Dynamical adaptive tensor method for the Vlasov-Poisson system

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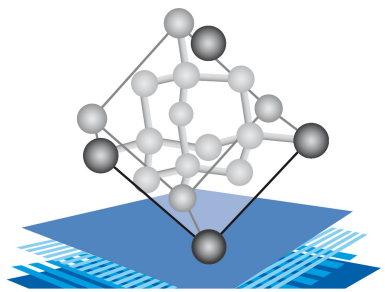

MATHerials

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Motivation: kinetic equations

[Dolbeault,2002]

The purpose of kinetic equations is the description of dilute particle gases at an intermediate scale between the microscopic scale and the hydrodynamical scale.

Dilute gases: system with a large number of particles, for which a description of the position and of the velocity of each particle is irrelevant, but for which the decription cannot be reduced to the computation of an average velocity at any time $t \in \mathbb{R}_+$ and any position $x \in \mathbb{R}^3$.

One wants to take into account more than one possible velocity at each point, and the description has therefore to be done at the level of the phase space (at a statistical level) by a distribution function

$$f(t,x,v) \qquad t \in \mathbb{R}_+, \quad x \in \mathbb{R}^3, \quad v \in \mathbb{R}^3$$

Normalization condition:

$$\int_{x\in\mathbb{R}^3} \int_{v\in\mathbb{R}^3} f(t,x,v)\, dv\, dx = 1.$$

Particle density:

$$\rho(t,x) = \int_{v\in\mathbb{R}^3} f(t,x,v)\, dv.$$

Transport equation

Since f describes the statistical evolution of the system of particles, f has to be constant along the characteristics $(X(t), V(t))$ in the phase space given by Newtonâs law:

$$\frac{dX}{dt} = V, \quad \frac{dV}{dt} = F(t, X(t))$$

where $F(t, X(t))$ is the force acting on a particle located at position $X(t)$ at time t.
If F derives from a potential $U(t, x)$, we have $F(t, x) = -\nabla_x U(t, x)$.

$$0 = \frac{d}{dt}\left(f(t, X(t), V(t))\right) = \partial_t f + V(t) \cdot \nabla_x f + F(t, X(t)) \cdot \nabla_v f.$$

Therefore, f has to satisfy the so-called transport equation

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

Vlasov-Poisson system

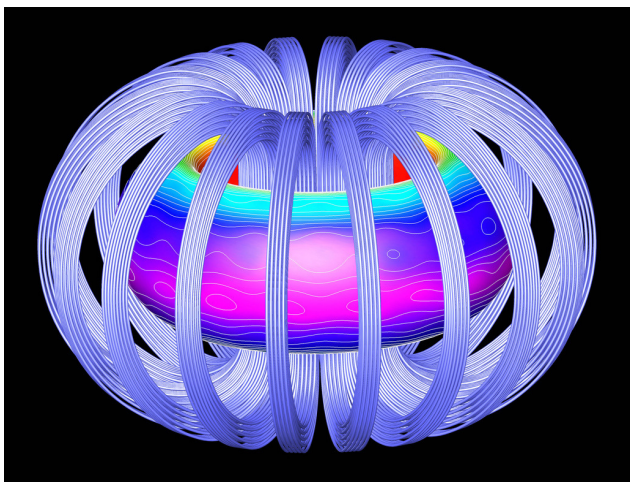
Mean-field approximation for electrically charged particles (electrons here):

Vlasov-Poisson (VP) system

$$\begin{cases} f(0,x,v) = f_0(x,v), \\ \partial_t f + v \cdot \nabla_x f + F(t,x) \cdot \nabla_v f = 0, \\ F(t,x) = -\nabla_x U(t,x), \\ \\ \Delta_x U(t,x) = 1 - \rho(t,x). \end{cases}$$

Applications:

- Plasma physics;
- Electron transport in semiconductors.



Vlasov-Poisson system

Time-dependent system of equations in $\mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3$:

$$\begin{cases} f(0,x,v) = f_0(x,v), \\ \partial_t f + v \cdot \nabla_x f + F(t,x) \cdot \nabla_v f = 0, \\ \Delta_x U(t,x) = 1 - \rho(t,x), \\ F(t,x) = -\nabla_x U(t,x). \end{cases} \tag{1}$$

[Lions, Perthame,1991]

Theorem

If $f_0 \in L^1(\mathbb{R}^3 \times \mathbb{R}^3) \times L^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ *satisfies the following condition*

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} |v|^m f_0(x,v)\, dx\, dv < +\infty \quad \text{for some } m > 3,$$

then, there exists a global strong non-negative solution f *to (1) so that*

$$f \in \mathcal{C}(\mathbb{R}_+; L^1(\mathbb{R}^3 \times \mathbb{R}^3)) \cap L^\infty(\mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3).$$

Classical numerical methods

Classical numerical methods:

- Stochastic particle methods (Particle In Cell): subject to statistical noise; [Birdsall, 1991], [Brackbill, 2016], [Cazeaux,Hesthaven,2014]
- Semi-lagrangian methods: used for 1D-1D and 2D-2D simulations, few 3D-3D calculations Crouseilles, Després, Faou, Sonnendrücker... ;
- Full eulerian methods: idem. [Filbet, Sonnendrücker, 2003]

What about tensor methods? [Kormann,2015] Tensor train format for semi-lagrangian method.

We wish to design a method which

- is based on a full eulerian method;
- allows for arbitrary spatial (or eventually velocity) domain geometries.

Let $\Omega_x, \Omega_v \subset \mathbb{R}^3$ and consider the resolution of (1) on $\Omega_x \times \Omega_v$ with appropriate boundary conditions (typically periodic or Dirichlet).

Tensor notation

For any functions $r : \Omega_x \to \mathbb{R}$ and $s : \Omega_v \to \mathbb{R}$, we use the notation

$$r \otimes s : \begin{cases} \Omega_x \times \Omega_v & \to & \mathbb{R} \\ (x, v) & \mapsto & r(x)s(v). \end{cases}$$

For any linear operator A (respectively B) acting on real-valued functions defined on Ω_x (respectively Ω_v), $A \otimes B$ is the linear operator acting on real-valued functions defined on $\Omega_x \times \Omega_v$ so that

$$(A \otimes B)(r \otimes s) = (Ar) \otimes (Bs), \quad \text{for all } r : \Omega_x \to \mathbb{R}, \quad s : \Omega_v \to \mathbb{R}.$$

Principle of the method

It is natural to think about tensor methods since

$$\partial_t f + \left(\sum_{i=1}^{3} \partial_{x_i} \otimes v_i + \sum_{i=1}^{3} F_i(x,t) \otimes \partial_{v_i} \right) f = 0.$$

Assume that

$$f_0(x,v) = \sum_{k=1}^{n_0} r_k^0(x) s_k^0(v) = \sum_{k=1}^{n_0} r_k^0 \otimes s_k^0(x,v).$$

Goal: find an approximation of $f(t,x,v)$ under a separated form

$$f(t,x,v) \approx \sum_{k=1}^{n_t} r_k(x,t) s_k(v,t),$$

using only 3D (and not 6D) linear problems.

Main tool: modified version of the POD/PGD method.

Hamiltonian structure of the Vlasov-Poisson system

Hamiltonian:

$$\mathcal{H} = \int_{x\in\Omega_x}\int_{v\in\Omega_v} \frac{1}{2}|v|^2 f(t,x,v)\,dxdv + \int_{x\in\Omega_x} \rho(t,x)U(t,x)\,dx.$$

Let us introduce the *reduced Poisson bracket* :

$$\{a,b\} := \nabla_x a\cdot\nabla_v b - \nabla_v a\cdot\nabla_x b.$$

As highlighted in t, the Vlasov-Poisson system can be rewritten as

$$\partial_t f = -\{f,h\},$$

where $h := \frac{1}{2}|v|^2 + U$ is the reduced hamiltonian.

Symplectic time-discretization scheme

Introduce a time step $\Delta t > 0$, and $t_m := m\Delta t$ for all $m \in \mathbb{N}^*$. For all $m \in \mathbb{N}^*$,

$$f^{(m)}(x, v) \approx f(t_m, x, v).$$

3-step symplectic scheme which respects the tensor structure of the equations:

$$\begin{cases} \left(I + \frac{\Delta t}{2} F^{(m)}(x) \cdot \nabla_v\right) f^{(m+1/3)} & = \left(I - \frac{\Delta t}{2} v \cdot \nabla_x\right) f^{(m)}, \\ \left(I + \frac{\Delta t}{2} v \cdot \nabla_x\right) f^{(m+2/3)} & = f^{(m+1/3)}, \\ f^{(m+1)} & = \left(I - \frac{\Delta t}{2} F^{(m+2/3)}(x) \cdot \nabla_v\right) f^{(m+2/3)}, \end{cases}$$

Fully discretized setting

Suppose that x-dependent (respectively v-dependent) functions are discretized using N_x (respectively N_v) degrees of freedom.

Fully discretized scheme:

$$\begin{cases} \left(I + \frac{\Delta t}{2} \sum_{i=1}^{3} F_{i,x}^{m} \otimes D_{i,v}\right) f^{(m+1/3)} & = \left(I - \frac{\Delta t}{2} \sum_{i=1}^{3} V_{i,v} \otimes D_{i,x}\right) f^{(m)}, \\ \left(I + \frac{\Delta t}{2} \sum_{i=1}^{3} V_{i} \otimes D_{i,x}\right) f^{(m+2/3)} & = I\, f^{(m+1/3)}, \\ I\, f^{(m+1)} & = \left(I - \frac{\Delta t}{2} \sum_{i=1}^{3} F_{i,x}^{m+2/3} \cdot \nabla_v\right) f^{(m+2/3)}, \end{cases}$$

where

$$I = I_x \otimes I_v \text{ is the mass matrix}$$

and $F_{i,x}^{m}, F_{i,x}^{m+2/3}, D_{i,x}, I_x \in \mathbb{R}^{N_x \times N_x}$ and $D_{i,v}, V_{i,v}, I_v \in \mathbb{R}^{N_v \times N_v}$, and $f^{(m)}, f^{(m+1/3)}, f^{(m+2/3)}, f^{(m+1)} \in \mathbb{R}^{N_x \times N_v}$.

Elementary step of the scheme

Each elementary step of this time-discretization scheme can be rewritten in the following form: for all $i \in \mathbb{N}^*$,

$$(I + \Delta t P)\, f^{(\frac{i+1}{3})} = (I + \Delta t Q)\, f^{(\frac{i}{3})}, \tag{2}$$

for some operators P and Q that can be written as the sum of at most 3 tensorized operators.

Thus, denoting by $\delta f := f^{(\frac{i+1}{3})} - f^{(\frac{i}{3})}$, (2) boils down to solving

$$(I + \Delta t P)\, \delta f = g, \tag{3}$$

where g is a sum of tensorized functions.

Full fixed-point iteration algorithm for (3): Start from an initial guess δf^0. For all $j \in \mathbb{N}^*$, compute

$$I\, \delta f^j = g - \Delta t P \delta f^{j-1}.$$

It would converge if $\|\Delta t P\| < 1$. This is not true in general in infinite dimension but can be obtained in a discretized setting up to choosing Δt sufficiently small.
However, this would lead to a decomposition of δf with a potentially very high number of tensorized functions...

Fixed-point POD/PGD

Let

- H_x and H_v be two Hilbert spaces;
- $I = I_x \otimes I_v$ where I_x (respectively I_v) is a bounded self-adjoint coercive operator on H_x (respectively on H_v);
- $P = \sum_{q=1}^{N} P_x^q \otimes P_v^q$ where $P_x^q \in \mathcal{L}(H_x)$ and $P_v^q \in \mathcal{L}(H_v)$;
- $g \in H_x \otimes H_v$.

Consider the following algorithm for the resolution of $(I + \Delta t P)\delta f = g$.

1. Start from the initial guess $\delta f^0 = 0$.
2. For all $n \in \mathbb{N}^*$, compute $(r_n, s_n) \in H_x \times H_v$ so that

$$(r_n, s_n) \in \underset{(r,s)\in H_x\times H_v}{\operatorname{argmin}} \|g - \Delta t P \delta f^{n-1} - I\, r \otimes s\|_{H_x\otimes H_v}. \tag{4}$$

3. Define $\delta f^n := \delta f^{n-1} + r_n \otimes s_n$.
4. Set $n := n + 1$ and go back to step 2.

Fixed-point POD/PGD

Extending results of [Cancès, E., Lelièvre,2013]

Proposition (E., Lombardi, 2016)

Let $\kappa := \max_{1 \leq q \leq N} \| I_x^{-1} P_x^q \otimes I_v^{-1} P_v^q \|$. *Then, the fixed-point POD/PGD algorithm converges provided that the following condition holds*

$$3 \Delta t N \kappa < 1. \tag{5}$$

Note that (5) is independent on the dimension of the spaces H_x and H_v.

In practice, problems of the form (4) are solved using a standard ALS procedure.

Back to the Vlasov-Poisson context

Instead, we use the following algorithm for the resolution of (3) in the fully discretized setting.
Let $\eta > 0$ be an error threshold.

1. Start from the initial guess $\delta f^0 = 0$.
2. For all $n \in \mathbb{N}^*$, compute $(r_n, s_n) \in \mathbb{R}^{N_x} \times \mathbb{R}^{N_v}$ so that

$$(r_n, s_n) \in \underset{(r,s)\in\mathbb{R}^{N_x}\times\mathbb{R}^{N_v}}{\operatorname{argmin}} \|g - \Delta t P \delta f^{n-1} - I\, r \otimes s\|_{\mathbb{R}^{N_x}\otimes\mathbb{R}^{N_v}}. \qquad (6)$$

3. Define $\delta f^n := \delta f^{n-1} + r_n \otimes s_n$.
4. If $\|r_n \otimes s_n\| < \eta$, then stop. Otherwise, $n := n + 1$ and go back to step 2.

Let $n_{\delta f}$ be the final value of n so that at the end of the algorithm

$$\delta f^{n_{\delta f}} = \sum_{k=1}^{n_{\delta f}} r_k \otimes s_k.$$

In practice, $n_{\delta f}$ is much lower than the rank which would have been obtained using a full fixed-point algorithm.

Recompression step

Assume that $f^{(\frac{i}{3})}$ was known under a separated form

$$f^{(\frac{i}{3})} = \sum_{k=1}^{n_{\frac{i}{3}}} \widetilde{r}_k \otimes \widetilde{s}_k.$$

Then, we have obtained an approximated representation of $f^{(\frac{i+1}{3})}$ with rank $n_{\frac{i}{3}} + n_{\delta f}$ given by

$$\overline{f}^{(\frac{i+1}{3})} = \sum_{k=1}^{n_{\frac{i}{3}}} \widetilde{r}_k \otimes \widetilde{s}_k + \sum_{k=1}^{n_{\delta f}} r_k \otimes s_k.$$

The final approximation of $\overline{f}^{(\frac{i+1}{3})}$ is given by

$$POD\left(\overline{f}^{(\frac{i+1}{3})}, \eta\right)$$

which amounts to computing:

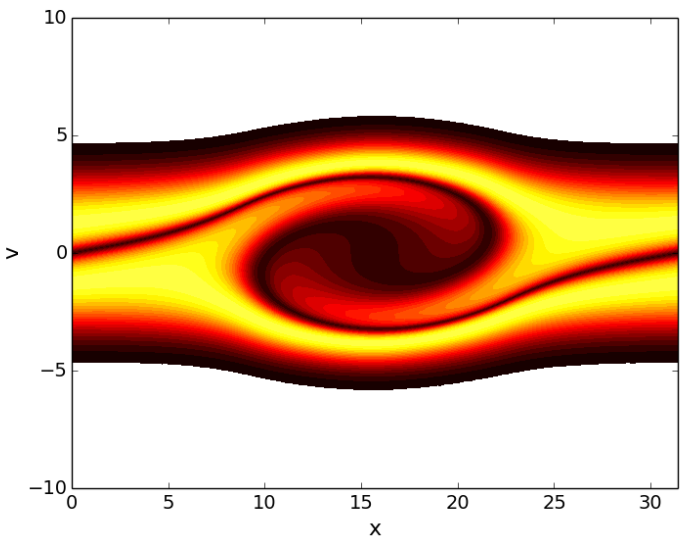
- the QR decomosition of two matrices, respectively of size $(n_{\frac{i}{3}} + n_{\delta f}) \times N_x$ and $(n_{\frac{i}{3}} + n_{\delta f}) \times N_v$;
- the SVD of a matrix of size $(n_{\frac{i}{3}} + n_{\delta f}) \times (n_{\frac{i}{3}} + n_{\delta f})$.

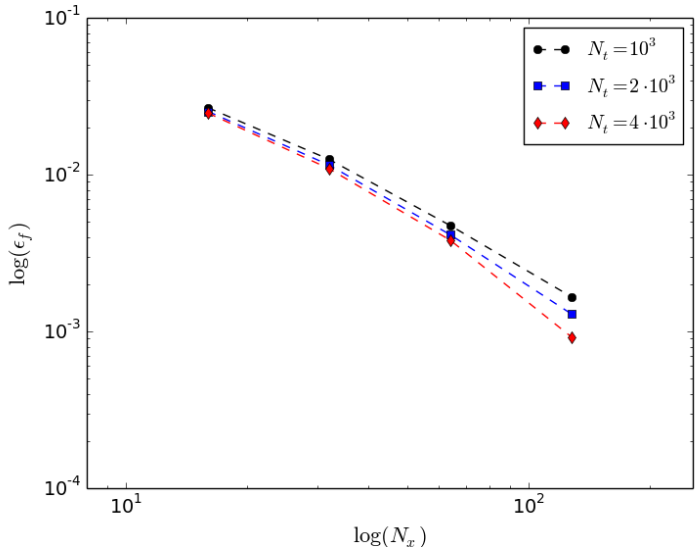
Good news

Two-stream instability test case.

1D-1D test case:

$$f_0(x,v) = (1+\beta\cos(kx))\left(\frac{1}{\sqrt{4\pi}}e^{-(v-v_0))2/2} + \frac{1}{\sqrt{4\pi}}e^{-(v+v_0))2/2}\right)$$

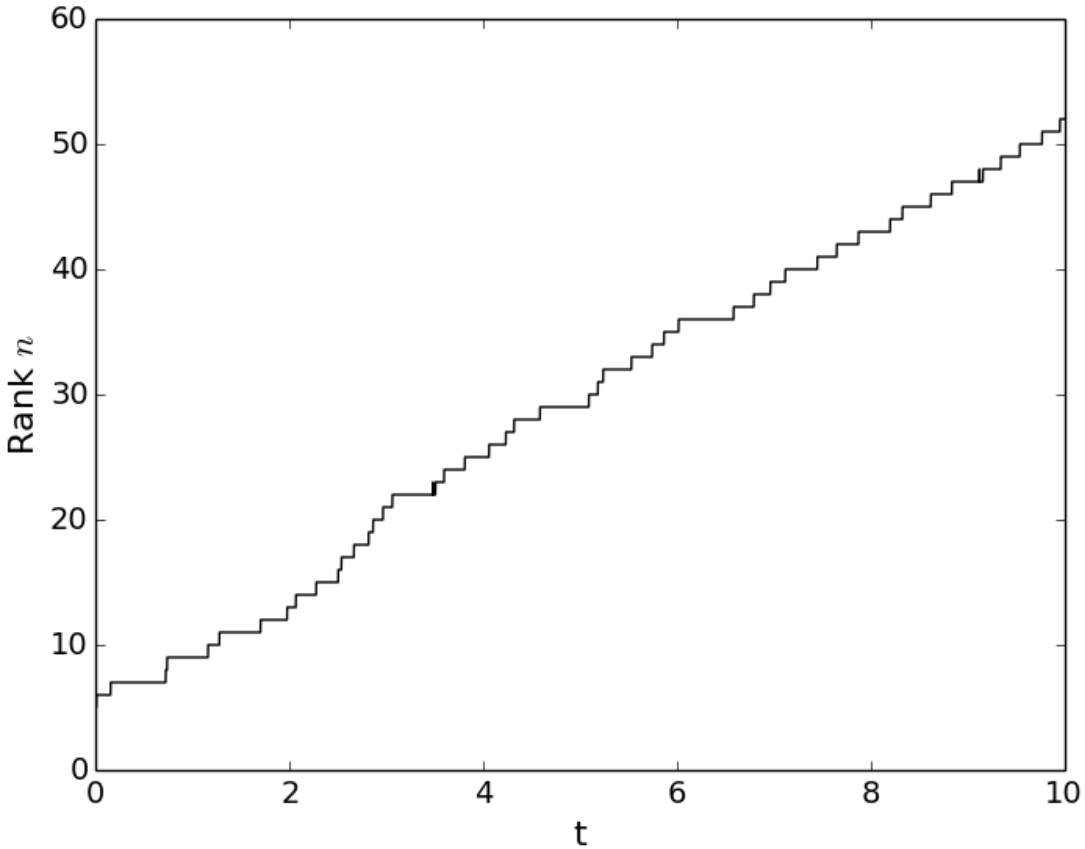




3D-3D test case

Bad news

Evolution of the ranks



Summary and perspectives

- Numerical tensor method which adaptively adapts the rank of the decomposition during time evolution for the Vlasov-Poisson system (fully eulerian method).
- Encouraging preliminary numerical results, even in 3D-3D.
- Numerical observation: the rank of the solution seems to increase linearly with time... which are not good news a priori for long time simulations!
- Parallelize and speed up the method: ongoing work on a domain decomposition method (joint work with Damiano Lombardi and Athmane Bakhta). Different separated representations of the solution on each subdomain automatically leads to a decrease of the rank.
- Rigorous error analysis of the method. “Cleaner” control of the approximation parameter η.
- Apply the algorithm to other types of kinetic equations (Vlasov-Maxwell, Boltzmann).

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