THEMATIC SEMESTER

Interacting particles, PDEs and applications

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https://indico.math.cnrs.fr/category/816

Particle Dynamics and PDEs: Connections and Applications

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Outline

A Gallery of Models

A Gallery of Models

Kinetic theory describes system using distribution function $f(t,x,v)$ with position $x \in \mathbb{R}^n$, velocity $v \in \mathbb{R}^n$, $n = 1, 2$ or 3 where

$$f(t,x,v)\,dx\,dv \;=\; \text{number of particles in phase-space volume}\,dx\,dv.$$

It is solution to the following transport equation

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

Often, we have $\nabla_v \cdot F = 0$, so that,

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

We define density, momentum and kinetic energy as

$$\begin{pmatrix} \rho(t,x) \\ \rho\,u(t,x) \\ e(t,x) \end{pmatrix} \;=\; \int_{\mathbb{R}^n} \begin{pmatrix} 1 \\ v \\ \dfrac{|v|^2}{2} \end{pmatrix} f(t,x,v)\,dv.$$

The Vlasov-Poisson Model

Electrostatic interaction

Consider the force on a particle of charge q:

$$F(t,x) = q\,E = -q\,\nabla_x \phi,$$

where ϕ solves the Poisson equation

This yields the Vlasov-Poisson system,

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \dfrac{q}{m} \nabla_x \phi \cdot \nabla_v f = 0, \\ -\Delta \phi = \dfrac{q}{\epsilon_0}\, \rho_f, \end{cases}$$

with

$$\rho_f(t,x) = \int_{\mathbb{R}^n} f(t,x,v)\, dv.$$

The Vlasov-Poisson Model

- Positivity : $f^{in} \geq 0$ implies that $f(t) \geq 0$, for all $t \geq 0$.
- Preservation of L^p norms for $1 \leq p \leq \infty$ since

$$\nabla_{(x,v)} \cdot (v, E(t,x)) \;=\; 0$$

we have

$$\|f(t)\|_{L^p} \;=\; \|f^{in}\|_{L^p}, \qquad \forall\, t \geq 0.$$

- Preservation of energy : for all $t \geq 0$.,

$$\mathcal{E}(t) := \frac{m}{2} \int_{\mathbb{T}^d \times \mathbb{R}^d} |v|^2 f(t,x,v)\, dv\, dx + \frac{\epsilon_0}{2} \int_{\mathbb{T}^d} |\nabla_x \phi(t,x)|^2 dx.$$

- Velocity moment estimates

$$m_p(t) = \int_{\mathbb{T}^d \times \mathbb{R}^d} |v|^p f(t,x,v)\, dx\, dv.$$

Landau damping

Vlasov-Poisson in the torus

Consider

$$\begin{cases} \partial_t f + v\,\partial_x f + \partial_x \phi\,\partial_v f = 0, \quad (x,v) \in \mathbb{T} \times \mathbb{R}, \\ -\partial_{xx}\phi = \rho_f - 1, \quad x \in \mathbb{T}, \end{cases}$$

Consider f_{eq} a space homogeneous equlibrium

$$f_{eq}(v) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{v^2}{2}\right)$$

and the initial datum

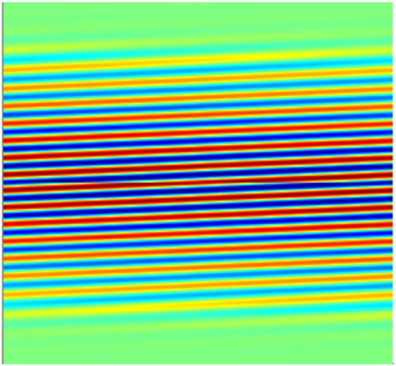
$$f_0(x,v) = (1 + \alpha \cos(kx))\, f_{eq}(v) \quad (x,v) \in \mathbb{T} \times \mathbb{R},$$

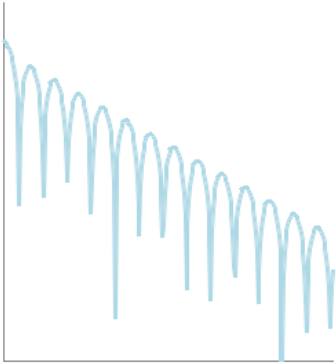
with $k = 0.5$. We study the time evolution of the potential energy

$$\mathcal{E}_{pot}(t) = \frac{1}{2} \int_{\mathbb{T}} |\partial_x \phi|^2 \, dx$$

Landau damping

Time evolution of the distribution function $f - f_{eq}$ in phase space (x, v) and the potential energy $\mathcal{E}_{pot}$.





Two stream instability

Vlasov-Poisson in the torus

Consider

$$\begin{cases} \partial_t f + v\,\partial_x f + \partial_x \phi\,\partial_v f = 0, & (x,v) \in \mathbb{T}\times\mathbb{R}, \\ -\partial_{xx}\phi = \rho_f - 1, & x \in \mathbb{T}, \end{cases}$$

with the initial datum for $(x,v) \in \mathbb{T}\times\mathbb{R}$

$$f_0(x,v) = \frac{n_0(x)}{2\sqrt{2\pi\,T_0}}\left[\exp\left(-\frac{|v-v_0|^2}{2T_0}\right) + \exp\left(-\frac{|v+v_0|^2}{2T_0}\right)\right],$$

with $v_0 = 1.5$, $T = 0.3$ and

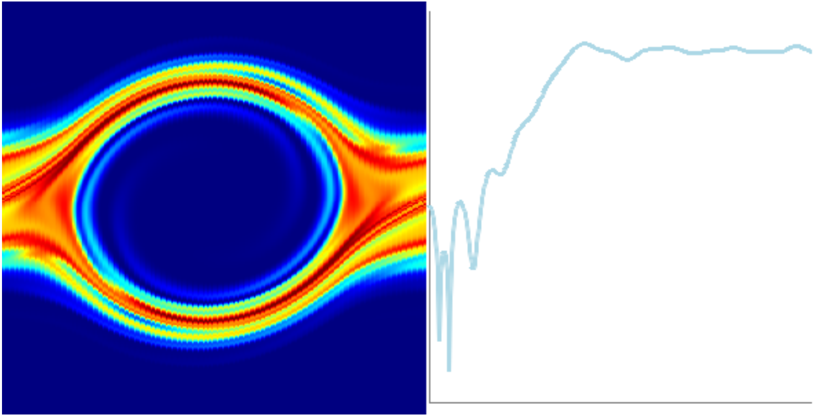
$$n_0(x) = 1 + 0.01\cos(kx)\,, \qquad x \in \mathbb{T},$$

with $k = 0.5$. We study the time evolution of the potential energy

$$\mathcal{E}_{pot}(t) = \frac{1}{2}\int_{\mathbb{T}} |\partial_x\phi|^2\,dx.$$

Two stream instability

Time evolution of the distribution function f in phase space (x, v) and the potential energy $\mathcal{E}_{pot}$.



Bump on the tail

Vlasov-Poisson in the torus

Consider

$$\begin{cases} \partial_t f + v\,\partial_x f + \partial_x \phi\,\partial_v f = 0, & (x,v) \in \mathbb{T} \times \mathbb{R}, \\ -\partial_{xx}\phi = \rho_f - 1, & x \in \mathbb{T}, \end{cases}$$

with the initial datum for $(x,v) \in \mathbb{T} \times \mathbb{R}$

$$f_0(x,v) = \frac{n_0}{\sqrt{2\pi}} \exp\left(-\frac{|v|^2}{2}\right) + \frac{n_b}{\sqrt{2\pi T_0}} \exp\left(-\frac{|v+v_0|^2}{2T_0}\right),$$

with $v_0 = 1.5$, $T = 0.3$ and $n_b = 0.1$

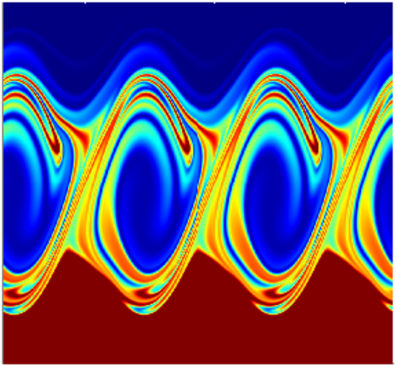
$$n_0(x) = 0.9 + 0.01\cos(kx)\,, \qquad x \in \mathbb{T},$$

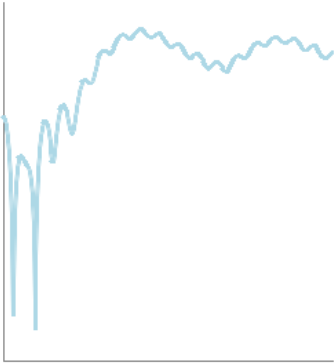
with $k = 0.5$. We study the time evolution of the potential energy

$$\mathcal{E}_{pot}(t) = \frac{1}{2}\int_{\mathbb{T}} |\partial_x \phi|^2\,dx.$$

Bump on the tail

Time evolution of the distribution function f in phase space (x, v) and the potential energy $\mathcal{E}_{pot}$.





The Vlasov-Maxwell Model

Electro-magnetic interaction

It includes magnetic field, which is important at high speeds with the Lorentz force:

$$F = q\big(E + v \times B\big).$$

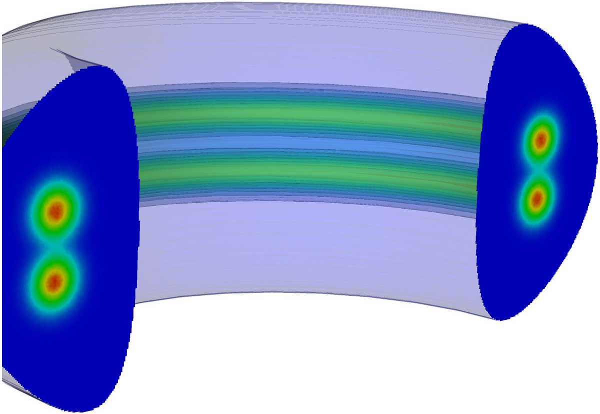
It yields to the Vlasov-Maxwell system

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + \dfrac{q}{m}(E + v \times B) \cdot \nabla_v f = 0, \\ \nabla \cdot B = 0, \quad \partial_t B + \nabla \times E = 0, \\ \nabla \cdot E = \dfrac{q}{\epsilon_0}\,\rho_f, \quad \dfrac{1}{c^2}\,\partial_t E - \nabla \times B = -\mu_0\, q\, J_f. \end{cases}$$

with

$$\rho_f = \int_{\mathbb{R}^n} f\, dv, \qquad J_f = \int_{\mathbb{R}^n} v\, f\, dv.$$

Magnetic confinement



- **Example : magnetic confinement in a tokamak**[a]

[a] PhD K. H. Trinh (advisors FF and L.M. Rodrigues) on Particle-In-Cells simulations.

A plasma is a multiscale problem and we aim to study its long time behavior

Aggregation equation

The aggregation equation appears in granular media models, swarming models for animal collective behavior, equilibrium states for self-assembly and molecules, and mean-field games in socioeconomics among others.

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\mathcal{K}[\rho]\, \rho) = 0, \\ \mathcal{K}[\rho] = \int_{\mathbb{R}^n} K(x, x')\, \rho(t, x')\, dx' \end{cases}$$

where the kernel K determines the interactions.
Often we choose

$$K(x, y) = -\nabla_x W(x - y),$$

which measures the interaction force that an infinitesimal particle located at $y \in \mathbb{R}^n$ will exert on a particle located at $x \in \mathbb{R}^n$.

Theory of characteristics

Example : free transport equation

Let us consider the equation

$$\partial_t f + v \cdot \nabla_x f = 0,$$

with $f(0, x, v) = f^{in}(x, v)$. The characteristic curve through y at $t = 0$ is $\gamma(t) = y + t\, v$ and the solution is constant along characteristics:

$$f(t, \gamma(t), v) = \text{constant}.$$

Theorem 2.1

For $f^{in} \in \mathscr{C}^1(\mathbb{R}^n \times \mathbb{R}^n)$, the Cauchy problem

$$\partial_t f + v \cdot \nabla_x f = 0,$$

with $f(0, x, v) = f^{in}(x, v)$ has a unique solution $f \in \mathscr{C}^1(\mathbb{R}_+ \times \mathbb{R}^{2n})$ given by

$$f(t, x, v) = f^{in}(x - tv, v).$$

Proof of Theorem

Uniqueness. Let f be a $\mathscr{C}^1$ solution, hence along $\gamma(t) = y + tv$:

$$\frac{d}{dt} f(t, y + tv, v) \;=\; \partial_t f + v \cdot \nabla_x f \;=\; 0.$$

Thus $f(t, y + tv, v) \;=\; f(0, y, v) \;=\; f^{in}(y, v)$.

Existence. Define $f(t, x, v) \;=\; f^{in}(x - tv, v)$, hence

- Clearly we have $f(0, x, v) = f^{in}(x, v)$.
- Moreover, a direct computation shows

$$\partial_t f + v \cdot \nabla_x f \;=\; 0.$$

An example : Phase Mixing

About the qualitative behavior of the solution. Phase mixing[1] is a damping mechanism due to shearing in the phase space $\mathbb{T} \times \mathbb{R}$ by the free-transport dynamics,

$$\partial_t f + v \cdot \nabla_x f = 0,$$

leading to decay of macroscopic quantities such as the charged density

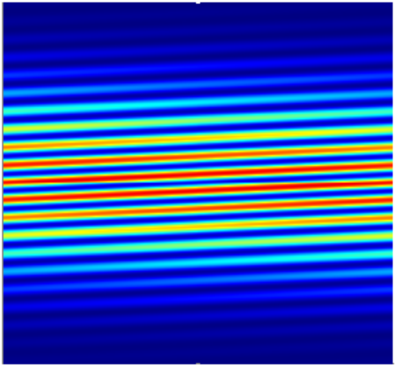
$$\rho(t,x) = \int_{\mathbb{R}} f(t,x,v)\, dv.$$

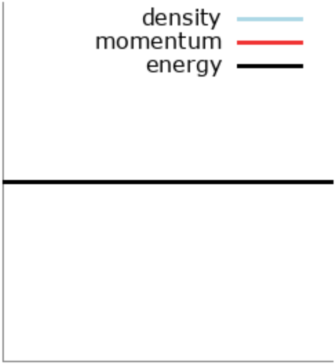
Indeed, the transport dynamics or shearing of each elementary mode $e^{ik\cdot x}$, for $k \in \mathbb{Z} \setminus \{0\}$, creates fast oscillation $e^{-ikt\cdot v}$ in v, which leads to rapid decay of macroscopic quantities, thanks to velocity averaging.

[1] C. Mouhot and C. Villani or T. Nguyen on Landau damping (2010-)

Illustration of Phase Mixing

Time evolution of the distribution function f in phase space (x, v) and the macroscopic quantities ρ, ρu and energy e.





Transport equation (non conservative form)

We set $z = (x, v)$ and $V(t, z) \in \mathbb{R}^d$ be a time-dependent vector field and consider the following linear transport equation

$$\begin{cases} \partial_t f + V(t,z) \cdot \nabla_z f = 0, \\ f(0,z) = f^{in}(z). \end{cases}$$

Assumptions:

(H1) $V \in \mathscr{C}([0,T] \times \mathbb{R}^d)$.
(H2) $\nabla_x V \in \mathscr{C}([0,T] \times \mathbb{R}^d)$.
(H3) Linear growth: $\|V(t,z)\| \leq \kappa (1 + \|z\|)$.

Definition of characteristic curves

Consider $\gamma(s)$ solving

$$\begin{cases} \dot{\gamma}(s) = V(s, \gamma(s)), \\ \gamma(t) = z. \end{cases}$$

Denote as $\gamma(s) = Z(s,t,z)$.

Existence of Characteristic Flow

Theorem 2.2

Under assumptions (H1)-(H3), for each (t, z), *there exists a unique solution*

$$s \mapsto Z(s, t, z) \in \mathscr{C}^1([0, T]; \mathbb{R}^d).$$

Moreover, $Z \in \mathscr{C}^1([0, T]^2 \times \mathbb{R}^d)$.

Theorem 2.3

The flow $Z(s, t, z)$ *satisfies:*

(i) *Flow property:* $Z(t_3, t_2, Z(t_2, t_1, z)) = Z(t_3, t_1, z)$.

(ii) $Z(s, t, \cdot)$ *is a* $\mathscr{C}^1$*-diffeomorphism.*

(iii) *Jacobian* $J(s, t, z) = \det(D_z Z(s, t, z))$ *satisfies*

$$\partial_s J = \nabla_z \cdot V(s, Z(s, t, z))\, J, \quad J(t, t, z) = 1,$$

that is, $J(s, t, z) = \exp\left(\int_t^s \nabla_z \cdot V(\tau, Z(\tau, t, z))\, d\tau\right)$.

Remarks on the compressibility of the flow

The Jacobian $J(s,t,z) = \det(D_z Z(s,t,z))$ measure the incompressibility of the flow

- When $J(s,t,z) \equiv 1$ means that the flow is incompressible, that is, $\nabla_z \cdot V = 0$ and the non-conservative equation can be written as

$$\begin{cases} \partial_t f + \nabla_z \cdot (V(t,z) f) = 0, \\ f(0,z) = f^{in}(z), \end{cases}$$

describing the conservation of mass

$$\int_{\mathbb{R}^d} f(t) dz = \int_{\mathbb{R}^d} f^{in} dz.$$

- When $J(s,t,z) \neq 1$ means that the flow is compressible. This equation cannot be written in a conservative form and mass is not conserved.

Solving the Transport Equation

We now use the flow to construct the solution.

Theorem 2.4

The unique $\mathscr{C}^1$ solution is

$$f(t,z) = f^{in}\left(Z(0,t,z)\right).$$

and $\|f(t)\|_{L^\infty} = \|f^{in}\|_{L^\infty}$.

Proof. Along the characteristic $Z(t,0,y)$:

$$\frac{d}{dt} f(t, Z(t,0,y)) = 0, \implies f(t, Z(t,0,y)) = f^{in}(y).$$

Change of variable $z = Z(t,0,y)$ gives the formula.

$$\partial_t Z(s,t,z) + \left(V(t,z)\cdot\nabla_z\right) Z(s,t,z) = 0.$$

This is the key identity used in the existence proof.

A simple example

Consider the linear transport equation

$$\partial_t f + v \cdot \nabla_x f + F(x, x) \cdot \nabla_v f = 0,$$

with

$$F(x) = -\left(1 + \frac{1}{1 + 5|x|^2}\right) x.$$

Characteristic curves are

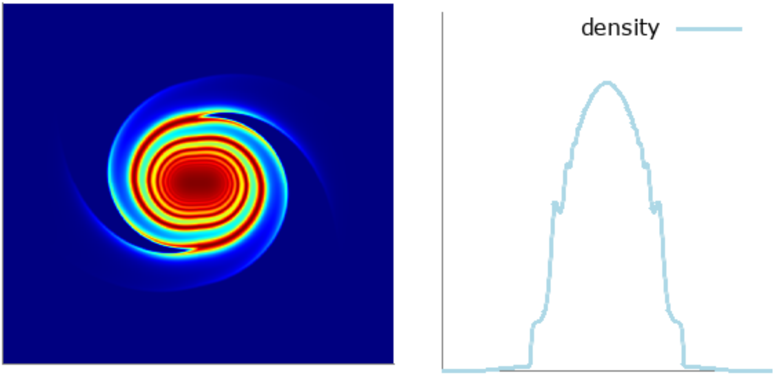
$$\frac{dx}{dt} = v, \quad \frac{dx}{dt} = F(x),$$

and we have

$$\frac{1}{2}\frac{d}{dt}\left(|x|^2 + |v|^2\right) = \frac{x \cdot v}{1 + 5|x|^2} \leq \frac{1}{2}\left(|x|^2 + |v|^2\right).$$

An example of non smooth initial datum

Time evolution of the distribution function f in phase space (x, v) and the density ρ.



Transport equation (conservative form)

Let $V(t,z) \in \mathbb{R}^d$ be a time-dependent vector field and consider the following linear transport equation

$$\begin{cases} \partial_t \mu + \nabla_z \cdot (V(t,z)\,\mu) \;=\; 0, \\ \mu(0,z) = \mu^{in}(z). \end{cases}$$

When μ^{in} is only a positive measure or $L^1(\mathbb{R}^d)$ function, we may define a notion of weak solution.

Definition of a weak solution

A weak solution of the Cauchy problem for the conservative transport equation an element of $\mu \in \mathscr{C}([0,T]; w - \mathcal{M}(R^d))$ that satisfies the initial condition and the equality

$$\int_0^T \int_{\mathbb{R}^d} (\partial_t + V(t,z) \cdot \nabla_z)\,\varphi(t,z)\,\mu(t,dz)\,dt = 0,$$

for each $\varphi \in \mathscr{C}^1_c((0,T) \times \mathbb{R}^d)$.

Transport equation (conservative form)

Definition of Push-Forward of Measures

If μ is a positive measure and $T : \mathbb{R}^d \to \mathbb{R}^d$ is measurable, the push-forward is $(T_{\#}\mu)(B) = \mu(T^{-1}(B))$.

The definition of $T_{\#}\mu$ can be equivalently recast as follows:

$$\int_{\mathbb{R}^d} 1_B(y)\, T_{\#}\mu(dy) = \int_{\mathbb{R}^d} 1_{T^{-1}(B)}(x)\, \mu(dx) = \int_{\mathbb{R}^d} 1_B(T(x))\, \mu(dx).$$

Theorem 2.5

The measure-valued solution in the weak sense is given by

$$\mu(t) = Z(t, 0, \cdot)_{\#}\mu^{in},$$

that is, for any test function $\varphi \in \mathscr{C}(\mathbb{R}^d)$, we have

$$\int_{\mathbb{R}^d} \varphi(z)\, \mu(t, dz) = \int_{\mathbb{R}^d} \varphi(Z(t, 0, y))\mu^{in}(dy).$$

Proof of existence and uniqueness.

Existence. Let $\varphi \in \mathscr{C}_c^1((0,T)\times\mathbb{R}^d)$ and define

$$\mathcal{I}(t) \;=\; \int_{\mathbb{R}^d} \varphi(t, Z(t,0,y))\, \mu^{in}(dy).$$

Then

$$\begin{aligned}\frac{\mathrm{d}\mathcal{I}}{\mathrm{d}t}(t) &= \int_{\mathbb{R}^N} \big(\partial_t\varphi + V\cdot\nabla_x\varphi\big)(t, Z(t,0,y))\, \mu^{in}(dy)\\ &= \int_{\mathbb{R}^N} \big(\partial_t\varphi(t,x) + V(t,x)\cdot\nabla_x\varphi(t,x)\big)\, \mu(t,dx).\end{aligned}$$

Integrating in time gives the weak formulation.

Uniqueness. Let μ be any weak solution. We define

$$\nu(t) \;:=\; Z(0,t,\cdot)_{\#}\mu(t).$$

Then fix $\psi \in \mathscr{C}_c^1(\mathbb{R}^d)$ and compute in the sense of distribution :

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^d} \psi(x)\, \nu(t,dx).$$

Using that

$$(\partial_t + V(t,z)\cdot\nabla_z)\,\psi(Z(0,t,z)) \;=\; 0.$$

Proof of existence and uniqueness

this implies

$$\frac{d}{dt}\int \psi(x)\,\nu(t,dx) \,=\, 0 \quad \text{in } \mathcal{D}'((0,T)),$$

hence $\nu(t) = \mu^{in}$, so $\mu(t) = Z(t,0,\cdot)_{\#}\mu^{in}$.

Support Control. Using linear growth of V:

$$|Z(s,t,y)| \leq (|y| + \kappa T)e^{\kappa T}$$

This ensures that the support of the function $(t,y) \mapsto \psi(Z(0,t,y))$ is compact, justifying all the integration by parts.

Regular Solutions in Conservative Form

Theorem 2.6

Let V satisfy (H1)-(H2)-(H3) and $f^{in} \in C^1(\mathbb{R}^d)$. Then

$$\partial_t f + \nabla_z \cdot (V(t,z)\, f) = 0, \quad f|_{t=0} = f^{in}$$

has a unique solution

$$f(t,z) \;=\; f^{in}\big(Z(0,t,z)\big)\, J(0,t,z)$$

where $J(s,t,z) = \det(D_z Z(s,t,z))$.

Uniqueness. Assume g satisfies the equation with $g|_{t=0} = 0$. Then

$$(\partial_t \;+\; V \cdot \nabla_z)\; g \;=\; -g\, \nabla_z \cdot V$$

Along characteristics:

$$\frac{d}{dt} g(t, Z(t,0,z)) \;=\; -g(t, Z(t,0,z))\; (\nabla_z \cdot V)\, (t, Z(t,0,z)).$$

With $g(0,z) = 0$, the solution of this ODE is $g \equiv 0$.

Regular Solutions in Conservative Form

Existence. We first define

$$f(t,z) \,=\, f^{in}\big(Z(0,t,z)\big)\, J(0,t,z)$$

- Initial condition holds because $J(0,0,z) = 1$.
- One verifies by direct (though technical) computation using the Jacobian evolution equation

$$J(s,t,z) = \exp\left(\int_t^s \nabla_z \cdot V\left(\tau, Z(\tau,t,z)\right)\, d\tau\right)$$

that f solves the conservative transport equation.

Moreover, we show the conservation of mass

$$\int_{\mathbb{R}^d} f(t,z)\, dz \,=\, \int_{\mathbb{R}^d} f^{in}(z)\, dz.$$

Summary of the first Lecture

- We have constructed smooth solution for transport equations and proved existence of uniquness using the flow.

$$\partial_t f + V(t, Z) \cdot \nabla_z f = 0.$$

- We have studied measure value solution for conservative transport equations and proved existence of uniquness using again the flow.

$$\partial_t \mu + \nabla_z \cdot (V(t, z)\, \mu) = 0.$$

- For smooth data, the solution remains smooth.
- Fixed point theorem for existence and uniqueness of solutions.

What is coming next?

- Mean field limit
- Particle methods

Toward nonlinear equation

Nonlinear transport equation

Often we deal with nonlinear transport equation on the form

$$\partial_t \mu + \nabla_z \cdot (V[\mu]\,\mu) = 0,$$

where the veolcity field $V[\mu]$ now depends on the measure μ.

We can prove existence and uniqueness of measure or smooth solution using the theory of characteristics using a fixed point algorithm : we set $V[\mu^0] = V[\mu^{in}]$ and solve for $n \geq 0$,

$$\partial_t \mu^{n+1} + \nabla_z \cdot \left(V[\mu^n]\,\mu^{n+1}\right) = 0.$$

- **This requires good *a priori* estimates on the velocity field $V[\mu^n]$.**

Some references

For the general theory on transport equations:

- F. Bouchut, F. Golse and M. Pulvirenti, Kinetic equations and asymptotic theory
- F. Golse, Lecture notes https://www.cmls.polytechnique.fr/perso/golse

For the general theory on Vlasov-Poisson and Vlasov-Maxwell systems

- Weak and renormalized solutions: Theory of Diperna-Lions ;
- smooth solutions for Vlasov-Poisson[2] and for Vlasov-Maxwell[3]
- Landau damping[4].

[2] Ukai and Okabe for 2D (1978), Pfaffelmoser for 3D (1992)

[3] Glassey-Strauss, then Bouchut, Golse and Pallard (2003)

[4] Bedrossian, Grenier and Mouhot, Landau damping: paraproducts and Gevrey regularity (2016) and Grenier, N'Guyen and Rodnianski, Landau damping for analytic and Gevrey data (2021)

From Classical Mechanics to nonlinear transport equations

N-body problem

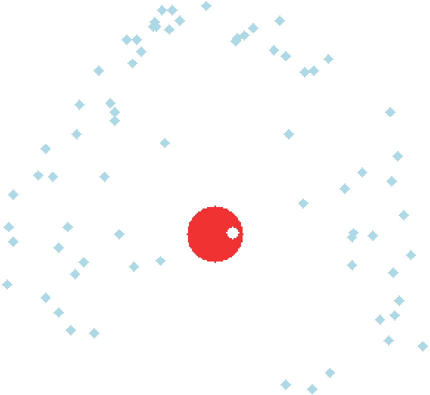
In physics, the N-body problem in three dimension is the problem of predicting the individual motions of a group of celestial objects interacting with each other gravitationally.
Consider the system for $1 \leq i \leq N$

$$\begin{cases} \dfrac{dX_i}{dt}(t) = V_i(t) \\ m_i \dfrac{dV_i}{dt}(t) \,=\, G \displaystyle\sum_{j \neq i} m_i \, m_j \nabla_X U\left(X_i(t) - X_j(t)\right), \end{cases}$$

where U is the Newtonian or Coulombian potential

$$U(X) \,=\, \frac{1}{|X|}, \qquad \nabla_X U = \frac{X}{|X|^3}.$$

A simulation of N-body problem



The interaction kernel K

Assume that

$$K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$$

satisfies the following assumptions. First K is skew-symmetric: for all z, $z' \in \mathbb{R}^d$,

$$K(z, z') = -K(z', z).$$

Besides,

$$K \in \mathscr{C}^1(\mathbb{R}^d \times \mathbb{R}^d; \mathbb{R}^d),$$

with bounded partial derivatives of order one.

In other words, there exists a constant $L \geq 0$ such that

$$\sup_{z' \in \mathbb{R}^d} |\nabla_z K(z, z')| \leq L, \qquad \sup_{z \in \mathbb{R}^d} |\nabla_{z'} K(z, z')| \leq L.$$

Remark. For practical applications, we should go beyond these assumptions and deal with singular kernels.

General Formalism in Classical Mechanics

Consider a system of N particles, whose state at time t is defined by phase space coordinates

$$z_1(t), \dots, z_N(t) \in \mathbb{R}^d.$$

Example

In the case of the Vlasov–Poisson system, the phase space is

$$\mathbb{R}^3 \times \mathbb{R}^3 \simeq \mathbb{R}^6,$$

so that $d = 6$, and $z_j = (x_j, v_j)$, where x_j and v_j are respectively the position and the velocity of the jth particle.

$$\frac{dz_i}{dt}(t) = \frac{1}{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} K(z_i(t), z_j(t)), \qquad i = 1, \dots, N.$$

The key idea in the mean field limit

Assume that the points $(z_j(t))_{1\le j\le N}$ are distributed at time t under the probability measure $f(t,dz)$ in the large N limit. Then,

$$\frac{1}{N}\sum_{j=1}^{N} K(z_i(t),z_j(t)) \to \int_{\mathbb{R}^d} K(z_i(t),z')\,f(t,dz'), \quad \text{as} \quad N\to+\infty.$$

This suggests replacing the N-particle system of differential equations with the single differential equation

$$\frac{dz}{dt}(t) \;=\; \int_{\mathbb{R}^d} K(z(t),z')\,f(t,dz').$$

One recognizes the equation of characteristics for

$$\partial_t f + \nabla_z\cdot(\mathcal{K}[f]\,f) \;=\; 0,$$

where

$$\mathcal{K}[f](t,z) \;:=\; \int_{\mathbb{R}^d} K(z,z')\,f(t,dz').$$

Definition of empirical measure

To each N-tuple

$$Z_N = (z_1, \dots, z_N) \in (\mathbb{R}^d)^N \simeq \mathbb{R}^{dN},$$

we associate the empirical measure defined as

$$\mu_{Z_N}(t) = \frac{1}{N} \sum_{i=1}^{N} \delta_{z_i(t)}$$

It describes the statistical distribution of the N-particle system in phase space.

We define the set of Borel probability measures on $\mathbb{R}^d$ with finite moment of order 1, that is,

$$\mathcal{P}_1(\mathbb{R}^d) := \left\{ p \in \mathcal{P}(\mathbb{R}^d) \text{ such that } \int_{\mathbb{R}^d} |z| \, p(dz) < \infty \right\}.$$

Empirical measure

We have for any $p \in \mathcal{P}_1(\mathbb{R}^d)$,

$$\mathcal{K}[p](z) := \int_{\mathbb{R}^d} K(z,z')\,p(dz').$$

Theorem 3.1

The Cauchy problem for the N-particle ODE system

$$\begin{cases} \dfrac{dz_i}{dt}(t) = \dfrac{1}{N}\displaystyle\sum_{j=1}^{N} K(z_i(t), z_j(t)), & i = 1,\ldots,N, \\ z_i(0) = z_i^{in}, \end{cases}$$

has a unique solution of class $\mathscr{C}^1$ on $\mathbb{R}$. Moreover, the empirical measure $\mu_{Z_N(t)}$ is a weak solution of

$$\begin{cases} \partial_t\mu + \nabla_z\cdot(\mathcal{K}[\mu]\,\mu) = 0, \\ \mu|_{t=0} = \mu^{in}. \end{cases}$$

Mean-field characteristic equation

Theorem 3.2

For each $\zeta^{in} \in \mathbb{R}^d$ and each Borel probability measure $\mu^{in} \in \mathcal{P}_1(\mathbb{R}^d)$, there exists a unique solution denoted by

$$t \mapsto Z(t, \zeta^{in}, \mu^{in}) \in \mathbb{R}^d$$

of class $\mathscr{C}^1$ of the problem

$$\begin{cases} \partial_t Z(t, \zeta^{in}, \mu^{in}) = \mathcal{K}[\mu(t)](Z(t, \zeta^{in}, \mu^{in})), \\ \mu(t) = Z(t, \cdot, \mu^{in})_{\#}\mu^{in}, \\ Z(0, \zeta^{in}, \mu^{in}) = \zeta^{in}. \end{cases}$$

Remark. The evolution of $t \mapsto Z(t, \zeta^{in}, \mu^{in})$ is set in the single-particle phase space $\mathbb{R}^d$, and not in the N-particle phase space. Observe that

$$z_i(t) = Z(t, z_i^{in}, \mu_{Z_N^{in}}), \qquad i = 1, \ldots, N.$$

Monge–Kantorovich distance

Given $\mu, \nu \in \mathcal{P}_1(\mathbb{R}^d)$, we define $\Pi(\mu,\nu)$ to be the set of Borel probability measures $\pi \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ with first and second marginals μ and ν respectively.

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} (\phi(x) + \psi(y))\, \pi(dx\, dy) = \int_{\mathbb{R}^d} \phi(x)\, \mu(dx) + \int_{\mathbb{R}^d} \psi(y)\, \nu(dy)$$

Definition 1

For each $\mu, \nu \in \mathcal{P}_1(\mathbb{R}^d)$, the Monge–Kantorovich distance $\mathrm{dist}_1(\mu,\nu)$ between μ and ν is defined by the formula[5]

$$\begin{aligned} \mathrm{dist}_1(\mu,\nu) &= \inf_{\pi \in \Pi(\mu,\nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} |x-y|\, \pi(dx\, dy) \\ &= \sup_{\substack{\phi \in \mathrm{Lip}(\mathbb{R}^d) \\ \mathrm{Lip}(\phi) \le 1}} \left| \int_{\mathbb{R}^d} \phi(z)\, \mu(dz) - \int_{\mathbb{R}^d} \phi(z)\, \nu(dz) \right| \end{aligned}$$

[5] C. Villani, Topics in Optimal Transportation

Dobrushin's estimate

Let ζ_1^{in}, $\zeta_2^{in} \in \mathbb{R}^d$, and μ_1^{in}, $\mu_2^{in} \in \mathcal{P}_1(\mathbb{R}^d)$. From Duhamel's formula

$$mathcall \; := \; Z(t,\zeta_1,\mu_1^{in}) - Z(t,\zeta_2,\mu_2^{in}) \; = \; \zeta_1 - \zeta_2 +$$

$$\int_0^t \left(\int_{\mathbb{R}^d} K(Z(s,\zeta_1,\mu_1^{in}),z')\mu_1(s,dz') - \int_{\mathbb{R}^d} K(Z(s,\zeta_2,\mu_2^{in}),z')\mu_2(s,dz') \right) ds.$$

So that

$$\begin{aligned} & Z(t,\zeta_1,\mu_1^{in}) - Z(t,\zeta_2,\mu_2^{in}) = \zeta_1 - \zeta_2 + \\ & \int_0^t \int_{\mathbb{R}^d\times\mathbb{R}^d} \Big(K(Z(s,\zeta_1,\mu_1^{in}),Z(s,\zeta_1',\mu_1^{in})) \\ & \qquad\qquad - K(Z(s,\zeta_2,\mu_2^{in}),Z(s,\zeta_2',\mu_2^{in})) \Big) \, \pi^{in}(d\zeta_1' d\zeta_2') \, ds. \end{aligned}$$

This last equality is the key observation in Dobrushin's argument, which explains the role of couplings of μ_1^{in} and μ_2^{in}.

Dobrushin's estimate

We introduce the notation

$$D[\pi](s) := \int_{\mathbb{R}^d \times \mathbb{R}^d} |Z(s,\zeta_1',\mu_1^{in}) - Z(s,\zeta_2',\mu_2^{in})| \, \pi(d\zeta_1' d\zeta_2').$$

Thus, the previous equality yields

$$|Z(t,\zeta_1,\mu_1^{in}) - Z(t,\zeta_2,\mu_2^{in})| \le |\zeta_1 - \zeta_2|$$

$$+L\int_0^t |Z(s,\zeta_1,\mu_1^{in}) - Z(s,\zeta_2,\mu_2^{in})| \, ds + L\int_0^t D[\pi^{in}](s)\, ds.$$

Integrating against $\pi^{in}(d\zeta_1 \, d\zeta_2)$, it gives

$$\begin{aligned} D[\pi^{in}](t) &\le D[\pi^{in}](0) + L\int_0^t D[\pi^{in}](s)\, ds + L\int_0^t D[\pi^{in}](s)\, ds \\ &= D[\pi^{in}](0) + 2L\int_0^t D[\pi^{in}](s)\, ds. \end{aligned}$$

Dobrushin's estimate

We can now state and prove Dobrushin's stability estimate.

Theorem 3.3 (Dobrushin's estimate)

Assume that the interaction kernel $K \in \mathscr{C}^1(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{R}^d)$ *satisfies our previous assumptions. Let* μ_1^{in}, $\mu_2^{in} \in \mathcal{P}_1(\mathbb{R}^d)$, *and let*

$$\mu_j(t) = Z(t, \cdot, \mu_j^{in})_{\#}\mu_j^{in}, \qquad j = 1, 2.$$

Then for all $t \in \mathbb{R}$,

$$\mathrm{dist}_1(\mu_1(t), \mu_2(t)) \leq e^{2L|t|}\ \mathrm{dist}_1(\mu_1^{in}, \mu_2^{in}).$$

Using that the emprirical measure is a measure solution to the PDE, we prove the mean field limit.

Some references

For the general theory on mean field limit

- R. Dobrushin[6]
- M. Hauray and P.-E. Jabin[7]
- D. Bresch, P.E. Jabin and J. Soler[8]

This approach applies, not only in classical mechanics, but alos in quantum mechanics

- Ch. Saffirio and N. Leopold[9]
- F. Golse and C. Mouhot[10]

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[6]Vlasov equations, Funct. Anal. Appl. 13 (1979), 115–123.
[7]N -particles approximation of the Vlasov equations with singular potential (2007)
[8]A new approach to the mean-field limit of Vlasov-Fokker-Planck equations (2025).
[9]Derivation of the Vlasov-Maxwell system from the Maxwell-Schrödinger equations with extended charges (2025), From the Hartree to the Vlasov dynamics: conditional strong convergence (2020)
[10]On the mean field and classical limits of quantum mechanics (2016).

Summary of the second Lecture

- We introduce classical mechanics systems of EODs

- We define the Monge-Kantorovich distance and introduce Dobrushin' estimates.

- Mean field limit.

What is coming next?

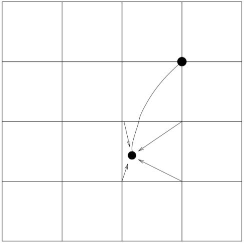
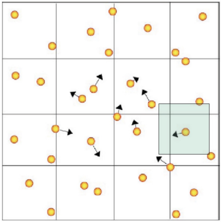
- Numerical methods for transport equation

- Nonlinear problems.

Particle and semi-Lagrangian methods

Backward Semi-Lagrangien method *vs.* Particle method

$$\partial_t f + V(t,z)\cdot\nabla_z f = 0 \qquad\qquad \partial_t \mu + \nabla_z\cdot(V(t,z)\mu) = 0$$

Backward Semi-Lagrangian	Particle method
	
$f_i^{n+1} = I[f^n]\left(Z^n(t^{n+1}, z_i)\right), \quad i\in\mathbb{Z}^d$	$\mu^{n+1}(z) = \sum_k \omega_k \delta(z - Z^{n+1}(t^n, z_k^n))$
For example $Z^n(t^{n+1}, z_i) = z_i - V(t^{n+1}, z_i)\Delta t$	For example $Z^{n+1}(t^n, z_k^n) = z_k^n + V(t^n, z_k^n)\Delta t$

Particle approximation for conservative equantion

We have already seen that

$$\mu_N(t,z) = \sum_{k=1}^{N} \omega_w \, \delta(z - Z_k)$$

with

$$\frac{dZ_k}{dt} = V(t, Z_k(t))$$

is a measure solution of the conservative transport equation.

Linear case

If we can solve exactly the equations of motion (which is sometimes the case when we only have a sufficiently simple applied field), the particle method gives the exact solution for an initial distribution function in the form of a sum of Dirac masses.

Nonlinear case $V = \mathcal{K}[\mu_N]$

It remains to compute the non local field $\mathcal{K}[\mu_N]$. It is costly !!

Approximation of the initial condition

(i) Determinist method: We define a mesh of the phase space (uniform or not). We take as the initial position of the particles (Z_k^0) the barycenters of the meshes and for weight ω_k associates the integral of μ^{in} on the corresponding mesh:

$$\omega_k = \int_{\mathbb{R}} \mu^{in}(z)\, dz$$

so that

$$\sum_k^N \omega_k = \int_{\mathbb{R}} \mu^{in}(z) dz.$$

(ii) Monte-Carlo method: We choose the initial positions randomly or pseudo-random according to the probability density associated with μ^{in}.

Convergence of the particle method in the linear case

Theorem 4.1 (Convergence analysis)

Assume that the velocity field $V \in \mathscr{C}^1(\mathbb{R}^\times \mathbb{R}^d, \mathbb{R}^d)$ *satisfies our previous assumptions and for all* $t \in \mathbb{R}$,

$$\|V(t,z) - V(t,z')\| \ \leq \ L\,\|z - z'\|, \qquad \forall\, z,\ z' \ \in \mathbb{R}^d.$$

Let μ^{in}, $\mu_N^{in} \in \mathcal{P}_1(\mathbb{R}^d)$. *Then for all* $t \in \mathbb{R}$,

$$\mathrm{dist}_1(\mu(t), \mu_N(t)) \leq e^{L|t|}\ \mathrm{dist}_1(\mu^{in}, \mu_N^{in}).$$

- show that

$$\|Z(t,z_1) - Z_N(t,z_2)\| \leq |z_1 - z_2| + L\int_0^t \|Z(s,z_1) - Z_N(s,z_2)\| ds.$$

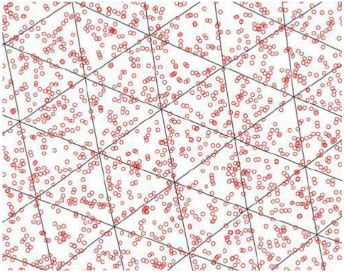
- for any coupling π^{in}, $D[\pi^{in}](t) \leq D[\pi^{in}](0) + L\int_0^t D[\pi^{in}](s)ds.$

Particle-mesh coupling

Warning....

The particle approximation μ_N of the distribution function does not make it possible to define a value of this function at all points in space.

- it is a problem to get strong convergence
- it is a problem for nonlinear PDE with interactions.



$\Longrightarrow$ a regularization step is necessary on a mesh.

To do this, we define convolution kernels and B-splines.

Particle-mesh coupling

B-splines by induction

We define the B-spline of order 0 which we will denote S^0 by

$$S^0(z) = \begin{cases} \frac{1}{h}, \text{ if } -h/2 \le z \le h/2 \\ 0, \text{ else.} \end{cases}$$

Higher order B-splines are then defined by: for all $m \ge 1$,

$$S^m(z) = \left(S^0\right)^{*m}(z) = S^0 \star S^{m-1}(z) = \frac{1}{h}\int_{z-h/2}^{z+h/2} S^{m-1}(x)\, dx.$$

Example

We get for instance for $m = 1$

$$S^1(z) = \frac{1}{h} \begin{cases} 1 - \frac{|z|}{h}, \text{ if } |z| \leq h \\ 0, \text{ else.} \end{cases}$$

or for second order $m = 2$

$$S^2(z) = \frac{1}{h} \begin{cases} \frac{1}{2}\left(\frac{3}{2} - \frac{|z|}{h}\right)^2, \text{ if } h/2 \leq |z| \leq 3h/2 \\ \frac{3}{4} - \left(\frac{z}{h}\right)^2, \text{ if } |z| \leq h/2 \\ 0, \text{ else.} \end{cases}$$

or at order $m = 3$

$$S^3(z) = \frac{1}{6h} \begin{cases} \left(2 - \frac{|z|}{h}\right)^3, \text{ if } h \leq |z| \leq 2h \\ 4 - 6\left(\frac{|z|}{h}\right)^2 + 3\left(\frac{|z|}{h}\right)^3, \text{ if } |z| \leq h \\ 0, \text{ else.} \end{cases}$$

Properties of B-spline functions.

B-splines verify the following important properties:

- Average unit

$$\int_{\mathbb{R}} S^m(x)dx = 1.$$

- Partition of the unit. For $x_j = jh$,

$$h \sum_j S^m(x - x_j) = 1.$$

- Parity

$$S^m(-x) = S^m(x), \qquad x \in \mathbb{R}.$$

Smooth Particle approximation

Consider

$$\partial_t \mu + \nabla_z \cdot (V(t,z)\mu) = 0.$$

We build the following approximation from the particle system

$$\begin{cases} \dfrac{dZ_k}{dt} = V(t, Z_k(t)), & 1 \le k \le N, \\ Z_k(0) = Z_k^0 \end{cases}$$

and define a smooth approximation f_N as

$$f_N(t,z) = \frac{1}{N}\sum_{k=1}^{N} S^m\left(z - Z_k(t)\right).$$

Warning. The distribution f_N is not anymore an exact solution of the transport equation.

Convergence analysis

We get the following result[11]

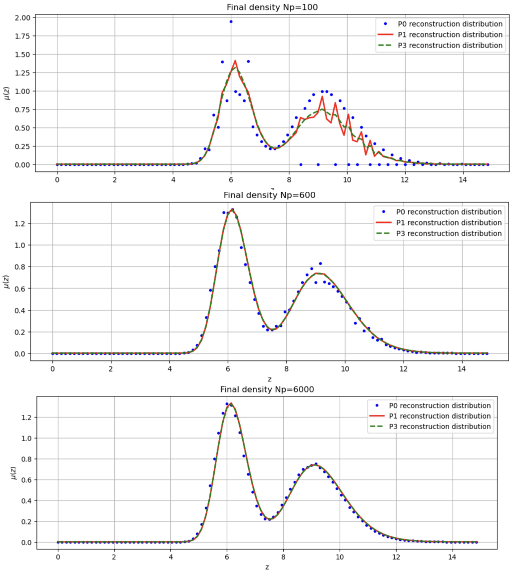
Theorem 2

Under the previous assumptions on the velocity field V and for $m \geq 0$, we consider f the solution to the transport equation and its approximation f_N. Then, we have

$$\sup_{t \in [0,T]} \|f(t) - f_N(t)\|_{L^p} \leq C \left(h^r \, \|f^{in}\|_{W^{r,p}} + \left(\frac{1}{N\,h}\right)^{m+1} \|f^{in}\|_{W^{m+1,p}} \right).$$

[11] P.-A. Raviart, An analysis of particle methods, Numerical methods in fluid dynamics (1983), A. Cohen and B. Perthame, Optimal approximations of transport equations by particle and pseudoparticle methods (2000)

Illustration : $hN = 1$, 6 and 60 for different splines



Application to Vlasov-Poisson

We consider again the electrostatic Vlasov–Poisson system:

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + E(t,x) \cdot \nabla_v f = 0, \\ E = -\nabla_x \phi, \\ -\Delta_x \phi = \rho - \rho_0, \end{cases}$$

where

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

Here:

- $f(t,x,v)$ is the particle distribution function,
- $\rho(t,x)$ is the charge density,
- $E(t,x)$ is the electric field.

The Particle-In-Cell method

We approximate the distribution function by macro-particles:

$$f_N(t, x, v) = \sum_{k=1}^{N} \omega_k \, \delta(x - X_k(t)) \, \delta(v - V_k(t)).$$

Here:

- $X_k(t)$ is the particle position,
- $V_k(t)$ is the particle velocity,
- ω_k is the particle weight.

The particles follow the characteristic equations:

$$\begin{cases} \dfrac{dX_k}{dt} = V_k, \\ \dfrac{dV_k}{dt} = E(t, X_k). \end{cases}$$

Projection / Interpolation steps

The charge density on the grid is computed by:

$$\rho_h(t,x) = \sum_{k=1}^{N} \omega_k \, S^m(xi - X_k).$$

Once ρ_h is known on the grid, we solve:

$$-\Delta\phi = \rho - \rho_0.$$

In 1D, a finite difference discretization gives:

$$-\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = \rho_i - \rho_0.$$

Then:

$$E_i = -\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}.$$

The electric field is now known on the grid but it must now be evaluated at particle positions.

$$E(X_k) = \sum_i E_i \, S^m(x_i - X_k).$$

This step is often called interpolation.

The particle trajectory

A popular scheme for the particle trajectory is the Verlet scheme : fix a time step $\Delta t > 0$ and $t^n = n\,\Delta t$, we have

$$\begin{cases} \dfrac{V_k^{n+1/2} - V_k^n}{\Delta t} = \dfrac{1}{2}\,E(t^n, X_k^n), \\ \dfrac{X_k^{n+1} - X_k^n}{\Delta t} = V_k^{n+1/2}, \\ \dfrac{V_k^{n+1} - V_k^{n+1/2}}{\Delta t} = \dfrac{1}{2}\,E(t^{n+1}, X_k^{n+1}). \end{cases}$$

Loop in time from time t^n to time t^{n+1}

1. We calculate the charge densities ρ_h and current J_h on the mesh.
2. We update the electromagnetic field with a classic mesh solver.
3. We calculate the fields at the positions of the particles.
4. The particles are advanced using a numerical scheme for the characteristics.

Properties of the Particle-In-Cell method

Conservation of mass for PIC[12]

$$\int_{\mathbb{R}} \rho_N(t,x)dx = \int_{\mathbb{R}} \rho_h(t,x)dx = \text{constant}.$$

Important issues are other conservations as conservation of charge

$$\partial_t \rho_h + \nabla_x \cdot J = 0.$$

and preservation of total energy

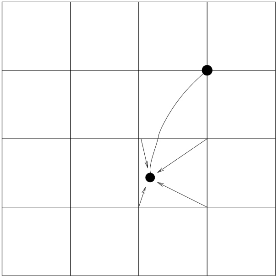
$$\mathcal{E}(t) = \frac{1}{2}\int_{\mathbb{T}\times\mathbb{R}} |v|^2 f_N(t,x,v)\; dx\, dv + \frac{1}{2}\int_{\mathbb{T}} |\nabla_x \phi|(t,x)dx = \text{constant}.$$

[12] C. K. Birdsall, A. B. Langdon (1991), G.-H. Cottet, P.-A. Raviart (1984)

The semi-Lagrangian method for non conservative transport

Now consider the transport equation

$$\partial_t f + V(t,z) \cdot \nabla_z f = 0$$



We use the fact that

$$f(t^{n+1}, z) = f(t^n, Z(t^n, t^{n+1}, z)),$$

that is

$$\|f(t)\|_{L^\infty} = \text{constant.}$$

But no conservation of mass except when $\nabla_z \cdot V(t,z) = 0$ meaning that the flow is incompressible.

The semi-Lagrangian method

At time $t^n = n\Delta t$, we know f_i^n on grid points z_i for $1 \leq i \leq N$.
We reconstruct the distribution function $f_h \in \mathscr{C}^2(\mathbb{T})$, based on B-splines as

$$f_h^n(z) \;=\; \sum_{j=1}^{N} \alpha_j \, S^3(z - z_j),$$

where the coefficients $(\alpha_j)_{1 \leq j \leq N}$ are determined by the interpolation conditions

$$f_i^n \;= f_h(z_i) \;=\; \sum_{j=1}^{N} \alpha_j \, S^3(z_i - z_j),$$

We solve the following backward in time system

$$\begin{cases} \dfrac{dZ}{dt} = \mathcal{K}[f_h](Z) \;=\; \displaystyle\int_{\mathbb{R}} K(Z, z')\, f_h(z')\, dz', \quad \text{on } t \in [t^n, t^{n+1}] \\ Z(t^{n+1}) \;=\; z_i, \quad 1 \leq i \leq N \end{cases}$$

and compute

$$f_i^{n+1} \;=\; f_h\left(Z(t^n, t^{n+1}, z_i)\right).$$

Time splitting method for the Vlasov-Poisson system

For the Vlasov-Poisson system

$$\partial_t f + v \cdot \nabla_x f + E \cdot \nabla_v f \; = \; 0.$$

We will decompose the equation into the following two parts: on

$$\partial_t f + v \cdot \nabla_x f \; = \; 0,$$

with v fixed, that is,

$$f_{k,i}^{n+1/2} = f_h(t^n, x_k - v_i \Delta t, v_i)$$

and then

$$\partial_t f + E \cdot \nabla_v f \; = \; 0,$$

with x fixed, that is,

$$f_{k,i}^{n+1} = f_h(t^{n+1/2}, x_k, v_i - \Delta t E^{n+1/2}(x_k)).$$

• These are then two advections with constant coefficients that can be solved more simply.

Error estimates for the semi-Lagrangian method

- A Strang splitting scheme may be applied to increase the order of accuracy.

We have the following result[13]

Theorem 3

Suppose that $E \in \mathscr{C}^2([0,T] \times \mathbb{T})$ *and* $f \in \mathscr{C}^3([0,T] \times \mathbb{T} \times \mathbb{R})$ *and consider* f_h *computed from the semi-Lagrangian method, then we have*

$$\|f - f_h\|_\infty \leq C\,(\Delta t^2 + \frac{h^2}{\Delta t}).$$

[13] N. Besse, N. Besse and M. Mehrenberger