Joint ICTP-IAEA College on Plasma Physics

Vlasov simulatons of plasma turbulence

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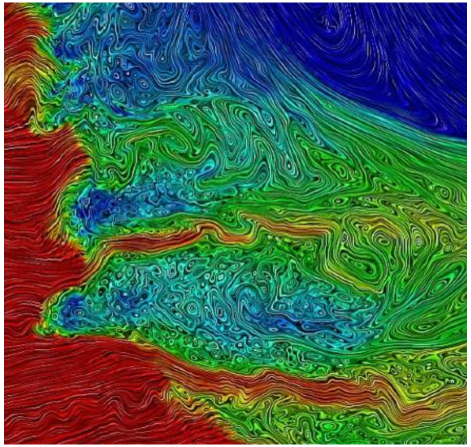

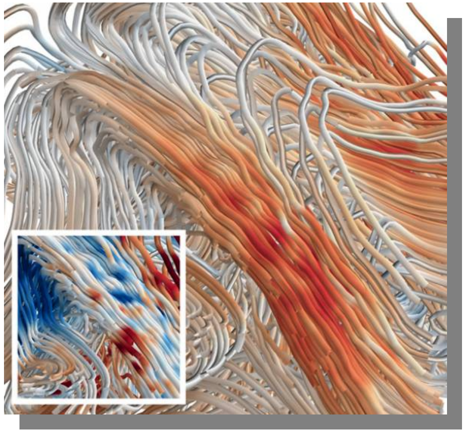

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DIPARTIMENTO DI FISICA

Structure of the course

Part I

Numerical methods for kinetic simulations of plasmas

Part II

Direct numerical simulations of plasma turbulence: Eulerian simulations

Part III

Comparison between simulations and observations;
Particle in cell simulations of turbulence

Part I

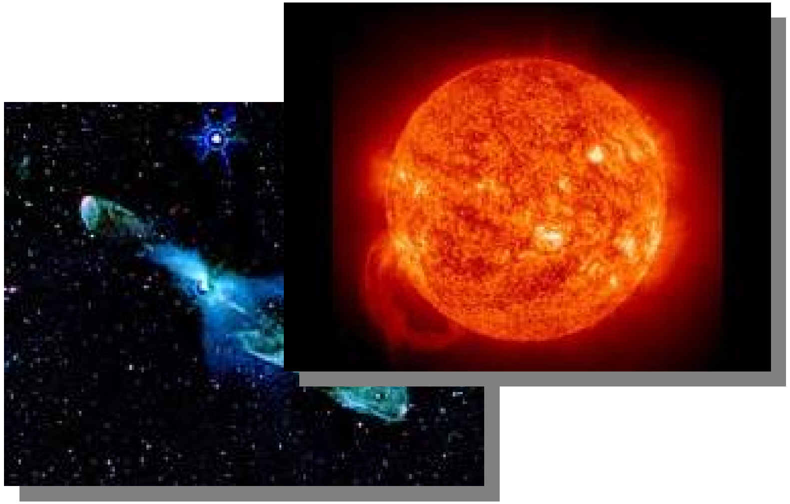
Numerical methods for kinetic simulations of plasmas

Outline of Part I

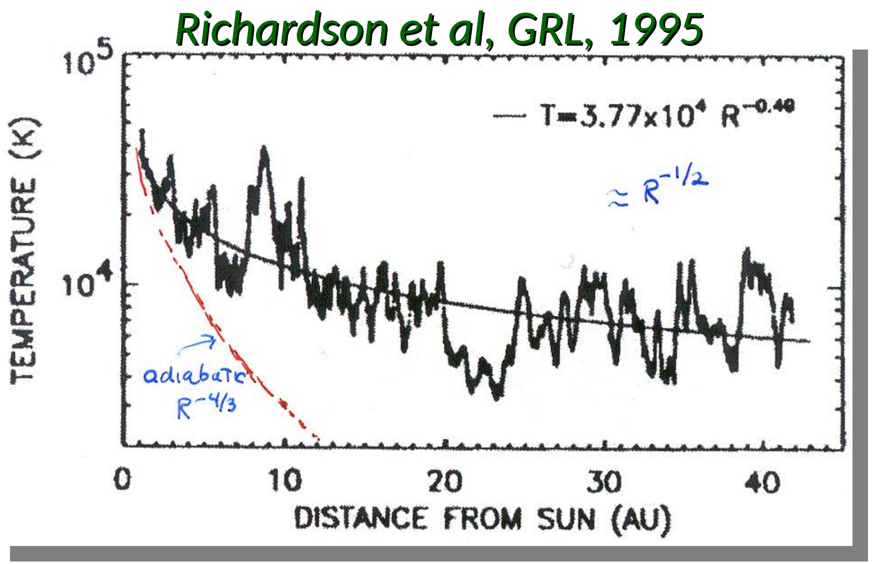
- Introduction to plasma complex dynamics
- Methods to simulate the Vlasov equation. Focus on the Eulerian approach
- Discretization of the equations, basic numerical schemes and numerical stability
- Advanced numerical schemes for simulations of plasma turbulence

Plasma in the Universe

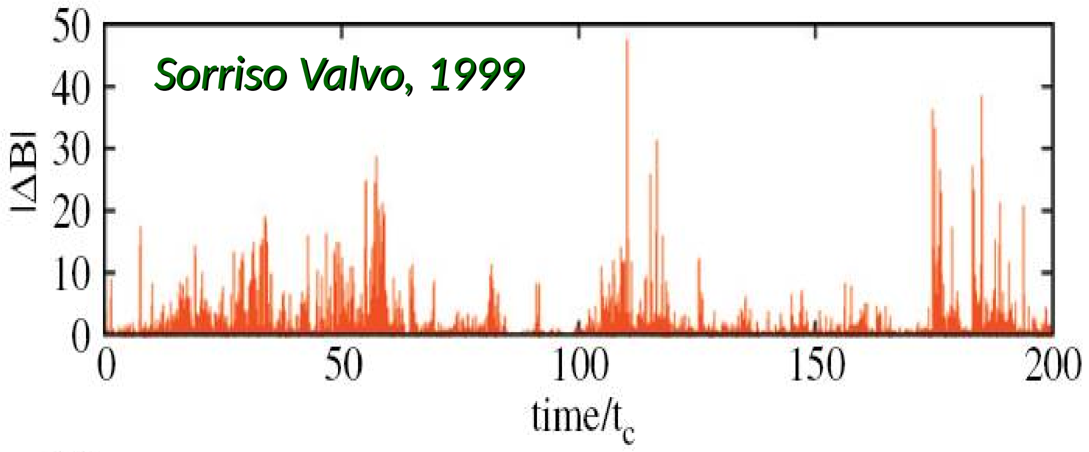
- A plasma is a ionized gas where charged particles interact via electromagnetic forces
- More than 99.9 % of matter in the Universe can be considered as a plasma
- Plasma is mostly collisionless
- Observations are somehow limited



Turbulence in space plasmas



Solar wind is turbulent and intermittent



Most of the plasma energization (plasma heating and particle acceleration) occurring in turbulent collisionless plasmas, such as those permeating the solar system is expected to occur at kinetic scales (scales ~ particle gyroradii and below)

How are plasmas heated and particle accelerated?

Temperature anisotropy in space plasmas

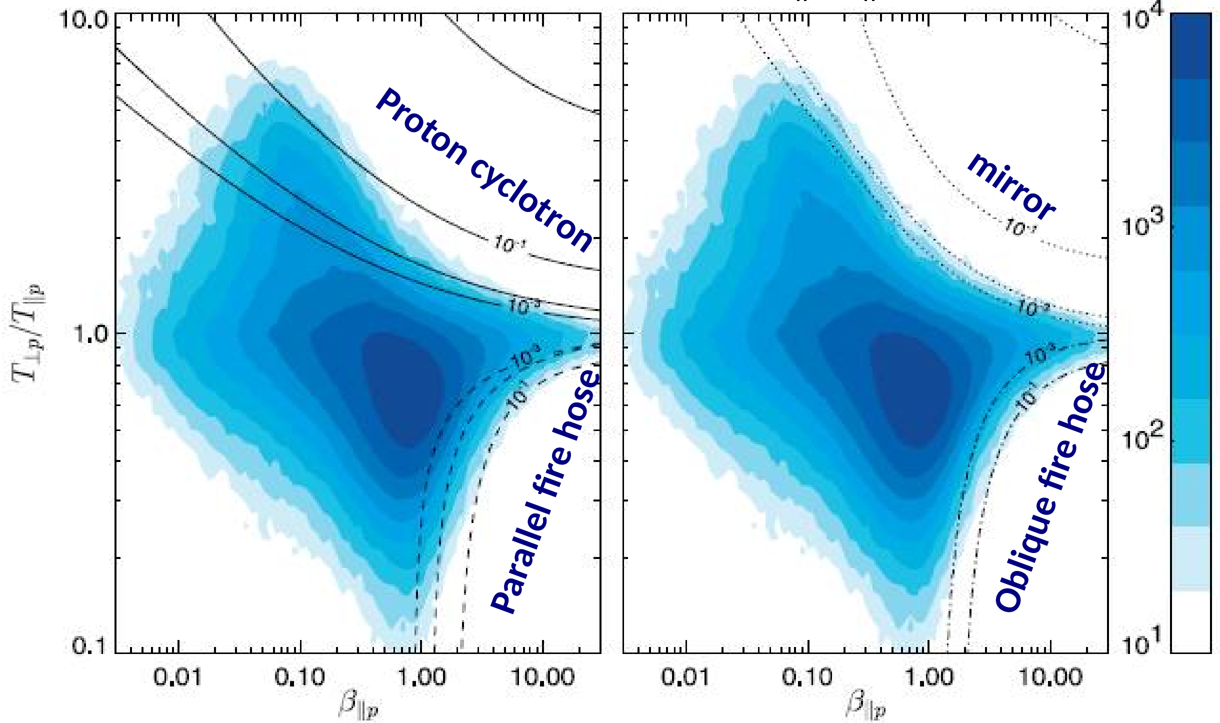
$$\Pi(\mathbf{x},t)=m\int\int\int[\mathbf{v}-\mathbf{V}_{bulk}(\mathbf{x},t)][\mathbf{v}-\mathbf{V}_{bulk}(\mathbf{x},t)]f(\mathbf{x},\mathbf{v},t)\,d^3v$$

$$\Pi=p_\perp I+(p_{\|}-p_\perp)\mathbf{b}\,\mathbf{b}$$

$$\mathbf{b}=\frac{\mathbf{B}}{|\mathbf{B}|}$$

$T_{||}$ and $T_\perp \equiv$
parallel and perpendicular proton temperatures with respect to the ambient *B*

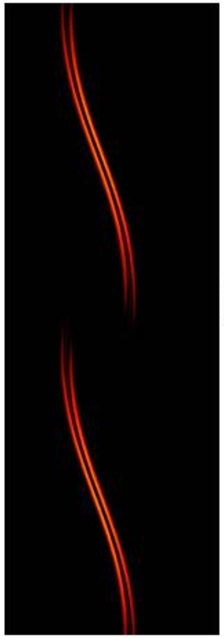
Distribution PDF($T_\perp/T_{||}$, $\beta_{||}$)



Hellinger et al. GRL (2006);
Kasper et al. JGR (2006);
Kasper et al., (2002)

Kinetic instabilities influence the solar wind → **Astrophysical plasmas are turbulent, intermittent and show many kinetic (non-fluid) phenomena** → **We need simulations!**

Simulations of Plasma Turbulence



Karimabadi et al, PoP, 2013

Kinetic equations for a collisionless plasma

The Vlasov-Maxwell system

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{v}\cdot\nabla f_\alpha + \frac{q_\alpha}{m_\alpha}\left[\mathbf{E} + \frac{\mathbf{v}\times\mathbf{B}}{c}\right]\cdot\nabla_v f_\alpha = 0 \longrightarrow f_\alpha = f_\alpha(\mathbf{x},\mathbf{v},t)$$

$$\int f_\alpha(\mathbf{x},\mathbf{v},t)d\mathbf{x}d\mathbf{v} = N_\alpha$$

$$\nabla\cdot\mathbf{B} = 0$$

$$\nabla\cdot\mathbf{E} = 4\pi\sum_\alpha q_\alpha\int f_\alpha(\mathbf{x},\mathbf{v},t)d\mathbf{v}$$

$$\nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t}$$

$$\nabla\times\mathbf{B} = \frac{4\pi}{c}\sum_\alpha q_\alpha\int \mathbf{v}f_\alpha(\mathbf{x},\mathbf{v},t)d\mathbf{v} + \frac{1}{c}\frac{\partial\mathbf{E}}{\partial t}$$

6D + time!

Two numerical philosophies

Method 1: the Eulerian approach

The Vlasov equation is solved directly for the particle distribution function, on a phase space grid. Moments (density and current) are evaluated by direct integration of the distribution function

- Zero noise
- Very computationally demanding because of memory limitations

Method 2: the Lagrangian approach

Vlasov is solved via a *Montecarlo* technique. The equations of motion of a large number of (macro) particles are solved and the distribution function is reconstructed. Maxwell equations are evaluated on a grid, through interpolation

- Very cheap from the computational point of view
- Numerical noise

We will use both methods, depending on the problem that we want to study. We will start with Method 1

Method 1: Eulerian

Full Vlasov–Maxwell

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{v}\cdot\nabla f_\alpha + \frac{q_\alpha}{m_\alpha}\left[\mathbf{E} + \frac{\mathbf{v}\times\mathbf{B}}{c}\right]\cdot\nabla_v f_\alpha = 0$$

$$\nabla\cdot\mathbf{B} = 0$$

$$\nabla\cdot\mathbf{E} = 4\pi\sum_\alpha q_\alpha\int f_\alpha(\mathbf{x},\mathbf{v},t)d\mathbf{v}$$

$$\nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t}$$

$$\nabla\times\mathbf{B} = \frac{4\pi}{c}\sum_\alpha q_\alpha\int \mathbf{v} f_\alpha(\mathbf{x},\mathbf{v},t)d\mathbf{v} + \frac{1}{c}\frac{\partial\mathbf{E}}{\partial t}$$

- Nonlinear integro-differential equation in 6D phase space + time
- Very hard and time demanding to solve numerically!
- To date, numerical solutions are available for approximated, reduced systems

easier

Hybrid Vlasov–Maxwell

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f + \frac{e}{m}\left[\mathbf{E} + \frac{\mathbf{v}\times\mathbf{B}}{c}\right]\cdot\nabla_v f = 0$$

$$\mathbf{E} = -\frac{\mathbf{u}\times\mathbf{B}}{c} + \frac{1}{nec}(\mathbf{j}\times\mathbf{B}) - \frac{1}{ne}\nabla P_e$$

$$\nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t}$$

$$\nabla\times\mathbf{B} = \frac{4\pi\mathbf{j}}{c}$$

$$n_e \simeq n_i \simeq n$$

$$P_e = P_e(n)$$

easier

1D-1V Vlasov–Poisson

$$\frac{\partial f_e}{\partial t} + v\frac{\partial f_e}{\partial x} - \frac{eE}{m}\frac{\partial f_e}{\partial v} = 0$$

$$\frac{\partial E}{\partial x} = 4\pi e\left[n_0 - \int f_e(x,v,t)dv\right]$$

Numerical technique for Eulerian-Vlasov

Vlasov equation is an advection equation in phase space

- Let us consider the 1D-1V case (we will discuss later the generalization to full phase space)

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + a\frac{\partial f}{\partial v} = \frac{\partial f}{\partial t} + \frac{\partial (vf)}{\partial x} + \frac{\partial (af)}{\partial v} = 0$$

$$f = f(x,v,t); \quad a = a(x)$$

- Let us focus on advection in *x* first (later we will discuss how to couple it to advection in *v*)

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0$$

$$f = f(x,t); \quad x \in [0,L]; \quad t \in [0,T]; \quad v = const.$$

$$f(x,0) = f_0(x); \quad f(0,t) = f(L,t), \ \ \forall t \in [0,T]$$

For simplicity, periodic boundary conditions

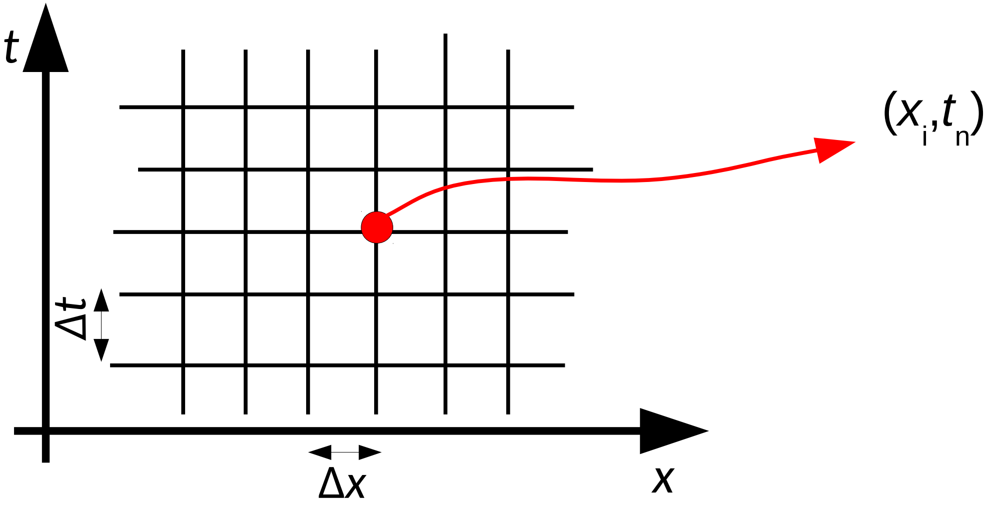
Three main steps:

1) Discretize (*x*,*t*) plane

2) Approximate derivatives in discretized plane (allowed operations are +,-,*x*,/)

3) Create algorithm to solve the equation

Spatial derivatives



Discretization:

$$x_i = (i-1)\Delta x; \quad i = 1, \cdots, N_x; \quad \Delta x = \frac{L}{N_x}$$

$$x_0 = 0, \quad x_{N_x} = L - \Delta x$$

$$t_n = n\Delta t; \quad n = 0, \cdots, N_t; \quad \Delta t = \frac{T}{N_t}$$

$$t_0 = 0, \quad t_{N_t} = T$$

Derivatives approximation (finite differences):

$$f(x_{i+1}) = f(x_i) + \Delta x \left(\frac{df}{dx}\right)_{x_i} + \frac{1}{2}\Delta x^2 \left(\frac{d^2 f}{dx^2}\right)_{x_i} + \frac{1}{3!}\left(\frac{d^3 f}{dx^3}\right)_{x_i} + o(\Delta x^4) \qquad (1)$$

$$f(x_{i-1}) = f(x_i) - \Delta x \left(\frac{df}{dx}\right)_{x_i} + \frac{1}{2}\Delta x^2 \left(\frac{d^2 f}{dx^2}\right)_{x_i} - \frac{1}{3!}\left(\frac{d^3 f}{dx^3}\right)_{x_i} + o(\Delta x^4) \qquad (2)$$

Euler forward

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} + o(\Delta x)$$

Euler backward

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f(x_i) - f(x_{i-1})}{\Delta x} + o(\Delta x)$$

$$(1) - (2) \Rightarrow \left(\frac{df}{dx}\right)_{x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + o(\Delta x^2)$$

$$(1) + (2) \Rightarrow \left(\frac{d^2 f}{dx^2}\right)_{x_i} = \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{\Delta x^2} + o(\Delta x^2)$$

} Centered differences

Phase error for finite differences

Let's consider the centered difference scheme:

$$\left(\frac{df}{dx}\right)_{x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + o(\Delta x^2)$$

Let's take for example:

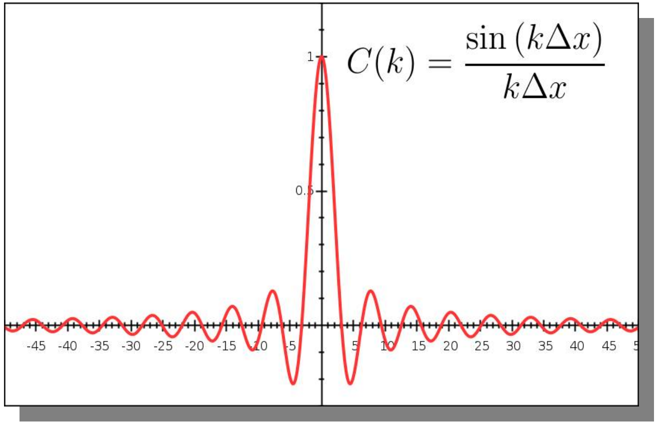
$$f(x) = \sin(kx) \Rightarrow f'(x) = k\cos(kx) \Rightarrow f'(x_i) = k\cos(kx_i)$$

By applying centered-difference formula one gets:

$$f'(x_i)^{num} = \frac{\sin[k(x_i+\Delta x)] - \sin[k(x_i-\Delta x)]}{2\Delta x} = \cos(kx_i)\left[\frac{\sin(k\Delta x)}{k\Delta x}\right] = C(k)f'(x_i)$$

When solving advection equations through finite difference schemes:

$$\frac{\partial f}{\partial t} + v\,C(k)\frac{\partial f}{\partial x} = 0$$



Keep phase error under control!

A naive try....

Explicit finite difference scheme

Euler forward — Centered

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = -v\left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}\right)$$

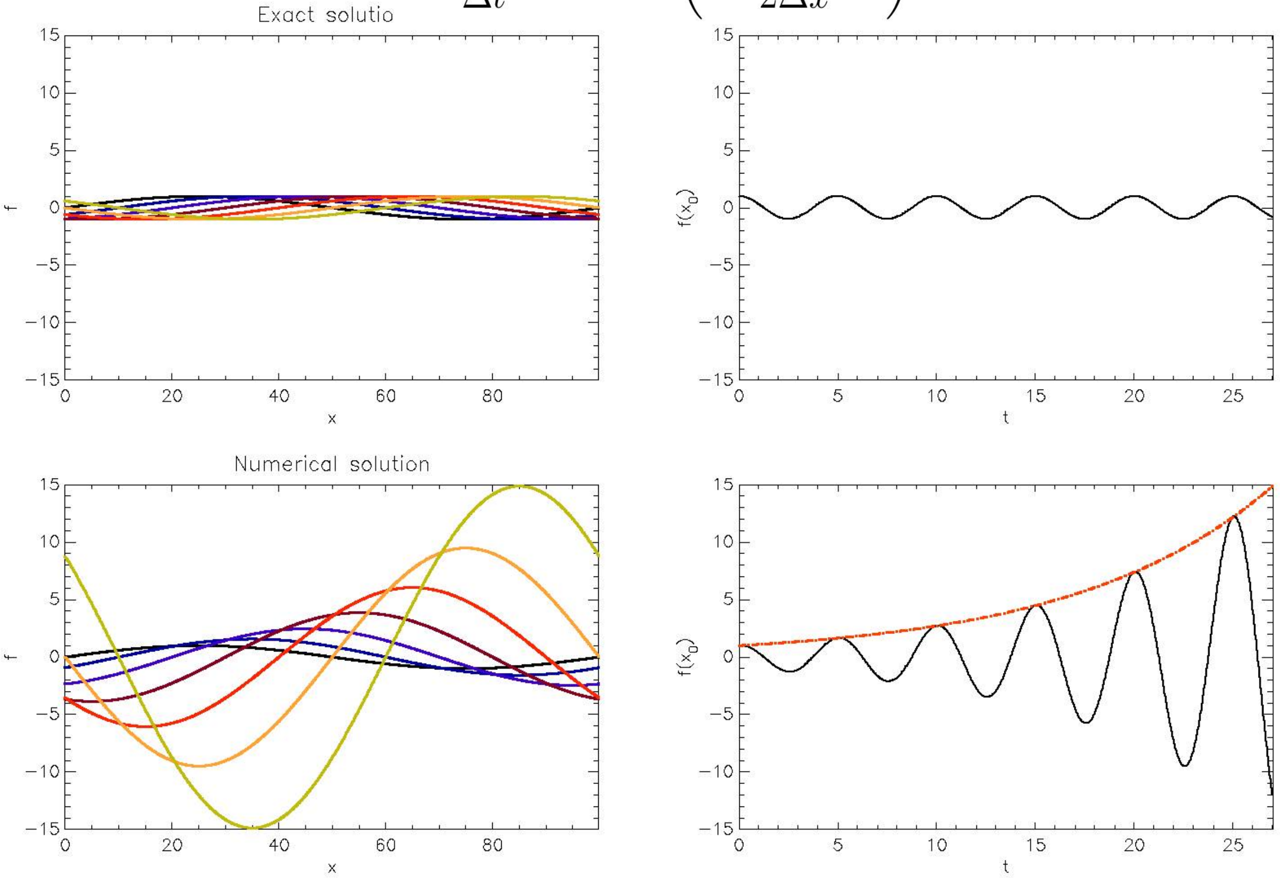
$$f_i^{n+1} = f_i^n - v\Delta t\left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}\right), \quad \forall i = 1, \cdots, N_x$$

A naive try → numerical instabilities

Explicit finite difference scheme

$$\frac{f_i^{n+1}-f_i^n}{\Delta t} = -v\left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}\right)$$

Different times in sequence (*black*, *blue*, .., *yellow*)→ (t_0, t_1, ..., t_N)



Something weird is going on, numerical solution is out of control!

Von Neumann stability analysis (1)

- Let us perform an analysis of the finite difference scheme by expressing the solution as a Fourier series

- Since the equation is linear, we only examine the behavior of a single mode. Consider a trial solution of the form

$$f^n(x_i)=\sum \hat{f}^n(k)e^{jkx_i}=\hat{f}^n(k)e^{ijk\Delta x} \quad \Rightarrow \quad f_i^n=\hat{f}^n e^{jik\Delta x}$$

- This is a spatial Fourier expansion. Plugging in the difference formula:

$$\hat{f}^{n+1}=\hat{f}^n-\frac{C}{2}\hat{f}^n\left(e^{jik\Delta x}-e^{jik\Delta x}\right); \quad C=\frac{v\Delta t}{\Delta x}$$

- Let us define the amplification Factor as:

$$A=\left|\frac{\hat{f}^{n+1}}{\hat{f}^n}\right|^2$$

A method is well-behaved or stable when A ≤ 1

Von Neumann stability analysis (2)

For our “forward-central scheme” one gets

$$A = [1 - jC\sin(k\Delta x)]^2 = 1 + C^2 \sin(k\Delta x)^2 \leq 1$$

Independently of the CFL number, all Fourier modes increase in magnitude as time advances
This method is unconditionally unstable...
We are in trouble!

Let us play a bit with our scheme

$$f_i^{n+1} = f_i^n - v\Delta t \left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}\right), \quad \forall i = 1, \cdots, N_x$$

Replace by average

$$f_i^{n+1} = \frac{(f_{i+1}^n + f_{i-1}^n)}{2} - v\Delta t \left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}\right)$$

Lax–Wendroff method

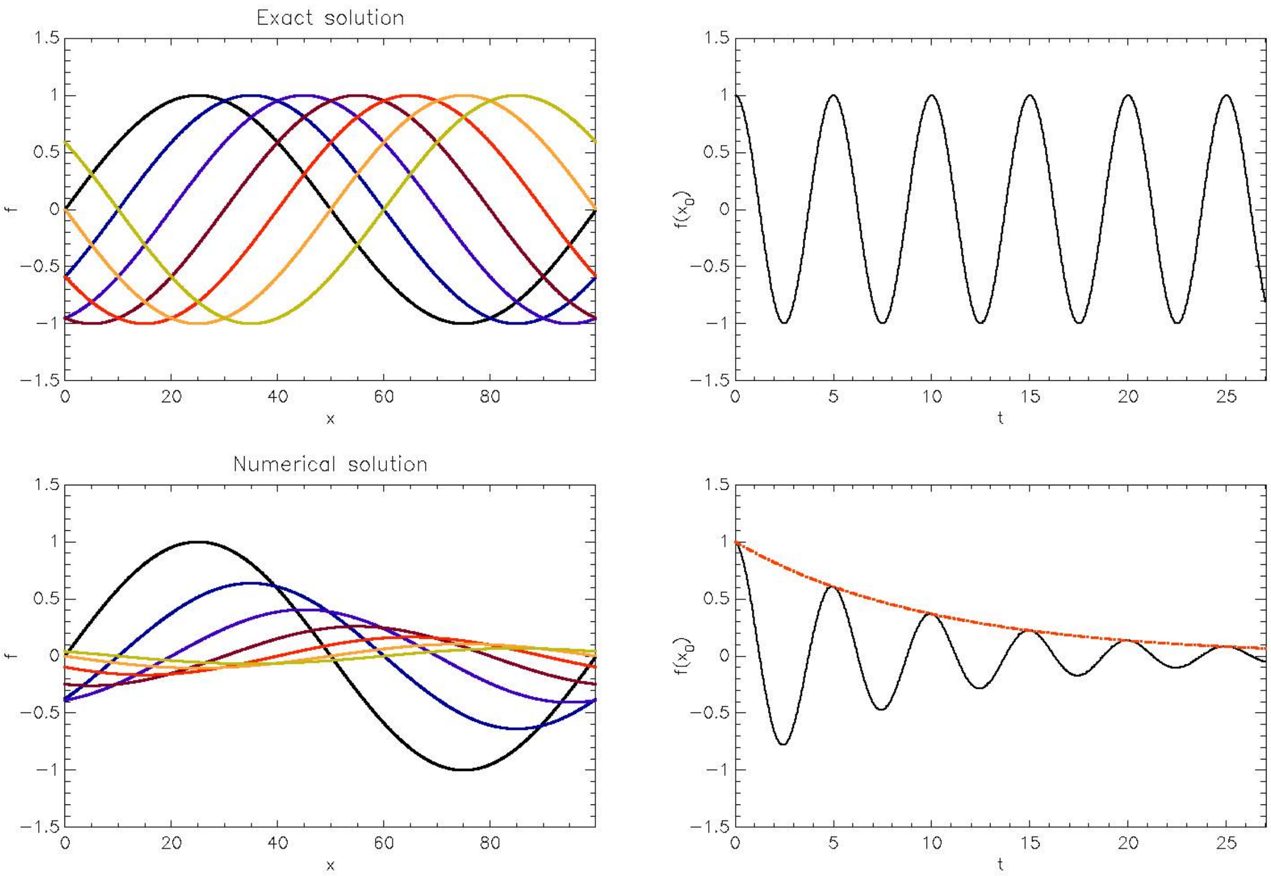
$$A \leq 1 \Rightarrow \Delta t \leq \frac{\Delta x}{|v|}$$

CFL stability condition

Check the CFL condition before running a simulation!

Lax-Wendroff solution

$$f_i^{n+1} = \frac{(f_{i+1}^n + f_{i-1}^n)}{2} - v\Delta t \left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} \right)$$



Signals are slowly decaying: What’s happening now?

Analysis of the Lax-Wendroff scheme

$$f_i^{n+1} = \frac{(f_{i+1}^n + f_{i-1}^n)}{2} - v\Delta t \left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} \right)$$

Rearranging the RHS

$$f_i^{n+1} = \frac{(f_{i+1}^n + f_{i-1}^n)}{2} - v\Delta t \left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} \right) + f_i^n - f_i^n \Rightarrow$$

$$\Rightarrow \quad f_i^{n+1} = \frac{(f_{i+1}^n + f_{i-1}^n - 2f_i^n)}{2\Delta x^2}\Delta x^2 - v\Delta t \left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} \right) + f_i^n \Rightarrow$$

$$\Rightarrow \quad \frac{f_i^{n+1} - f_i^n}{\Delta t} + v \left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} \right) - \frac{(f_{i+1}^n + f_{i-1}^n - 2f_i^n)}{2\Delta x^2} \frac{\Delta x^2}{\Delta t} = 0$$

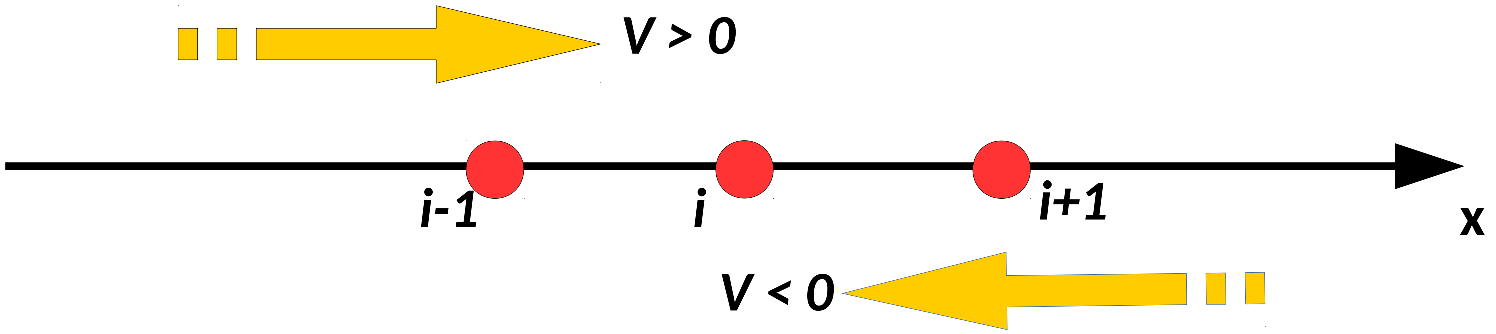
$$\Delta t,\ \Delta x \to 0$$

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - \nu \frac{\partial^2 f}{\partial x^2} = 0; \quad \nu = \frac{\Delta x^2}{2\Delta t}$$

We have an additional term!
We are not solving anymore the original equation

Check the consistency of an algorithm before running a simulation

Upwind schemes (first-order Godunov method)



$$f_i^{n+1} = f_i^n - |v|\Delta t\left(\frac{f_i^n - f_{i-1}^n}{\Delta x}\right), \qquad v > 0$$

$$f_i^{n+1} = f_i^n + |v|\Delta t\left(\frac{f_{i+1}^n - f_i^n}{\Delta x}\right), \qquad v < 0$$

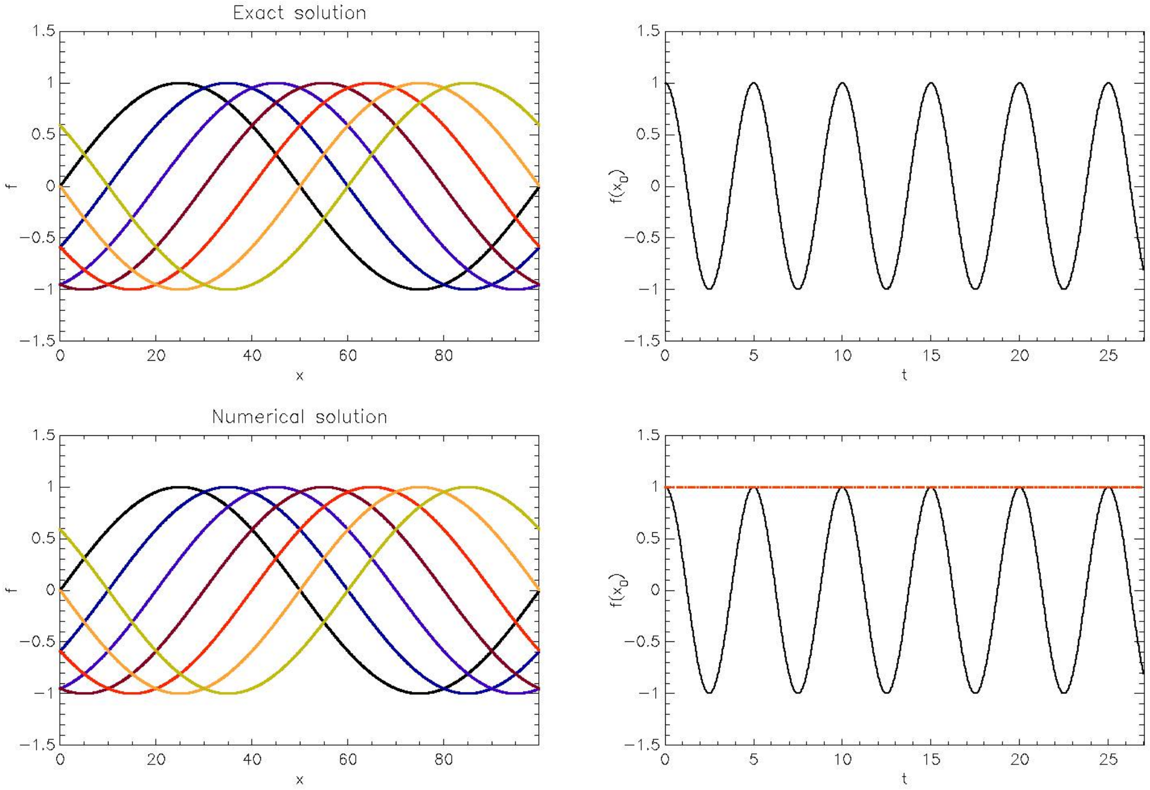
$$A \leq 1 \Rightarrow \Delta t \leq \frac{\Delta x}{|v|}$$

CFL stability condition

Upwind schemes (first-order Godunov method)

$$f_i^{n+1} = f_i^n - |v|\Delta t\left(\frac{f_i^n - f_{i-1}^n}{\Delta x}\right), \qquad v > 0$$

$$f_i^{n+1} = f_i^n + |v|\Delta t\left(\frac{f_{i+1}^n - f_i^n}{\Delta x}\right), \qquad v < 0$$



Upwind schemes work quite well!

Van Leer scheme (higher order accuracy)

Widely adopted for integration of the Vlasov equation

Van Leer, JCP, 1974, 1977a, 1977b, 1979; Mangeney+, JCP, 2000

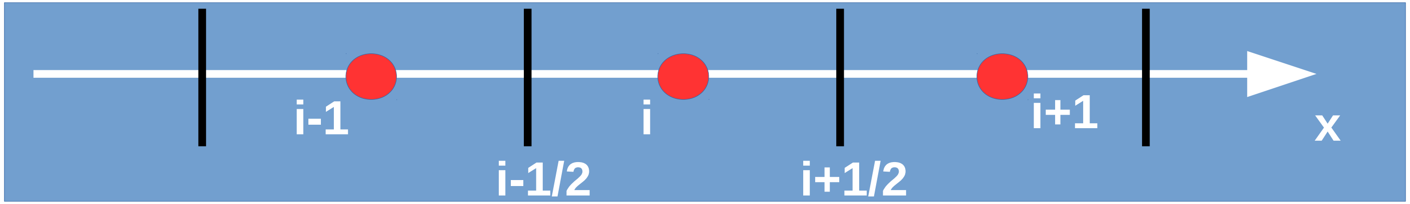
$$\bar{f}_i(t) = \frac{1}{\Delta x}\int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} f(x,t)\ dx$$

The unknowns are the spatial averages of the function itself

Averaging and integrating advection equation in time gives:

$$\bar{f}_i(t+\Delta t) = \bar{f}_i(t) - \frac{v\Delta t}{\Delta x}\int_t^{t+\Delta t} dt' \int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} \frac{\partial f(x,t')}{\partial x}\ dx =$$

$$= \bar{f}_i(t) - \frac{v\Delta t}{\Delta x}\int_t^{t+\Delta t} dt' \left[f\left(x_i+\frac{\Delta x}{2},t'\right) - f\left(x_i-\frac{\Delta x}{2},t'\right)\right]$$



Implicit scheme

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} = -v\left(\frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}\right)$$

Explicit scheme

$$\left.\frac{\partial f}{\partial t}\right|_{t_n} \quad forward \qquad \left.\frac{\partial f}{\partial t}\right|_{t_{n+1}} \quad backward$$

$$f_i^{n+1} = f_i^n - v\Delta t\left(\frac{f_{i+1}^{n+1} - f_{i-1}^{n+1}}{2\Delta x}\right) \Rightarrow$$

$$\left(-\frac{v\Delta t}{2\Delta x}\right) f_{i-1}^{n+1} + f_i^{n+1} + \left(\frac{v\Delta t}{2\Delta x}\right) f_{i+1}^{n+1} = f_i^n$$

LHS: Linear combination of unknowns: **fully implicit schemes**

Implicit schemes

$$-\alpha f_{i-1}^{n+1} + f_i^{n+1} + \alpha f_{i+1}^{n+1} = f_i^n; \quad \forall i = 1, \cdots, N_x; \quad \alpha = \frac{v\Delta t}{\Delta x}$$

$$\left(M \right) \left(f_i^{n+1} \right) = \left(f_i^n \right)$$

The solution for *f* at step *n+1* is obtained by solving this linear system, through standard linear algebra routines

Example: N_x=6 and periodic boundary conditions

$$M = \begin{bmatrix} 1 & \alpha & 0 & 0 & 0 & -\alpha \\ -\alpha & 1 & \alpha & 0 & 0 & 0 \\ 0 & -\alpha & 1 & \alpha & 0 & 0 \\ 0 & 0 & -\alpha & 1 & \alpha & 0 \\ 0 & 0 & 0 & -\alpha & 1 & \alpha \\ \alpha & 0 & 0 & 0 & -\alpha & 1 \end{bmatrix}$$

M is a tridiagonal matrix with full corners

Fully implicit schemes are unconditionally STABLE!
... but there is a big matrix to invert!

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Phase space integration: the splitting scheme

Let's go back to our 1D-1V Vlasov equation

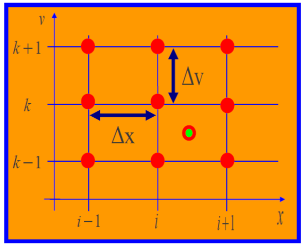
$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + a\frac{\partial f}{\partial v} = \frac{\partial f}{\partial t} + \frac{\partial (vf)}{\partial x} + \frac{\partial (af)}{\partial v} = 0$$

$$f = f(x,v,t); \quad a = a(x)$$

Now we know how to solve advection equations. Let's split the evolution in 2 parts:

$$\frac{\partial f_x}{\partial t} + v\frac{\partial f_x}{\partial x} = 0 \qquad f_x(t+\Delta t) = \Lambda_x(\Delta t) f_x(t)$$

$$\frac{\partial f_v}{\partial t} + a\frac{\partial f_v}{\partial v} = 0 \qquad f_v(t+\Delta t) = \Lambda_v(\Delta t) f_v(t)$$



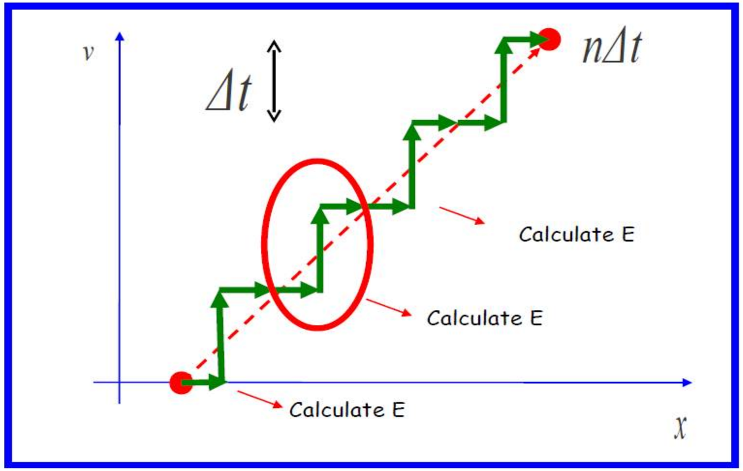
Couple f_x*(x,t)* and f_v*(x,t)* to get a solution for *f(x,v,t)*:

$$f(n\Delta t) = \{\Lambda_x(\Delta t/2)\Lambda_v(\Delta t)\Lambda_x(\Delta t/2)\}^n f_0 + o(\Delta t^3)$$

The splitting scheme

Cheng & Knorr, JCP, 1976;

Generalized to 6D in *Mangeney et al. JCP, 2000*



Take-home messages from Part I

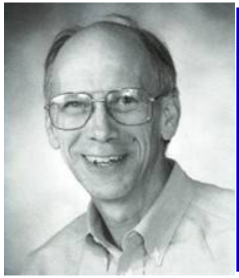
- Equations that describe the plasma in a self-consistent way are very complex and computationally demanding

- There are two approaches to study plasma dynamics: the Eulerian (solve Eq.s for the distribution function) and the Lagrangian approach (solve equations for particles)

- Basic numerical scheme do not work properly. Test your scheme BEFORE running "important simulations"

- Advanced, high order methods give satisfactory results

- Numerical simulations are complementary to observational data. Understanding the reality cannot rely on simulations or observation alone, comprehension is given by a right balance among the two.



"Calculators can only calculate - they cannot do mathematics."

J. A. Van de Walle