Wavelet based density estimation for noise reduction in plasma simulation using particles

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Outline

- Introduction (physical point of view)
- Introduction (statistical point of view)
- WBDE
- Application to 1+1D Vlasov-Poisson
- Application to 2+2D Vlasov-Poisson (preliminary)
- Conclusion & Outlook

Introductions

Plasma simulation using particles

In hot plasmas **the collision frequency is low** with respect to a variety of interesting phenomena (including turbulence).

→ solve **Newton's equations**, with

simulated « mesoparticles » $N_p << N$ **ions and/or electrons**

To avoid $O(N_p^2)$ complexity, the charge and current have to be somehow **coarse-grained** before computing the electromagnetic fields.

Features of particle simulations

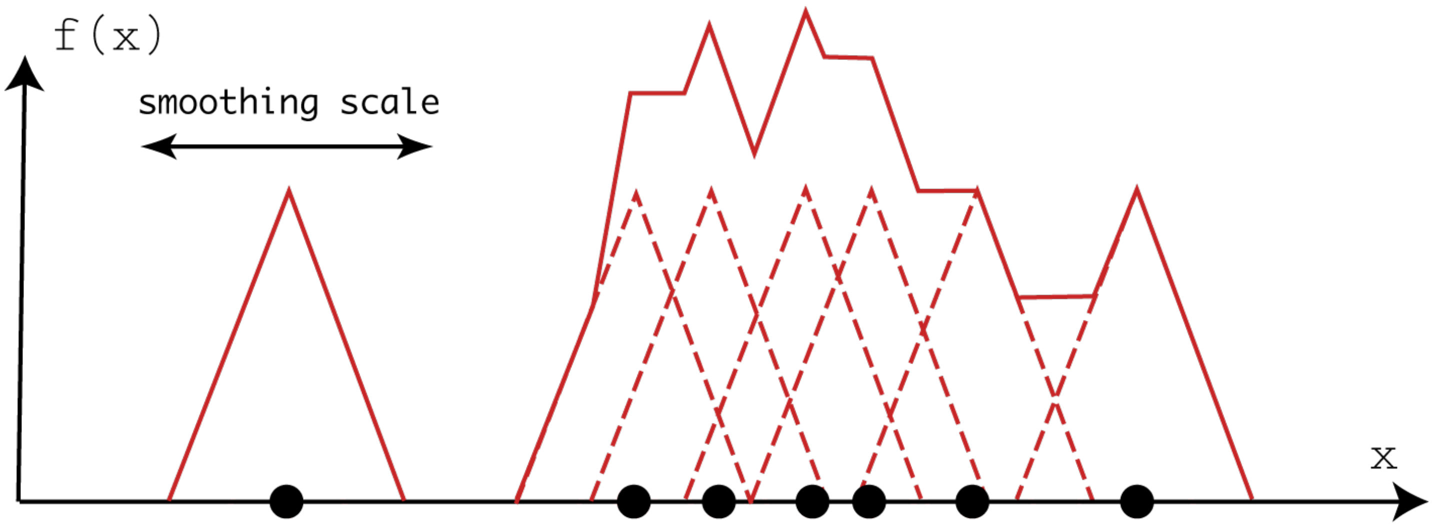
- N body problem $\rightarrow$ particle trajectories are not integrable,
- individual particle positions cannot be predicted,
- accurate predictions can only be expected for global quantities,
- we focus on the **single particle distribution function**, f.

A smoothness issue?

- The main source of numerical errors is the imperfect reconstruction of the EM fields (other source: time discretization),
- reconstruction is imperfect because there are not enough particles,
- in other words the estimated f is « rougher » than is should,
- hence the fields are themselves too rough/spiky, and the effective collisionality of the plasma is increased,
- we should smooth f to improve the simulation !
- (Note for later: the deterministic f can also have rough features that we want to keep.)

Finite size particles

- A better reconstruction of the EM fields can be obtained by assuming that the particles each represent a **cloud** of charge instead of a point charge,
- this will avoid artificial collisions, at the expense of loosing fine grained details of the PDF. (similar to LES)



The same story told from the statistical point of view

- in fact we are trying to to solve the Vlasov equation by discretizing it using a set of Lagrangian markers (**not physical particles!**),
- based on marker positions, we are looking for **the best candidate** for f
- since particle positions are likely to be “random” due to the chaotic dynamics, why not try

statistical estimation ?

Statistical independance hypothesis

- the interaction between markers has two effects of a very different nature :
  - collisionless effect : time evolution of f
  - “collisional effect” : build-up of correlations between positions of numerical particles (pair correlations + higher order)
- we assume that correlations remain small,

→ marker positions can be interpreted as independent realizations of a random variable with probability density f.

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→ marker positions can be interpreted as independent realizations of a random variable with probability density f.

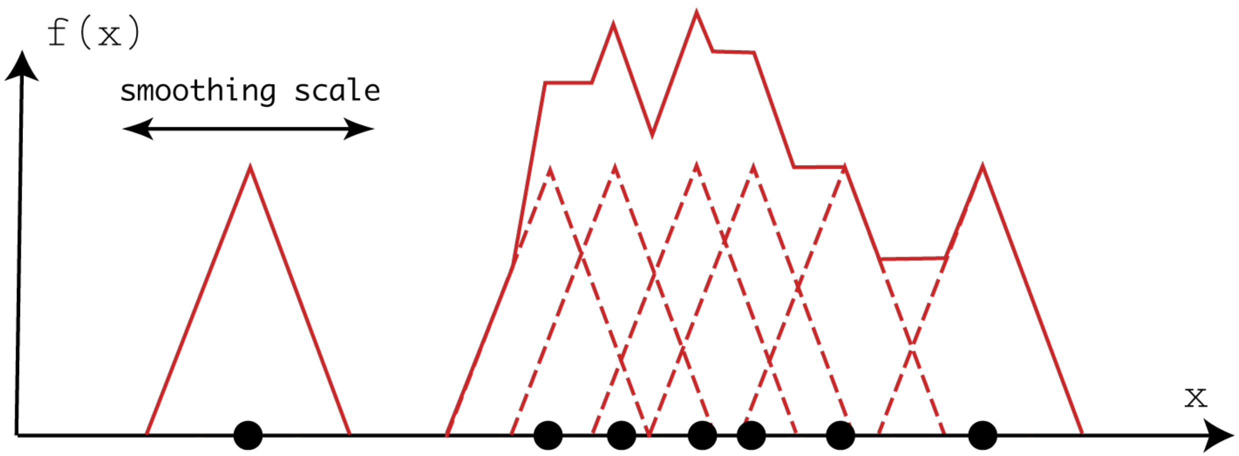
This simple approximation completely determines the system.

Kernel density estimation

The nonparametric density estimation issue is in most cases addressed by kernel density estimation (Parzen 1962):

the delta distribution corresponding to each marker is convoluted with a localized kernel function with unit integral.

→ we come back to our starting point: finite size particles!



How can we improve this scheme ?

- Main issue: unknown local regularity of the underlying Vlasov solution, hence **unknown smoothing scale**.

- We can circumvent this problem by using **nonlinear wavelet thresholding**, which adapts locally to the regularity of the PDF.

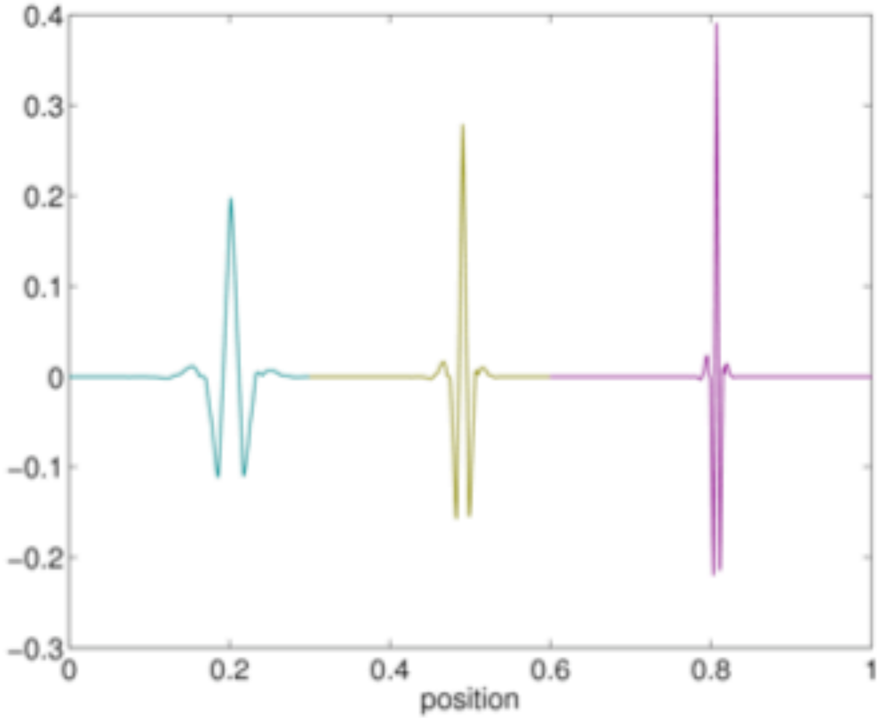
  → Wavelet-based density estimation (WBDE)

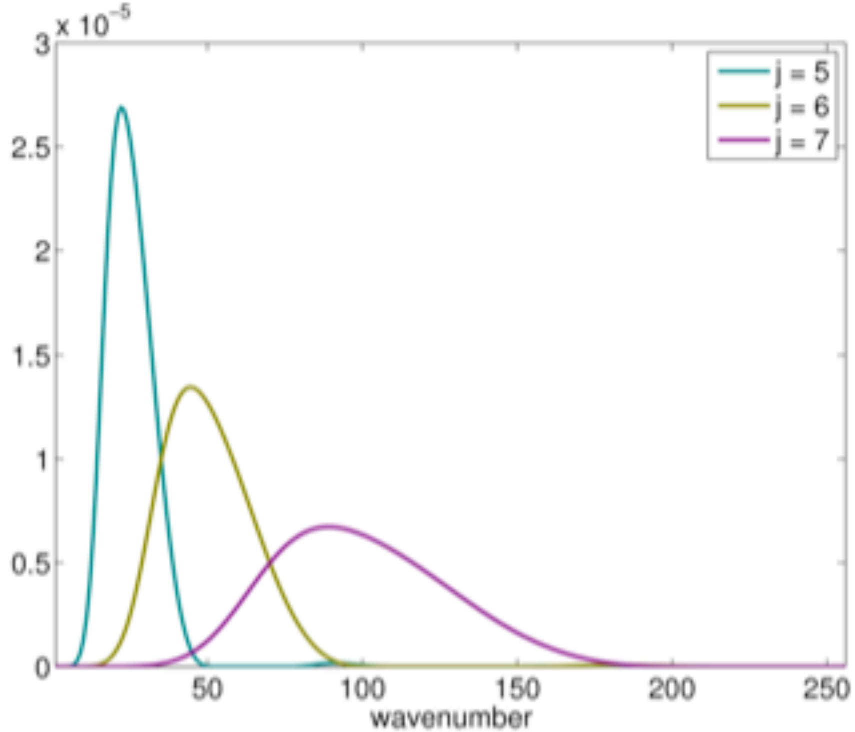
- a good threshold scaling can be predicted based on the statistical independance hypothesis (Donoho et al., 1996)

Wavelet-based density estimation

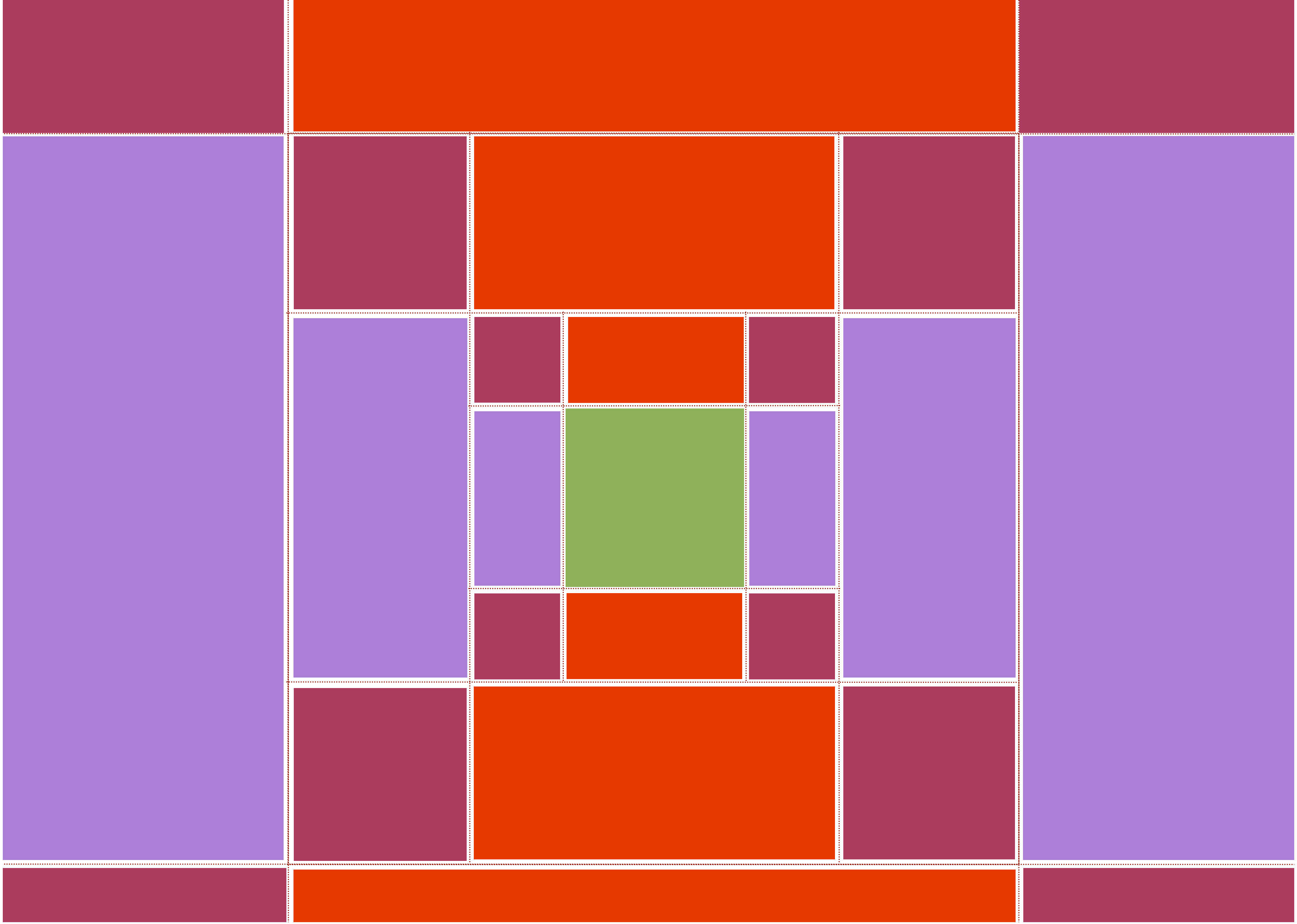
Wavelet bases

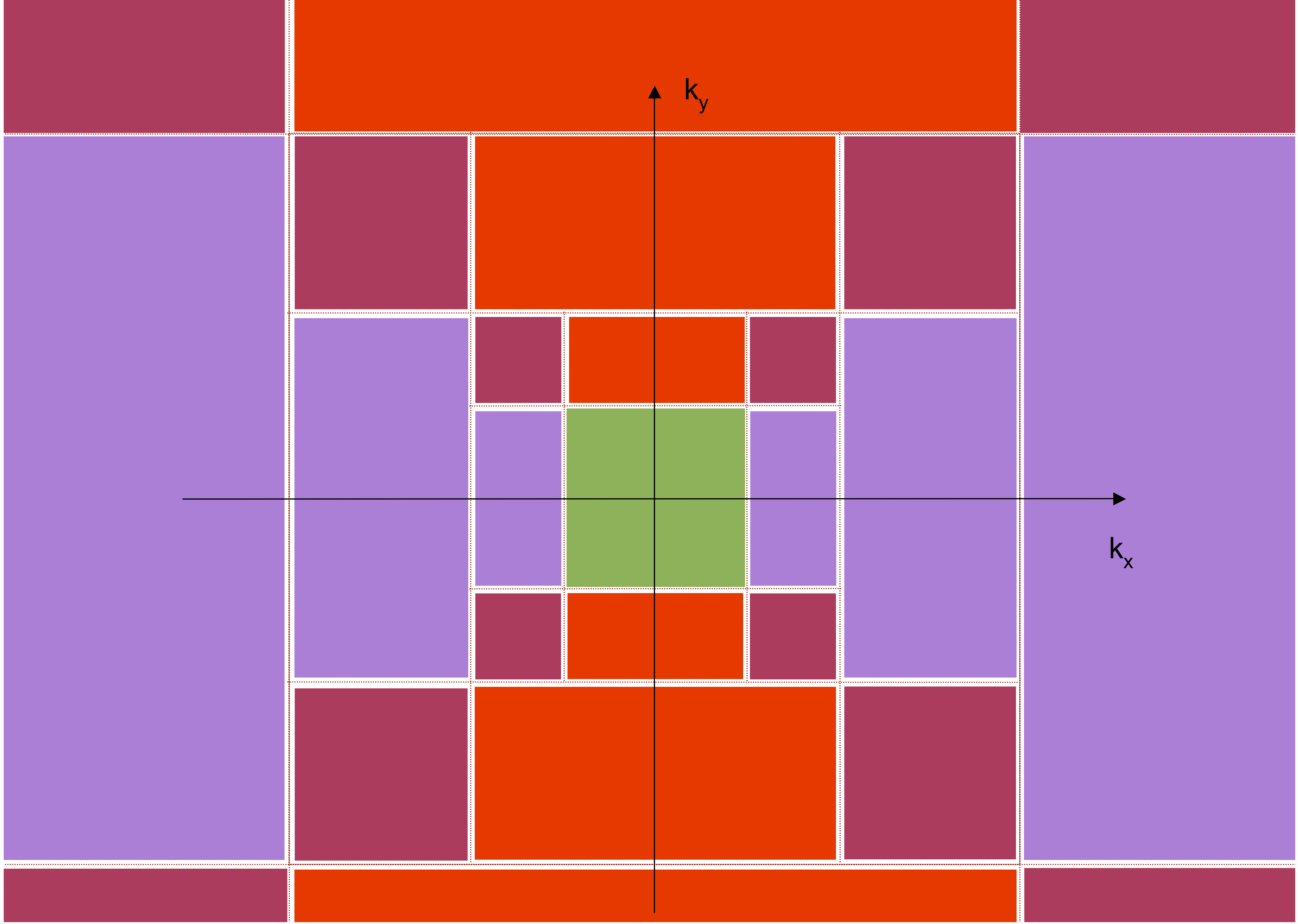
orthogonal wavelet bases on the real line are obtained by dilating and translating a single, well chosen oscillating function



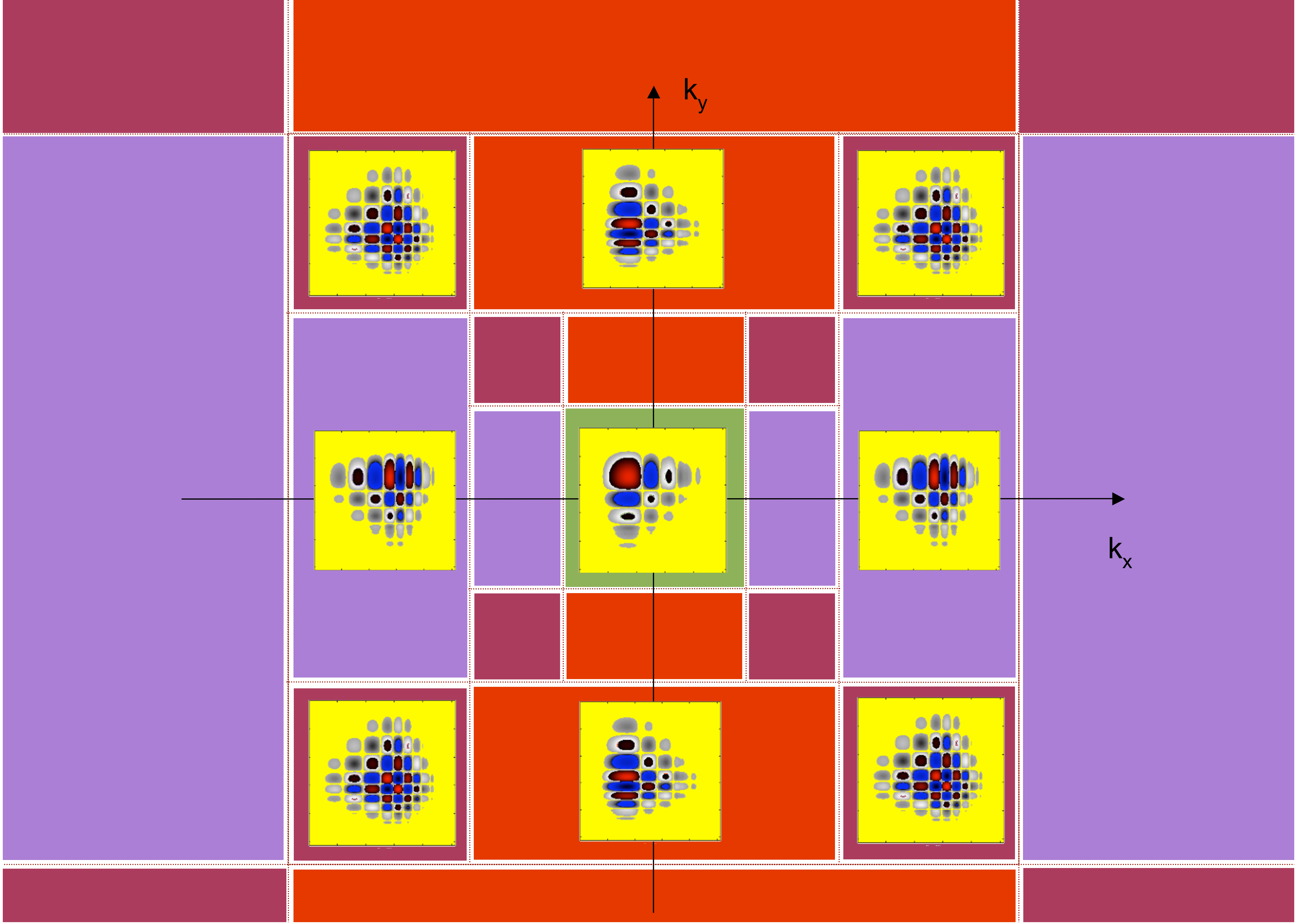


wavelets are indexed by their scale j and position i, which we regroup under the notation λ.





k_y
k_x

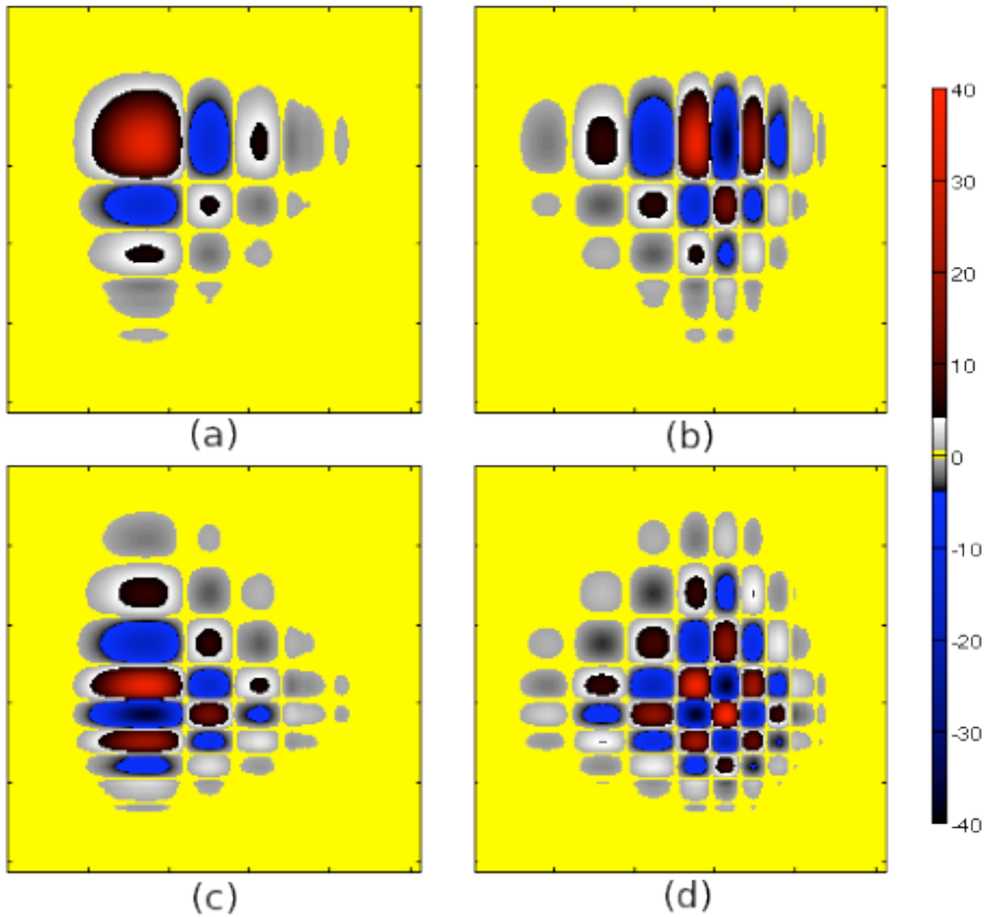


k_y
k_x

Choice of wavelet family

For the present study we have used the orthogonal 6th order **Daubechies wavelets:**

- 6 vanishing moments
- filters of length 12
- continuously differentiable



Empirical wavelet coefficients

The empirical density function can be written as a sum of Dirac distributions:

$$f^{\delta}(\mathbf{x}) = \frac{1}{N_p} \sum_{n=1}^{N_p} \delta(\mathbf{x} - \mathbf{X}_n)$$

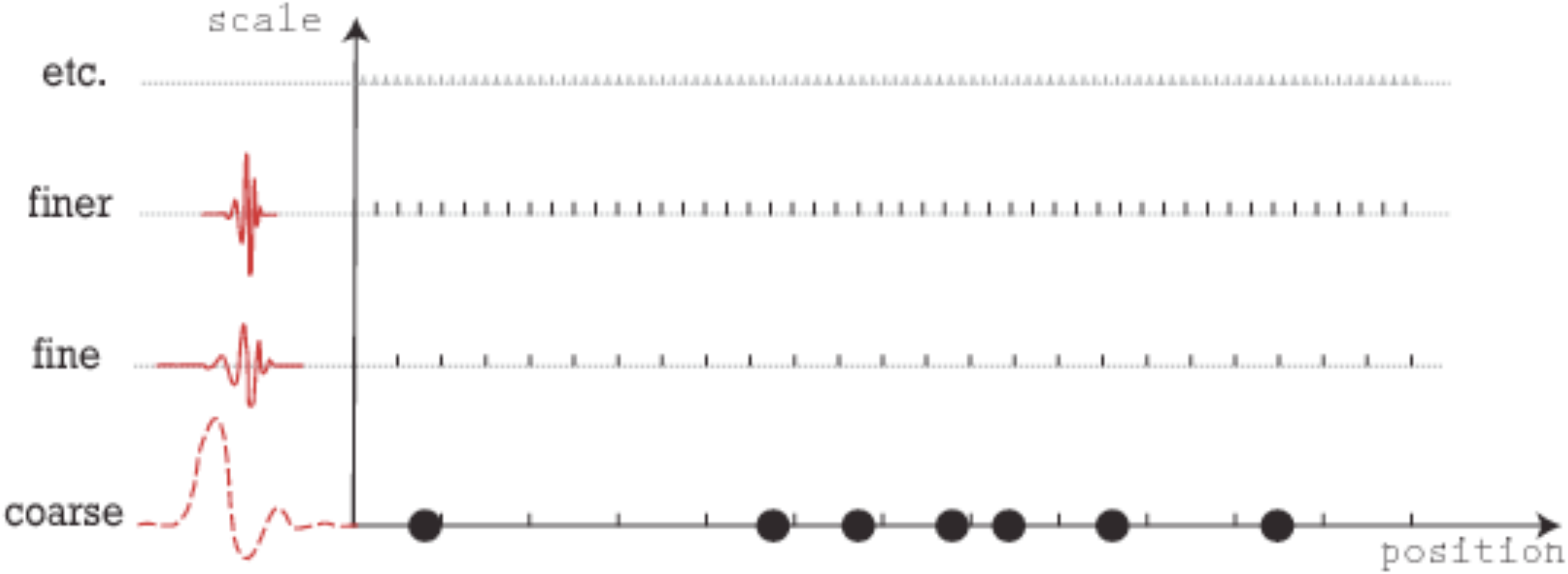
The empirical wavelet (resp. scaling function) coefficients are by definition the wavelet (resp. scaling function) coefficients of f^{δ}:

$$\overline{f}_{\lambda} \;=\; \langle f^{\delta} \mid \varphi_{\lambda} \rangle = \frac{1}{N_p} \sum_{n=1}^{N_p} \varphi_{\lambda}(X_n)$$

$$\tilde{f}_{\lambda} \;=\; \langle f^{\delta} \mid \psi_{\lambda} \rangle = \frac{1}{N_p} \sum^{N_p} \psi_{\lambda}(X_n)$$

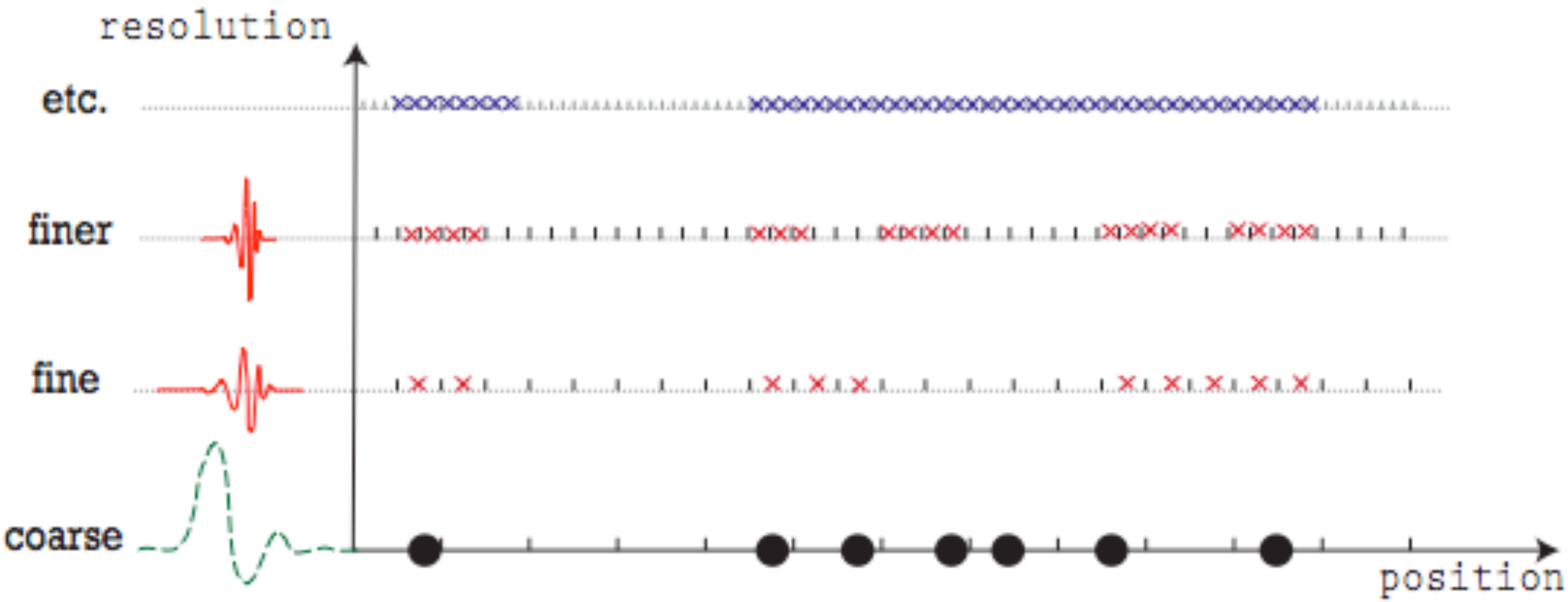
Wavelet representation of the PDF

$$f = \sum_{\lambda \in \Lambda_{\phi, L}} \overline{f}_\lambda \phi_\lambda + \sum_{\lambda \in \Lambda_{\psi, L}} \tilde{f}_\lambda \psi_\lambda$$



Wavelet thresholding

Denoising consists in retaining only a subset of the empirical wavelet coefficients in the reconstruction.



WBDE algorithm

1. Construct a histogram on a regular grid

2. Approximate the empirical wavelet coefficients by those of the histogram

3. Process the empirical wavelet coefficients as follows
   (N_p is the number of particles):

FINE
discard all

J $$2^{dJ} := \frac{N_p}{\log_2 N_p}$$

nonlinear
threshold

keep only coefficients such that $\left|\tilde{f}_\lambda^H\right| \geq \sqrt{\frac{j}{4N_p}}$

L $$2^{dL} := N_p^{\frac{1}{3}}$$

COARSE

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additional scales that could not be captured by a linear procedure

L $\quad 2^{dL} := N_p^{\frac{1}{3}}$

COARSE

Applications

Methodology

- **Postprocess** the results of simulations done using classical methods,
- **comparisons: histogram** and **proper orthogonal decomposition** methods,
- whenever possible, compute the L^2 **error** with respect to a reference solution (obtained using a higher number of particles).

POD method

- Construct a histogram and consider it as a matrix M, then compute the SVD of M:

$$M = {}^tUSV$$

- Set all but a few large singular values to zero,
- Reconstruct the distribution function.

1+1D Bump-on-tail instability

Vlasov-Poisson electron plasma with uniform ion background.

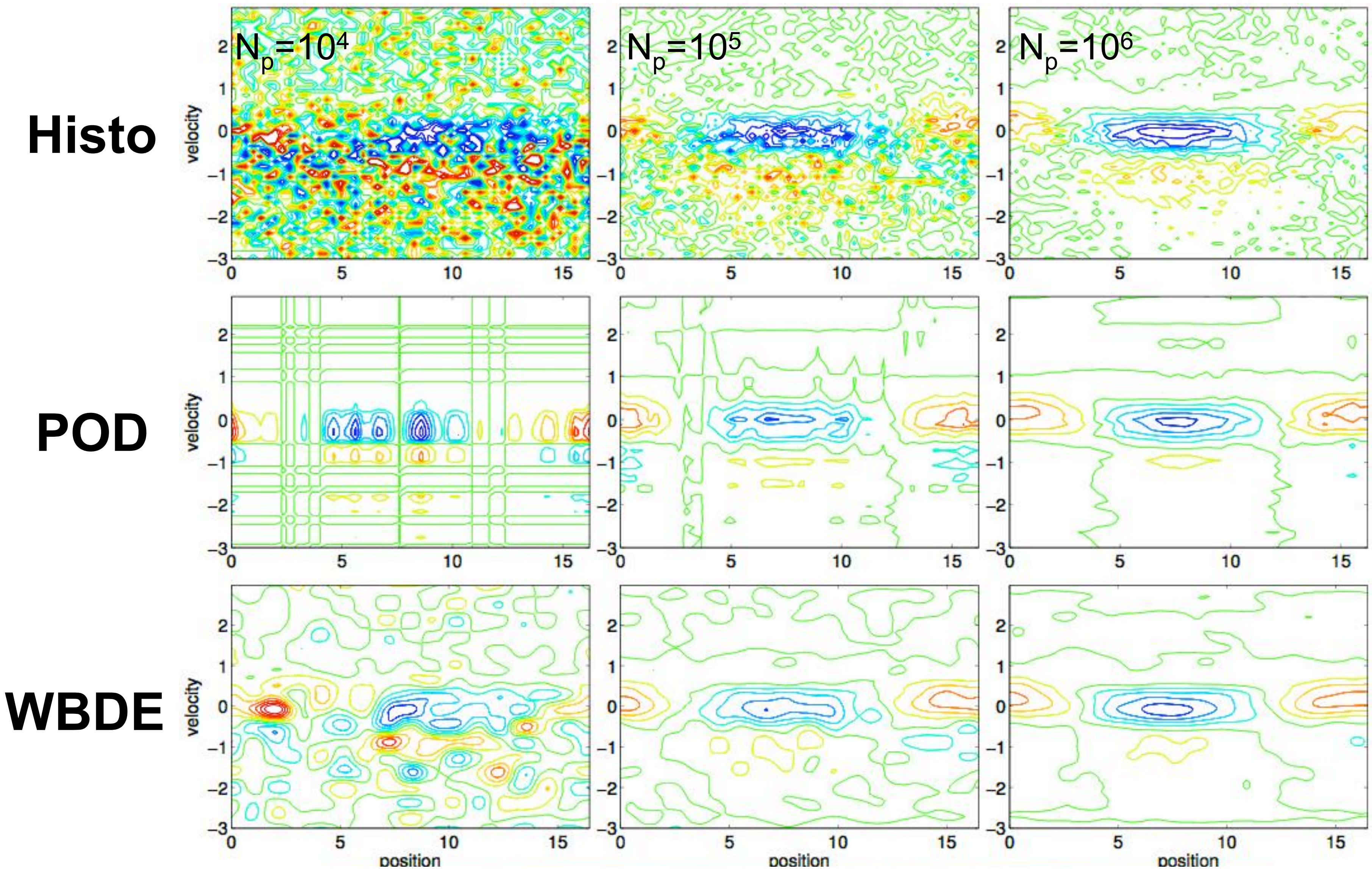
Particle-in-cell code with triangular charge assignment function

Initial condition: uniform in space, velocity distribution with a slightly unstable tail

$$f_0(x,v) = \frac{2}{3\pi\zeta}\frac{1-2qv+2v^2}{(1+v^2)^2}$$

$q = 1.25$
$N_p = 10^4, 10^5, 10^6$
domain size 16.52 fits the most unstable mode

1+1D Bump-on-tail instability



1+1D Bump-on-tail instability

Normalized L^2 error

between the reconstructed distribution functions and the histogram obtained from the simulation with $N_p=10^6$ particles:

		$N_p = 10^4$	$N_p = 10^5$
histogram	f_H	0.443	0.140
POD	f_P	0.163	0.090
WBDE	f_W	0.173	0.086

1+1D Two-streams instability

Initial condition: two counter-propagating, uniform in space monokinetic electron beams.

The initial condition is deterministic…oups

there is initially no noise to remove !!

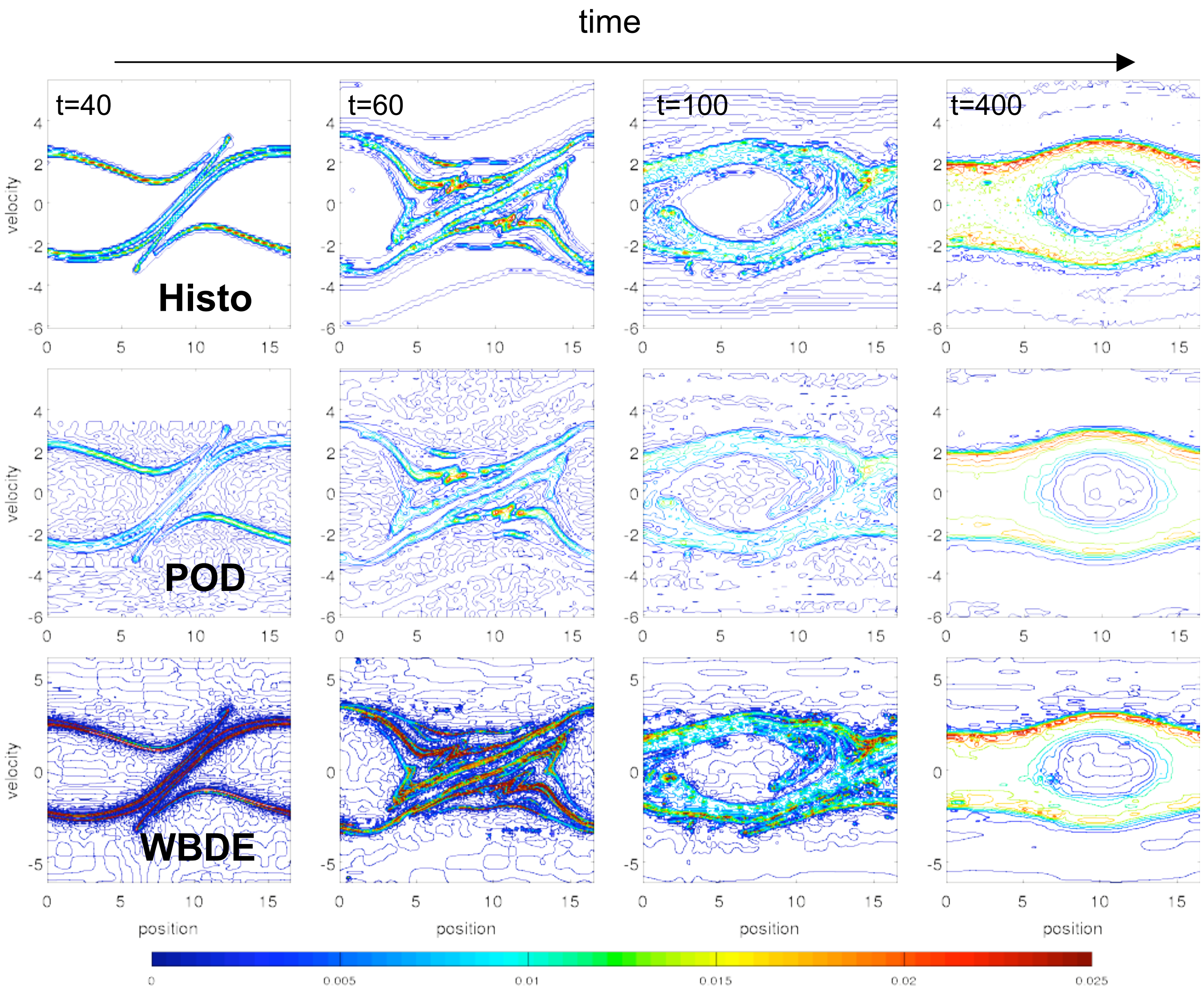
But noise appears due to the instability.

How will the method handle this ?

1+1D Two-streams instability

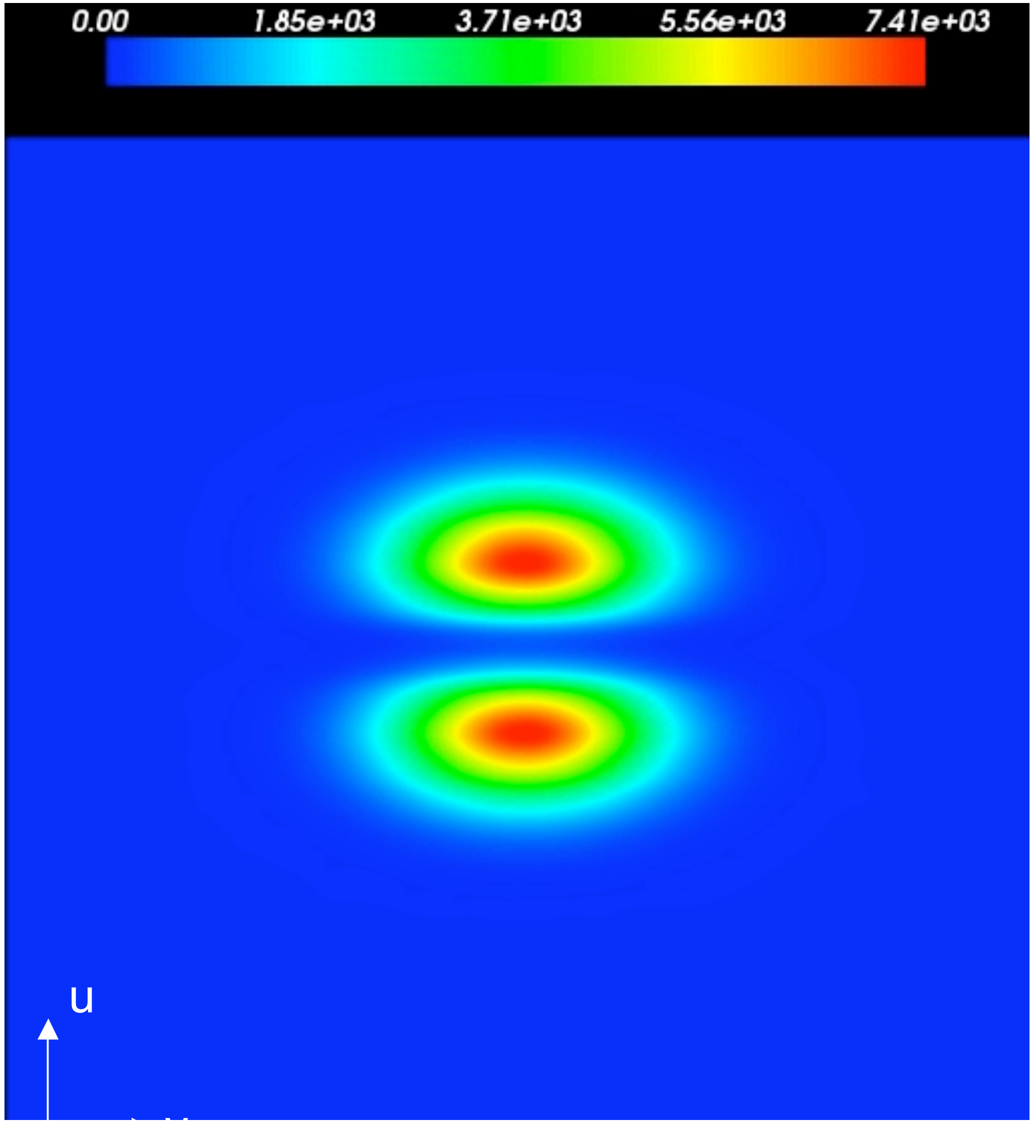
Self-consistent noise builds up due to the nonlinear dynamics.

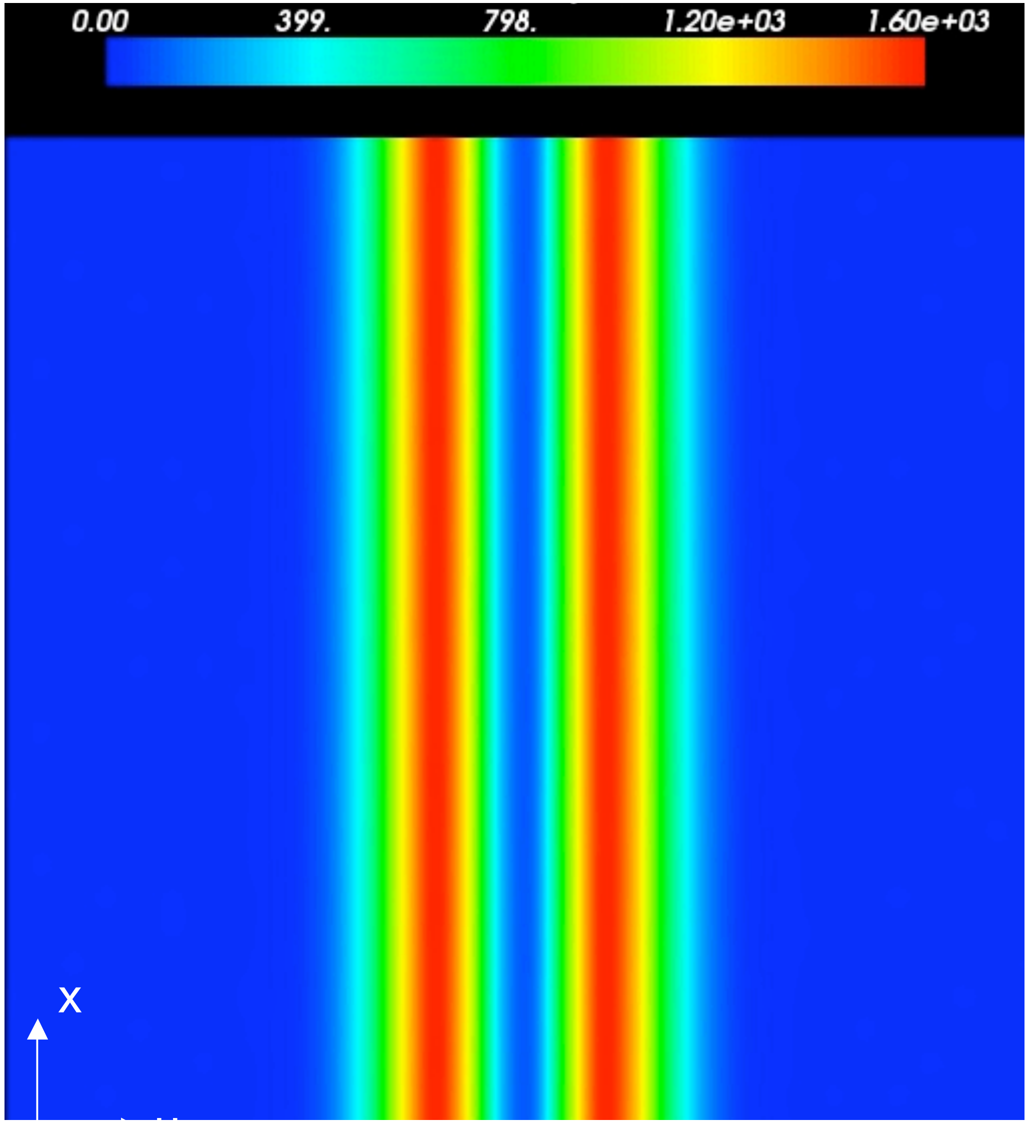
- At short times, WBDE preserves the **sharpness** of the solution.
- At late times (t=400), the estimates given by POD and WBDE are **smoother** than the histogram because part of the noise has been cured.



2+2D Two-streams instability

Initial condition



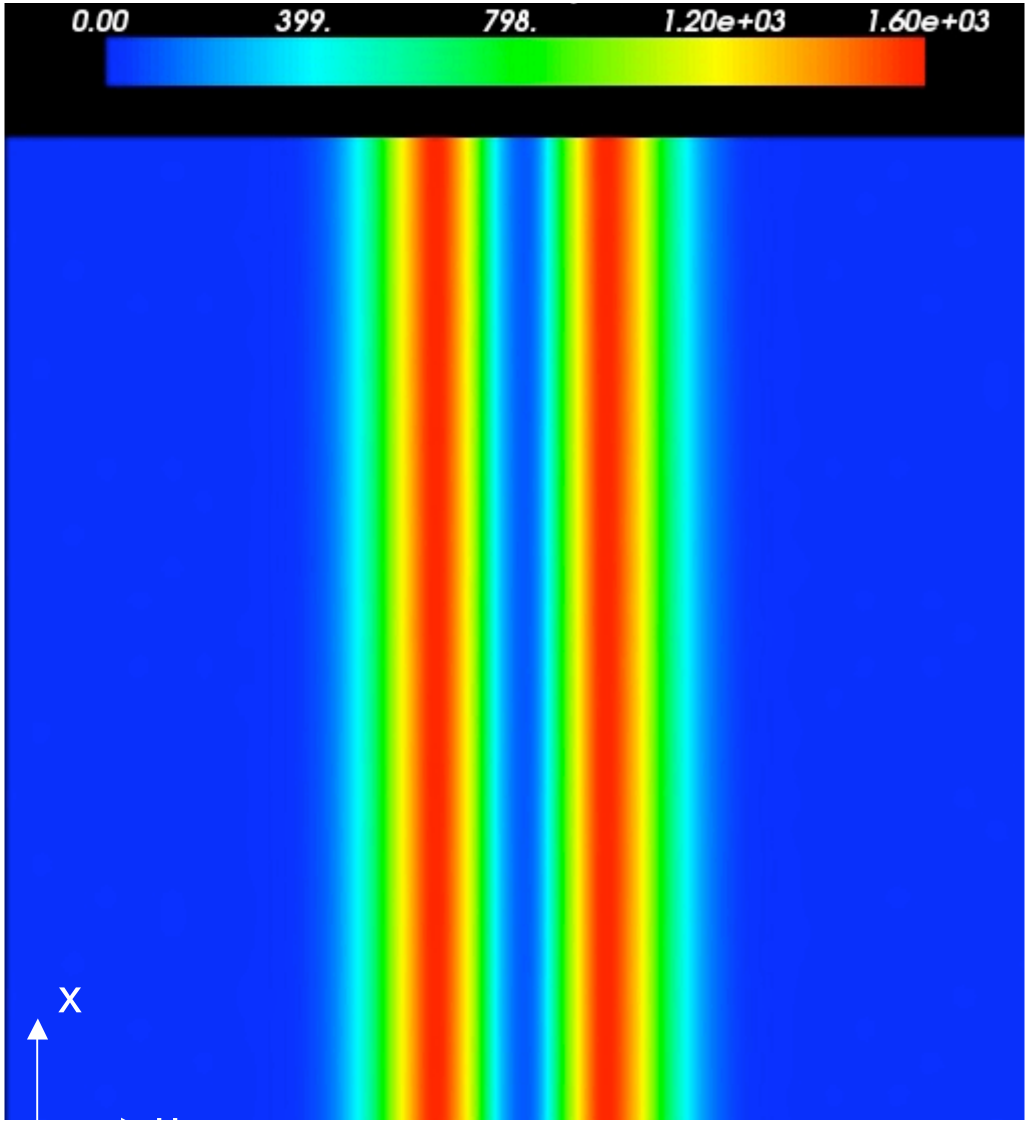


2+2D Two-streams instability

As before we postprocess the results of a particle-in-cell simulation.

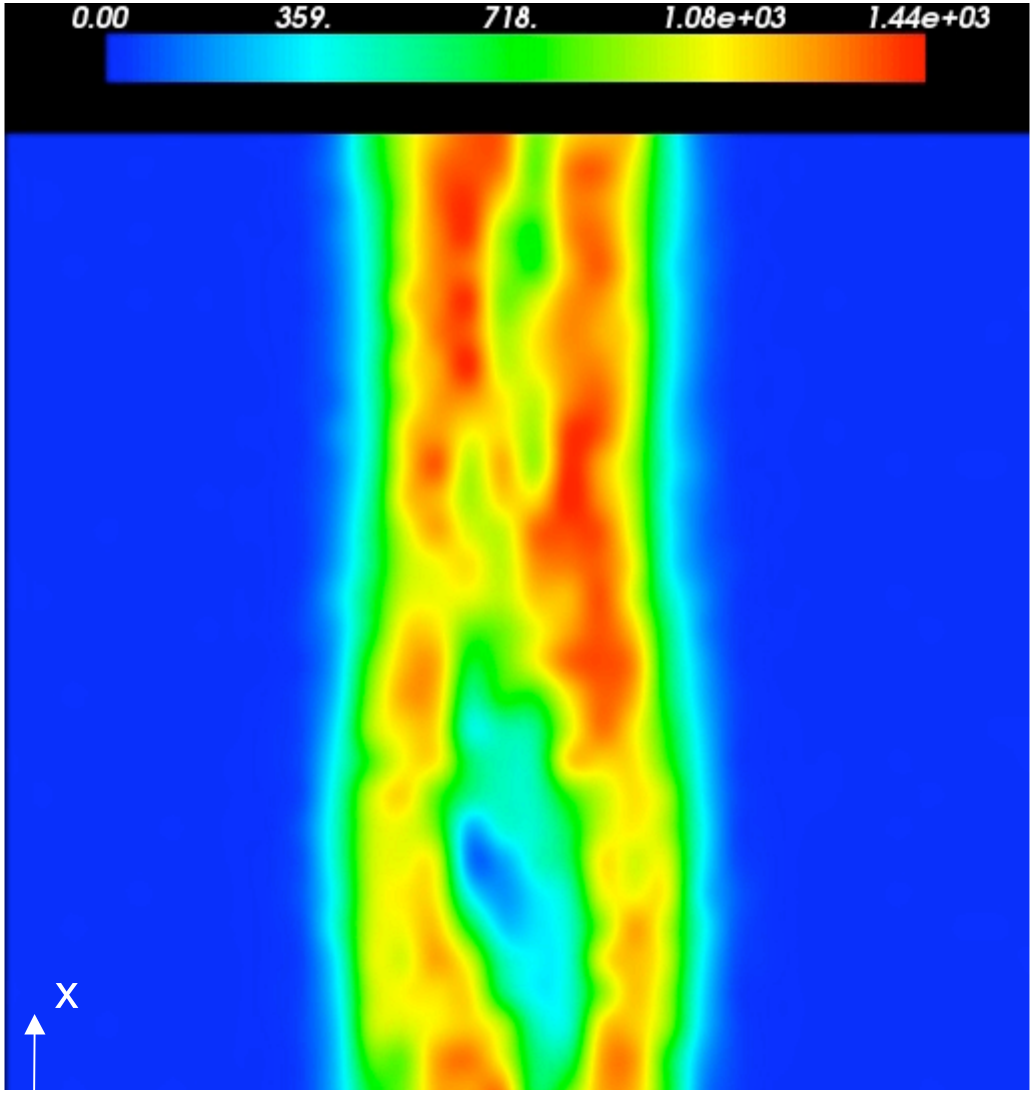
Number of particles:
N_p = 323 000

Grid resolutions:
Ng = 32^4 for the histogram
and
Ng = 128^4 for WBDE

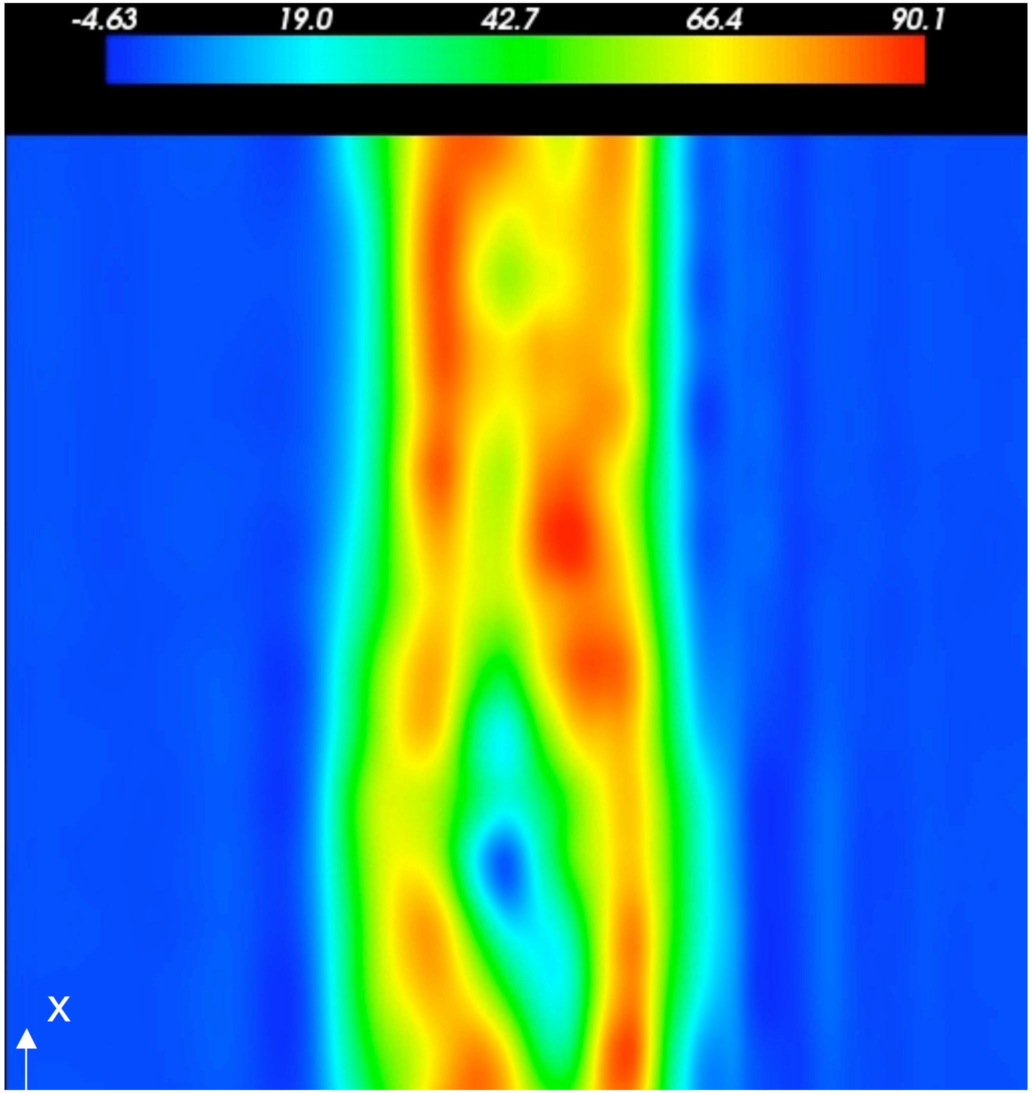


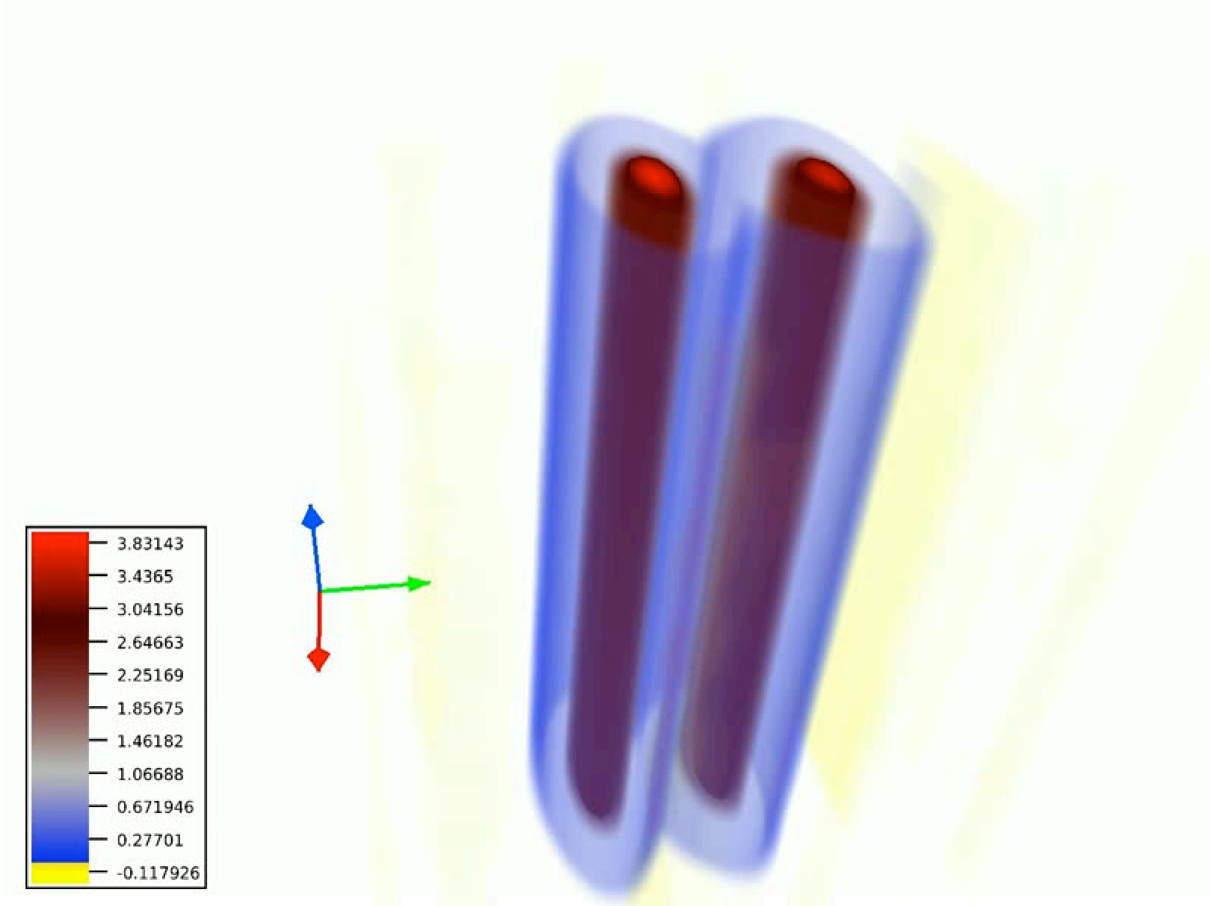
Comparison after nonlinear evolution

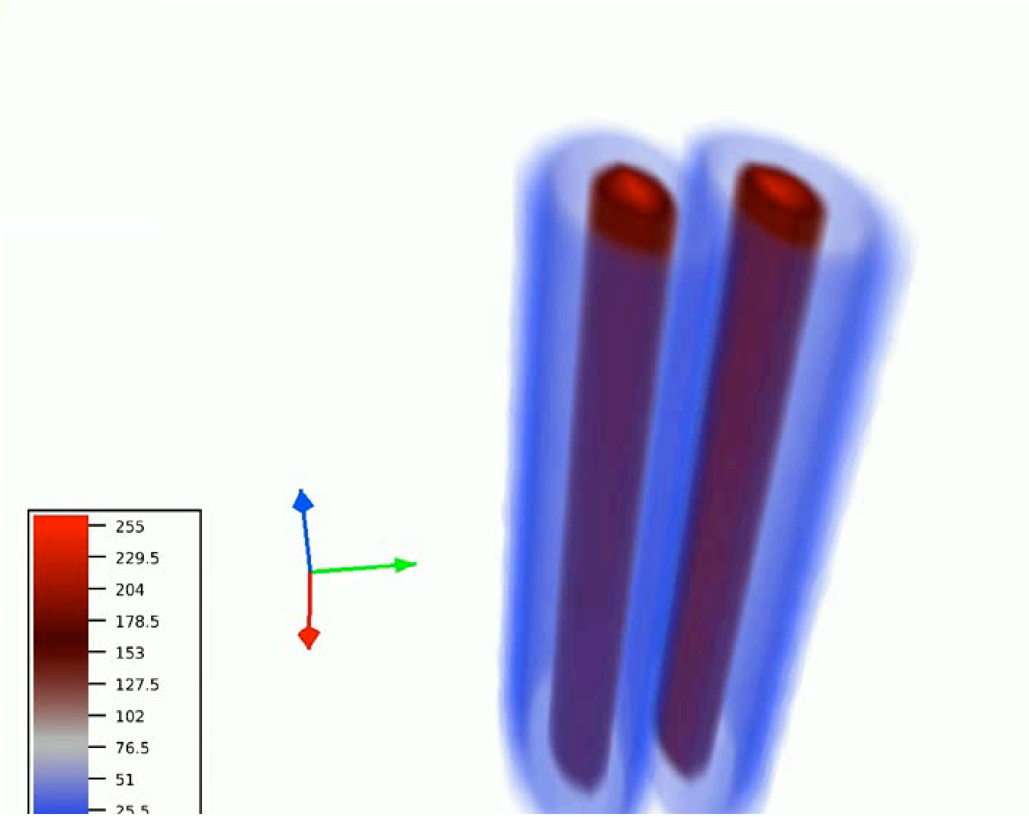
Histogram



WBDE




3.83143
3.4365
3.04156
2.64663
2.25169
1.85675
1.46182
1.06688
0.671946
0.27701
-0.117926


255
229.5
204
178.5
153
127.5
102
76.5
51
25.5

Outlook

Outlook

- continue work on the 2+2D case (vary number of particles),
- assess the importance of the artefacts introduced by WBDE (e.g. **negative density**),
- avoid histograms completely by computing the empirical wavelet coefficients directly (Daubechie's cascade algorithm?),
- develop an electrostatic PIW (particle-in-wavelets) code, by using the WBDE method at each timestep to estimate the potential (in the electrostatic case it's possible to denoise directly the charge field instead of f).

Thank you !

and also thanks to:

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Don Spong
Steve Cowley

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for their cool Winter School.

Ad break

C++, d-dimensional

parallel wavelet transform library

available for download at

http://justpmf.com/romain/kicksey_winsey

under the GPL license

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