Particle-In-Cell simulations for highly oscillatory Vlasov-Poisson system

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Modeling and Numerical Methods for Hot Plasmas II
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Outline

Outline

4d Vlasov-Poisson equation – strong magnetic field

For $\varepsilon \to 0$ solve numerically in $t_f \sim 1$ and $t_f \sim 1/\varepsilon$

$$\begin{cases} \partial_t f^\varepsilon + \mathbf{v} \cdot \nabla_{\mathbf{x}} f^\varepsilon + \left(\mathbf{E}^\varepsilon + \frac{1}{\varepsilon}\mathbf{v}^\perp\right) \cdot \nabla_{\mathbf{v}} f^\varepsilon = 0, \\ \mathbf{E}^\varepsilon(\mathbf{x}, t) = -\nabla_{\mathbf{x}}\phi^\varepsilon, \quad -\Delta_{\mathbf{x}}\phi^\varepsilon = \int_{\mathbb{R}^2} f^\varepsilon d\mathbf{v} - n_i, \\ f^\varepsilon(\mathbf{x}, \mathbf{v}, t = 0) = f_0(\mathbf{x}, \mathbf{v}), \end{cases}$$

where

- $f^\varepsilon = f^\varepsilon(t, \mathbf{x}, \mathbf{v})$ particles distribution function
- Position $\mathbf{x} = (x_1, x_2)$, Velocity $\mathbf{v} = (v_1, v_2)$, and $\mathbf{v}^\perp = (-v_2, v_1)$

- **Strong** and constant magnetic field in the x_3 direction
- $\mathbf{E}^\varepsilon(\mathbf{x}, t)$ evolves in the plane $\perp$ to the magnetic field.

E. Frénod, E. Sonnendrücker, M3AS, 2000. Drift phenomenon on a long time scale due to the self-consistent electric field $\perp$ to the strong magnetic field.

4d Vlasov-Poisson equation – strong magnetic field

For $\varepsilon \to 0$ solve numerically in $t_f \sim 1$ and $t_f \sim 1/\varepsilon$

$$\begin{cases} \partial_t f^\varepsilon + \mathbf{v} \cdot \nabla_\mathbf{x} f^\varepsilon + \left(\mathbf{E}^\varepsilon + \frac{1}{\varepsilon} \mathbf{v}^\perp \right) \cdot \nabla_\mathbf{v} f^\varepsilon = 0, \\ \mathbf{E}^\varepsilon (\mathbf{x}, t) = -\nabla_\mathbf{x} \phi^\varepsilon, \quad -\Delta_\mathbf{x} \phi^\varepsilon = \int_{\mathbb{R}^2} f^\varepsilon d\mathbf{v} - n_i, \\ f^\varepsilon (\mathbf{x}, \mathbf{v}, t = 0) = f_0 (\mathbf{x}, \mathbf{v}), \end{cases}$$

Difficulties:

- nonlinear coupling
- high frequency oscillations induced by $\frac{1}{\varepsilon}$.
- $\varepsilon \sim 0$ but not uniformly.

Existing methods for similar problems

- reduce the dimensionality, by decoupling slow and fast dynamics and finding an invariant: Littlejohn (1979), Hahm (1988), Brizard (1995) etc. Frénod, Lutz (2014), Lutz (2014)
- homogenization – the two-scale limit (Frénod, Sonnendrücker 1998, 2001, 2009) : $f^\varepsilon \longrightarrow F$ when $\varepsilon \longrightarrow 0$.
  The limit solves an equation `free of oscillations`.
- micro/macro decomposition (identify the limit model + reformulation):
  – double scale reformulation of the equation
  (Crouseilles-Lemou-Méhats, 2013)

  – Two-Scale-Asymptotic-Preserving-Schemes
  (Frénod-Crouseilles-H.-Mouton, 2011)

Particle-In-Cell method

- The unknown is approximated by a collection of **macroparticles** $(\mathbf{X}_k(t), \mathbf{V}_k(t))$

$$f^{\varepsilon}_{N_p}(t,\mathbf{x},\mathbf{v}) = \sum_{k=1}^{N_p} \omega_k \, \delta(\mathbf{x} - \mathbf{X}_k(t)) \, \delta(\mathbf{y} - \mathbf{V}_k(t))$$

which move along the characteristic curve of Vlasov equation:

$$\begin{cases} \mathbf{X}'(t) = \mathbf{V}(t), \\ \mathbf{V}'(t) = \frac{1}{\varepsilon}\mathbf{V}^{\perp}(t) + \mathbf{E}^{\varepsilon}(t, \mathbf{X}(t)), \end{cases}$$

- Random initial particles.
  - deposit particles on the grid ⇒ the grid density (the RHS of Poisson equation).
  - solve Poisson equation on the grid ⇒ the grid electric field **E**.
  - interpolate **E** in each particle.
  - push particles with this field.

Highly oscillatory solutions

- When $\mathbf{E} \equiv 0$, the solution is

$$\mathbf{X}(t) = \mathbf{x}_0 + \varepsilon \mathbf{v}_0^{\perp} - \varepsilon \mathcal{R}\left(\frac{t}{\varepsilon}\right) \mathbf{v}_0^{\perp}$$
$$\mathbf{V}(t) = \mathcal{R}\left(\frac{t}{\varepsilon}\right) \mathbf{v}_0$$

where $\mathcal{R}(\tau) = \begin{pmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{pmatrix}$ and $\mathbf{x}_0 + \varepsilon \mathbf{v}_0^{\perp}$ is the guiding center.

- When the electric field $\mathbf{E}$ is not zero => **stiff** solutions (evolving on two disparate time scales)

General problem

Solve numerically **stiff** ODEs where stifness arises from the **linear** term

$$y'(t) = \frac{1}{\varepsilon} L y(t) + F(t, y(t)).$$

Aim:

- perform long-time simulation of the ODE with large time steps with respect to the oscillation.
- the numerical scheme needs to work uniformly when $\varepsilon \to 0$.
- the numerical scheme needs to be stable and accurate for any initial condition.

The solution is

$$y_{n+1} = e^{(\Delta t/\varepsilon) L} y_n + e^{(\Delta t/\varepsilon) L} \int_{t_n}^{t_{n+1}} e^{(t_n - \tau)/\varepsilon L} F(\tau, y(\tau)) \, d\tau.$$

- the stiff part is solved exactly.
- Q.: How to derive approximations to the integral term?

M. Hochbruck, A. Ostermann, *Exponential integrators*, 2010.

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Outline

Back to the PIC scheme for the Vlasov-Poisson system

$$\mathbf{X}'(t) = \mathbf{V}(t), \qquad \mathbf{X}(0) = \mathbf{x}_0$$

$$\mathbf{V}'(t) = \frac{1}{\varepsilon}\mathbf{V}^{\perp}(t) + \mathbf{E}^{\varepsilon}(t, \mathbf{X}(t)), \qquad \mathbf{V}(0) = \mathbf{v}_0$$

where $\mathbf{E}^{\varepsilon}$ is either given or computed by the Poisson equation.

The **exponential integrator** in **velocity**:

- $\mathbf{V}(t) = e^{\frac{t-s}{\varepsilon}L}\,\mathbf{V}(s) + e^{\frac{t-s}{\varepsilon}L}\int_s^t e^{\frac{s-\tau}{\varepsilon}L}\,\mathbf{E}^{\varepsilon}(\mathbf{X}(\tau), \tau)\, d\tau.$
- $\mathbf{X}(t) = \mathbf{X}(s) + \int_s^t \mathbf{V}(\tau)\, d\tau.$

where

$$L = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \text{and} \quad e^{\tau L} = \mathcal{R}(\tau)$$

The new time-stepping scheme

We want $\Delta t \gg \varepsilon$. Find the integer N and the real o s.t.

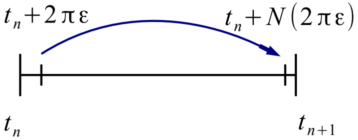
$$\Delta t = N \cdot (2\pi\varepsilon) + o$$

We approximate the integral term by

$$\int_{t_n}^{t_n + N(2\pi\varepsilon)} \mathcal{R}\left(\frac{t_n - \tau}{\varepsilon}\right) \mathbf{E}^{\varepsilon}\left(\mathbf{X}\left(\tau\right), \tau\right) d\tau \simeq N \cdot \int_{t_n}^{t_n + 2\pi\varepsilon} \ldots d\tau$$

Assumption: $\tau \longrightarrow \mathbf{E}^{\varepsilon}\left(\mathbf{X}\left(\tau\right), \tau\right) \simeq 2\pi\varepsilon$-periodic.

$$\begin{pmatrix} \mathbf{X}(t_n + N \cdot 2\pi\varepsilon) \\ \mathbf{V}(t_n + N \cdot 2\pi\varepsilon) \end{pmatrix} = \begin{pmatrix} \mathbf{X}_n \\ \mathbf{V}_n \end{pmatrix} + N \begin{pmatrix} \mathbf{X}(t_n + 2\pi\varepsilon) - \mathbf{X}_n \\ \mathbf{V}(t_n + 2\pi\varepsilon) - \mathbf{V}_n \end{pmatrix}.$$

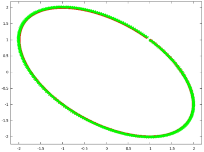


First test-case: 4d linear Vlasov equation

Verification in a linear case:

$$\mathbf{E}^{\varepsilon}(\mathbf{x}, t) = \begin{pmatrix} 2x_1 + x_2 \\ x_1 + 2x_2 \end{pmatrix}$$

- identify the **slow motion** $\sim \sin(\sqrt{3}\varepsilon\, t)$ and **fast motion** $\sim \cos(t/\varepsilon)$



$\varepsilon = 0.01$, $(1,1,1,1)$ initial condition **far** from the slow manifold, final time $t = 360$.

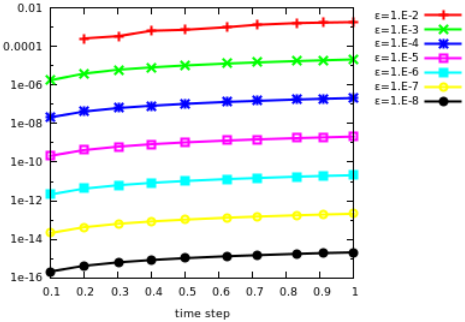
- tests with initial conditions close to/far from the slow manifold (that particular solution (or i.c.) for which the fast oscillations dissappear.)
- **global errors** at short time ($t = 10$) and long time ($t = 1/\varepsilon$)

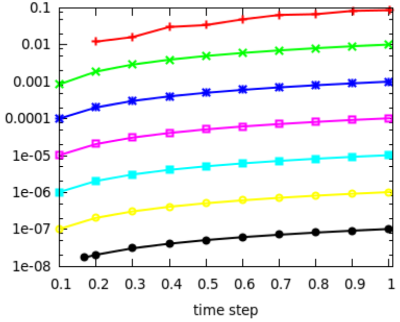
4d linear Vlasov equation: global errors

	Δt =1E-1	Δt =2E-1	Δt =5E-1	Δt =8E-1	Δt =1
ε=1.E-2	1	3	7	12	15
ε=1.E-4	159	318	795	1 273	1 591
ε=1.E-6	15 915	31 830	79 577	127 323	159 154

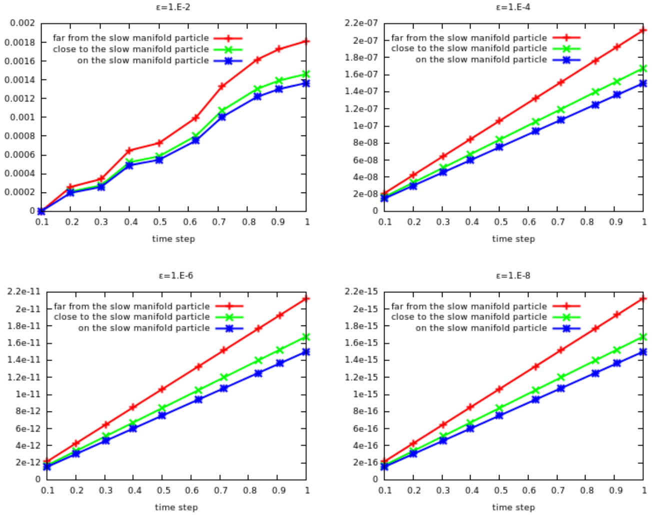
Table: The whole number of rapid full tours enclosed in a time step of the scheme

uniformly accurate when ε vanishes





Global errors at final time 10: $\varepsilon = 10^{-2},\ 10^{-4},\ 10^{-6},\ 10^{-8}$



- the same order of error for different initial conditions.
- similar behaviour at long times ($\sim 1/\varepsilon$).

Second test-case: the Vlasov-Poisson system

1. Compare in **short** time ($t \sim 1$)

$$\partial_t f^\varepsilon + \mathbf{v} \cdot \nabla_\mathbf{x} f^\varepsilon + \left(\mathcal{E}^\varepsilon + \frac{1}{\varepsilon} \mathbf{v}^\perp \right) \cdot \nabla_\mathbf{v} f^\varepsilon = 0 \quad + \text{Poisson}$$

and the reduced model

$$\partial_t f_{GC} + \varepsilon \mathbf{E}^\perp \cdot \nabla_\mathbf{x} f_{GC} = 0 \quad + \text{Poisson.}$$

2. Compare in **long** time ($t \sim 1$)

$$\partial_t g^\varepsilon + \frac{1}{\varepsilon} \left(\mathbf{v} \cdot \nabla_\mathbf{x} g^\varepsilon + \left(\mathcal{E}^\varepsilon + \frac{1}{\varepsilon} \mathbf{v}^\perp \right) \cdot \nabla_\mathbf{v} g^\varepsilon \right) = 0 \quad + \text{Poisson}$$

and the limit model

$$\partial_t g_{GC} + \mathbf{E}^\perp \cdot \nabla_\mathbf{x} g_{GC} = 0 \quad + \text{Poisson.}$$

Vlasov-Poisson: long and short time equations

1. **Long** time ($\sim 1/\varepsilon$) accuracy against the Guiding Center model

$$g^{\varepsilon}(\mathbf{x},\mathbf{v},t) = f^{\varepsilon}(\mathbf{x},\mathbf{v},\frac{t}{\varepsilon}) \Rightarrow \begin{cases} \partial_t g^{\varepsilon} + \frac{1}{\varepsilon}\Big(\mathbf{v}\cdot\nabla_{\mathbf{x}} g^{\varepsilon} + \Big(\mathcal{E}^{\varepsilon} + \frac{1}{\varepsilon}\mathbf{v}^{\perp}\Big)\cdot\nabla_{\mathbf{v}} g^{\varepsilon}\Big) = 0 \\ + \text{ Poisson} \end{cases}$$

When $\varepsilon \to 0$ then $\int g^{\varepsilon} d\mathbf{v} \to g_{GC}$ where

$$\partial_t g_{GC} + \mathbf{E}^{\perp}\cdot\nabla_{\mathbf{x}} g_{GC} = 0 \quad + \text{ Poisson.}$$

(Golse–Saint-Raymond 1999; Frénod–Sonnendrücker 2000, Bostan 2010)

2. **Short** time (~ 1) accuracy against the short time Guiding Center model

$$f^{\varepsilon}_{GC}(\mathbf{x},t) = g_{GC}(\mathbf{x},\varepsilon t) \Rightarrow \begin{cases} \partial_t f^{\varepsilon}_{GC} + \varepsilon \mathbf{E}^{\perp}_{\varepsilon}\cdot\nabla_{\mathbf{x}} f^{\varepsilon}_{GC} = 0 \\ + \text{ Poisson} \end{cases}$$

Vlasov-Poisson: short and long time simulations

1. **Short** test case: Landau damping (periodic boundary condition on $[0, 4\pi] \times [0, 1]$)

$$f_0\,(\mathbf{x}, \mathbf{v}) = \frac{1}{2\pi}\Big(1 + 0.1\ \cos\,(x_1/2)\Big)\ \exp\left(-\frac{v_1^2 + v_2^2}{2}\right).$$

2. **Long** test case: Kelvin-Helmholtz (periodic boundary condition on $[0, 4\pi] \times [0, 2\pi]$)

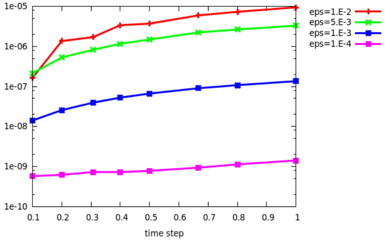
$$f_0(\mathbf{x}, \mathbf{v}) = \frac{1}{2\pi\, T_1\, T_2}\Big(\sin(x_2) + 0.05\ \cos(x_1/2)\Big)\ \exp\left(-\frac{v_1^2 + v_2^2}{2}\right).$$

Global errors in time of the $L_2([0, T_1] \times [0, T_2])$ norm of the densities

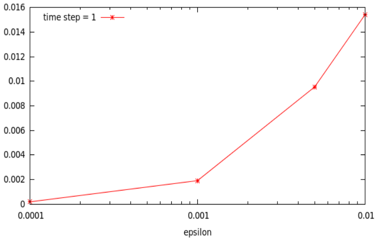
4d VP: Global errors at time = 4

Short time simulations: comparisons with

a reference solution ($\Delta t = 2\pi\varepsilon/100$)



the (short time) Guiding Center model

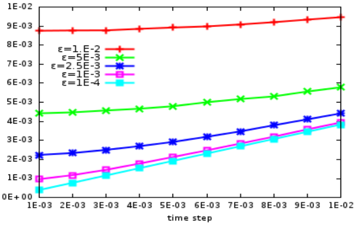


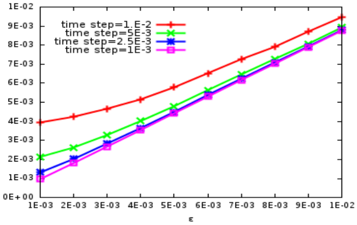
	Δt =1E-1	Δt =2E-1	Δt =5E-1	Δt =8E-1	Δt =1
ε=1.E-2	1	3	7	12	15
ε=1.E-3	15	31	79	127	159
ε=1.E-4	159	318	795	1273	1591

Table: The whole number of rapid full tours enclosed in a time step of the scheme

4d VP: Global errors at time = 5

Long time simulations : Kelvin-Helmholtz instability





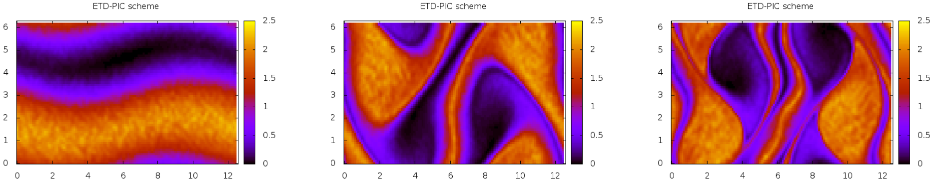
Asymptotic Preserving behaviour with respect to the Guiding Center model

	Δt=1E-3	Δt=3E-3	Δt=5E-3	Δt= 7E-3	Δt=1E-2
$\varepsilon =$5.E-3	6	19	31	44	63
$\varepsilon =$2.5E-3	25	76	127	178	254
$\varepsilon =$1.E-3	159	477	795	1 114	1 591
$\varepsilon =$1.E-4	15 915	47 746	79 577	111 408	159 154

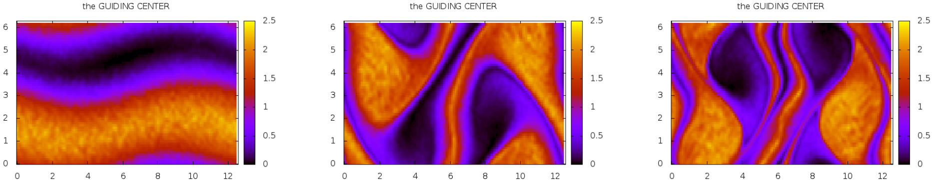
Table: The whole number of rapid full tours enclosed in a time step of the scheme

ε-Vlasov-Poisson solution vs. Guiding Center solution

$\Delta t = 0.01$, $\varepsilon = 0.005$ $(N = 63)$ the scheme $\uparrow$ Guiding Center $\downarrow$ densities



$t_f = 5$ 15 20



Outline

Aim

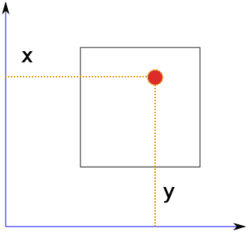
1. Compare the time scheme to a reference solution of the oscillatory Vlasov-Poisson system in long time.
2. **Additional aim**: Show numerically the convergence result (Vlasov-Poisson vs. guiding center simulations)

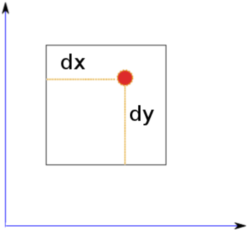
- high computational cost for the reference solution (classical time schemes)
  Difficulties:
  - we address noise by using a large number of particles.
  - conventional PIC suffers from often data motion (memory/CPU).
- need to optimize the PIC implementation
  K. J. Bowers: J. Comput. Phys. (2001).
  D. Tskhakaya, R. Schneider: J. Comput. Phys. (2007).

Implementation in SeLaLib (the Semi Lagrangian Library),
`http://selalib.gforge.inria.fr/`

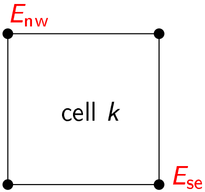
Main ingredients (1/2)

Data structures: data used together should be stored together






```
type :: sll_particle_2d
   sll_int32  :: ic
   sll_real32 :: dx
   sll_real32 :: dy
   sll_real64 :: vx
   sll_real64 :: vy
   sll_real32 :: q
end type sll_particle_2d
```



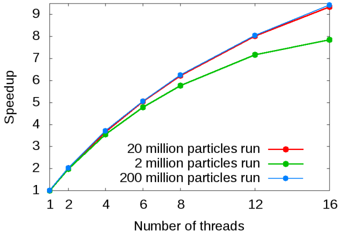

```
type charge_accumulator_cell_2d
   sll_real64 :: q_sw
   sll_real64 :: q_se
   sll_real64 :: q_nw
   sll_real64 :: q_ne
end type charge_accumulator_cell_2d
```

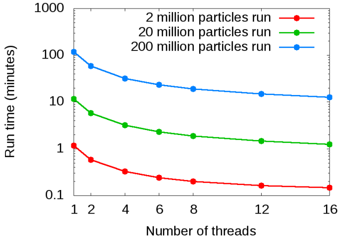
Main ingredients (2/2)

1. Cell index + local offset for particle representation:
   - reduced memory size
   - reduces the nb of arithmetical operations during the interpolation and the charge deposition
2. Cell-based $\mathbf{E}$ and ρ:
   - allows to advance particles with a minimum of accessed memory streams.
   - additional steps to convert to/from grid arrays: $\mathbf{E}_{i,j} \longrightarrow \mathbf{E}_{accum}(k)$ and $\rho_{accum}(k) \longrightarrow \rho_{i,j}$ (the cost is $\sim$ to $N_{\mathbf{cells}}$)
3. Particle sorting (to be done periodically):
   - maximize sequential particle processing
4. Parallelization: multiprocess (MPI) + multithread (OpenMP)

Performance: speedup

Landau damping test-case 1000 iterations, a grid of 512 x 16 cells.
Verification: conservation of the total energy, electric field energy.

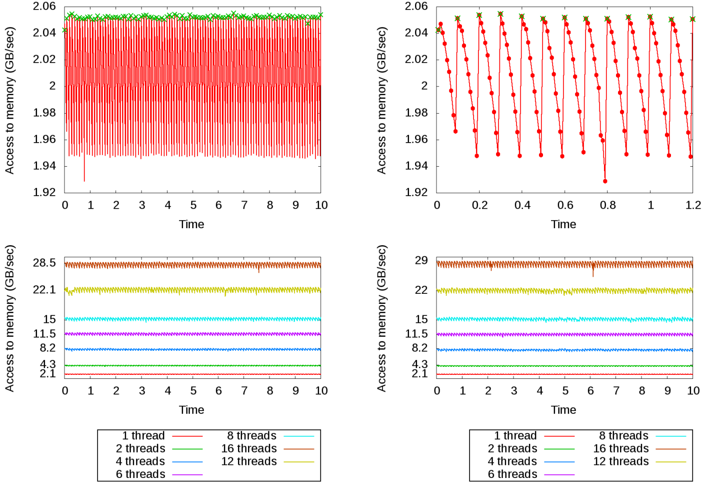




Threads	Time (seconds)	Speedup
1	703.2	1.0
2	348.2	2.02
4	191.5	3.67
6	139.2	5.05
8	112.9	6.23
12	87.7	8.02
16	75.3	9.34

Performance: memory bandwidth

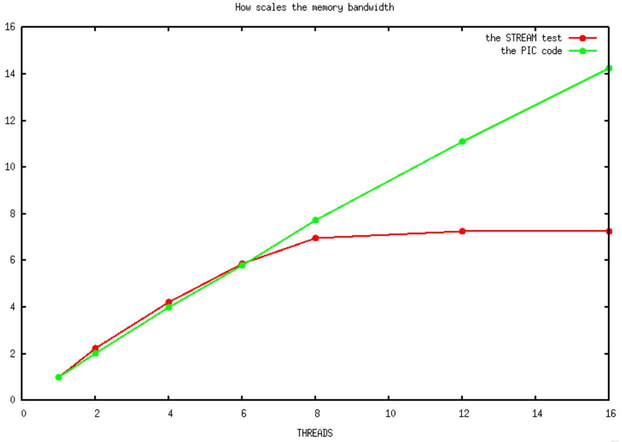
N (nb of loads/stores) $*$ 32B/time of particle push



2 million (left) and 20 million (right) particles runs.

Performance: MB Stream benchmark

The `stream` test : 10 GB/s on single core and 75 GB/s /16 threads.
Use of 2 processes and several threads.
20 million particles run.



Performance

Million of particles processed per second : $N_p * N_{iter}/T$.

Simulation\Threads	1	2	4	8	16
2 million particles	28.5	56.8	101.7	165.2	224.3
20 million particles	28.4	57.4	104.4	177.1	265.6
200 million particles	28.0	56.9	103.5	174.4	263.8

Vlasov-Poisson/guiding center model

Long time (~ 1) simulations of

$$\begin{cases} \partial_t g^\varepsilon + \frac{1}{\varepsilon}\left(\mathbf{v}\cdot\nabla_\mathbf{x} g^\varepsilon + \left(\mathcal{E}^\varepsilon + \frac{1}{\varepsilon}\mathbf{v}^\perp\right)\cdot\nabla_\mathbf{v} g^\varepsilon\right) = 0 \\ + \text{Poisson} \end{cases}$$

and the limit model

$$\partial_t g_{GC} + \mathbf{E}^\perp \cdot \nabla_\mathbf{x} g_{GC} = 0 \quad + \text{Poisson}.$$

Kelvin-Helmholtz instability: periodic-periodic boundary conditions on $[0,4\pi]\times[0,2\pi]$, Poisson (solved by FFT). Random initialization of

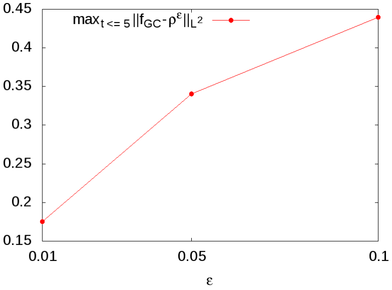
$$f_0(\mathbf{x},\mathbf{v}) = \frac{1}{2\pi}\Big(\sin(x_2) + 0.05\,\cos(x_1/2)\Big)\exp\left(-\frac{v_1^2+v_2^2}{2}\right).$$

Numerical results

10 million particles, 256×128 cells.

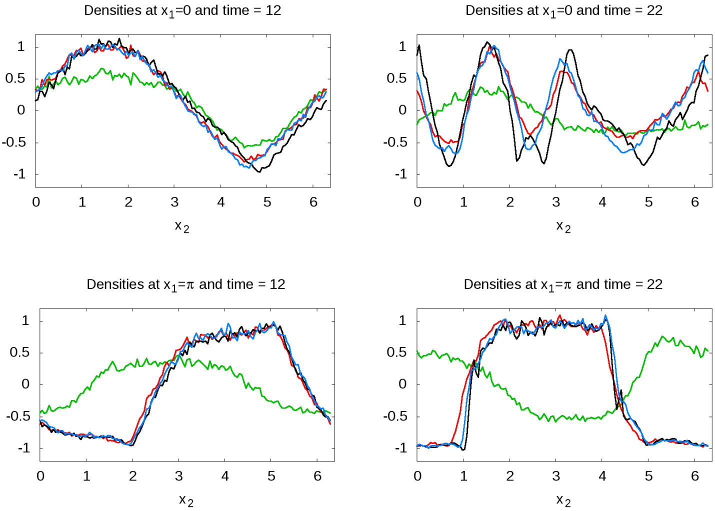
- for VP: Reference solution with leap-frog, $\delta t = 2\pi\varepsilon^2/80$
- for GC: RK2 with $\Delta t = 0.01$.

Global error at time $t = 5$: $||g_{GC} - \rho^\varepsilon||_{L^2}$



Numerical results

guiding center, VP with $\varepsilon = 0.05$, VP with $\varepsilon = 0.1$, VP with $\varepsilon = 0.5$



Conclusion and Outlook

- E. Frénod, S.H., M. Lutz, E. Sonnendrücker, CiCP, 2015.
- E. Chacon-Golcher, S. H., M. Lutz, preprint HAL.

Short and long time simulation for oscillatory 4d Vlasov-Poisson:

- allows large time steps with respect to the rapid period.
- produce accurate numerical solutions for different small values of ε with the same computational cost.
- achieve high efficiency in PIC simulation with many particles.
- compute reference solution for oscillatory VP with accuracy.

- compare the time scheme to a reference solution in long time.
- consider slowly varying magnetic field B.
- improve the algorithm
- towards the 6d model

THANK YOU !