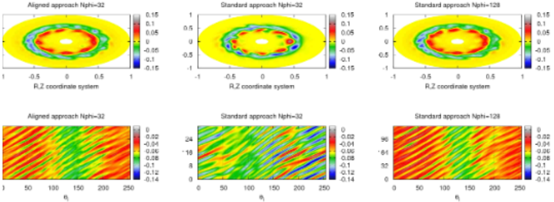
- drift kinetic model in cylinder geometry
- corresponds to `Grandgirard et al 2006`, when $b_\theta = 0$
- Poloidal cut $f(t, r, \theta, z = 0, v = 0)$
- Mode $(m = 10, n = -9)$ the most unstable (aligned method, LAG17) $255 \times 512 \times \mathbf{32} \times 128$ (256 proc), 4000 itérations $\Delta t = 2$, on helios, supercomputer, 21 heures.



Application : gyrokinetic simulation in Gysela

- Gain of factor 4 in Gysela (gyrokinetic code, CEA Cadarache)
- $256 \times 256 \times N_\varphi \times 48$
- Initialization with a bath of modes
- Degree 4, and cubic splines in θ and other interpolations





$N_\varphi = 32$, aligned $\quad N_\varphi = 32$, standard $\quad N_\varphi = 128$, standard

CEMRACS projects

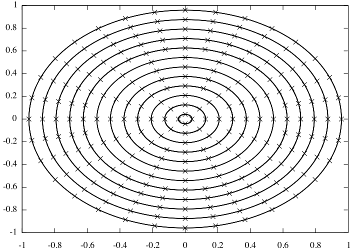
PICSL project

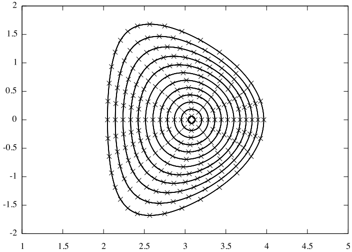
Participants : Yann Barsamian, Joackim Bernier, Sever Histoaga, M. M., Pierre Navaro

- Two species kinetic simulations
  - Vlasov-Poisson $2D \times 2D$ (cartesian geometry)
    - Landau
    - Test case of M. Badsi & M. Herda, Cemracs, 2014
  - Drift kinetic simulations $3D \times 1D$ (polar geometry)
  - Adding of Maxwell solver (equivalent to Poisson)
- Numerical methods :
  - Particle in Cell (PIC)
  - Semi-Lagrangian (SL)
- Tasks
  - Testcase description and dispersion analysis
  - Code development in Selalib library
  - Performance and numerical convergence

TARGET project

Participants : Nicolas Bouzat, Camilla Bressan, Virginie Grandgirard, Guillaume Latu, M. M.
Aim : adapt SL codes to new type of meshes like





Conclusion/Perspectives

- Progress in the method FCISL initiated by M. Ottaviani
  - Analysis for 2D advection ; new proof of stability of SL schemes
  - Validation on an adapted drift kinetic model
  - Validation in Gysela
- Perspectives
  - Study of other reconstructions : splines, Hermite, SLDG
  - More realistic configurations
  - Adaptation of the geometry / multi species (cf PICSL and TARGET)
- Other works
  - SL for BGK model
  - SL for stabilization of a network of strings
  - Gyroaverage operator and Padé approximants