Adaptive Methods for the Vlasov Equation

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Outline

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Kinetic models for plasmas and particle beams

In the sequel we shall consider only the collisionless relativistic Vlasov-Maxwell equations

$$\frac{\partial f_s}{\partial t} + \frac{\mathbf{p}}{m_s \gamma_s} \cdot \nabla_x f_s + q_s(\mathbf{E} + \frac{\mathbf{p}}{m_s \gamma_s} \times \mathbf{B}) \cdot \nabla_p f_s = 0,$$

$$\partial_t \mathbf{E} - c^2 \nabla \times \mathbf{B} = -\frac{\mathbf{J}}{\epsilon_0}, \qquad \nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0},$$

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0, \qquad \nabla \cdot \mathbf{B} = 0,$$

where $\gamma_s^2 = 1 + \frac{|\mathbf{p}|^2}{m_s^2 c^2}$ and the source terms are computed by

$$\rho = \sum_s q_s \int f_s \, d\mathbf{p}, \qquad \mathbf{J} = \sum_s \frac{q_s}{m_s} \int f_s \frac{\mathbf{p}}{\gamma_s} \, d\mathbf{p}.$$

In some cases Maxwell's equations can be replaced by a reduced model like Poisson's equation.

Outline

Invariants of Vlasov-Maxwell system

- Invariance along characteristics:

$$\frac{d}{dt} f(X(t), P(t), t) = 0$$

where $\dot{X} = \frac{P}{m\gamma}$, $\dot{P} = q(E(X(t), t) + \frac{P(t)}{m\gamma} \times B(X(t), t))$.

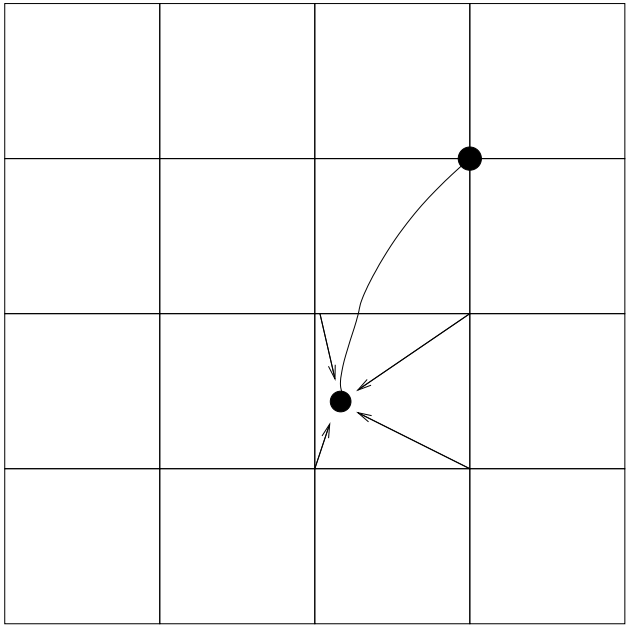
- Energy: $\int f(\gamma - 1)\, dx\, dp + \frac{1}{2}(\int (E^2 + B^2)\, dx$.
- L^q norms: $\int f^q\, dx\, dp$.
- Phase space volume: $\int_V f(x, p, t)\, dx\, dp$.
  - Conservative form of Vlasov equation

$$\frac{\partial f}{\partial t} + \nabla_{x,p} \cdot (Ff) = 0,$$

with $F = (\frac{p}{\gamma m}, E + \frac{p}{\gamma m} \times B)$ so that $\nabla_{x,p} \cdot F = 0$.

Outline

The backward semi-Lagrangian Method



- f conserved along characteristics
- Find the origin of the characteristics ending at the grid points
- Interpolate old value at origin of characteristics from known grid values
  $\longrightarrow$ High order interpolation needed

- Typical interpolation schemes.
  - Cubic spline [Cheng-Knorr 1976, Sonnendrücker-Roche-Bertrand-Ghizzo 1998]
  - Cubic Hermite with derivative transport [Nakamura-Yabe 1999]

Comparison of PIC and Eulerian methods

- Particle-In-Cell (PIC) method is the most widely used.
  - Pros:
    - Good qualitative results with few particles.
    - Very good when particle dynamics dominated by fields which do not depend on particles (e.g. in accelerators when self field small compared to applied field).
    - More efficient when dimension is increased (phase-space = 6D).
  - Cons Hard to get good precision : slow convergence, numerical noise, low resolution at high velocities.
- Grid based Vlasov methods
  - Pros High-order method, same resolution everywhere on grid.
  - Cons Needs huge computer ressources in 2D or 3D.

Outline

Problems with grid based methods

- Numerical diffusion
- Curse of dimensionality: N^d grid points needed in d dimensions on uniform grids.
  Number of grid points grows exponentially with dimension
  $\longrightarrow$ killer for Vlasov equation where d up to 6.
  Memory needed
  - In 2D, 16384^2 grid $\longrightarrow$ 2 GB
  - In 4D, 256^4 grid $\longrightarrow$ 32 GB
  - In 6D, 64^6 grid $\longrightarrow$ 512 GB
- Adaptive algorithm is a must in higher dimensions

Outline

A typical beam simulation

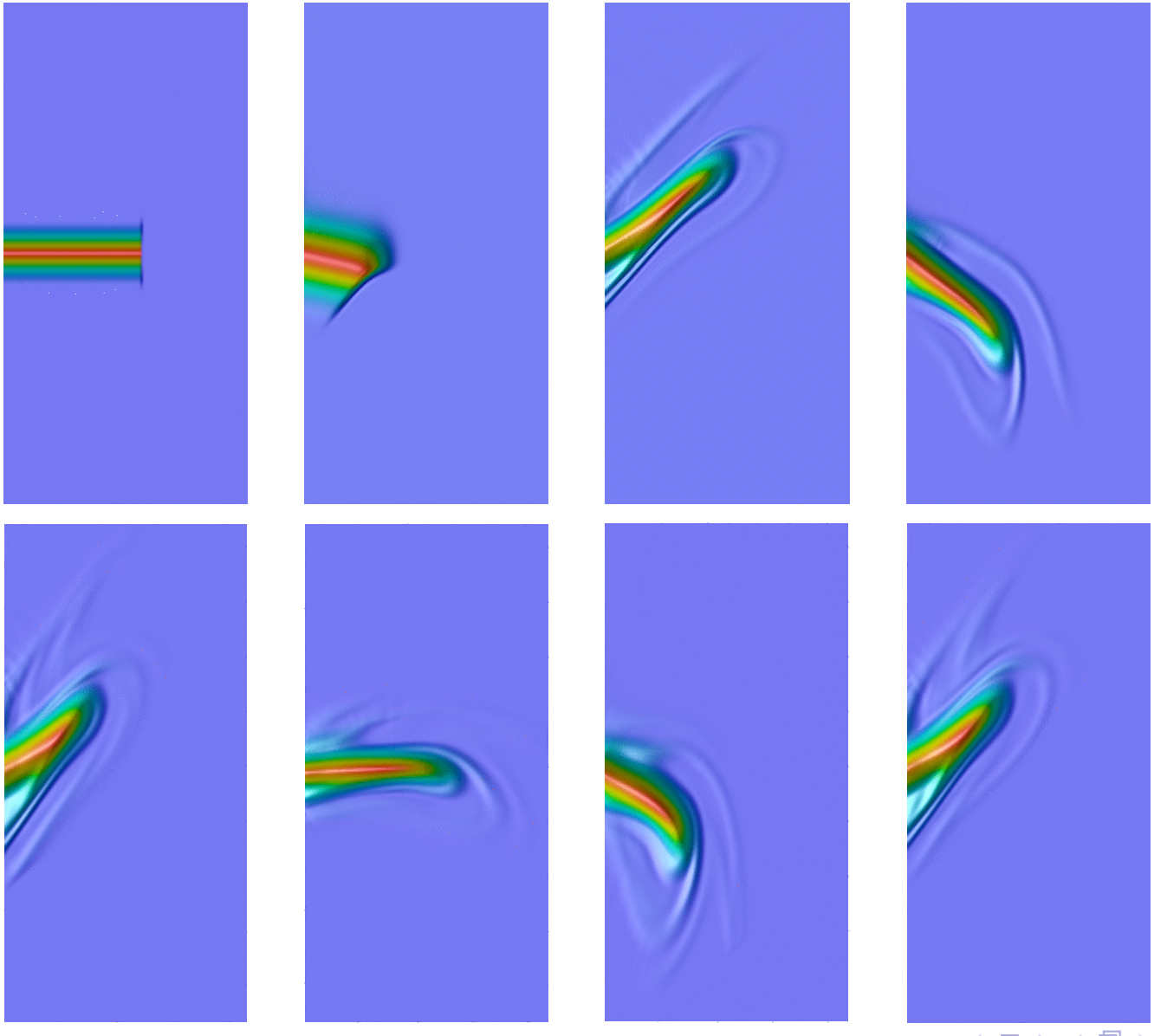
Semi-Gaussian beam in periodic focusing channel

- Applied field $\vec{B} = (-\frac{1}{2}B'(z)x,\ -\frac{1}{2}B'(z)y,\ B(z))$, with $B(z) = \frac{B_0}{2}(1 + \cos(\frac{2\pi z}{s}))$, with $B_0 = 2\,T$ and $S = 1\,m$.
- Semi-Gaussian beam of emittance $\epsilon = 10^{-3}$,

$$f_0(r, v_r, P_\theta) = \frac{n_0}{\pi a^2}\ \exp(-\frac{v_r^2 + (P_\theta/(mr))^2}{2v_{th}^2}),$$

where $P_\theta = mrv_\theta + mB(z)\frac{r^2}{2}$, $n_0 = \frac{I}{qv_z}$, $I = 0.05\,A$ and $E = 80\,MeV$ so that $v_z = 626084\,ms^{-1}$.

Semi-Gaussian beam in periodic focusing channel

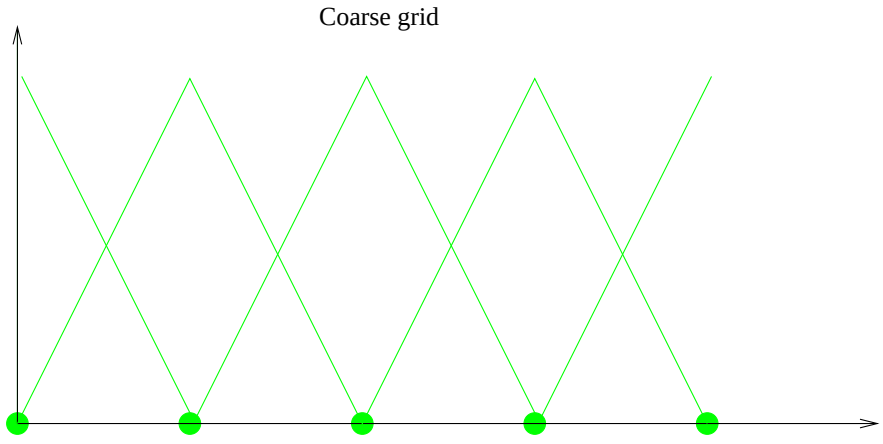


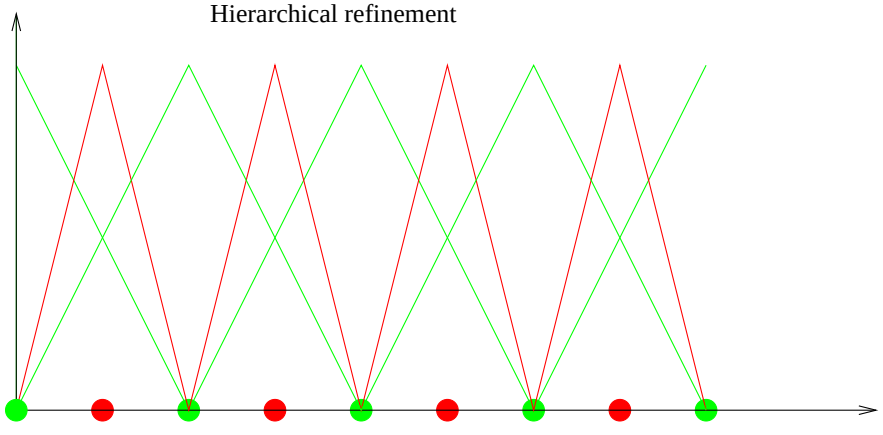
Outline

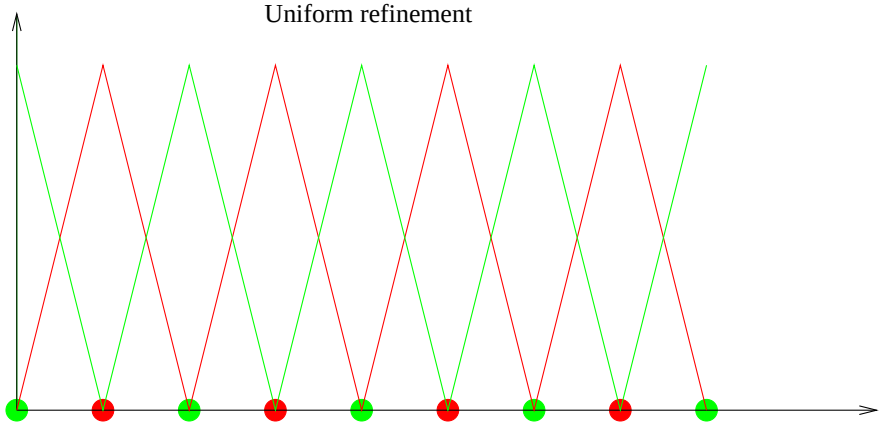
Adaptive semi-Lagrangian method

- Semi-Lagrangian method consists of two stages : advection and interpolation
- Interpolation can be made adaptive : approximate f^n with as few points as possible for a given numerical error using non linear approximation.
- Construct approximation layer by layer, starting from coarse approximation and adding pieces to improve precision where needed, using nested grids.
- It is possible to modify hierarchical decomposition so as to exactly conserve mass and any given number of moments even when grid points are removed.

Uniform and Hierarchical Refinements







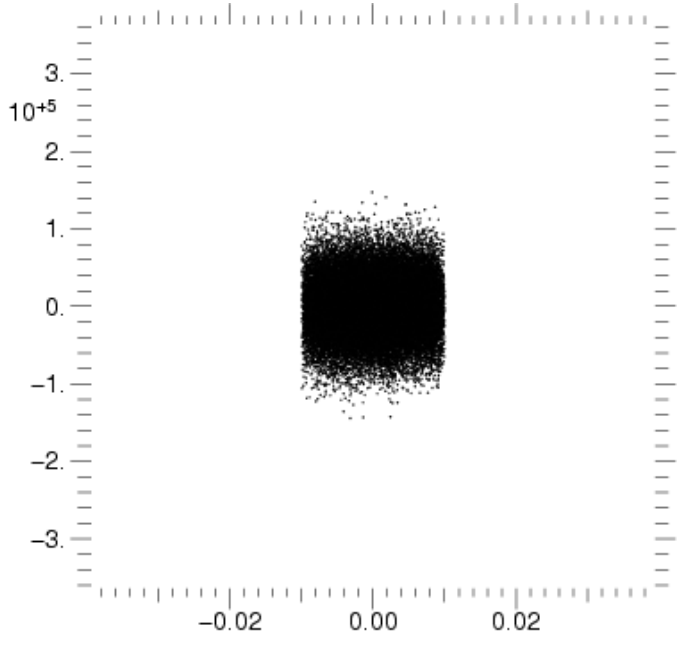
Nonlinear approximation

- Decomposition of f_{j+1} in uniform and hierarchical basis

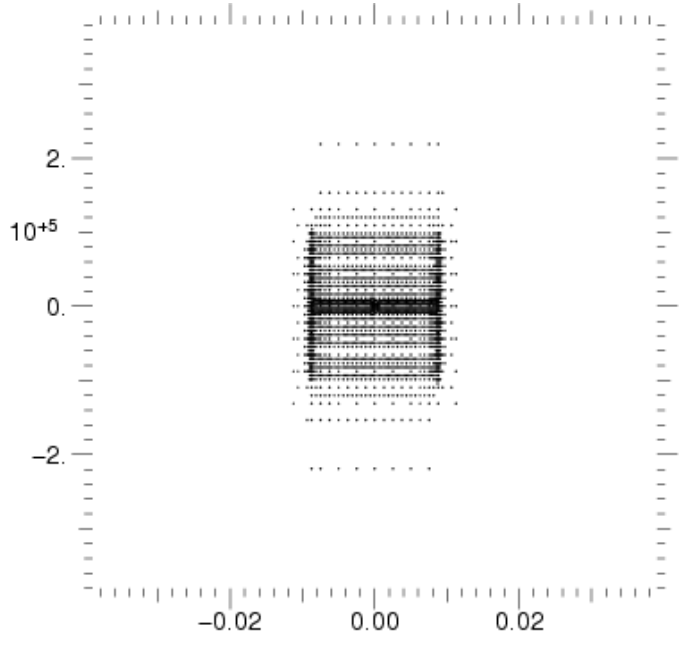
$$\begin{aligned} f_{j+1} &= \sum_k c_k^{j+1} \varphi_k^{j+1} \text{ (uniform)} \\ &= \sum_k c_k^j \varphi_k^j + \sum_k d_k^j \psi_k^j \text{ (hierarchical)} \end{aligned}$$

- In hierarchical decomposition coefficients d_{2i+1} at fine scale are small if f is close to affine in $[x_{2i}, x_{2i+2}]$.
- Linear (uniform) approximation consists in using a given number of basis functions independently of approximated function f.
- Nonlinear approximation consists in keeping the N highest coefficients in hierarchical decomposition (depends on f) [De Vore 1998]
  Only grid points where f varies most are kept.

Localization of points



PIC code



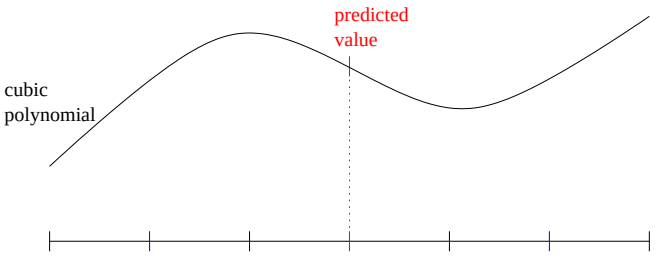
non linear approximation

Construction of a hierarchical approximation

- Hierarchical approximation is constructed by defining an interpolation method enabling to go from coarse grid to fine grid.
- Two methods have been tried:
  1. Interpolating wavelets based on Lagrange polynomial interpolation. Classical wavelet compression technique. Addressed moment conservation issues [Gutnic-Haefele-Paun-Sonnendrücker 2004, Gutnic-Haefele-Sonnendrücker 2006].
  2. Hierarchical approximation based on finite element interpolants. More local, cell based $\rightarrow$ simpler and potentially more efficient parallelization. [Campos Pinto-Mehrenberger 2003].

Hierarchical expression of f_{j+1} of interpolating wavelets

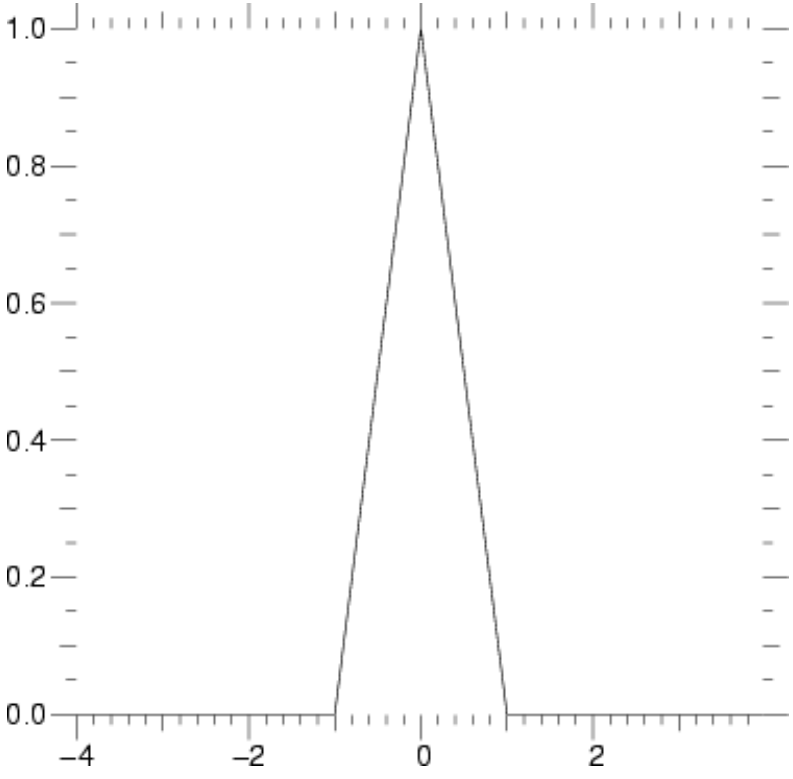
- Consider Gridfunction f_j defined by its values c_k^j on G^j of step 2^{-j}.



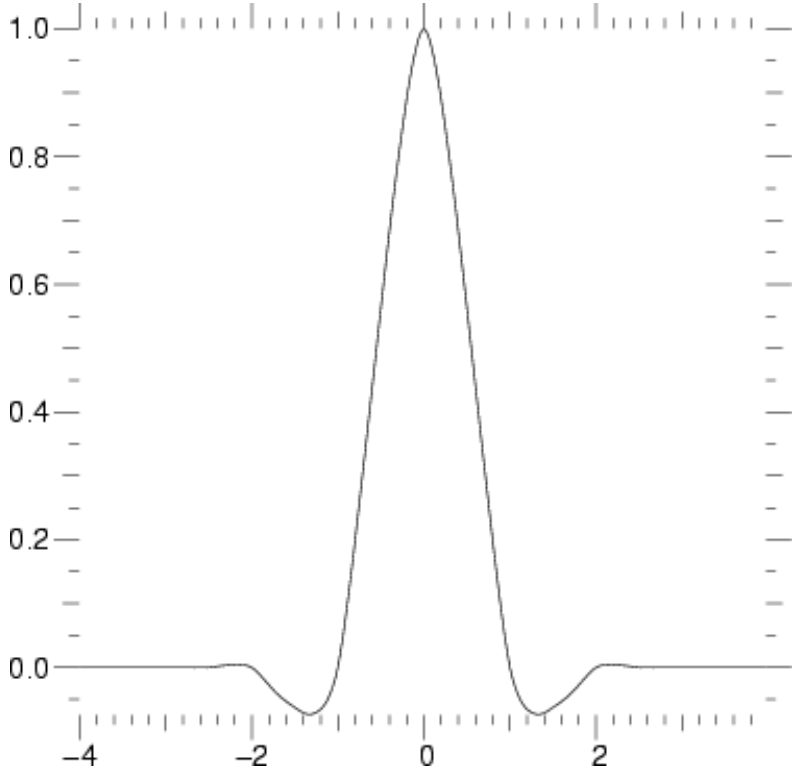
- Define dyadic refinement procedure via interpolation operator, e.g. Lagrange interpolation

- Refinement procedure linear with respect to c_k^j so that on can introduce basis functions φ_k^j defined by infinite refinement of $\delta_{k,n}$

Basis functions = Scaling functions



linear Lagrange interpolation



cubic Lagrange interpolation

Multiresolution Analysis (MRA)

Our ad hoc hierarchical procedure fits into the mathematical framework of multiresolution analysis (wavelets) [Cohen 2003].

- A multiresolution analysis is a sequence of subspaces $(V_j)_{j\in\mathbb{Z}}$ of $L^2(\mathbb{R})$ verifying the following properties
  - There exists a function φ called scaling function such that $t \mapsto \varphi(2^j t - k)_{k\in\mathbb{Z}}$ forms a basis of V_j.
  - The spaces V_j are nested $V_j \subset V_{j+1}$. Hence

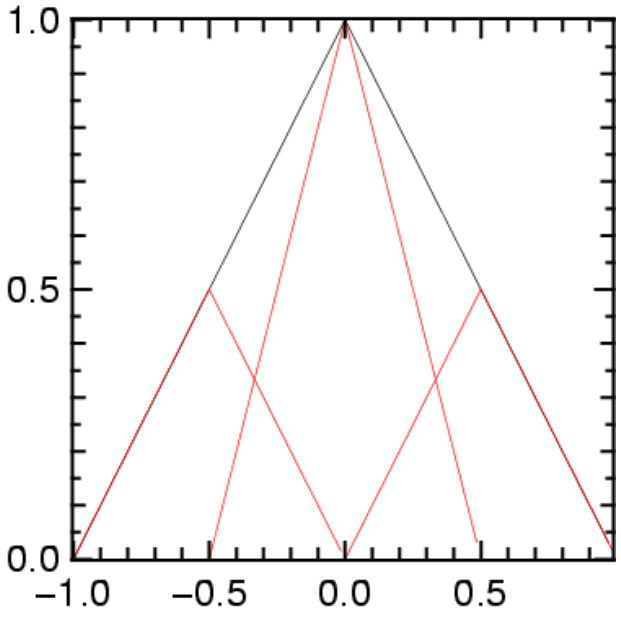
$$\varphi(t) = \sum_{n\in\mathbb{Z}} h_n \varphi(2t - n).$$

  - $\cap_j V_j = \{0\}$ et $\overline{\cup_j V_j} = L^2(\mathbb{R})$.

Example : the Schauder multiresolution analysis

- Scaling function defined by

$$\varphi(t) = \max(0, 1 - |x|)$$



  - The space V_j is the set of functions which are linear on each of the intervals $[k2^{-j}, (k+1)2^{-j}[$.
  - Scaling relation

$$\varphi(t) = \frac{1}{2}\varphi(2t+1) + \varphi(2t) + \frac{1}{2}\varphi(2t-1).$$

Filter

- Multiresolution analysis completely defined by scaling relation

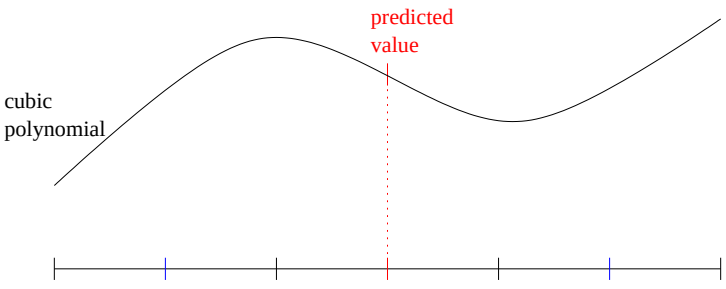
$$\varphi(t) = \sum_{n\in\mathbb{Z}} h_n \varphi(2t - n).$$

  - Scaling function completely defined by coefficients $(h_n)_{n\in\mathbb{Z}}$.
    - Properties of $(h_n)_{n\in\mathbb{Z}}$ translate on properties on φ.
  - Express that $V_0 \subset V_1$, and by change of scale $V_j \subset V_{j+1}$.
- Fourier transform of scaling relation

$$\hat{\varphi}(2\omega) = \frac{1}{2} m(\omega)\hat{\varphi}(\omega), \qquad \text{where } m(\omega) = \sum_{n\in\mathbb{Z}} h_n e^{-in\omega}.$$

  - In frequency domain change of scale corresponds to filtering by filter m.

Case of interpolating wavelets



- Interpolation procedure yields scaling relation.
- For Lagrange interpolation, denoting by $\varphi_k^j = \varphi(2^j \cdot -k)$, we get

$$\varphi_k^j = \varphi_{2k}^{j+1} + \sum_{n=1-N}^{N} a_n \varphi_{2k+1+n}^{j+1}.$$

e.g in case of linear interpolation $N = 1$, $a_0 = a_1 = \frac{1}{2}$.

The supplementary space

- It is natural to look for W_j such that $V_{j+1} = V_j \oplus W_j$. Only one possibility if orthonality is required, infinitely many else.
- W_j will be uniquely defined by the projection $P_j : V^{j+1} \to V^j$.
- One convenient choice is to use the restriction for P_j, i.e.

$$P_j(f) = \sum_k f(x_k^j)\varphi_k^j(x) = \sum_k \langle f, \delta_k^j \rangle \varphi_k^j(x).$$

- $\tilde{V}^j = span((\delta_k^j)_k)$ defines set of nested space with scaling relation $\delta_k^j = \delta_{2k}^{j+1}$, thus another MRA.

Expression of f_{j+1} in V_{j+1} and $V_j \oplus W_j$

- A basis of W_j will consist of $(\varphi^{j+1}_{2k+1})_k$.
- Compare f_{j+1} to its restriction on G^j:
  - equal at even grid points
  - define d^j_k as

$$d^j_k = c^{j+1}_{2k+1} - P_{2N-1}(x^{j+1}_{2k+1}) = c^{j+1}_{2k+1} - \sum_{n=1-N}^{N} a_n c^{j+1}_{2k+2n}.$$

- $f_{j+1} \in V_{j+1}$ can be expressed equivalently as

$$\begin{aligned} f_{j+1} &= \sum_k c^{j+1}_k \varphi^{j+1}_k \\ &= \sum_k c^j_k \varphi^j_k + \sum_k d^j_k \psi^j_k \end{aligned}$$

Biorthogonal wavelets (1)

The interpolating scaling functions (basis of V_j) and wavelets (basis of W_j) fit in the framework of biorthogonal wavelets

- Introduced by Cohen, Daubechies and Fauveau (1992).
- Biorthogonal wavelets defined by set of four L^2 functions $\varphi, \tilde{\varphi}, \psi, \tilde{\psi}$ called respectively scaling function, dual scaling function, wavelet and dual wavelet.
- φ and $\tilde{\varphi}$ are defined by their scaling relations

$$\varphi(x) = \sum_{n \in \mathbb{Z}} h_n \varphi(2x - n),$$

$$\tilde{\varphi}(x) = \sum_{n \in \mathbb{Z}} \tilde{h}_n \tilde{\varphi}(2x - n).$$

Biorthogonal wavelets (2)

- Then ψ and $\tilde{\psi}$ are defined by

$$\psi(x) = \sum_{n\in\mathbb{Z}} g_n \varphi(2x-n) \quad \text{with } g_n = (-1)^{n+1}\tilde{h}_{1-n},$$

$$\tilde{\psi}(x) = \sum_{n\in\mathbb{Z}} \tilde{g}_n \tilde{\varphi}(2x-n) \quad \text{with } \tilde{g}_n = (-1)^{n+1} h_{1-n}.$$

- The following space decompositions are associated to the biorthogonal wavelets

$$V_{j+1} = V_j \oplus W_j, \qquad \tilde{V}_{j+1} = \tilde{V}_j \oplus \tilde{W}_j.$$

where $(\varphi(2^j \cdot -k))_k$ span V_j and $(\psi(2^j \cdot -k))_k$ span W_j.

Biorthogonal wavelets (3)

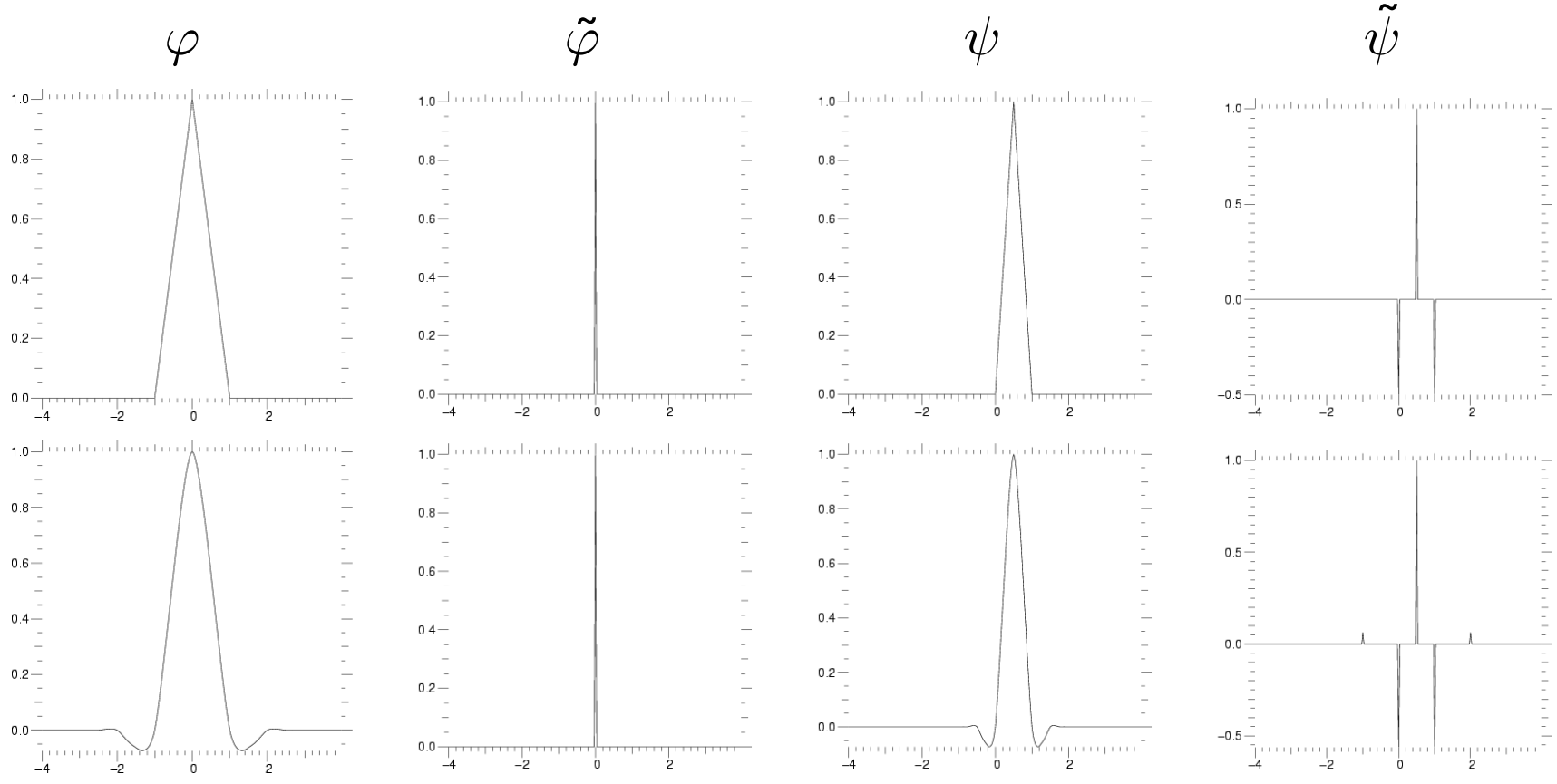
- Bases are biorthogonal:
  $\langle \varphi, \tilde{\varphi}(\cdot - k) \rangle = \delta_{0,k}, \quad \langle \varphi, \tilde{\psi}(\cdot - k) \rangle = 0.$
- Projections of f onto V_j and W_j defined by their coefficients

$$c_k^j = \langle f, \tilde{\varphi}_k^j \rangle, \quad d_k^j = \langle f, \tilde{\psi}_k^j \rangle, \quad \text{where } \varphi_k^j = \varphi(2^j \cdot - k).$$

- $f_{j+1} \in V_{j+1}$ can be expressed equivalently as

$$\begin{aligned} f_{j+1} &= \sum_k c_k^{j+1} \varphi_k^{j+1} \\ &= \sum_k c_k^j \varphi_k^j + \sum_k d_k^j \psi_k^j \end{aligned}$$

Scaling functions and wavelets



Case of interpolating wavelets: $\psi_k^j = \varphi_{2k+1}^{j+1}$, $\tilde{\varphi} = \delta$.

Thresholding

- Consider following expression: $f_{j+1} = \sum_k c_k^j \varphi_k^j + \sum_k d_k^j \psi_k^j$.
- Adaptivity introduced by neglecting the terms in this expansion such that $|d_k^j| < \epsilon_j$.
- Error commited can be easily estimated $\|d_k^j \psi_k^j\|_{L^p} = |d_k^j| 2^{-\frac{j}{p}} \|\psi\|_{L^p} < \epsilon_j 2^{-\frac{j}{p}} \|\psi\|_{L^p}$.
- Moments of f_{j+1} can be conserved by appropriately modifying ψ: taking $\psi^m = \psi - \sum_k s_k \varphi(\cdot - k)$ with $(s_k)_k$ chosen such that $\int x^l \psi^m(x)\, dx = 0$ for $0 \leq l \leq m$.
  $\rightarrow$ modifies the supplementary space W_j of V_j in V_{j+1}.

Computation of sources for Maxwell's equations

- The coupling of Vlasov with Maxwell lies in part on the computation of the charge and current densities from the distribution function

$$\rho = \sum_s q_s \int f_s \, d\mathbf{p}, \qquad \mathbf{J} = \sum_s \frac{q_s}{m_s} \int f_s \frac{\mathbf{p}}{\gamma_s} \, d\mathbf{p},$$

  where f_s is approximated by its wavelet decomposition.
- In practice for the computation of ρ, one needs to be able to compute

$$\int \phi_k^j(p) \, dp, \text{ and } \int \psi_k^j(p) \, dp$$

  $\longrightarrow$ Straightforward.

Computation of **J**

- A little bit more complicated for **J** where we need

$$\int \phi_k^j(p)\frac{p}{\gamma(p)}\,dp, \text{ and } \int \psi_k^j(p)\frac{p}{\gamma(p)}\,dp.$$

- As γ is a non linear function of p, no exact integration.
- We chose to approximate $\frac{1}{\gamma}$ by its polynomial interpolation (of degree 2 or 3), in order to boil down the problem to the computation of moments of wavelet and scaling function, which we know how to do.
- Full algorithm in [Besse, Latu, Ghizzo, S, Bertrand, JCP 2008].

The Algorithm for the Vlasov-Maxwell Problem

- **Initialisation**: decomposition and compression of f_0.
- **Computation** of electromagnetic field from Maxwell.
- **Prediction** of the grid $\tilde{G}$ (for important details) at the next time step following the characteristics forward. Retain points at level just finer.
- **Construction of** $\hat{G}$: grid where we have to compute values of f^{n+1} in order to compute its wavelet transform.
- **Transport-interpolation** : follow the characteristics backwards in x and interpolate using wavelet decomposition.
- **Wavelet transform of** f^{n+1}: compute the c_k and d_k coefficients at the points of $\tilde{G}$.

Rem: No splitting in this case. Generally done for Vlasov-Poisson.

Computer science issues

- Multiresolution code a lot harder to make efficient that uniform grid counterpart.
- Careful work on data structures and code optimization needed.
- Data structures:
  - Adaptive grid G
  - Distribution function F
  - Wavelet decomposition D
- Wall clock time depends mostly on data access speed.
- Try and make it as fast as possible for code optimization.
- For cache optimization data needs to be accessed by level or by physical position in different parts of the algorithm.

Optimization of data structure (2D)

- Hash tables efficient for memory reduction and random access, but not for ordered walk through by level with access to adjacent levels.
- Use sparse data structure based on two levels of dense arrays instead of hash-table
  - first array contains all grid points up to some intermediate level
  - second array which is allocated where needed contains all the grid points from this intermediate up to the finest level
  - all grid points can be accessed with at most one indirection pointer
- Computing time decreased by a factor of 3 in 2D

Optimization of data structure (4D)

- Data structure based on two levels of dense arrays (used in 2D code) consumes too much memory for large grid sizes (more than 128^4).
- Data structure based on hexadecatree is used but instead of storing one level per node, we store two levels per node, i.e. $16^2 = 256$ points.

Parallelization

- Two kinds of data locality because wavelet transform accesses grid points by levels.
- One single domain decomposition $\Rightarrow$ complex data shape access.
- Code was parallelized using OpenMP targeting shared memory computers to avoid calling communication subroutines.
- Efficiency on SGI Origin 3800 at 500 MHz for large grid (2D code)

1 proc	16 proc	32 proc	64 proc
100%	89%	79%	66%

Comparison dense vs. adaptive

- Comparison with optimize solver on uniforme mesh in 2D phase space for semi-Gaussian beam for different mesh sizes ($2^k \times 2^k$).

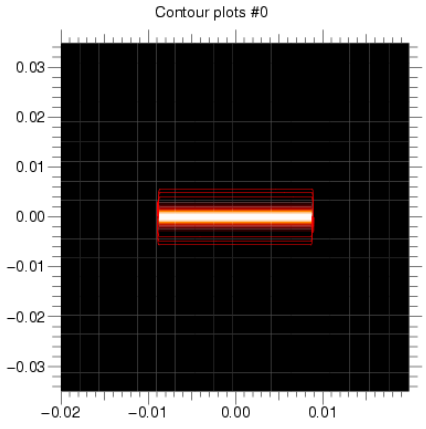
k	10	11	12	13	14
mesh size (MB)	8	32	128	512	2048
Loss 2D (s)	0.11	0.44	2.70	24.20	138.60
Obiwan 2D (s)	0.33	0.83	2.46	3.70	8.90

- Adaptive code becomes faster for very fine grids.
- Same remark for 4D code. Enables to take grids of 512^4 that uniform mesh solver cannot handle.

Transport of a 5 MeV proton beam

- Beam parameters:
  - Lattice consists of 60 periods of length $L = 1\ m$. Field given by
    $$B(z) = \alpha(1 + \cos(2\pi z/L)^2), \alpha = 1.12\ T.$$
  - $I = 1.9\ A \Rightarrow K = 10^{-4}$, $\epsilon_{KV} = 10^{-5}\pi\ m \cdot rad$.
  - $\sigma_0 = 2.3\ rad$ per period, $\sigma = 0.45\ rad$ per period $\Rightarrow \frac{\sigma}{\sigma_0} \approx 0.2$
- Numerical parameters:
  - 512×512 fine grid. Grid point suppression threshold 10^{-4}.
  - 50 time steps per lattice period.

+50% mismatch in all of r, v_r and I



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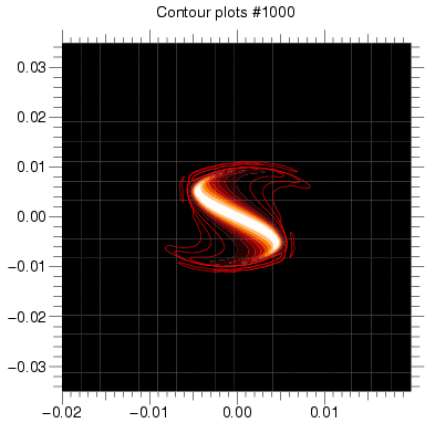
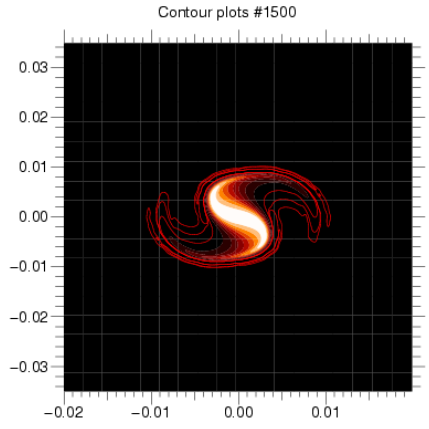
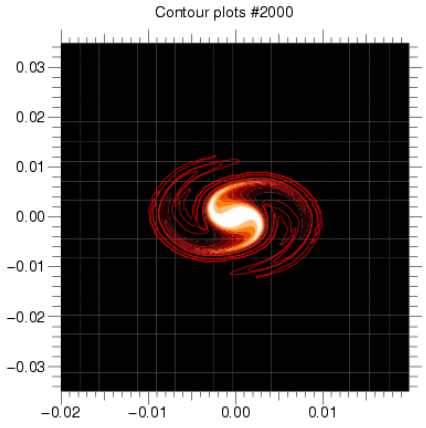


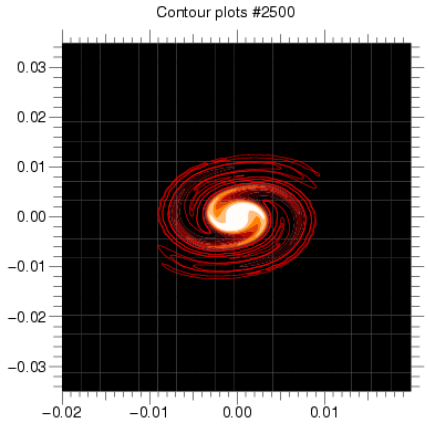
20 periods



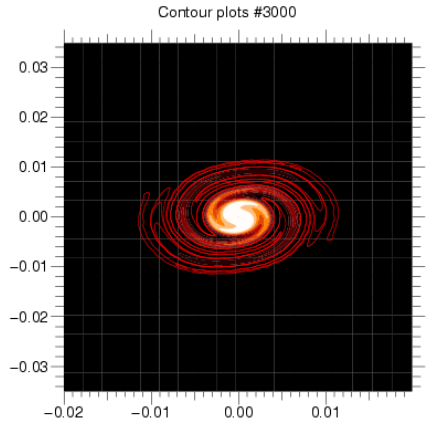
30 periods



40 periods

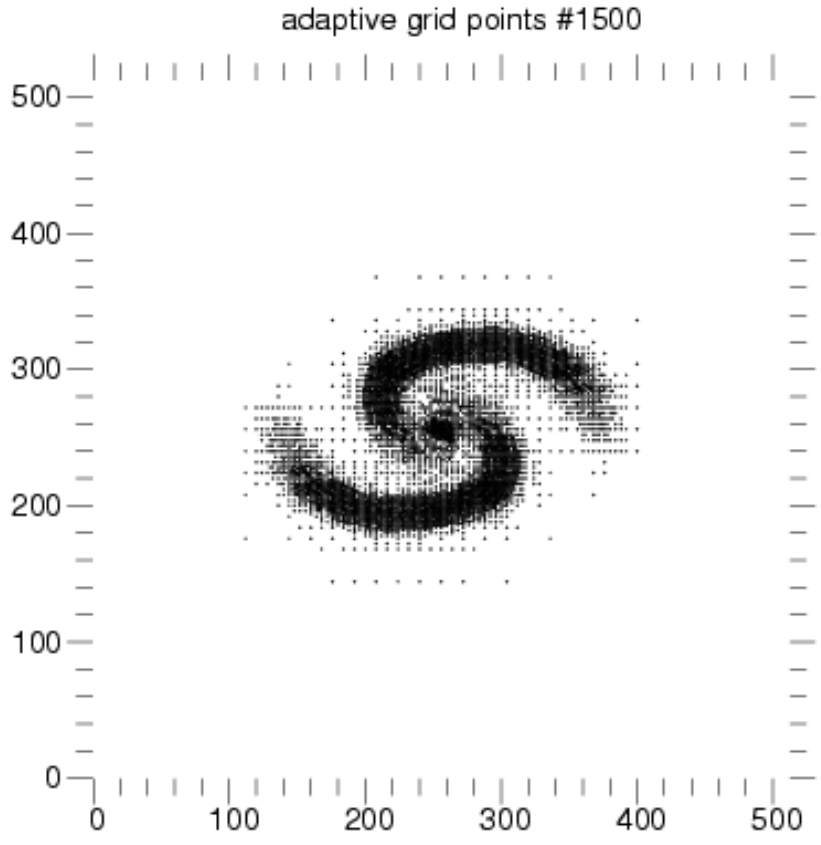


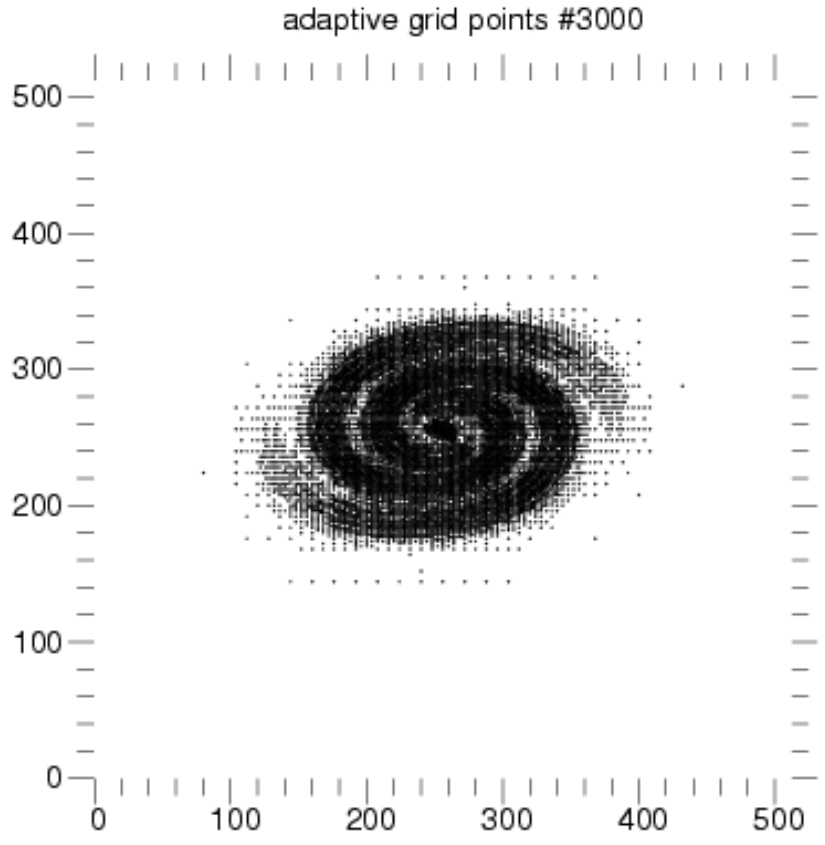
50 periods



60 periods

Localization of grid points after 30 and 60 periods





Parametric Vlasov-Maxwell instability (1/3)

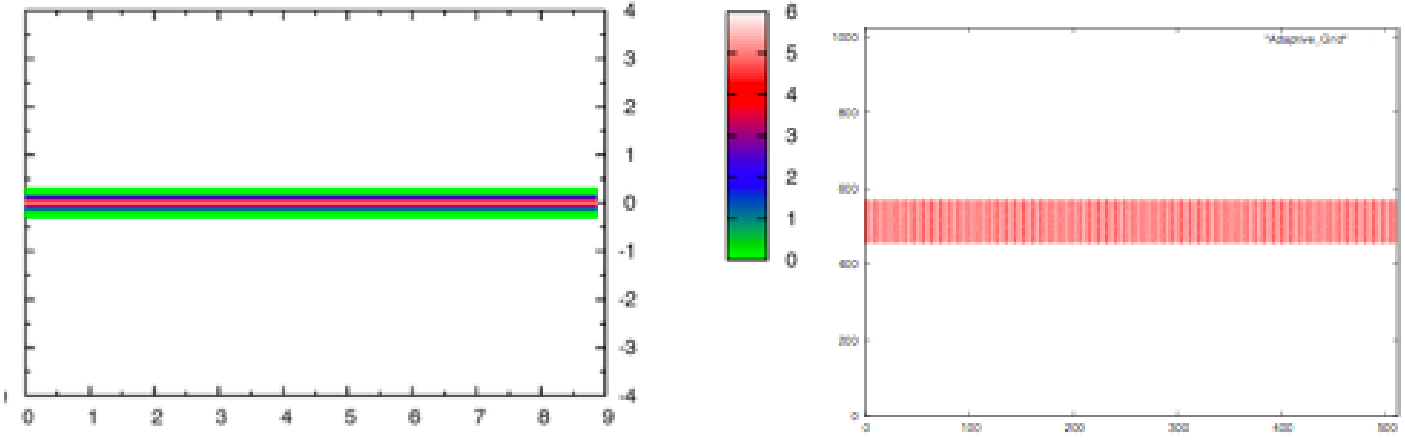


Figure 5: Snapshots at $t = 0\omega_p^{-1}$ of the distribution function in phase-space (x, p_x) and the associated adaptive grid for the parametric instability

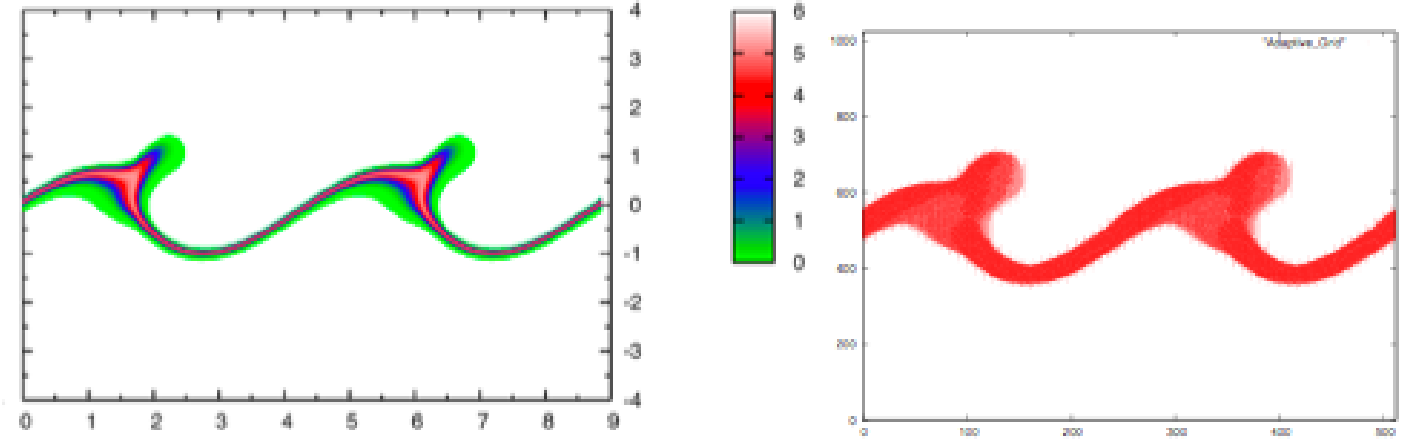


Figure 6: Snapshots at $t = 90.24\omega_p^{-1}$ of the distribution function in phase-space (x, p_x) and the associated adaptive grid for the parametric instability

Parametric Vlasov-Maxwell instability (2/3)

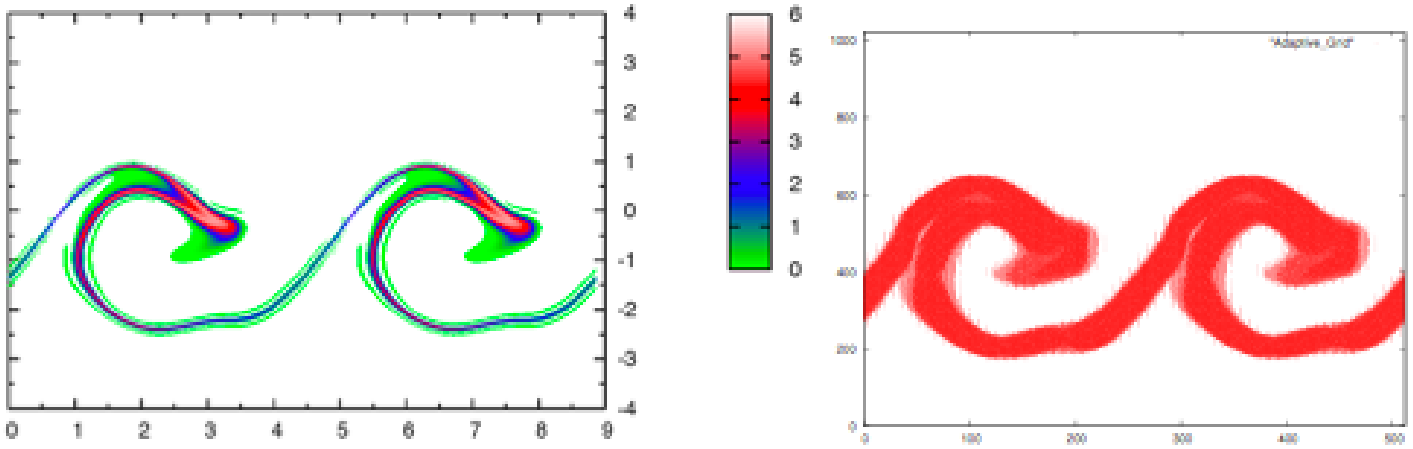


Figure 7: Snapshots at $t = 93.71\omega_p^{-1}$ of the distribution function in phase-space (x, p_x) and the associated adaptive grid for the parametric instability

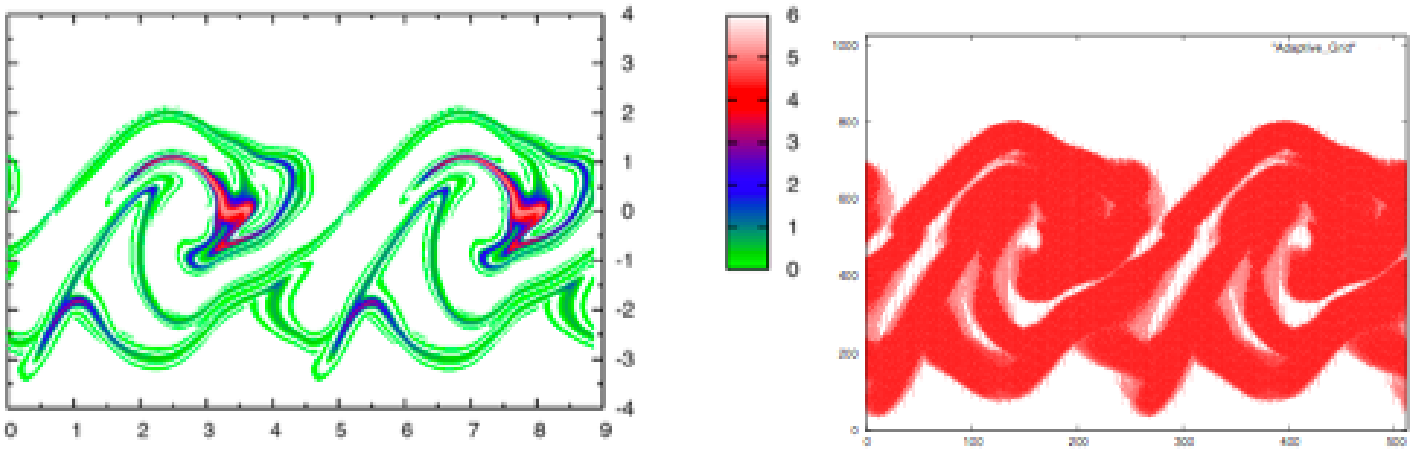


Figure 8: Snapshots at $t = 100.65\omega_p^{-1}$ of the distribution function in phase-space (x, p_x) and the associated adaptive grid for the parametric instability

Parametric Vlasov-Maxwell instability (3/3)

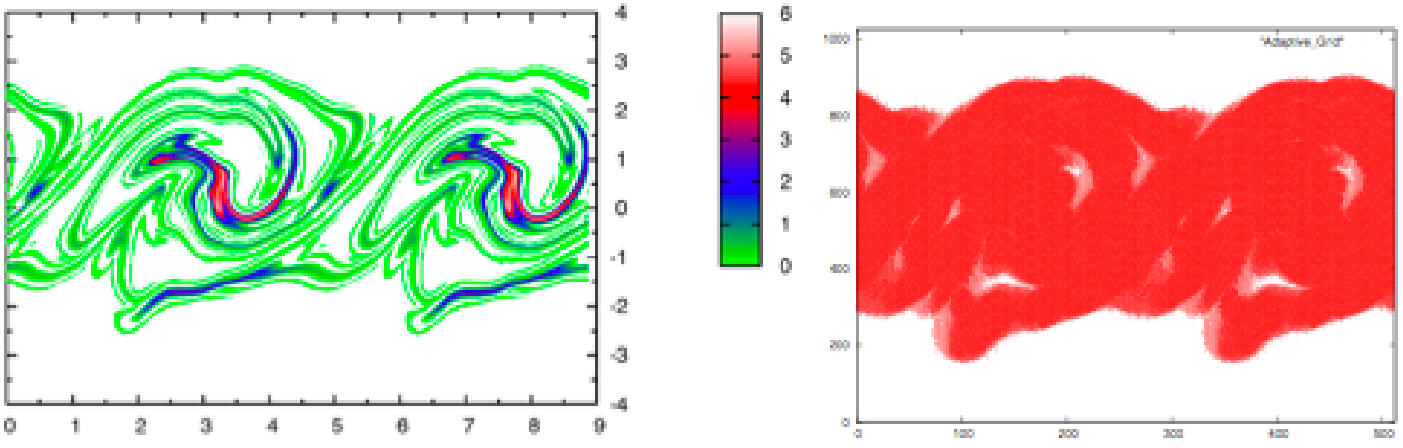


Figure 9: Snapshots at $t = 104.13\omega_p^{-1}$ of the distribution function in phase-space (x, p_x) and the associated adaptive grid for the parametric instability

Laser wake-field (1/2)

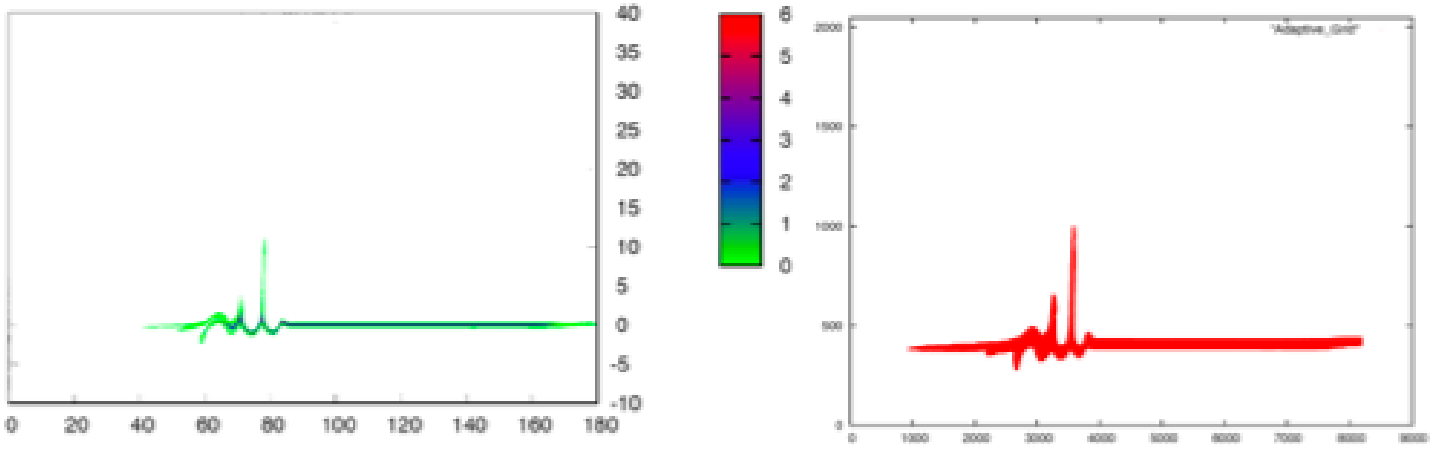


Figure 14: Snapshots at $t = 88.\omega_p^{-1}$ of the distribution function in phase-space (x, p_x) and the associated adaptive grid for the laser-wake field

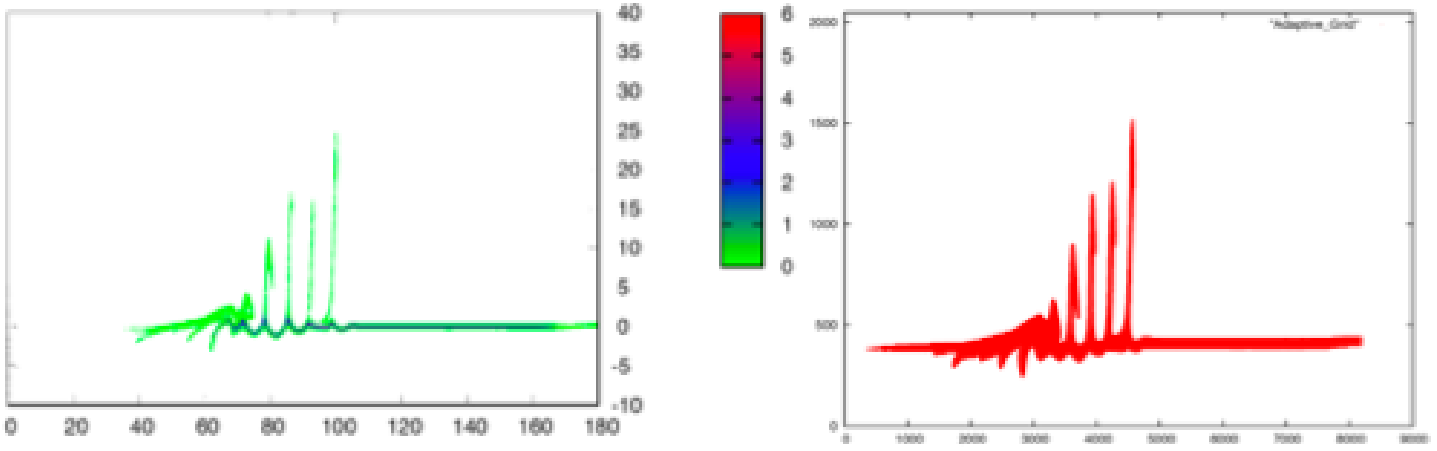


Figure 15: Snapshots at $t = 110.\omega_p^{-1}$ of the distribution function in phase-space (x, p_x) and the associated adaptive grid for the laser-wake field

Laser wake-field (2/2)

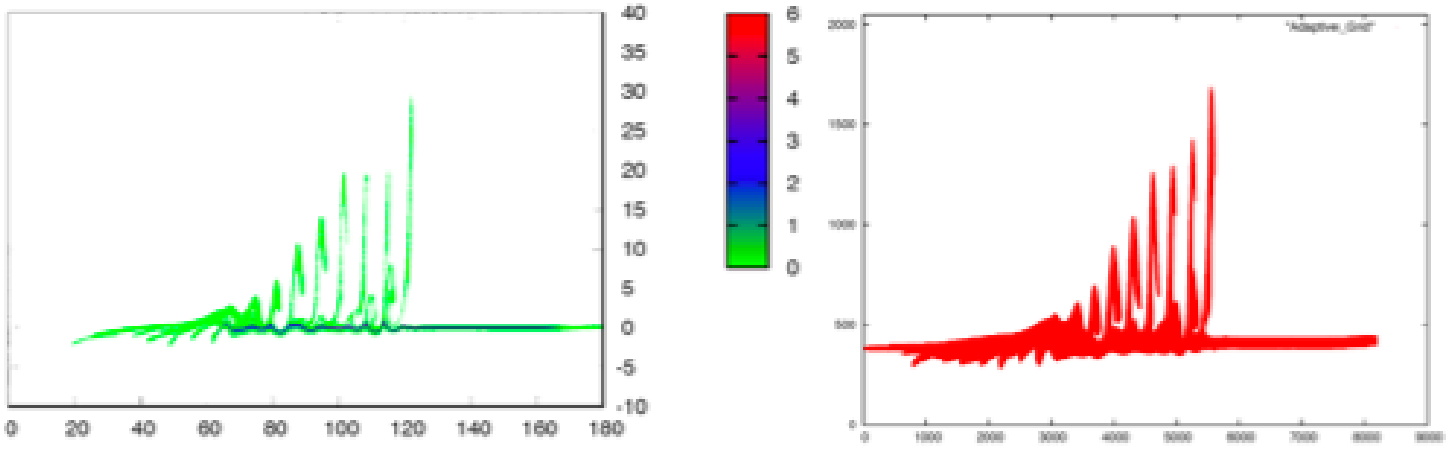


Figure 16: Snapshots at $t = 132.\omega_p^{-1}$ of the distribution function in phase-space (x, p_x) and the associated adaptive grid for the laser-wake field

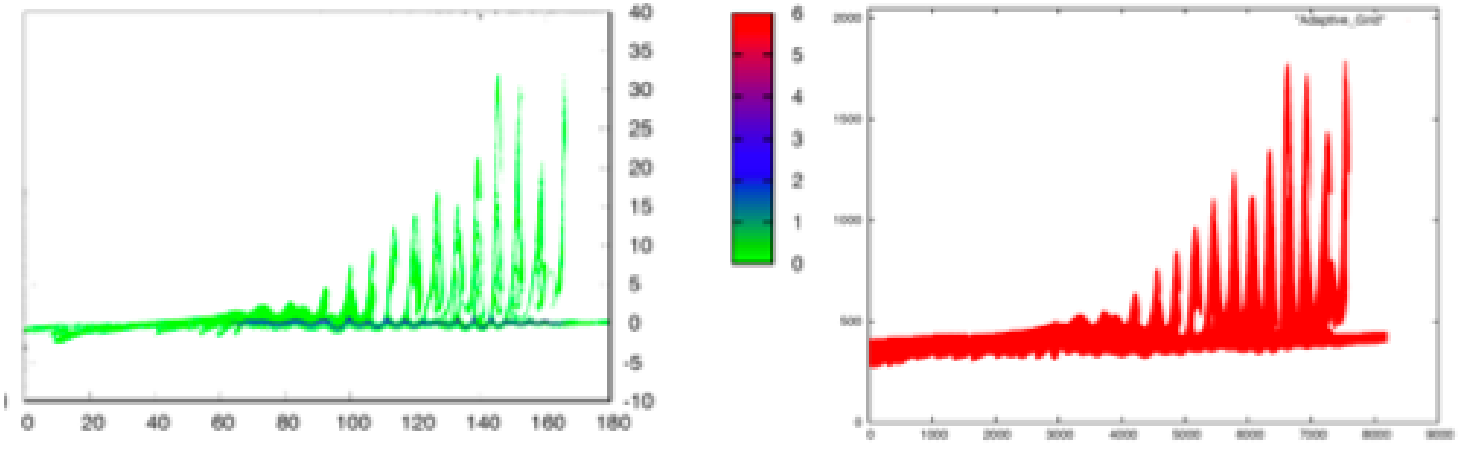


Figure 17: Snapshots at $t = 176.\omega_p^{-1}$ of the distribution function in phase-space (x, p_x) and the associated adaptive grid for the laser-wake field

Conclusions

- Grid based Vlasov solvers are a valuable tool to have in one's simulation toolbox.
- No noise. Better representation in low density regions of phase space.
- Adaptive grid strategy can be made efficient by careful optimization.
- 2D (4D phase-space) code is now running and can perform realistic simulations of transverse phase space.
- Adaptive solvers make it possible to access very fine resolutions needed at some regions in the computation domain.
- Likely that such methods can be applied to $2D\frac{1}{2}$ and $3D$ in the future.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