From particle methods to hybrid semi- Lagrangian schemes

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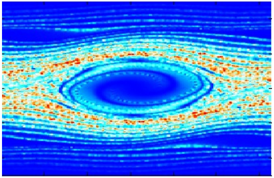
Introduction

Particle methods

Widely used for transport equations, especially for kinetic equations

- Quite easy to implement, even for high dimensions
- Lower computational cost than Eulerian methods (DG, Backward or Forward semi-Lagrangien schemes...)
- Main drawback : noisy solutions



Outline

1. Particle methods
2. LTP method
3. FBL method

Particle methods

Transport equation (conservative form)

$$\partial_t \rho + \nabla \cdot (a\rho) = 0, \qquad \rho(0,\cdot) = \rho^0 \tag{1}$$

with $a : \mathbb{R}^+ \times \mathbb{R}^d \to \mathbb{R}^d$ smooth ($a_i \in \mathrm{L}^\infty(0,T;W^{1,\infty})$).

Principle of particle methods

If $\rho^0(x) = \delta(x - x_0)$, then the measure solution of (1) is given by

$$\rho(t,x) = \delta(x - X_{0,x_0}(t))$$

where $X_{s,x_0}(t) = F^{s,t}(x_0)$ is the charateristic line starting from x_0 :

$$\begin{cases} \dfrac{d}{dt} X_{s,x_0}(t) & = a(t, X_{s,x_0}(t)) \\ X_{s,x_0}(s) & = x_0 \end{cases}$$

Particle methods

Consequence: discretization of (1)

- We choose $(\omega_k^0, x_k^0)_{1\leq k\leq N}$ such that $\rho^0(x) \sim \rho_h^0 = \sum_{k=1}^{N} \omega_k^0 \delta(x - x_k^0)$

  For example (deterministic initialization)

  $$x_k^0 = h\mathbf{k} \quad (\mathbf{k} \in \mathbb{Z}^d), \qquad \omega_k^0 = \rho^0(x_k^0)$$

- Then the solution $\rho(t,x)$ is approximated by

  $$\rho_h(t,x) = \sum_{k=1}^{N} \omega_k^0 \delta(x - X_k(t)) \qquad \text{with} \qquad \begin{cases} X_k'(t) = a(t, X_k(t)) \\ x_k(0) = x_k^0 \end{cases}$$

Remark

For equation $\partial_t \rho + \nabla \cdot (a\rho) + a_0 \rho = 0$ the weights evolve according to

$$\omega_k'(t) + a_0(t, X_k(t))\omega_k(t) = 0, \qquad \omega(0) = \omega_k^0$$

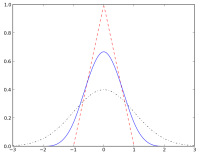
Regularization

Convolution kernel

Let $\varepsilon > 0$ and φ_ϵ such that $\int_{\mathbb{R}^d} \varphi_\varepsilon(x)\,dx = 1, \qquad \varphi_\varepsilon \rightharpoonup_{\varepsilon\to 0} \delta, \qquad \varphi_\varepsilon$ even.

Typically, we take $\varphi_\varepsilon(y) = \dfrac{1}{\varepsilon^d}\varphi\left(\dfrac{y}{\varepsilon}\right)$, with

- φ a spline fonction (B1 or B3)
- or φ a troncated Gaussian

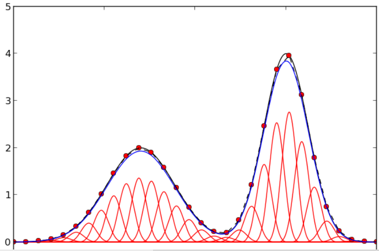


φ

Smooth particle approximation of ρ

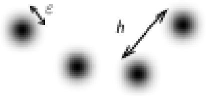
$$\rho_{h,\varepsilon}(t,x) = \sum_{k=1}^{N} \omega_k \varphi_\varepsilon(x - x_k(t))$$

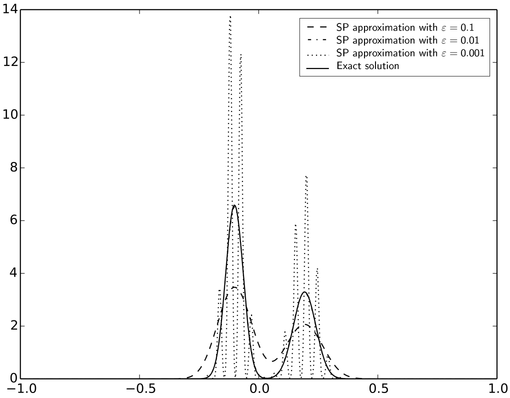
$$(\omega_k \simeq \int_{x_k^0 - h/2,\, x_k^0 + h/2} \rho^0(t)\,dt)$$



Smooth Particles methods

Choice of ε ?





Convergence of smooth Particles methods

Error estimate for a given velocity a [Raviart]

If $\varphi \in \mathcal{W}^{m,1}$ is such that $\int \varphi = 1$, $\int |x|^r |\varphi(x)|\,dx < +\infty$ and for a certain $m > 0$, $r > 0$

$$\int x_1^{k_1} \dots x_d^{k_d} \varphi(x_1, \dots, x_d)\,dx = 0, \quad |k| = k_1 + \dots + k_d \leq r - 1$$

then the following error estimate hold :

$$\|\rho_{h,\varepsilon} - \rho\|_{L^\infty(0,T)\times\mathbb{R}^d} \leq C_T \left(\varepsilon^r |\rho^0|_{W^{r,\infty}} + \left(\frac{h}{\varepsilon}\right)^m |\rho^0|_{W^{m,\infty}} \right)$$

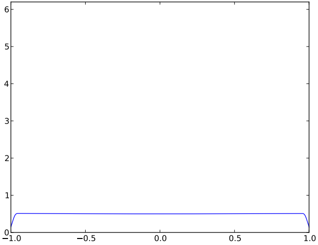
- With $h \sim \varepsilon$, weak convergence of the density only
- For a given ε, strong convergence requires $h \ll \varepsilon$ ($h \sim \varepsilon^{1/q}$, $q < 1$)
  - $\Rightarrow$ require a huge number of particles N ($N \sim \frac{1}{h^d}$)
  - $\Rightarrow$ implies extended particle overlapping

Exemple of a "noisy" Smooth Particle simulation

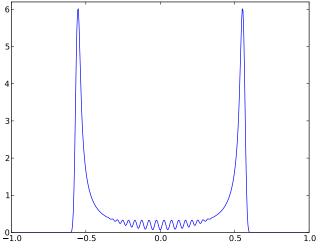
Numerical resolution with a SP method of the 1D-aggregation equation

$$\begin{cases} \partial_t \rho + \dfrac{\partial}{\partial x}(\rho u) = 0 \\ u(t,x) = -W' \star \rho \\ \rho(0,x) = \rho^0(x) \end{cases} \quad (2)$$

where $W(x) = \frac{|x|^a}{a} - \frac{|x|^b}{b}$, $(a,b) = (4, 2.5)$, with $N = 100$ particles, $\varepsilon = h$.



$\rho^0_{h,\varepsilon}$



$\rho^n_{h,\varepsilon}$ at steady state, with SP method

Denoising particle methods

Periodical remapping with $\varepsilon \sim h$

- re-initialize the particles on a phase-space grid.
- new particles = regular nodes

$$\rho_h^{\mathrm{n}}(x) = \sum_k \omega_k \varphi_h(x - X_k^n) \quad \longrightarrow \quad \rho_h^{\mathrm{n,\ remap}}(x) = A_h(\rho_h^{\mathrm{n}}) = \sum_k \omega_k^{\mathrm{remap}} \varphi_h(x - x_k^0)$$

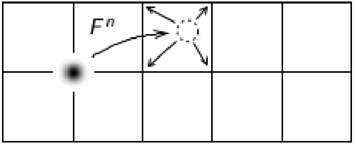
with $\omega_k^{\mathrm{remap}} = a_{k,h}(\rho_h^{\mathrm{n}})$ depends of values of ρ_h^{n} on a local stencil around x_k^0.

$\Rightarrow$ oscillations are smoothed out

... but numerical diffusion is introduced

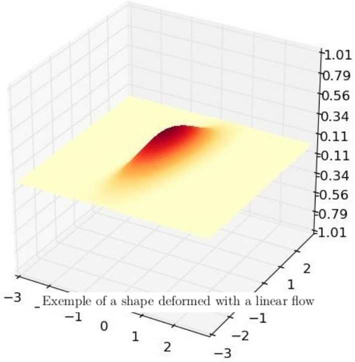
Same idea : Remeshed Particle Method/ Forward Semi-Lagrangien schemes

- Crouseilles, Respaud, Sonnendrücker 2008
- Cottet, Etancelin, Perignon, Picard, 2014 ; Cottet 2018



LTP (LTPIC) method

- Original idea of Perthame and Cohen (2000) : tranform the shape φ_ε of particles in order to better follow the flow
- LTP (and QTP) method developped in the context of the Vlasov-Poisson system (divergence free flow) by M. Campos-Pinto (JSC 2014, JCP 2014).



Exemple of a shape deformed with a linear flow

Idea of LTP method

- The solution of equation (1) is given by $\rho(t) = F_{\text{ex}}^{0,t} \# \rho^0$, i.e :

$$\rho(t,x) = j^{t,0}(x)\rho^0(F_{\text{ex}}^{t,0}(x))$$

with

$$\rho^0 \sim \rho_h^0 = \sum_k \omega_k \varphi_{h,k}^0, \qquad \varphi_{h,k}^0(x) = \frac{1}{h^d}\varphi\left(\frac{x - x_k^0}{h}\right)$$

- Introduce a linearization of the forward flow around x_k^0

$$F_{\text{lin},k}^{0,t} : x \to x_k(t) + \bar{J}_k^t(x - x_k^0), \qquad \bar{J}_k^t = J^{0,t}(x_k^0)$$

and transforme the shape of each particle according to the linearized flow

$$\varphi_{h,k}^t = F_{\text{lin},k}^{0,t} \# \varphi_h^0$$

Then

$$\varphi_{h,k}^t(y) = \frac{1}{\det(\bar{J}_k^t)} \varphi_h\Big(\underbrace{(\bar{J}_k^t)^{-1}}_{\text{deformation}} (y - x_k(t)) \Big)$$

LTP representation of $\rho(t^n, \cdot)$

$$\rho_h^n(x) = \sum_k \omega_k \varphi_{h,k}^n(x) \qquad \text{with} \qquad \varphi_{h,k}^n(x) = \frac{1}{h_k^n}\varphi\left(\frac{D_k^n}{h}(x - x_k^n)\right)$$

- D_k^n : "Deformation matrix"; $D_k^0 = I_{d\times d}$
- h_k^n : "volume of particles"; $h_k^0 = h^d$

Computation of the approximated Jacobian matrix

- Compute $D_k^n = D_k^{n-1}(J_k^{n-1})^{-1}$, where $J_k^{n-1} \simeq J^{t^{n-1},t^n}(x_k^{n-1})$,

using for example $$\frac{J^{s,t}}{dt}(x) = du(t, F^{s,t}(x))J^{s,t}(x)$$

- or directe FD using current positions of particles approximation

$$D_k^n = \left[\left(\frac{x_{k+e_j}^n - x_{k-ej}^n}{2h}\right)_{1\le i,j\le d}\right]^{-1},$$

Passiv flow

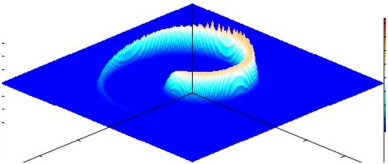
Theorem [M. Campos-Pinto, 2014]

If $\rho^0 \in W^{1,\infty}(\mathbb{R}^d)$, $a \in L^\infty([0,T], W^{2,\infty})$ and $\mathrm{div}(a) = 0$, with $x_k^n = F_{\mathrm{ex}}^{0,t_n}(x_k^0)$ then

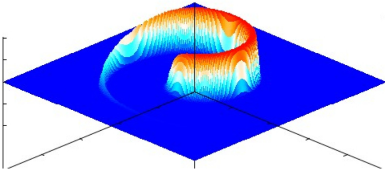
$$\|\rho_h^n - \rho_{\mathrm{ex}}^n\|_\infty \leq Ch \qquad (C = C(T, \|\rho^0\|_{W^{1,\infty}},))$$

Example : reversible "swirling" velocity field (LeVeque)

$$u_{SW,T}(t,x) = \cos\left(\frac{\pi t}{T}\right) \mathrm{curl}\,(\phi_{SW}(x)), \qquad \phi_{SW}(x) = \frac{-1}{\pi} \sin^2(\pi x_1) \sin^2(\pi x_2)$$



SP solution



LTP solution

$$N_{part} = 4 \cdot 10^4,\ t = T/2,\ \Delta_{remap} = 10\Delta t$$

Passiv flow : idea of the proof

- Approximation operator : $A_h : \rho^0 \mapsto \rho_h^0(x) = \sum_k \omega_k \varphi_{h,k}^0(x)$ such that

$$\|A_h\rho^0 - \rho^0\|_{L^\infty} \leq Ch|\rho^0|_{W^{1,\infty}}$$

- Let denote $S_{h,k}^0 = \mathrm{Supp}(\varphi_{h,k}^0)$ and

$$\Sigma_{h,k}^n = F_{\mathrm{ex}}^{0,t_n}(S_{h,k}^0) \cup F_{h,k}^{0,t_n}(S_{h,k}^0)$$

- Overlapping ($\mathcal{K}_n(x)$: set of overlapping particles at location x) :

$$\kappa_n := \sup_{x\in\mathbb{R}^d} \#\mathcal{K}_n(x), \qquad \mathcal{K}_n(x) := \{k \in \mathbb{Z}^d,\ x \in \Sigma_{h,k}^n\}.$$

- Error on the Forward flow :

$$\bar{e_F}^n = \sup_k \|F_{\mathrm{ex}}^{0,t_n} - F_{h,k}^{0,t_n}\|_{L^\infty(S_{h,k}^0)}$$

Vlasov-Poisson system

$$\frac{\partial f}{\partial t} + v \cdot \partial_x f + E \cdot \partial_v f = 0, \qquad \partial_x E(t,x) = 1 - \int_{\mathbb{R}} f(t,x,v)\,dv$$

$f(t,x,v)$: density function in electron, $t \in [0,T]$

Hypothesis

- E given by

$$E(t,x) = \int_0^L K(x,y)\left(1 - \int_{\mathbb{R}} f(t,y,v)\,dv\right) dy,$$

- bounded support in v-dimension, L-periodic with respect to x
- $f^0 \in \mathcal{W}^{2,\infty}(\mathbb{R}^2)$
- global neutrality relation

$$\int_0^L \left(\int_{\mathbb{R}} f^0(x,v)\,dv - 1\right) dx = 0.$$

Vlasov-Poisson system

Theorem [GH Cottet, PA Raviart, 1984]

Using SP method, one has

$$\sup_{t\in[0,T]} \|E_h(t) - E(t)\|_{L^\infty} + \sup_k \|Z_k^h(t) - F_{\text{ex}}^{0,t}(z_k^0)\| \leq C_T\, h$$

Theorem [M. Campos-Pinto, F.C, 2014]

Using LTP method, one has

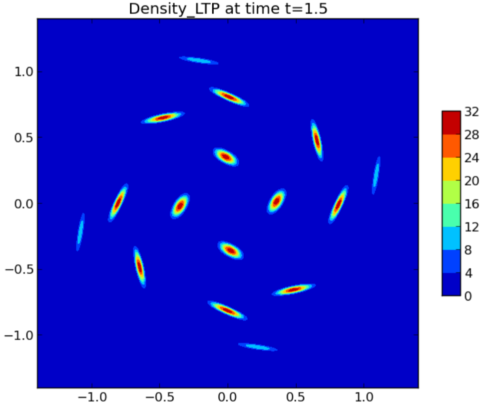
$$\sup_{0\leq n\leq T/\Delta t} \|E_h^n + 1/2 - E(t_{n+1/2})\|_{L^\infty} + \sup_k \|z_k^n - F_{\text{ex}}^{0,t_n}(z_k^0)\| \leq C_T\,(h^2 + \Delta t^2)$$

and provided $\Delta t \lesssim \sqrt{h}$, the particle approximation of the phase space density satisfies

$$\|f_h^n - f_{\text{ex}}^n\|_{L^\infty(\mathbb{R}^2)} \lesssim h + \frac{\Delta t^2}{h}$$

Loss of locality in LTP method

Evolution of the shapes of particles



$\Rightarrow$ necessity of periodical remappings

FBL method

We consider here the equation

$$\partial_t \rho + a \cdot \nabla \rho = 0, \qquad \rho(0, \cdot) = \rho^0 \tag{3}$$

The exact solution is given by

$$\rho(t, x) = \rho^0 \left(F^{t,0}(x) \right) \tag{4}$$

Idea

Use a approximation of the backward flow $F^{t,0}(x)$ (for all x) directly in (4) !!

FBL method

- "Particles" are pushed forward like in Particles methods : $(x_k^n)_k$
- Reconstruct of the backward flow at time t_n on a grid $(\xi_i)_{i\in\mathbb{Z}^d}$:

$$F^{t_n,0}(\xi_i) \simeq B_i^n := F^{t_n,0}_{h,k^*(n,i)}$$

where

$$k^*(n,i) := \mathrm{argmin}_k \|x_k^n - \xi_i\|$$

and

$$F^{t_n,0}_{h,k^*(n,i)} : x \mapsto x_k^0 + D_k^n(x - x_k^n), \qquad D_k^n \simeq (J_{F_{\mathrm{ex}}^{0,t_n}}(x_k^0))^{-1}$$

- (optional) Reconstruct a backward flow for all x with a partition of unity $\sum_i S_h(x-\xi_i) = 1$, and

$$B_h^n(x) = \sum_i B_i^n(x) S_h(x - \xi_i)$$

- Define a FBL approximation of ρ^n by

$$\rho_h^n(x) = \rho^0\left(B_h^n(x)\right)$$

FBL method for a passiv flow

Theorem [M. Campos-Pinto, F.C, 2016]

The FBL approximation of order 1 (LFBL) satisfy

$$\|\rho_h^n - \rho_{\text{ex}}^n\|_\infty \leq Ch^2$$

Key argument

LTP estimate is based on the bound

$$|\omega_k| \|\varphi_h(F_{h,k}^{t_n,0}(x)) - \varphi_h(F_{\text{ex}}^{t_n,0}(x))\| \leq |\omega_k| |\varphi_h|_{\text{lip}} \|F_{h,k}^{t_n,0} - F_{\text{ex}}^{t_n,0}\|_{L^\infty(S_{h,k}^n)} \lesssim \frac{1}{h} \bar{e_F}^n$$

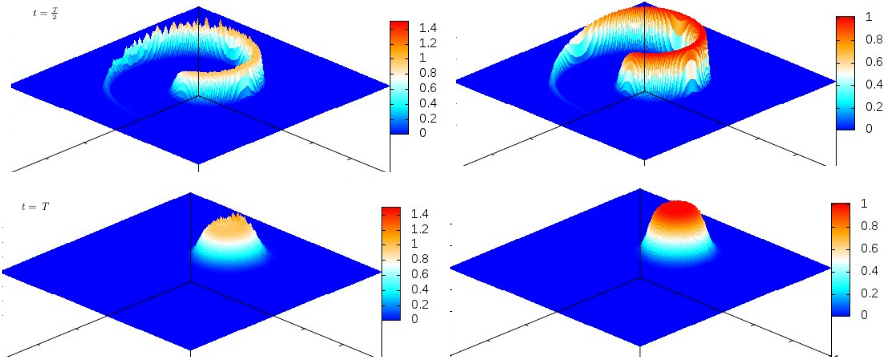
whereas for FBL we have

$$\|\rho_0(B_h^n(x)) - \rho_0(F_{\text{ex}}^{t_n,0}(x))\| \lesssim \|\rho^0\|_{\text{lip}} \bar{e_F}^n$$

FBL method

Example : reversible "swirling" velocity field $u_{SW,T}$

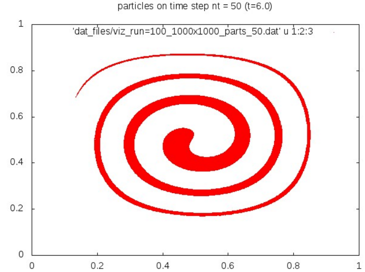
$N_{part} = 4 \cdot 10^4,\ T = 5,\ \Delta t = 0.05,\ \Delta t_{remap} = 1.5$

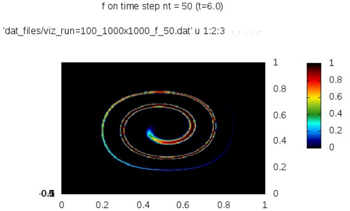


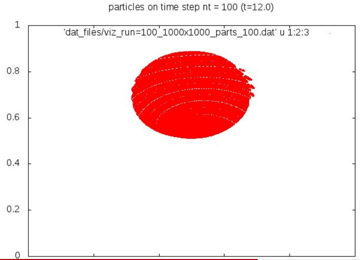
LTP solution FBL solution

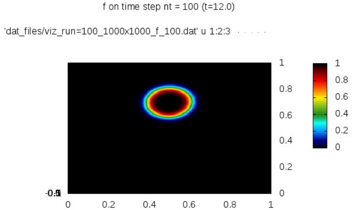
FBL method

$$N_{part} = 10^6,\ T = 12,\ \Delta t = 0.12,\ \Delta t_{remap} = 2$$



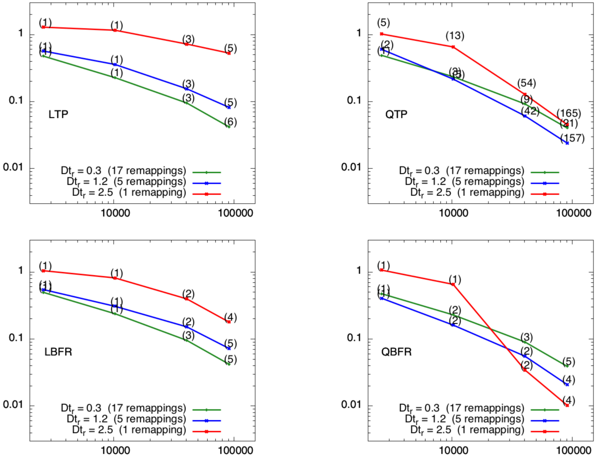






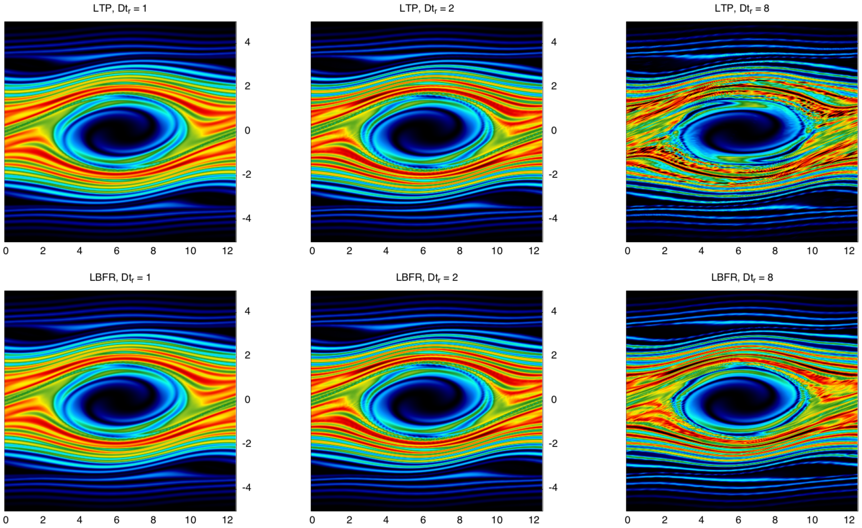
FBL method

Error estimates for the reversible "swirling" velocity field $u_{SW,T}$



FBL for Vlasov-Poisson system

Two stream instability $f_0(x,v) = (1 + \epsilon\cos(kx))\, v^2 \frac{1}{\sqrt{2\pi}} e^{-v^2/2}$, $\epsilon = 0.5$, $T = 45$.



Conclusion

- LTP methods improve accuracy ... but still need remappings
- QTP even better ... but very costly
- FBL methods: enhanced locality, less remappings are needed

Next prospects

- Multiscale method
- Extension to diffusion equation and Vlasov Fokker-Planck
  - linear Fokker Planck-Planck-Landau operator $PF(f)(v) = \nabla_v \cdot (\nabla_v f(v) + vf(v))$
  - non linear kernel $L_\phi(f)(v) = \nabla_v \cdot ((a_\phi \star f)\nabla_v f(v) - (b_\phi \star f)f(v))$

References

- M. Campos-Pinto, Towards smooth particles methods without smoothing, JSC 2014.
- M. Campos- Pinto, E. Sonnendrücker, A. Friedman, S. Lund, D. Grote, Noiseless Vlasov-Poisson simulations with linearly transformed particles, JCP 2014.
- M. Campos- Pinto, FC, Uniform convergence of a linearly transformed particle method for the Vlasov-Poisson system, SINUM 2016.
- M. Campos- Pinto, J. Carrillo, FC, Y.-P. Choi Convergence of a linearly transformed particle method for aggregation equations, Num. Math., 2018.
- M. Campos- Pinto, FC, From particle methods to hybrid semi-Lagrangian schemes. SMAI-JCM, 2018.

Thank you for your attention!