On the role of domain discretization in phase-mixing Hamiltonian systems

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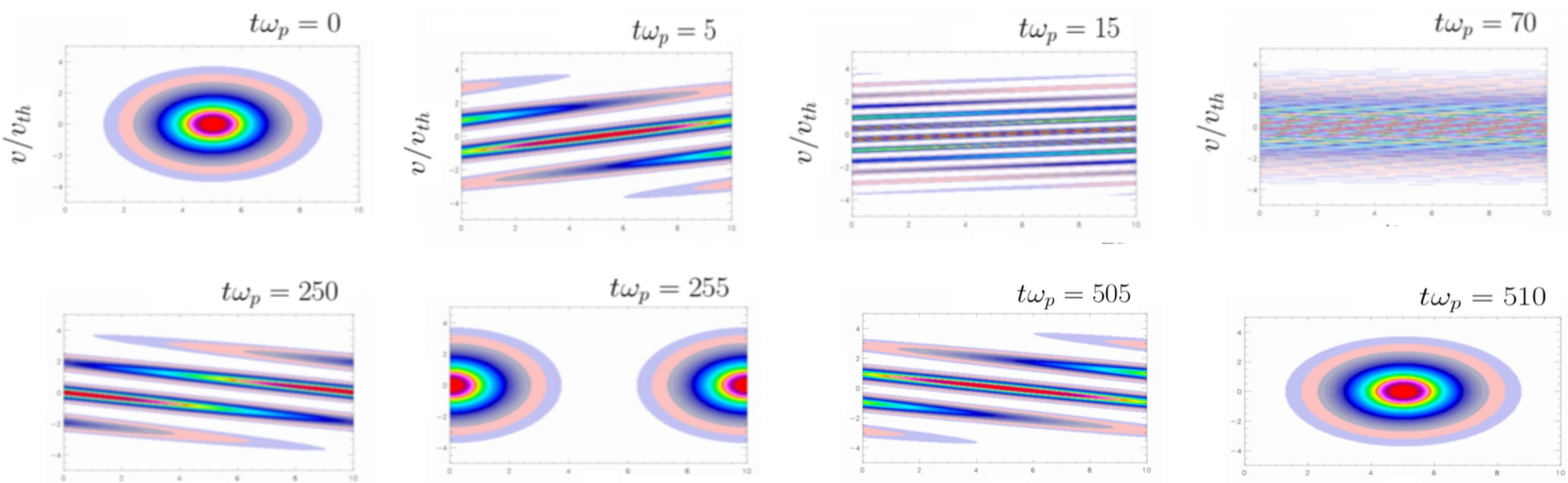
Institut Jean Lamour

Motivation : what about recurrence in Hamiltonian systems ?

- *Poincare recurrence in a free advection problem in 1D-1V phase-space*



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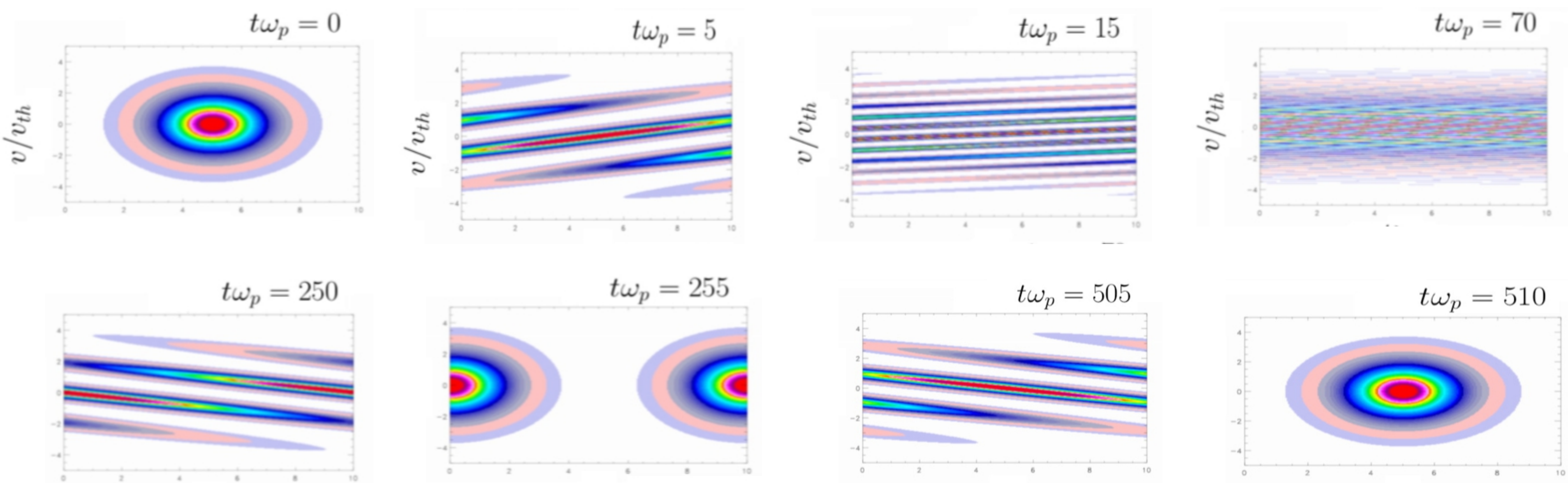

- *Poincare recurrence theorem*

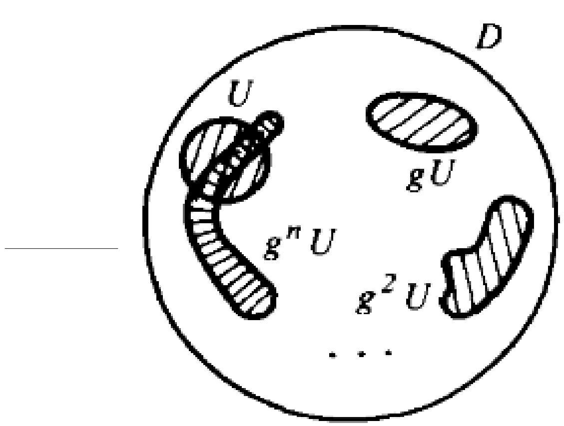

Figure 51   Theorem on returning

PROOF OF POINCARÉ'S THEOREM. We consider the images of the neighborhood U (Figure 51):

$$U, gU, g^2U, \ldots, g^nU, \ldots$$

All of these have the same volume. If they never intersected, D would have infinite volume. Therefore, for some $k \geq 0$ and $l \geq 0$, with $k > l$,

$$g^kU \cap g^lU \neq \varnothing.$$

Therefore, $g^{k-l}U \cap U \neq \varnothing$. If y is in this intersection, then $y = g^nx$, with $x \in U (n = k - l)$. Then $x \in U$ and $g^nx \in U (n = k - l)$. □

[Mathematical Methods of Classical Mechanics, V.I. Arn'old, Springer (1978); 1st edition (1974)]

Relevance of Poincare's recurrence to Hamiltonian flows...

$$\nabla = \begin{pmatrix} \dfrac{\partial}{\partial q} \\ \\ \dfrac{\partial}{\partial p} \end{pmatrix} \qquad \mathbf{V} = \begin{pmatrix} \dot{q} \\ \\ \dot{p} \end{pmatrix} \qquad \partial_t f + \mathbf{V} \cdot \nabla f = 0$$

In Hamiltonian systems => Liouville's theorem $\nabla \cdot \mathbf{V} = 0$

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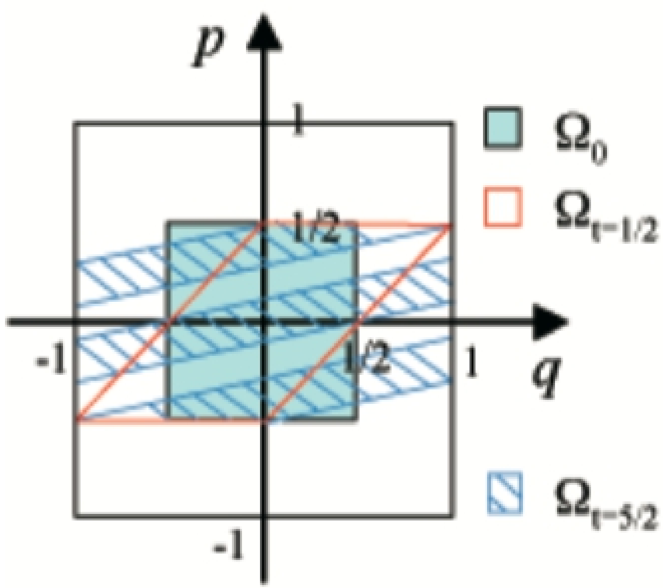
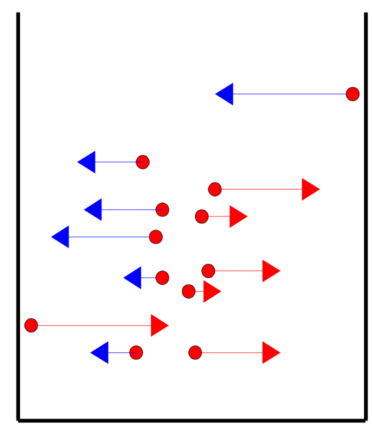
..and a classical exercise of statistical mechanics



$\simeq$

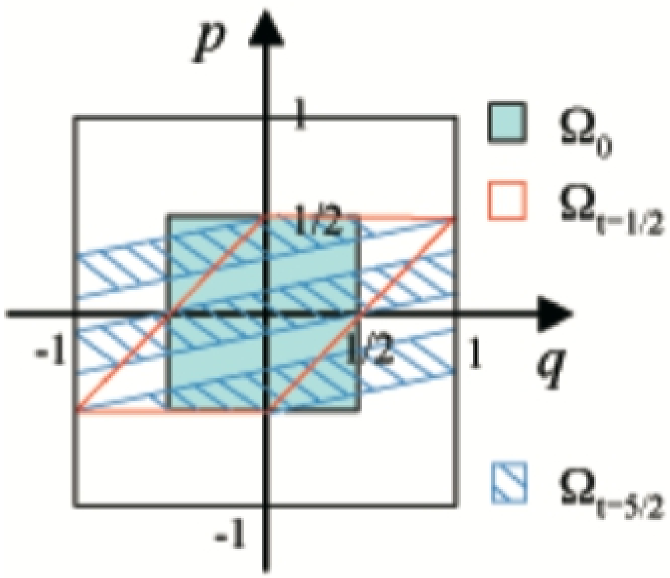


$$\dot{q} = \frac{p}{m}$$

$$\left\{ \begin{array}{l} \dot{p} = 0 \\ p \rightarrow -p \\ \text{(reflecting walls)} \end{array} \right.$$

[see ex. 3.5, p.72 in Statistical Mechanics, K. Huang, Wiley & Sons (1987);]

Free advection in the continuum model : no recurrence



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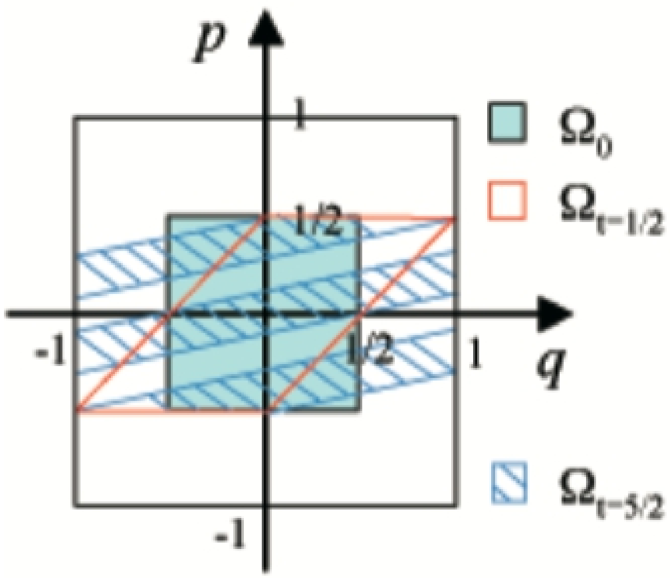
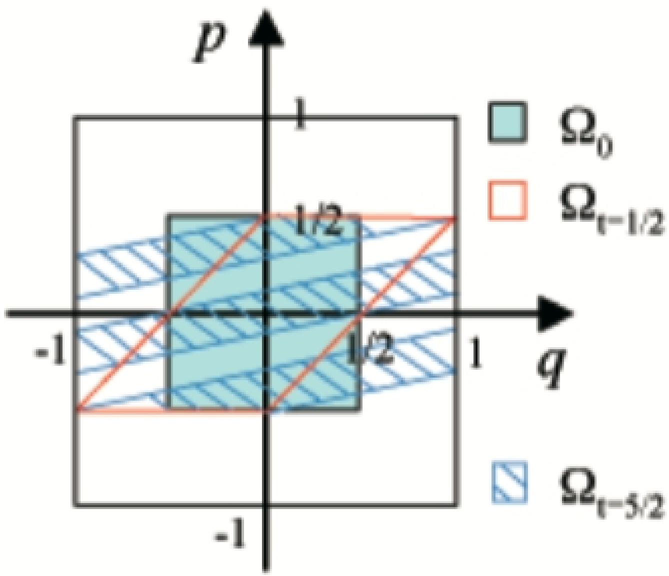


$$\partial_t f + \mathbf{V}\cdot\nabla f = 0 \quad \Rightarrow \quad \frac{\omega}{k} = V = \frac{p}{m}$$

$$\hat{f}(\omega, k; p) = \int_{-L_q/2}^{L_q/2} dq \int_0^{\infty} dt c^{i(\omega t - kq)} f(q, p, t)$$

Free advection in the continuum model : no recurrence



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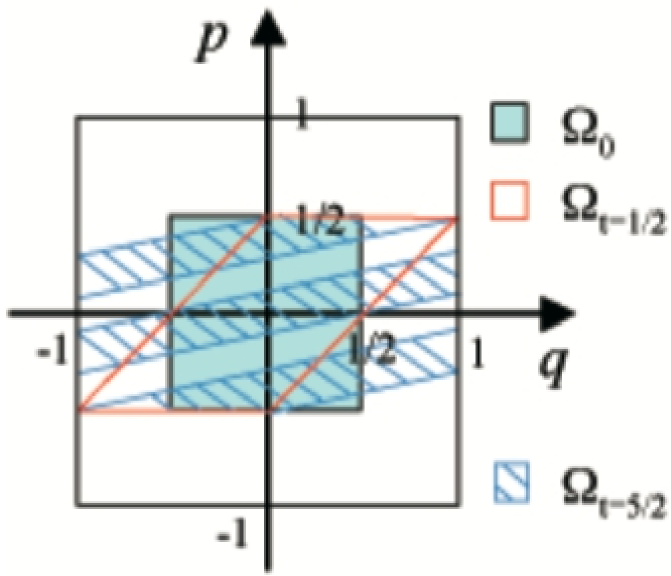
Filamentation
in momentum
space

Free advection in the continuum model : no recurrence



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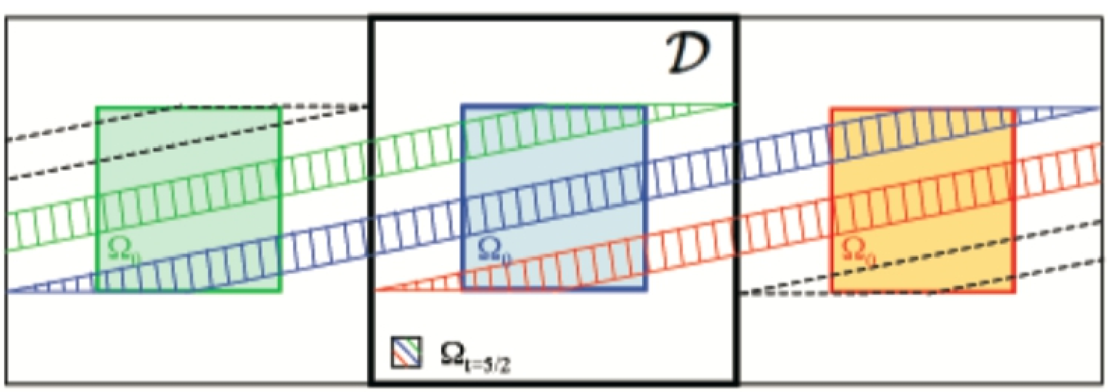
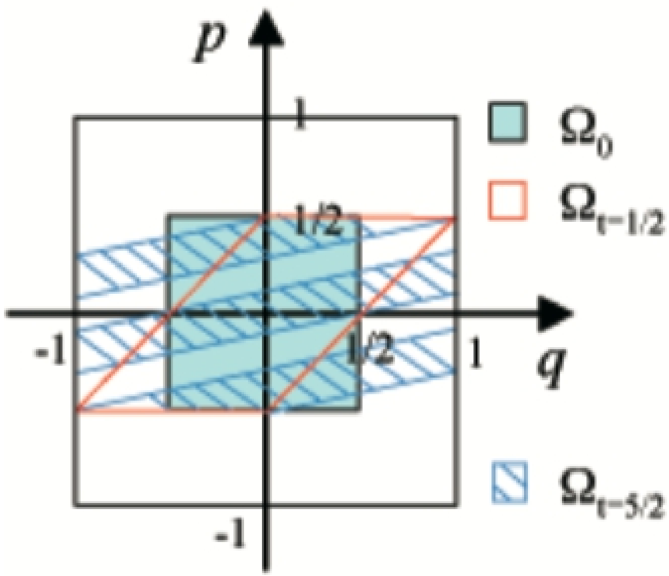
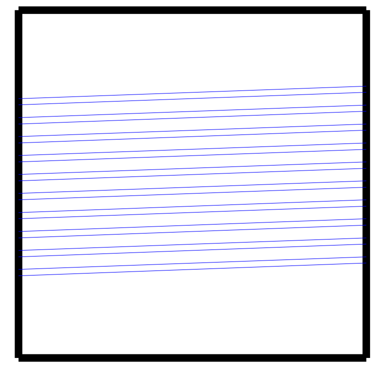
Filamentation in momentum space



Free advection in the continuum model : no recurrence



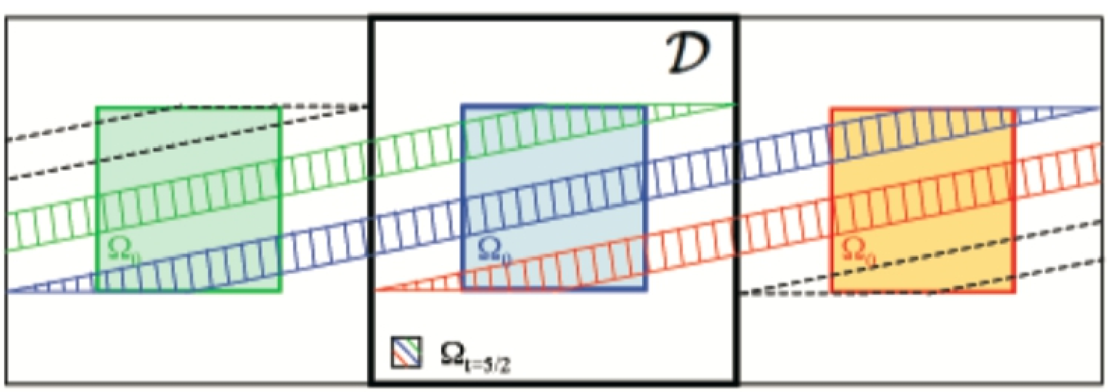
$t \to \infty$

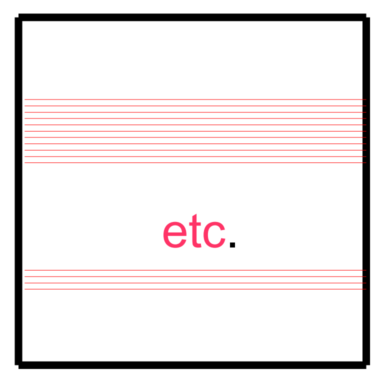


$\Omega_{t\to\infty}$

$\alpha \sim 1/t$

$\neq$





$\Omega_{t=\infty}$

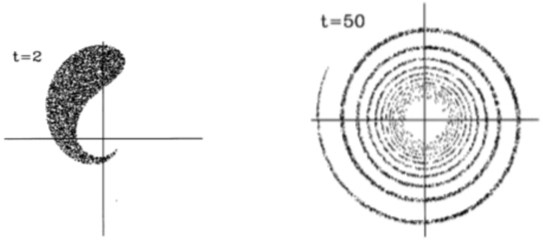
$\alpha = 0$

Some characterization of the phase-mixing process

- *Some essential features of filamentation and its role on phase-mixing have been already discussed by [Lynden-Bell, MNRAS 1962],[S Tremaine, MNRAS 1999] . Phase-mixing "per se" has been mostly discussed in terms of the so-called "mixing theorem" and of its consequences for relaxation toward equilibrium states (e.g., [S. Tremaine et al., MNRAS 1986], [W. Dehnen, MNRAS 2005])*

  I. *Mixing theorem (Tremaine et al., 1986)*

  II. *Decrease of effective dimension (Tremaine 1999)*



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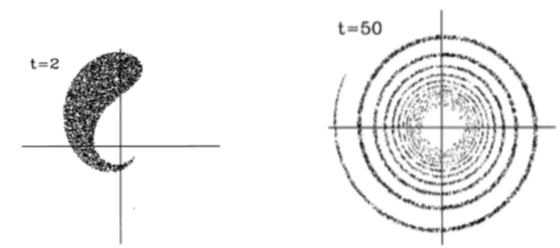
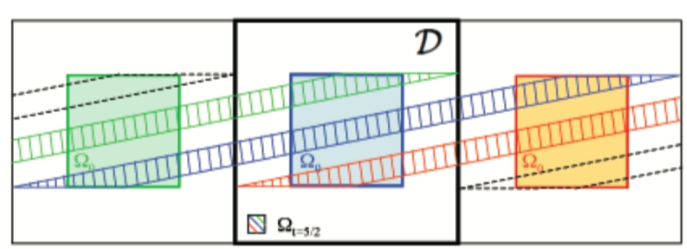


- *Here we find more useful to distinguish between "filamentation" (small scale generation) and what we can name "spatial folding" (bounded domain required)*

  - *"filamentation"* ⟶ *"kinematic cooling"*

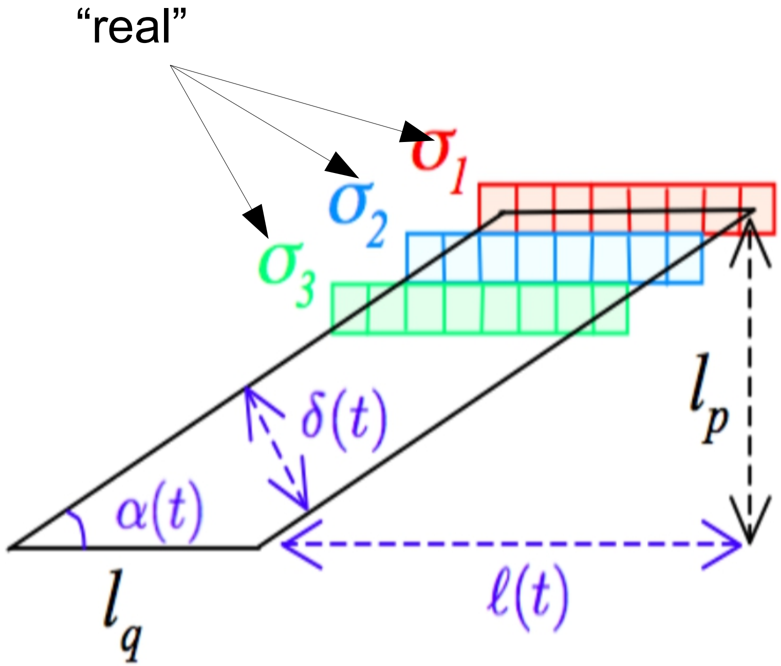
    (introducing ensemble averages with respect to q and p, a Temperature $T_{f,L}$ can be defined)

  - *"spatial folding"* ⟶ *"kinematic heating"*

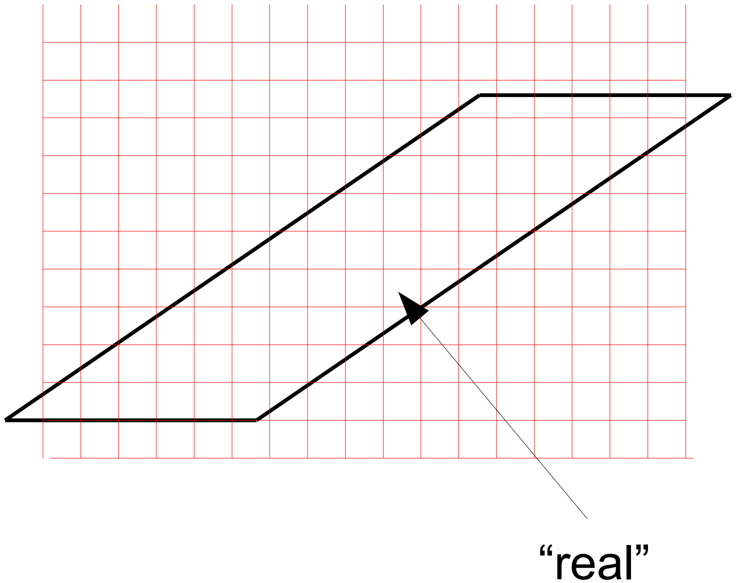


Free advection in the discrete model :
How is discretization done ?

Discretization of the distribution
(*"Lagrangian" discretization:*
PIC-like)



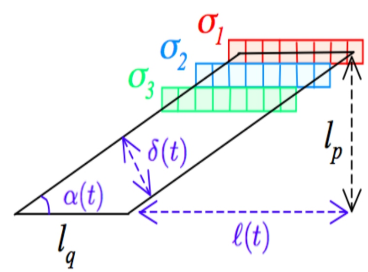
Discretization of the domain
(*"Eulerian" discretization:*
Non-particle codes)



Discretization in the Lagrangian framework : consequences

$$\delta q \neq 0$$

$$\delta p \neq 0$$

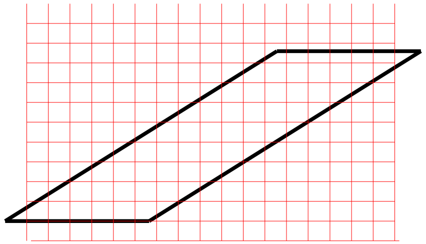


- *Recurrence is* made *possible, with period* $\tau_r = \dfrac{(2mL_q)^{N_p}}{\mathrm{lcm}\{\prod_j^{N_p} p_j\}}$
- Topological connection can be violated (but that's also why PIC codes are “good” for particle acceleration)
- A “metric Coarse Graining” (in the sense of [A.N. Gorban (2006)]) takes place, which can be generally associated to some kind of collisional dissipation (no entropy increase if particle collisions are disregarded by assuming them “transparent one to each other”).
- *Kinematic cooling due to filamentation is halted after* $t \sim ml_q / \delta p$ since

$$\min\{T_{f,L}\} = \frac{\delta p^2}{12 m k_B}$$

(“thermal noise” introduced by momentum discretization*)*

Discretization in the Eulerian framework : consequences



- *N.B. : Some kind of numerical smoothing is required once sub-grid filaments are generated*

"Eulerian Coarse Graning" required

- Exact *recurrence is in principle forbidden*: an "error" in returning exists, which is related to the excess mass function (first introduced by [Tremaine et al. MNRAS 1986] to measure the amount of mixing)

$$D[f] \equiv \int_{\bar{f}>f} (\bar{f}(q,p,t) - f(q,p,t))dqdp,$$

- Topological connection is respected (cf. filamentation problems in non-particle Vlasov codes)

- A "measure (or Ehrenfest's) Coarse Graining" (see [A.N. Gorban (2006)]) takes place. The role and form of coarse graining depends on the kind of "smoothing" (i.e. "average" over a cell) which has been chosen. *It always implies a loss of information and an entropy increase*, which also depends on the rate at which the measure CG is performed ([Gorban, PRE (2001), [Dhenen, MNRAS 2005]])

- A "*thermal noise*" of different nature with respect to the Eulerian case can take place once sub-grid filaments are generated but it *depends on the "rate of thinning" of the filaments.* It always introduces what we can call a "*measure heating*". A minimum kinetic temperature is nevertheless defined by the grid and is, again:

$$\min\{T_{f,L}\} = \frac{\delta p^2}{12 m k_B}$$

Some implications for PIC and non-particle Vlasov models

$$\frac{\partial}{\partial t} f(\boldsymbol{x},\boldsymbol{v},t) + \boldsymbol{v} \cdot \frac{\partial}{\partial \boldsymbol{x}} f^\alpha(\boldsymbol{x},\boldsymbol{v},t) + \frac{q^\alpha}{m^\alpha}\left(\boldsymbol{E} + \frac{\boldsymbol{v}\times\boldsymbol{B}}{c}\right) \cdot \frac{\partial}{\partial \boldsymbol{v}} f^\alpha(\boldsymbol{x},\boldsymbol{v},t) = \underbrace{o(g)}_{\to 0}$$

Discretization of the distribution
(*PIC codes*)

- *A finite, numerical $g_{PIC} \neq 0$ factor is intrinsically introduced by discretization :*
  [Feix & Bertrand, Tr. Th. Stat. Phys. 2005]

$$\boxed{g_{PIC} \equiv \left(n_{sp}(\delta q)^{D_q}\right)^{-1}}$$

- The general arguments about Lagrangian discretization apply

Discretization of the domain
(*Non-particle codes*)

- Although simulations are initialized with a formally $g_{Eul} = 0$ factor, a *$g_{Eul} \neq 0$ is generated because of sub-grid filamentation. It depends on the measure CG process.*

$$g_{Eul} = ?$$

- The general arguments about Eulerian discretization apply

Summary

- By distinguishing between *filamentation* and *spatial folding* we have pointed out the roles the two have in a phase-mixing processes, notably related to a *kinematic cooling* and to a *kinetic cooling*, respectively.
- By considering an ideal example, we have discussed some features which make *discretization of a Lagrangian and of an Eulerian domain different one from each other*, notably related to the t*wo different mechanisms of coarse graining* which take place in the two approaches.

Future work and perspectives

- Interesting implications for investigating the complementarety between PIC and non-particle codes → *more work required so to extend the analysis of the free advection case to*, e.g., the *Vlasov-Poisson system* (work in course of development..)

- A comparison between different kinds of "measure coarse graining" in non-particle Vlasov codes would be interesting → *use of AMR Vlasov-Poisson codes* [Deriaz & Periani,SIAM 2018] *and of semi-Lagrangian Vlasov code VLEM* [Sarrat, Ghizzo, Del Sarto, Serrat, EPJD 2017] (planned..)

References (wanna be...)

- D. Del Sarto, P. Bertrand, A. Ghizzo "Domain discretization, filamentation and Poincare recurrence in phase-mixing Hamiltoinan systems" – to be submitted to PRE
- "The Vlasov Equation I. History and General Properties", P. Bertrand, D. Del Sarto, A. Ghizzo, ISTE Editions 2019.
- "The Vlasov Equation III. Numerical Models", P. Bertrand, D. Del Sarto, A. Ghizzo, ISTE Editions – scheduled before end 2019.