Noiseless Vlasov-Poisson simulations with polynomially transformed particles

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— jointwork with —

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—

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Outline

1. Motivation
2. Smooth particle methods for linear transport
   - The standard particle method (eg, PIC)
   - The remapped particle method (FSL)
   - The polynomially-transformed particle method (LTP and QTP)
   - Convergence estimates
   - Implementation options
3. Application to Vlasov-Poisson
   - Strong Landau Damping
   - Charge deposition in LTPIC
4. Dynamic remapping strategy
   - Heuristic criterion
   - Local error indicators
   - Application to Vlasov-Poisson
5. Conclusion, future steps

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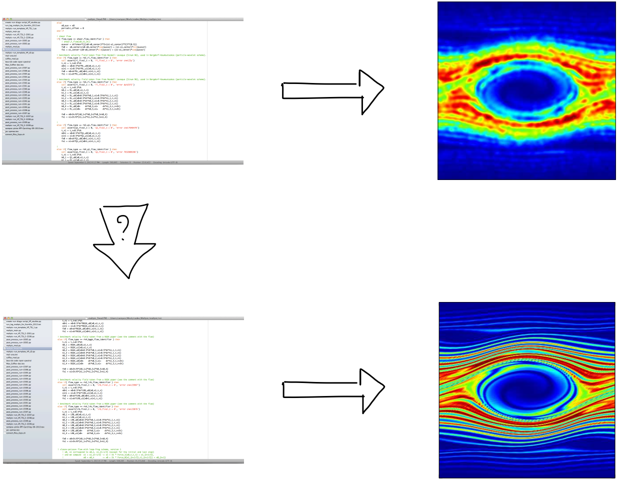
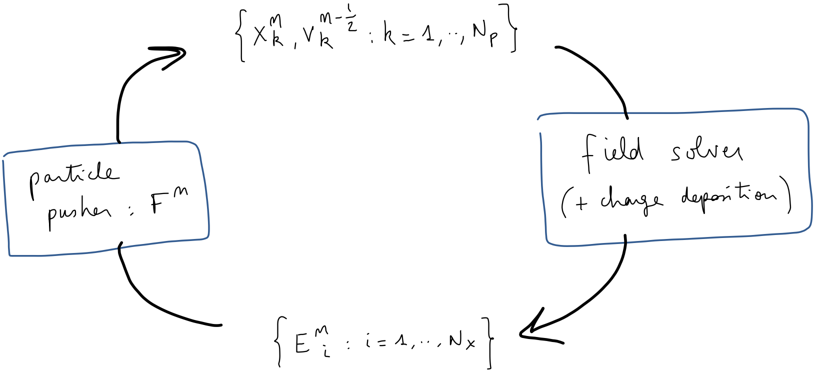
Motivation : denoising of PIC codes



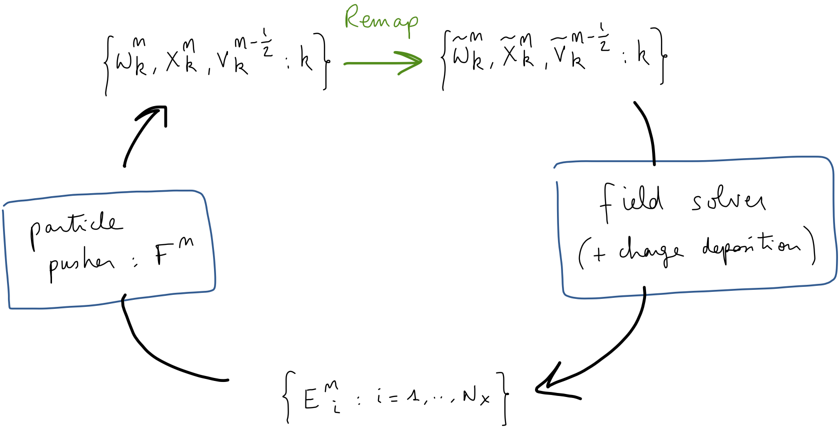
▷ Goal : denoise a PIC code with a minimal amount of changes...

Motivation : denoising of PIC codes, cont'd



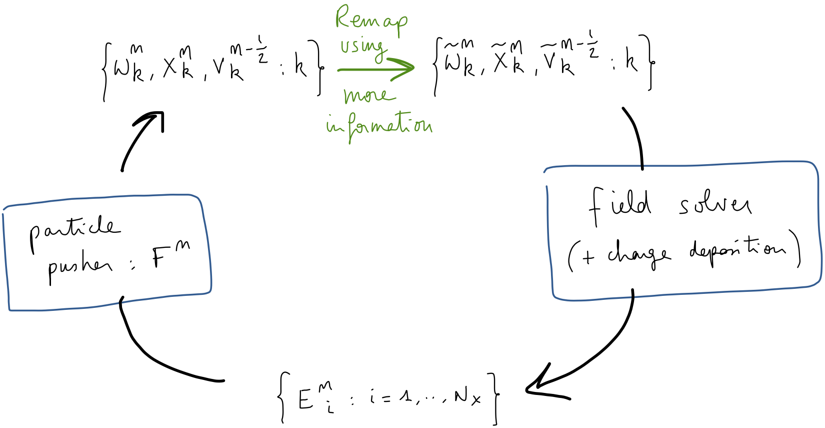
▷ Rough picture of a PIC code (electrostatic)

Motivation : denoising of PIC codes, cont'd



▷ Standard approach to denoising = FSL (remapped PIC) : often too diffusive

Motivation : denoising of PIC codes, cont'd



▷ Our solution to denoising : remap PIC, using more information from the flow

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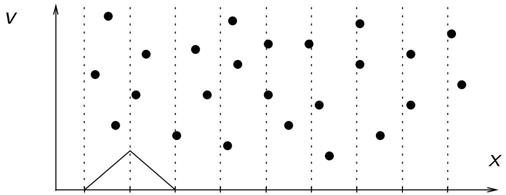
PIC method, sketched



particle positions :

$(x_k^n, v_k^n), \; k \le N_p$

grid cells :

$x_i, \; i \le N_c$

- Particle representation of the phase-space density :

$$f^n_{N_c,N_p}(x,v) = \sum_k w_k \delta_{(x_k^n, v_k^n)} \quad \text{or} \quad f^n_{h,\varepsilon}(x,v) = \sum_k w_k \varphi_\varepsilon(x - x_k^n, v - v_k^n)$$

- Nonlinear (eg Vlasov-Poisson) transport :

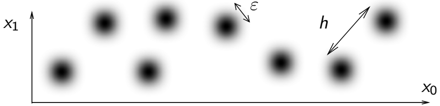
$$(x_k^{n+1}, v_k^{n+1}) = F^n(x_k^n, v_k^n)$$

Particles are pushed forward, eg with $F^n : (x,v) \mapsto (x + \Delta t v, v + \Delta t E^n(x))$

Why are there oscillations in the solutions ?

- Probabilistic initialization
- Underlying deterministic method : "ε-smoothed" (blob) particle method

$$\varphi_\varepsilon(x) = \frac{1}{\varepsilon^d}\varphi\left(\frac{x}{\varepsilon}\right)$$



- Standard analysis (Beale & Majda, Raviart, 80's) :
  - Error estimates :

$$\|f^n_{h,\varepsilon} - f^n\|_{L^\infty} \le \sup_x |\langle f^n_h - f^n, \psi_{x,\varepsilon}\rangle| + \|f^n * \varphi_e - f^n\|_{L^\infty} \lesssim \left(\frac{h}{\varepsilon}\right)^2 + \varepsilon^2$$

  - weak convergence for arbitrary ε, h
  - strong convergence requires $\varepsilon \sim h^q$ with $q < 1$
- In the weighted PIC scheme, $(\varepsilon, h) \leftarrow (N_c, N_p)$
  - For moderate values ($q \approx 0.8$) $\Longrightarrow$ $N_p/N_c \sim (N_c)^{\approx 1.5}$, too expensive !

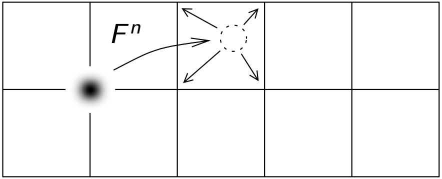
$\Longrightarrow$ Need to transport the particles with higher accuracy

Outline

Hybrid method : particles with remappings (Denavit, FSL)

$$f_h^n(x) = \sum_k w_k^n \varphi_h(x - x_k^n), \quad \text{h} : \begin{cases} \text{distance between particles } (x_k^0 = hk) \\ \text{scale of the particles } (\varepsilon = h) \end{cases}$$

- Transport as above : $x_k^{n+1} = F^n(x_k^n)$,
- Remap periodically : re-initialize the particles on a phase-space grid.
  - New particles = regular nodes
  - Remappings smooth out the oscillations but also introduce numerical diffusion



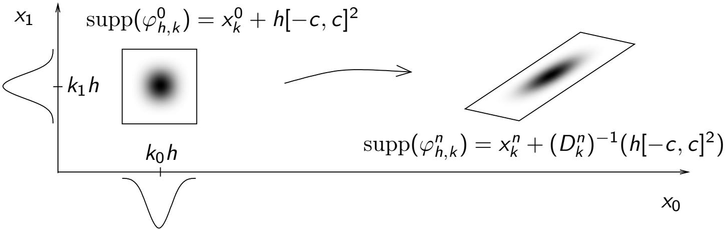
▷ High order projections, adaptive grids to reduce the numerical diffusion, see e.g., (Bergdorf and Koumoutsakos, 2006), (Wang, Miller and Collela, 2011)...

Outline

The linearly-transformed particle (LTP) method

- Each particle has a weight w_k^n, a center x_k^n and a deformation matrix D_k^n

$$f_h^n(x) = \sum_{k \in \mathbb{Z}^d} w_k^n \varphi_h(D_k^n(x - x_k^n))$$



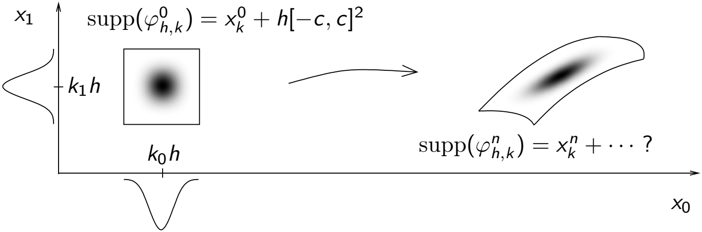
- LTP transport = exact transport of the particle for the linearized flow
  - in practice, apply the forward flow F^n on a local stencil around each particle
  - also need to remap to avoid arbitrary stretching

▷ Previous approaches
  - formal methods by (Hou, 1990), (Cohen and Perthame, 2000)
  - in plasma simulation, Complex Particle Kinetics by (Bateson and Hewett, 1998), (Hewett, 2003), (Alard and Colombi 2005)...

The quadratically-transformed particle method (QTP)

- Each QTP has the attributes of an LTP + additional matrices $(Q_k^n)_i$, $i = 0, 1$

$$f_h^n(x) \approx \sum_{k \in \mathbb{Z}^d} w_k^n \varphi_h\Big(D_k^n(x - x_k^n) + \frac{1}{2}\sum_{l_1, l_2}\big((Q_k^n)_{i,l_1,l_2}(x - x_k^n)_{l_1}(x - x_k^n)_{l_2}\big)_{i=0,1}\Big)$$



- QTP transport = push of the center + quadratic deformation of the shape
  - in practice, apply the forward flow F^n on a local stencil around each particle
  - also need to remap to avoid arbitrary stretching
  - particle support must be defined with some care

▷ New method

Outline

Polynomial particle transport : definition

- principle : transport the particle $\varphi^0_{h,k}(x) := \varphi_h(x - x^0_k)$ with

$$\bar{T}_h^{n,(r)} \varphi^0_{h,k}(x) := \varphi_h(\bar{B}_{h,k}^{n,(r)}(x) - x^0_k), \qquad \bar{B}_{h,k}^{n,(r)} \approx \bar{B}^n$$

- order 0 (PIC / FSL) : use

$$\bar{B}_{h,k}^{n,(0)}(x) := x^0_k + (x - x^n_k) \qquad \text{with} \quad x^n_k := \bar{F}^n(x^0_k)$$

- order 1 (LTP) : use

$$\bar{B}_{h,k}^{n,(1)}(x) := x^0_k + D^n_k(x - x^n_k) \qquad \text{with} \quad (D^n_k)_{i,j} := \partial_j (\bar{B}^n)_i (x^n_k)$$

- order 2 (QTP) : use

$$\bar{B}_{h,k}^{n,(2)}(x) := x^0_k + D^n_k(x - x^n_k) + \frac{1}{2}\Big(\sum_{l_1,l_2} (Q^n_k)_{i,l_1,l_2}(x - x^n_k)_{l_1}(x - x^n_k)_{l_2}\Big)_{i=0,1}$$

with

$$(Q^n_k)_{i,l_1,l_2} := \partial_{l_1,l_2}(\bar{B}^n)_i(x^n_k)$$

Polynomial particle transport : convergence estimates

Denote the backward flow error by

$$e^n_{B,(r)}(h) := \sup_{k\in\mathbb{Z}^d} \|\bar{B}^{n,(r)}_{h,k} - \bar{B}^n\|_{L^\infty(\Sigma^n_{h,k})} \qquad \text{where} \qquad \Sigma^n_{h,k} \approx \mathrm{supp}(\varphi^n_{h,k})$$

Theorem

The LTP ($r = 1$) and QTP ($r = 2$) transport operators satisfy

$$\|(T_{(r)} - T_{\mathrm{ex}})f^0_h\|_{L^\infty} \lesssim \Big(1 + \frac{e^n_{B,(1)}(h)}{h}\Big)^d \frac{e^n_{B,(r)}(h)}{h}\|f^0\|_{L^\infty}$$

for QTP particles restricted to domains of the form
$\Sigma^n_{h,k} := \bar{F}^{n,(1)}_{h,k}(B_{\ell^\infty}(x^0_k, h\tilde{\rho}^n_{h,k}))$ *with* $\tilde{\rho}^n_{h,k} := \rho^0 + \frac{1}{h}e^n_{B,(2),k}(h)$

Corollary

$$\|(T_{(r)} - T_{\mathrm{ex}})f^0_h\|_{L^\infty} \lesssim h^r C(F,r)\|f^0\|_{L^\infty}$$

Proof : The backward flow errors satisfy $e^n_{B,(r)}(h) \lesssim h^{r+1}|\bar{F}^n|^{r+1}_1|\bar{B}^n|_{r+1}$ □

Outline

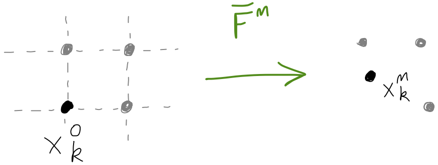
Option # 1 : the incremental approach

($\bar{F}^{n+1}$ = fwd flow on $[0, t_{n+1}] = F^n \bar{F}^n$)

- PIC/FSL : compute the particle centers $x_k^n := \bar{F}^n(x_k^0)$
  - initialize
    $$x_k^0 := kh$$
  - update
    $$x_k^{n+1} := F^n(x_k^n)$$
- LTP : compute the above + Jacobian matrices $D_k^n := \partial_j(\bar{B}^n)_i(x_k^n)$
  - initialize
    $$D_k^0 := I$$
  - update
    $$D_k^{n+1} := D_k^n(J_k^n)^{-1}$$
- QTP : compute the above + Hessian matrices $(Q_k^n)_{i,j_1,j_2} := \partial_{j_1,j_2}(\bar{B}^n)_i(x_k^n)$
  - initialize :
    $$Q_k^0 := 0$$
  - update

$$(Q_k^{n+1})_i := (J_k^n)^{-T}(Q_k^n)_i(J_k^n)^{-1} - \sum_j (D_k^n)_{i,j}(J_k^n)^{-T}\Big(\sum_{j'}((J_k^n)^{-1})_{j,j'}(H_k^n)_{j'}\Big)(J_k^n)^{-1}$$

Option # 2 : the direct approach



- Principle : instead of updating the approx. flow derivatives D_k^n or Q_k^n, push a local stencil of markers around each particle,

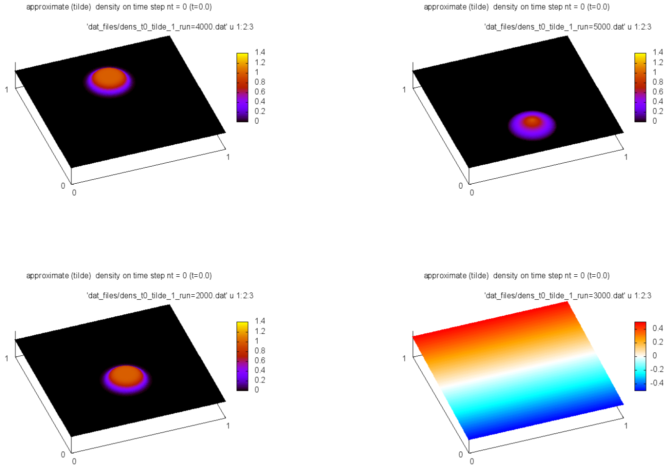
$$x_{k,i}^n \quad \mapsto \quad x_{k,i}^{n+1} := F^n(x_{k,i}^n), \quad i = 0, \dots, I$$

- $\rightarrow$ FD approximations of the Jacobian and Hessian matrices of $\bar{F}^n$ and $\bar{B}^n$
- $\rightarrow$ straightforward estimates for the local backward flow errors

$$e_{B,(r)}^n(h) := \sup_k \| \bar{B}_{h,k}^{n,(r)} - \bar{B}^n \|_{L^\infty(\Sigma_{h,k}^n)} \approx \sup_k \max_i \| \bar{B}_{h,k}^{n,(r)}(x_{k,i}^n) - x_{k,i}^0 \|$$

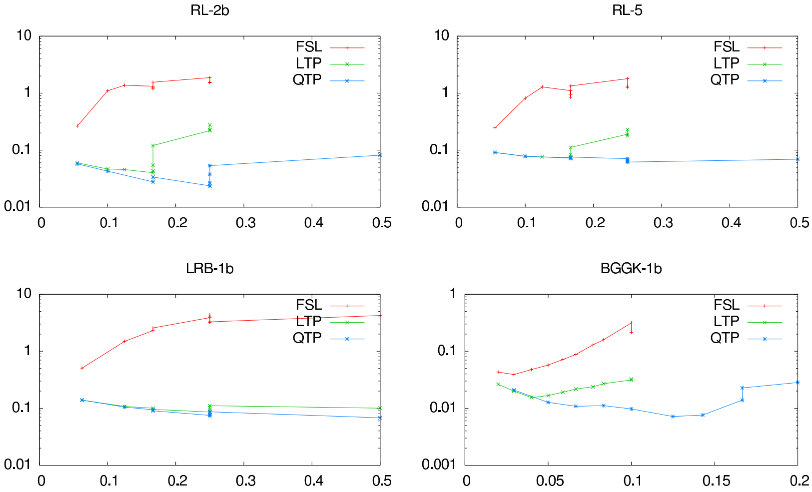
Test cases for linear transport

- 256x256 particles and RK4 numerical flow with $\Delta t = T/100$.



Numerical accuracy and robustness

- Final L^∞ errors vs. average remapping period



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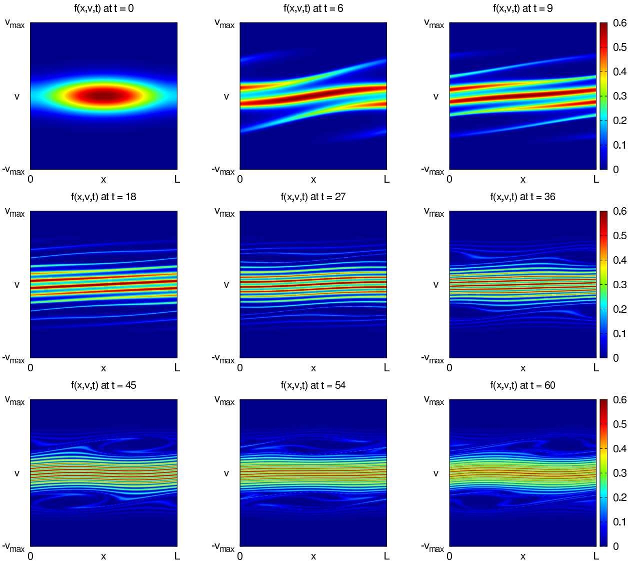
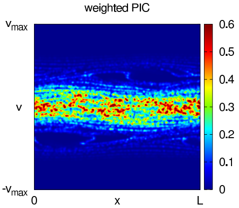
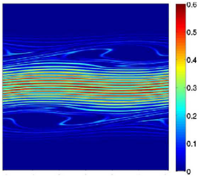
Strong Landau Damping : evolution in phase space



Strong Landau Damping : comparison of different schemes

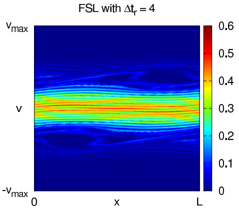
PIC
(weighted)
$\Delta t = 1/8$
$N_c = 128$
$N_p = 256 \times 256$
$\approx 400,000$ dofs

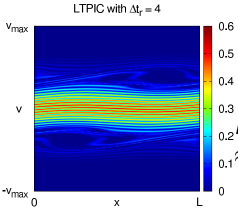




BSL-DG
(5th-order)
$\Delta t \approx 1/30$
mesh =
128×256
$\approx 500,000$ dofs

FSL
$\Delta t = 1/8$
$N_c = 64$
$N_p = 256 \times 256$
$\approx 400,000$ dofs





LTPIC
$\Delta t = 1/8$
$N_c = 64$
$N_p = 256 \times 256$
$\approx 400,000$ dofs

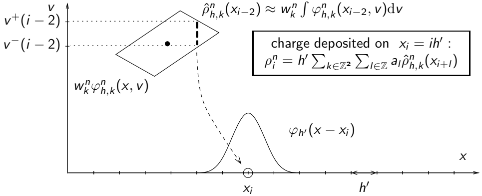
- BSL-DG taken from (Rossmanith and Seal, JCP 2011)

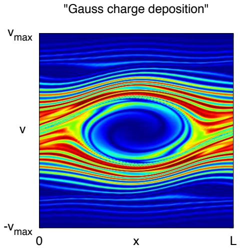
Outline

Scheme n.1 : "Gauss charge deposition"

- Apply numerical quadratures along v slices to estimate the charge density

$$\rho_h^n(x) \approx \int f_h^n(x,v)\,\mathrm{d}v = \sum_{k\in\mathbb{Z}^2} w_k^n \int \varphi_h(D_k^n(x-x_k^n, v-v_k^n))\,\mathrm{d}v$$



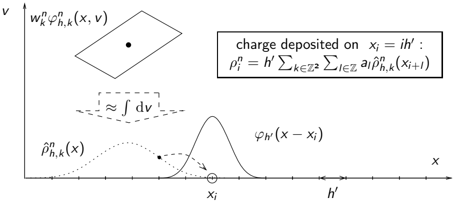


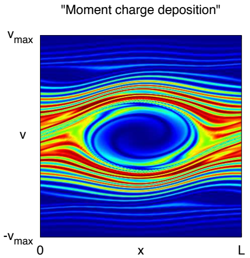
(64 cells, 256 x 256 particles)

Scheme n.2 : "Moment charge deposition"

- Replace each "v-integrated particle" by a B-spline with same 3 moments

$$\rho_h^n(x) \approx \int f_h^n(x,v)\,\mathrm{d}v = \sum_{k\in\mathbb{Z}^2} w_k^n \int \varphi_h(D_k^n(x - x_k^n, v - v_k^n))\,\mathrm{d}v$$



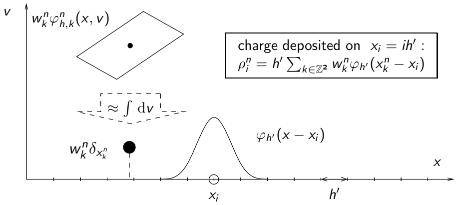


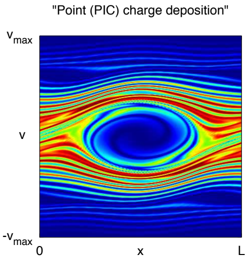
(64 cells, 256 x 256 particles)

Scheme n.3 : "Point charge deposition"

- Replace each "v-integrated particle" by a B-spline with same 2 moments !

$$\rho_h^n(x) \approx \int f_h^n(x,v)\,\mathrm{d}v = \sum_{k\in\mathbb{Z}^2} w_k^n \int \varphi_h(D_k^n(x-x_k^n, v-v_k^n))\,\mathrm{d}v$$





(64 cells, 256 x 256 particles)

Outline

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Remapped scheme

- A_h : B-spline (quasi)-interpolation on the cartesian grid $\{x_k^0 := hk, k \in \mathbb{Z}^2\}$,

$$A_h f(x) := \sum_k w_k(f)\varphi_h(x - x_k^0)$$

- T_h^n : transport operator on $[t_n, t_{n+1}]$

$$T_h^n : f_h^n = \sum_k w_k^n \varphi_h(D_k^n(\cdot - x_k^n)) \mapsto f_h^{n+1} = \sum_k w_k^{n+1}\varphi_h(D_k^{n+1}(\cdot - x_k^{n+1}))$$

with $\quad w_k^{n+1} := w_k^n, \quad x_k^{n+1} := F^n(x_k^n), \quad D_k^{n+1} := D_k^n J_k^n.$

- denote

$$n_0 = 0, \quad n_1, \quad \dots, \quad n_I \quad \text{and} \quad \tau_i := t_{n_i}$$

the time steps where the particle density is remapped on the cartesian grid ($\tilde{f}_h^{n_i} := A_h f_h^{n_i}$). Then the remapped particle scheme $S_h^{n_0,n} : f_h^{n_0} \mapsto f_h^n$ reads

$$S_h^{n_0,n} = S^{n_1,n} T_h^{n_0,n_1} A_h.$$

Heuristic remapping criterion

- The global error $e_h^{n_0,n} := \|(S_h^{n_0,n} - T_{\rm ex}^{n_0,n})f_h^{n_0}\|_{L^\infty}$ satisfies

$$
\begin{aligned}
e_h^{n_0,n} &\le \|(S_h^{n_1,n} - T_{\rm ex}^{n_1,n})f_h^{n_1}\|_{L^\infty} + \|T_{\rm ex}^{n_1,n}(T_h^{n_0,n_1} - T_{\rm ex}^{n_0,n_1})A_h f_h^{n_0}\|_{L^\infty} \\
&\qquad + \|T_{\rm ex}^{n_0,n}(A_h - I)f_h^{n_0}\|_{L^\infty} \\
&\le e_h^{n_1,n} + \|(T_h^{n_0,n_1} - T_{\rm ex}^{n_0,n_1})A_h f_h^{n_0}\|_{L^\infty} + \|(A_h - I)f_h^{n_0}\|_{L^\infty} \\
&\le \sum_{i=0}^{I-1} \Big(\|(T_h^{n_i,n_{i+1}} - T_{\rm ex}^{n_i,n_{i+1}})A_h f_h^{n_i}\|_{L^\infty} + \|(A_h - I)f_h^{n_i}\|_{L^\infty} \Big)
\end{aligned}
$$

- Typically,
  - remapping error is (roughly) independent on the strategy,
  - transport error may have exponential growth w.r.t. $\Delta\tau_i := t_n - \tau_i$
- Heuristic : balance the errors, i.e., remap $f_h^n \mapsto A_h f_h^n$ when

$$\mathcal{E}(\|(T_h^{n_i,n} - T_{\rm ex}^{n_i,n})A_h f_h^{n_i}\|_{L^\infty}) \ge \mathcal{E}(\|(A_h - I)f_h^n\|_{L^\infty})$$

- using the local flow errors, remap f_h^n if

$$C_{\rm balance}\Big(1 + \frac{e_B^n(h)}{h}\Big)^d \frac{e_B^n(h)}{h}\|f_h^{n_i}\|_{L^\infty} \ge h|f_h^n|_1$$

Outline

Estimating the transport error

- Direct estimate : the transport error satisfies

$$\|(T_h^{n_i,n} - T_{\rm ex}^{n_i,n})f_h^{n_i}\|_{L^\infty} \lesssim \Big(1 + \frac{e_B^n(h)}{h}\Big)^d \frac{e_B^n(h)}{h} \|f_h^{n_i}\|_{L^\infty}$$

  where $e_B^n(h)$ is the backward flow error,

$$e_B^n(h) := \sup_{k\in\mathbb{Z}^2} \|\bar{B}_{h,k}^n - \bar{B}_{\rm ex}^n\|_{L^\infty(\bar{\Sigma}_{h,k}^n)}$$

- Flow-based estimate (LTP) : with the 1st order particle method, we have

$$e_B^n(h) \lesssim h^2 |\bar{B}_{\rm ex}^n|_1^2 |B_{\rm ex}^n|_2$$

- Velocity-based estimate (LTP) : For $n_i \le n$, let

$$\beta(n_i, n) := (t_n - \tau_i) exp(3(t_n - \tau_i)|u|_{1,\tau_i,t_n})|u|_{2,\tau_i,t_n}.$$

  Then

$$e_B^n(h) \lesssim h^2 \beta(n_i, n)$$

Estimating the remapping error

- Remapping error estimate (not optimal)

$$\|(A_h - I) f_h^n\|_{L^\infty} \leq h c_A |f_h^n|_1$$

- To estimate in practice the smoothness of f_h^n we assume for simplicity that $f_h^n(x,y) \approx f_h^{n_i} \circ F^{-1}(x,y) =: f_h^{n_i}(\hat{x},\hat{y})$, and observe that

$$\begin{aligned} \partial_x f_h^n(x,y) &\approx \partial_x f_h^{n_i}(\hat{x},\hat{y}) \partial_x F^{-1}(x,y)_x + \partial_y f_h^{n_i}(\hat{x},\hat{y}) \partial_x F^{-1}(x,y)_y \\ &\approx \partial_x f_h^{n_i}(\hat{x},\hat{y}) (J_{F^{-1}}(x,y))_{x,x} + \partial_y f_h^{n_i}(\hat{x},\hat{y}) (J_{F^{-1}}(x,y))_{y,x} \end{aligned}$$

so that (using $D_k^n \approx J_{F^{-1}}(x_k^n)$)

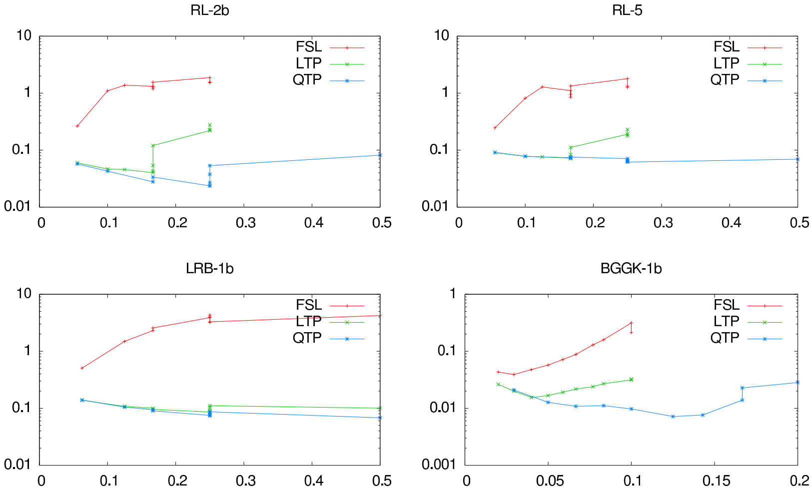
$$\|\partial_x f_h^n\|_{L^\infty} \approx \sup_{k \in \mathbb{Z}^2} |\partial_x f_h^n(x_k^n)| \approx \sup_{k \in \mathbb{Z}^2} |\partial_x f_h^{n_i}(x_k^0)(D_k^n)_{0,0} + \partial_y f_h^{n_i}(x_k^0)(D_k^n)_{1,0}|$$

We estimate $\|\partial_x f_h^n\|_{L^\infty}$ similarly, hence

$$|f_h^n|_1 := \|\partial_x f_h^n\|_{L^\infty} + \|\partial_y f_h^n\|_{L^\infty} \approx \sum_{j=0,1} \sup_{k \in \mathbb{Z}^2} |\partial_x f_h^{n_i}(x_k^0)(D_k^n)_{0,j} + \partial_y f_h^{n_i}(x_k^0)(D_k^n)_{1,j}|$$

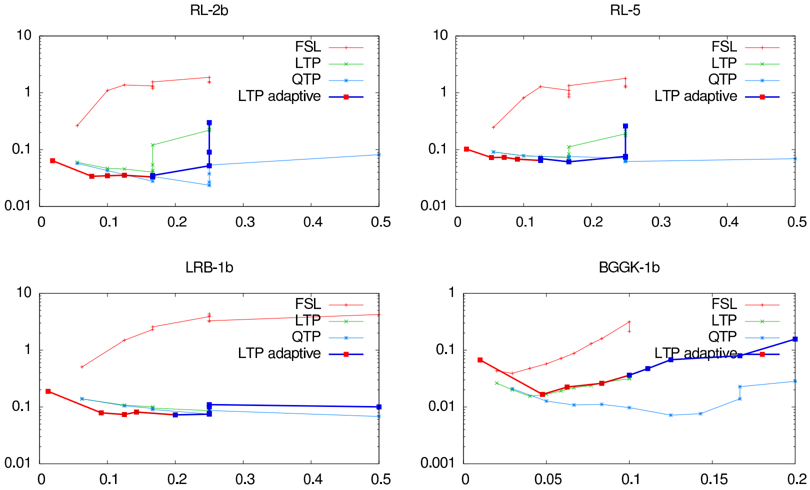
Optimal remapping periods : static strategy (again)

- Final L^∞ errors vs. average remapping period



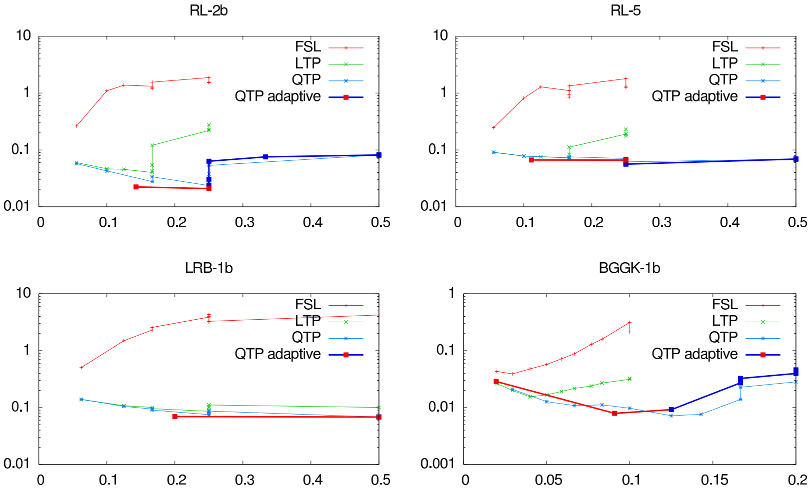
Optimal remapping periods : adaptive strategy (LTP)

- Final L^∞ errors vs. average remapping period



Optimal remapping periods : adaptive strategy (QTP)

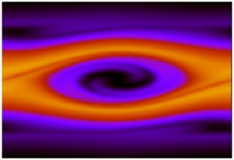
- Final L^∞ errors vs. average remapping period



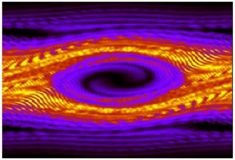
Outline

Vlasov-Poisson (TSI) with dynamic remappings : FSL

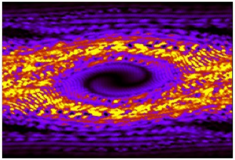
FSL, Dt_r = Dt



FSL, Dt_r = 15 Dt

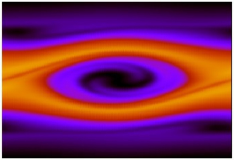


FSL, Dt_r = 30 Dt

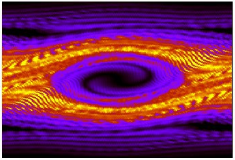


Vlasov-Poisson (TSI) with dynamic remappings : FSL

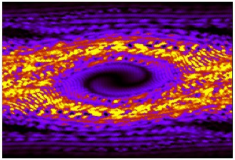
FSL, Dt_r = Dt



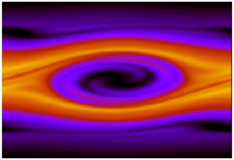
FSL, Dt_r = 15 Dt



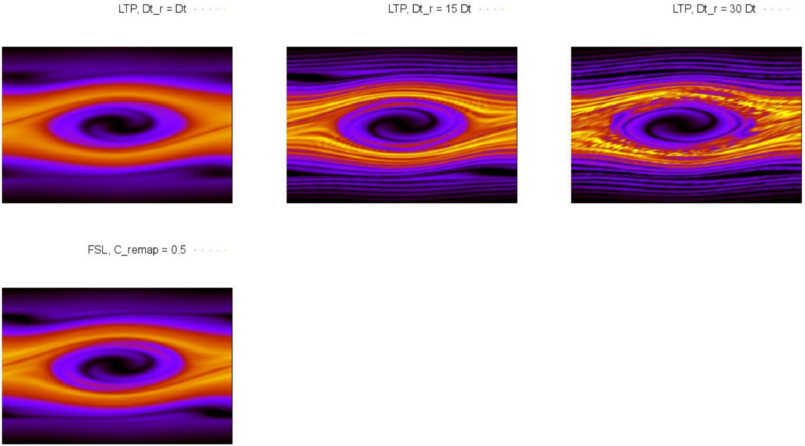
FSL, Dt_r = 30 Dt



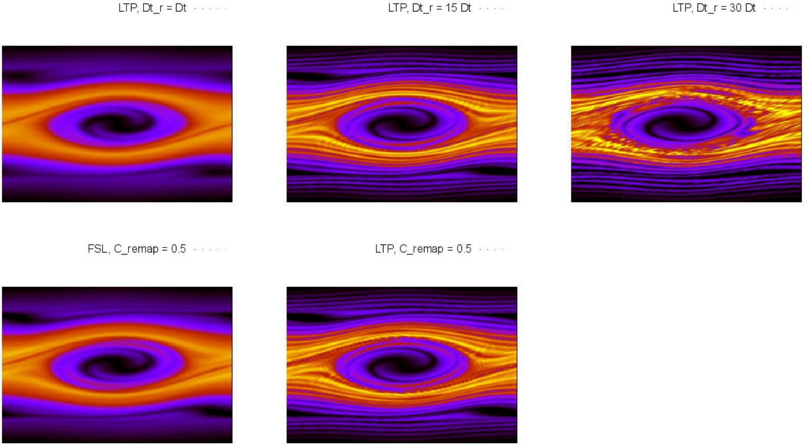
FSL, C_remap = 0.5



Vlasov-Poisson (TSI) with dynamic remappings : LTP

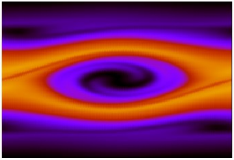


Vlasov-Poisson (TSI) with dynamic remappings : LTP

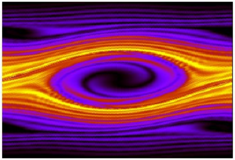


Vlasov-Poisson (TSI) with dynamic remappings : QTP

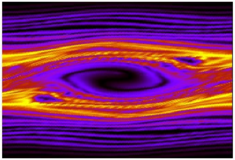
QTP, Dt_r = Dt



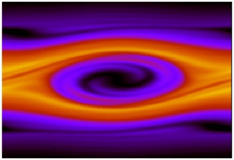
QTP, Dt_r = 15 Dt



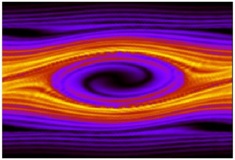
QTP, Dt_r = 30 Dt



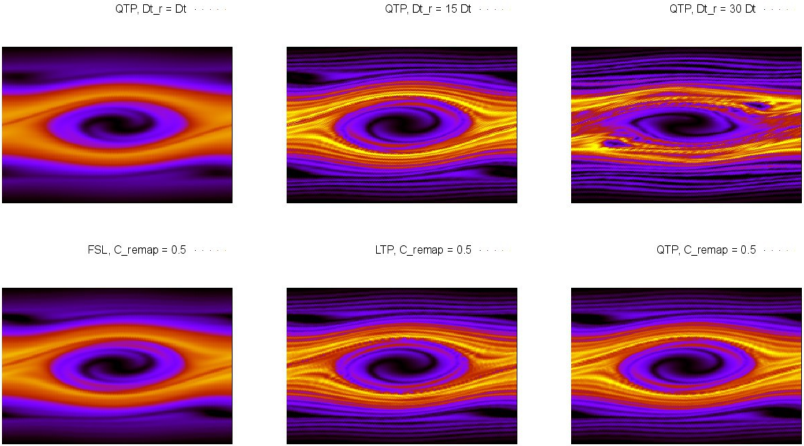
FSL, C_remap = 0.5



LTP, C_remap = 0.5

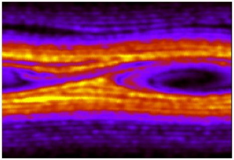


Vlasov-Poisson (TSI) with dynamic remappings : QTP

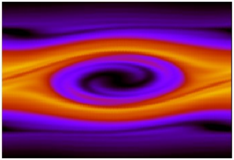


Vlasov-Poisson (TSI) with dynamic remappings : summary

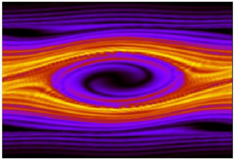
PIC



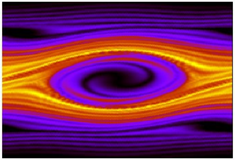
FSL, C_remap = 0.5



LTP, C_remap = 0.5



QTP, C_remap = 0.5

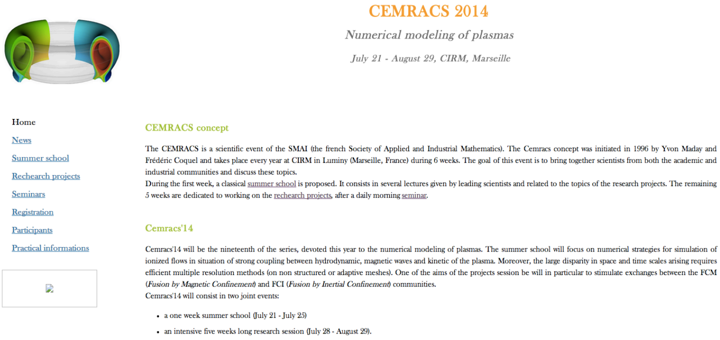


Outline

Clonclusion and future steps

- New particle scheme follows hybrid path :
  - algorithms similar to PIC
  - computational cost ?
  - accuracy similar to noiseless, state-of-the-art grid-based schemes
  - well suited for parallel codes
  - tractable error estimates, allow for adaptive remapping
- Advantages compared to "remapped PIC" (FSL) :
  - higher accuracy
  - lower remapping frequencies $\Longrightarrow$ more robust, less diffusive
- References
  - MCP (2012 - 2013, submitted) *Smooth particles methods without smoothing*
  - MCP, E. Sonnendrücker, A. Friedman, S. Lund, D. Grote (submitted) *Noiseless Vlasov-Poisson simulations with linearly transformed particles*
- Future steps :
  - Error analysis for coupled solvers
  - Multilevel particles
  - Extensions to other models (VP 2d, VM) and larger codes

Next year : CEMRACS 2014 summer school on Fusion



CEMRACS 2014

Numerical modeling of plasmas

July 21 - August 29, CIRM, Marseille

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CEMRACS concept

The CEMRACS is a scientific event of the SMAI (the french Society of Applied and Industrial Mathematics). The Cemracs concept was initiated in 1996 by Yvon Maday and Frédéric Coquel and takes place every year at CIRM in Luminy (Marseille, France) during 6 weeks. The goal of this event is to bring together scientists from both the academic and industrial communities and discuss these topics.
During the first week, a classical summer school is proposed. It consists in several lectures given by leading scientists and related to the topics of the research projects. The remaining 5 weeks are dedicated to working on the recheatch projects, after a daily morning seminar.

Cemracs'14

Cemracs'14 will be the nineteenth of the series, devoted this year to the numerical modeling of plasmas. The summer school will focus on numerical strategies for simulation of ionized flows in situation of strong coupling between hydrodynamic, magnetic waves and kinetic of the plasma. Moreover, the large disparity in space and time scales arising requires efficient multiple resolution methods (on non structured or adaptive meshes). One of the aims of the projects session be will in particular to stimulate exchanges between the FCM (*Fusion by Magnetic Confinement*) and FCI (*Fusion by Inertial Confinement*) communities.
Cemracs'14 will consist in two joint events:

- a one week summer school (July 21 - July 25)
- an intensive five weeks long research session (July 28 - August 29).

- July 21 - 25 : 1 week summer school on numerical models for fusion plasmas
- July 28 - August 29 : five weeks intensive research sessions
- To submit/join a project, contact
  - Boniface NKonga (Nice) : boniface.nkonga@unice.fr
  - Hervé Guillard (Inria Nice) : herve.guillard@inria.fr
  - Frédérique Charles (Paris 6) : charles@ann.jussieu.fr
  - me : campos@ann.jussieu.fr
  - ... or google "Cemracs 2014"