

THEMATIC SEMESTER

Interacting particles, PDEs and applications



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Particle Dynamics and PDEs: Connections and Applications

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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

$f(t, x, v) dx dv =$ 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

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

The Vlasov-Poisson Model

Electrostatic interaction

Consider the force on a particle of charge q :

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

where ϕ solves the Poisson equation

This yields the Vlasov-Poisson system,

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

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

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

- 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

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

Consider f_{eq} a space homogeneous equilibrium

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

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

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

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 $n_b = 0.1$

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

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:

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

It yields to the Vlasov-Maxwell system

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

with

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

- **Example : magnetic confinement in a tokamak^a**

^aPhD 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 $f^{in} \in \mathcal{C}^1(\mathbb{R}^n \times \mathbb{R}^n)$, 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 $f \in \mathcal{C}^1(\mathbb{R}_+ \times \mathbb{R}^{2n})$ given by

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

Proof of Theorem

Uniqueness. Let f be a \mathcal{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 mixing¹ 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.

¹C. 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) $V \in \mathcal{C}([0, T] \times \mathbb{R}^d)$.

(H2) $\nabla_x V \in \mathcal{C}([0, T] \times \mathbb{R}^d)$.

(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

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

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

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 \mathcal{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 \mathcal{C}^1 solution is

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

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

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.

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

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

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

and we have

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

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 is an element of $\mu \in \mathcal{C}([0, T]; w - \mathcal{M}(\mathbb{R}^d))$ 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 $\varphi \in \mathcal{C}_c^1((0, T) \times \mathbb{R}^d)$.

Transport equation (conservative form)

Definition of Push-Forward of Measures

If μ is a positive measure and $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$ 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 $\varphi \in \mathcal{C}(\mathbb{R}^d)$, 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 $\varphi \in \mathcal{C}_c^1((0, T) \times \mathbb{R}^d)$ and define

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

Then

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

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

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

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

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

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

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

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

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

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 uniqueness 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 uniqueness 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 velocity 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 $n \geq 0$,

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

- **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-Poisson² and for Vlasov-Maxwell³
- Landau damping⁴.

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

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

⁴Bedrossian, 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 $1 \leq i \leq N$

$$\left\{ \begin{array}{l} \frac{dX_i}{dt}(t) = V_i(t) \\ m_i \frac{dV_i}{dt}(t) = G \sum_{j \neq i} m_i m_j \nabla_x U(X_i(t) - X_j(t)), \end{array} \right.$$

where U is the Newtonian or Coulombian potential

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

A simulation of N-body problem

General Formalism in Classical Mechanics

The interaction kernel K

Assume that

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

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

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

Besides,

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

with bounded partial derivatives of order one.

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

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

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 j th particle.

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

The key idea in the mean field limit

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

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

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

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

Empirical measure

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

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

has a unique solution of class \mathcal{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 \mathcal{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

$$z_i(t) = Z(t, z_i^{in}, \mu_{z_N^{in}}), \quad i = 1, \dots, N.$$

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 $\text{dist}_1(\mu, \nu)$ between μ and ν is defined by the formula⁵

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

⁵C. Villani, Topics in Optimal Transportation

Dobrushin's estimate

Let $\zeta_1^{in}, \zeta_2^{in} \in \mathbb{R}^d$, and $\mu_1^{in}, \mu_2^{in} \in \mathcal{P}_1(\mathbb{R}^d)$. From Duhamel's formula

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

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

So that

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

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

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

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

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

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

Dobrushin's estimate

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

Theorem 3.3 (Dobrushin's estimate)

Assume that the interaction kernel $K \in \mathcal{C}^1(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{R}^d)$ satisfies our previous assumptions. Let $\mu_1^{in}, \mu_2^{in} \in \mathcal{P}_1(\mathbb{R}^d)$, and let

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

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

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

Using that the empirical 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. Dobrushin⁶
- M. Hauray and P.-E. Jabin⁷
- D. Bresch, P.E. Jabin and J. Soler⁸

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

- Ch. Saffirio and N. Leopold⁹
- F. Golse and C. Mouhot¹⁰

⁶Vlasov equations, *Funct. Anal. Appl.* 13 (1979), 115–123.

⁷N -particles approximation of the Vlasov equations with singular potential (2007)

⁸A new approach to the mean-field limit of Vlasov-Fokker-Planck equations (2025).

⁹Derivation 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)

¹⁰On 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.

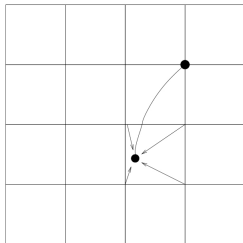
Particle and semi-Lagrangian methods

Backward Semi-Lagrangian method vs. Particle method

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

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

Backward Semi-Lagrangian

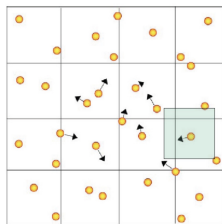


$$f_i^{n+1} = I[f^n](Z^n(t^{n+1}, z_i)), \quad i \in \mathbb{Z}^d$$

For example

$$Z^n(t^{n+1}, z_i) = z_i - V(t^{n+1}, z_i)\Delta t$$

Particle method



$$\mu^{n+1}(z) = \sum_k \omega_k \delta(z - Z^{n+1}(t^n, z_k^n))$$

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 equation

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 $V \in \mathcal{C}^1(\mathbb{R} \times \mathbb{R}^d, \mathbb{R}^d)$ satisfies our previous assumptions and for all $t \in \mathbb{R}$,

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

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

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

- show that

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

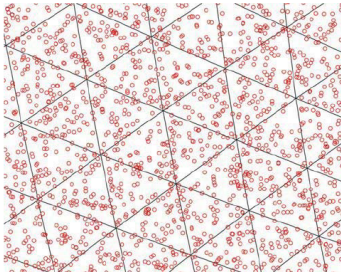
- for any coupling π^{in} , $D[\pi^{in}](t) \leq D[\pi^{in}](0) + L \int_0^t D[\pi^{in}](s) ds.$

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.



⇒ a regularization step is necessary on a mesh.

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

***B*-splines by induction**

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

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

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

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

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

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

Smooth Particle approximation

Consider

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

We build the following approximation from the particle system

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

and define a smooth approximation f_N as

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

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

We get the following result¹¹

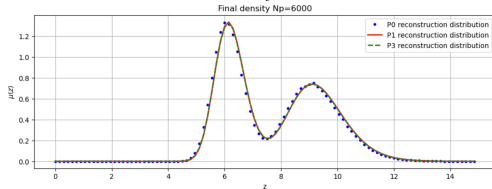
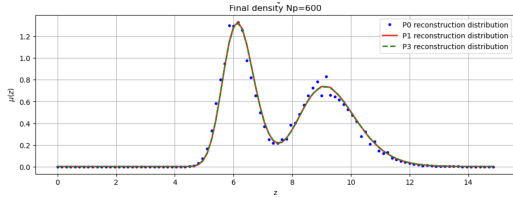
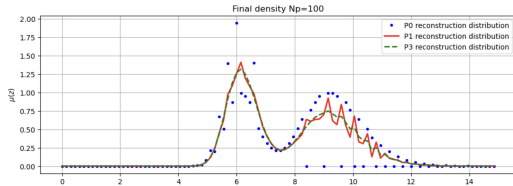
Theorem 2

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

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

¹¹P.-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:

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

Projection / Interpolation steps

The charge density on the grid is computed by:

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

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

$$\left\{ \begin{array}{l} \frac{V_k^{n+1/2} - V_k^n}{\Delta t} = \frac{1}{2} E(t^n, X_k^n), \\ \frac{X_k^{n+1} - X_k^n}{\Delta t} = V_k^{n+1/2}, \\ \frac{V_k^{n+1} - V_k^{n+1/2}}{\Delta t} = \frac{1}{2} E(t^{n+1}, X_k^{n+1}). \end{array} \right.$$

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 PIC¹²

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

Important issues are other conservations as conservation of charge

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

and preservation of total energy

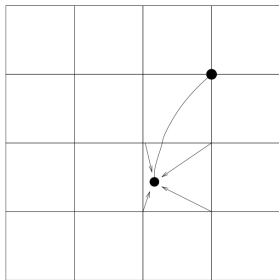
$$\mathcal{E}(t) = \frac{1}{2} \int_{\mathbb{T} \times \mathbb{R}} |v|^2 f_N(t, x, v) dx dv + \frac{1}{2} \int_{\mathbb{T}} |\nabla_x \phi|(t, x) dx = \text{constant}.$$

¹²C. 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 $f_h \in \mathcal{C}^2(\mathbb{T})$, 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

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

and compute

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

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 result¹³

Theorem 3

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

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

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