Adaptive Numerical Vlasov Simulation of Intense Beams

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New INRIA project CALVI devoted to the development of simulation and visualization tools for plasma physics and beam physics. Involves applied mathematicians, computer scientists and plasma physicists from Nancy and Strasbourg.

http://math.u-strasbg.fr/calvi

The quest

Improve numerical methods for intense beam simulation

- Room for improvement ?
  - PIC methods.
  - Grid based methods for the Vlasov equation.
- Towards efficient grid based methods
  - Moving phase space grid.
  - Hierarchical approximation.

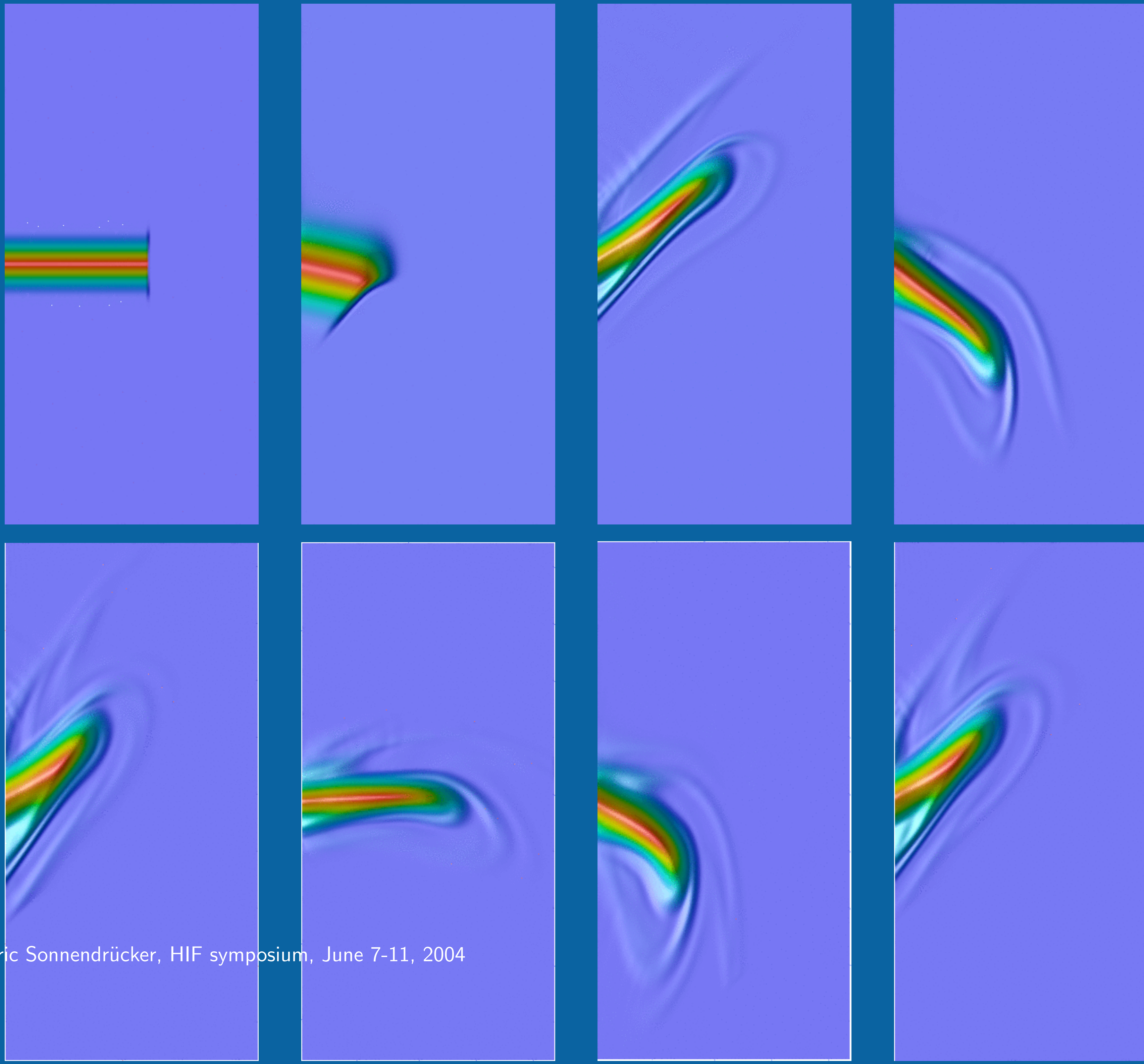
A typical beam simulation

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 $v_z = 626084\,ms^{-1}$.



The model

- Beam particles are described by distribution function $f(x, v, t)$.
- Distribution function $f(x, v, t)$ is solution of the Vlasov equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + \frac{q}{m} (E + v \times B) \cdot \nabla_v f = 0,$$

generally coupled with the Poisson or Maxwell equations.

- Goal: get an accurate numerical solution of this model.

Numerical methods

- Particle In Cell (PIC)
- Direct Vlasov solution on phase space grid

Principle of PIC methods

- Approximate initial distribution function by random sample of equally weighted macro-particles.
- Advance macro-particles using equations of motion.
- Regularize f in physical space to compute ρ and J on grid for coupling with field solver.
- Approximation of f can be expressed as

$$f_h(x,v,t) = \sum_p w_p S(x - x_p(t))\delta(v - v_p(t)).$$

Problems with PIC methods

- Numerical noise.
- Most particles localized in zones of high f.
  $\longrightarrow$ poor statistics in low density regions of phase space
  $\longrightarrow$ very hard to get accurate description of phenomena like halo.

Techniques for improvement

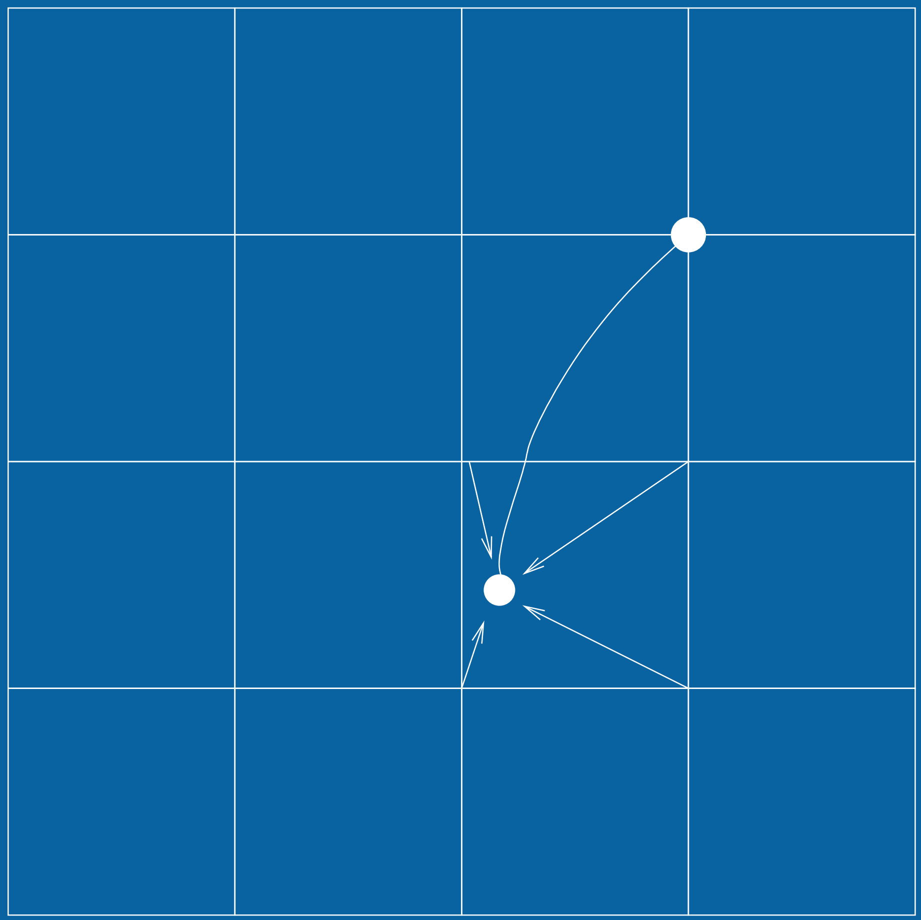
- Statistical noise reduction techniques:
  - Average over several runs with different initial samples.
  - δf methods. Decompose $f = f_0 + \delta f$ and use particle approximation only for perturbation (Lee, Qin,... , Friedman). Decreases noise where $\delta f << f_0$.
- Weighted PIC methods:
  - Draw uniform sample of macro-particles over phase-space and give them a weight according to value of distribution function at their location.
  - Problem: Mixing of high weight and low weight particles $\longrightarrow$ resample.

Methods based on a phase space grid

- Many different kinds of methods have been investigated!
- Prefer hybrid methods taking into account particle motion.
- Semi-Lagrangian method:
  - backward - forward
  - point based - cell based

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



Problems with grid based methods

- Numerical diffusion
- Curse of dimensionality: N^d grid points needed in d dimensions. Number of grid points grows exponentially with dimension
  $\longrightarrow$ killer for Vlasov equation where d up to 6.

Paths to improvement

- Moving grid techniques:
  use grid which follows closely global motion (envelope motion).

- Hierarchical approximation:
  Instead of approximating f on uniform grid, use nested grids and keep only N highest coefficients.

Moving computational domain

- For beam simulations large gain can already be expected by moving computation box.
- Computation box could be determined from envelope.
- Expect much easier implementation.
- Splitting algorithm would not work anymore.

Towards the moving grid algorithm

The semi-Lagrangian method consists in two conceptually different steps:

1. **Advection step:** follow particle trajectories. *completely independent of the grid and most naturally performed in the physical space*

2. **Interpolation step:** Interpolation grid needed to reconstruct the distribution function at every point in phase space at one given time step, needs not be the same at two different time steps. Ideal if grid points exactly on particle trajectories.

Desired features of efficient solver

- Use **optimal number of grid points** to reconstruct distribution function f at any given time with a given accurary.
- Minimize number of wasted grid points (computations in zones of vanishing f).
- Have grid points follow particle trajectories $\longrightarrow$ minimize interpolation errors.

The transform method

- Define at each time step an invertible mapping φ_t from a logical grid to the physical grid.
- This mapping needs to be known or constructed automatically.
- Distribution function on logical grid $f^*(x^*, v^*, t) = f(\varphi_t(x^*, v^*), t)$. $*$ denotes quantities on logical grid.
- f^* satisfies the following conservation property

$$f^*(x^*, v^*, t) = f^*(X^*(s; x, v, t), V^*(s; x, v, t), s)$$

Beam simulation in transverse phase space

Find transform following beam envelope.
e.g. RMS equivalent ellipse satisfies

$$\tan 2\theta = \frac{2\langle xx'\rangle}{\langle x^2\rangle - \langle x'^2\rangle},$$

$$a = \sqrt{2(\cos^2\theta\langle x^2\rangle + \sin^2\theta\langle x'^2\rangle + 2\sin\theta\cos\theta\langle xx'\rangle)},$$
$$b = \sqrt{2(\sin^2\theta\langle x^2\rangle + \cos^2\theta\langle x'^2\rangle - 2\sin\theta\cos\theta\langle xx'\rangle)}.$$

Numerical results

Toy problem: transverse axisymmetric Vlasov-Poisson equation with vanishing canonical angular momentum. This problem reads

$$\frac{\partial f}{\partial t} + v_r \frac{\partial f}{\partial r} + (F_{app} + \frac{q}{m} E_r) \frac{\partial f}{\partial v_r} = 0,$$

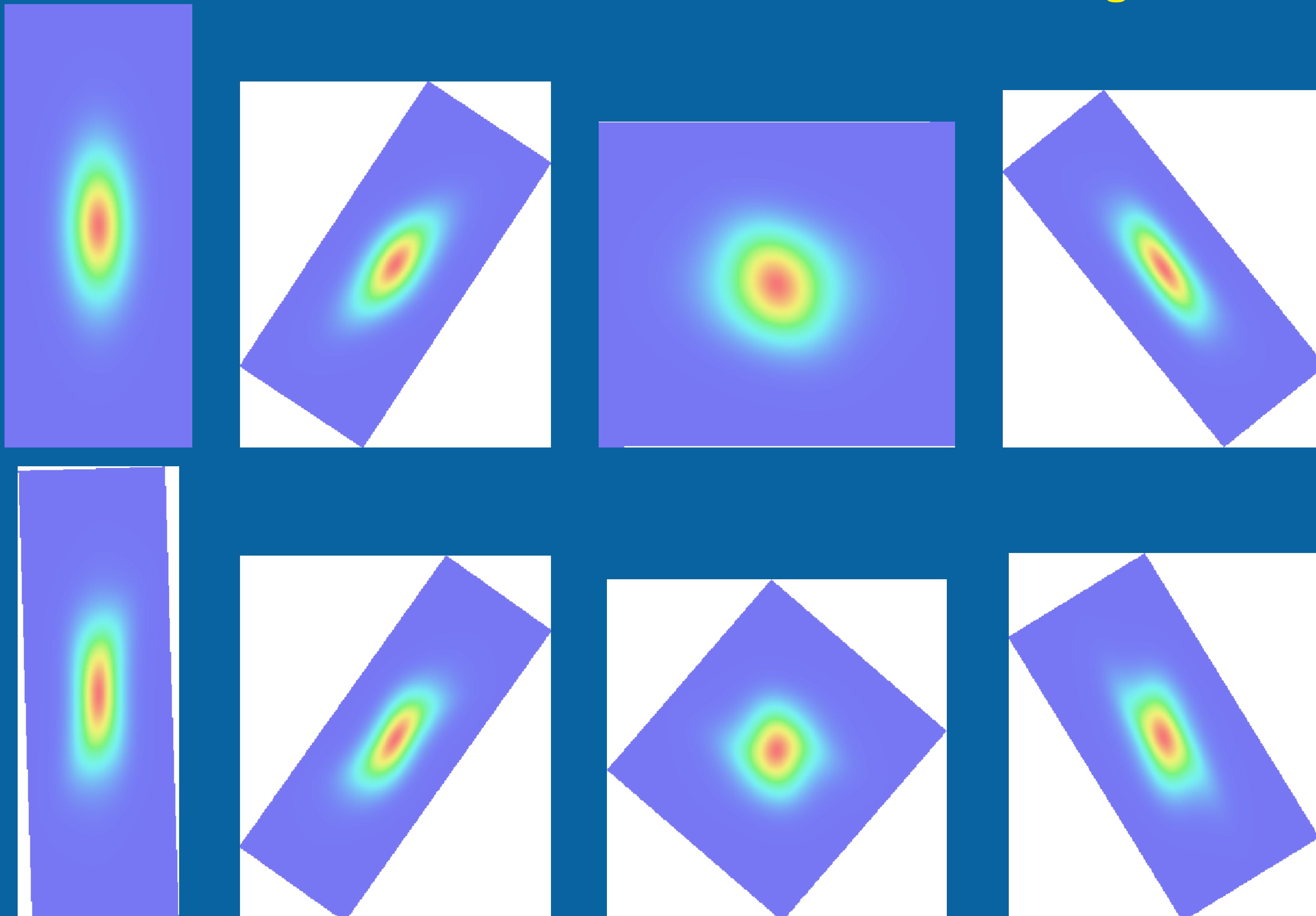
$$\frac{1}{r} \frac{d}{dr}(r E_r) = \rho = \int f \, dv_r.$$

Examples with important envelope motion.

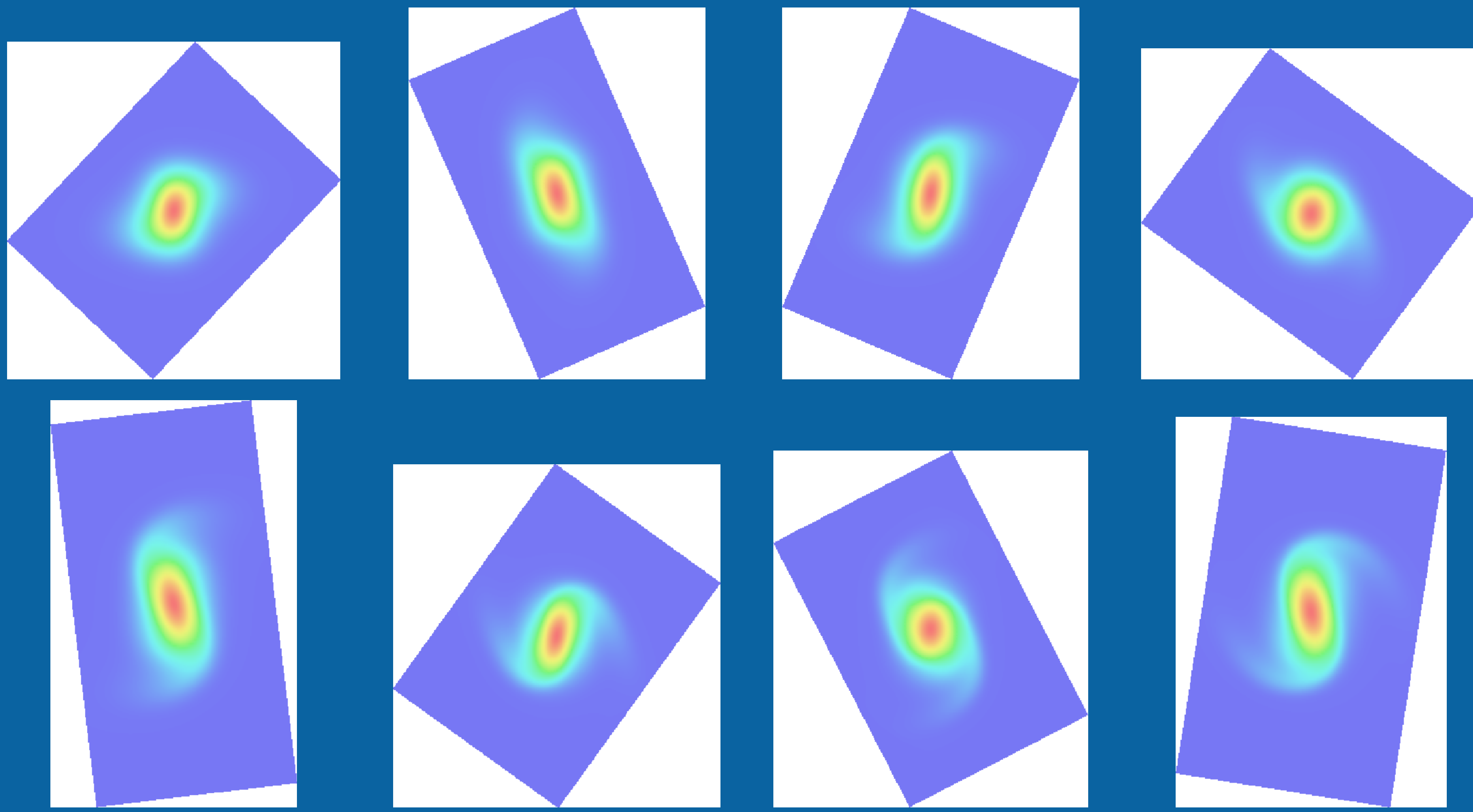
1. Mismatched beam in a uniform focusing channel.

2. Matched beam in a periodic focusing channel.

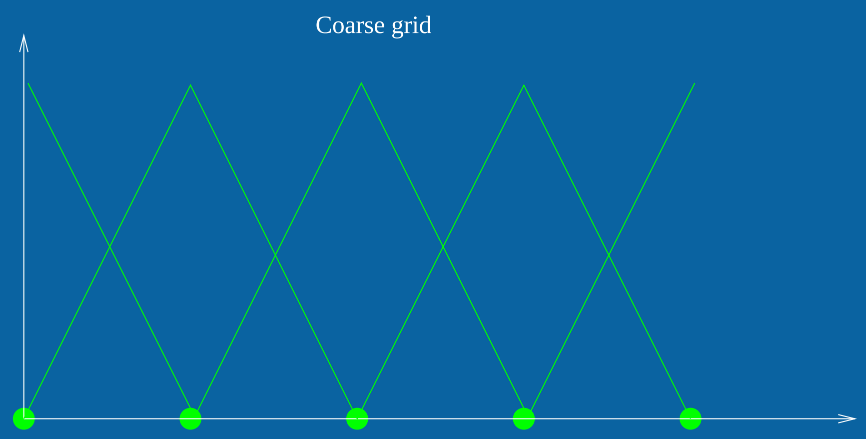
Evolution of mismatched Gaussian beam in uniform focusing channel

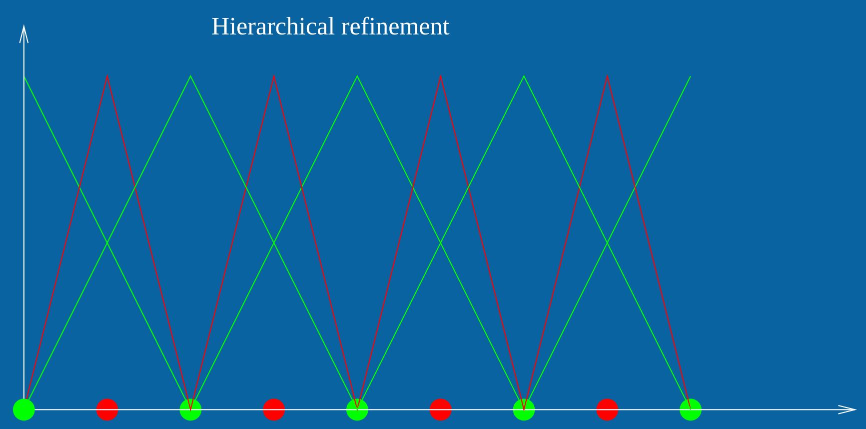


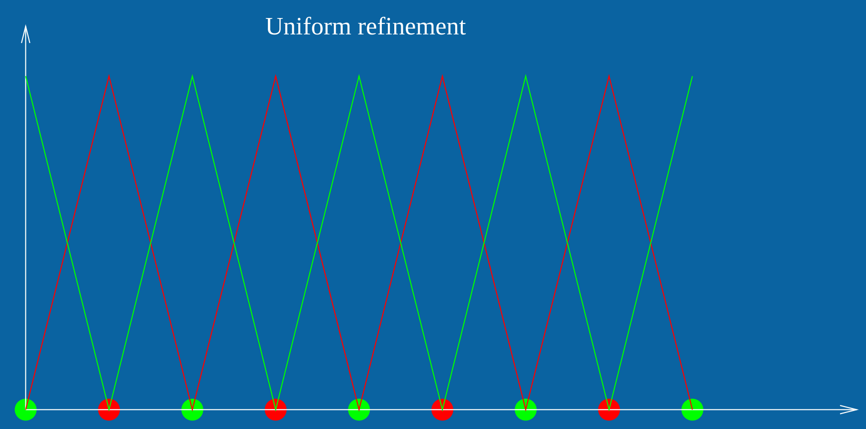
Evolution of matched Gaussian beam in periodic focusing channel



Hierarchical decomposition







Hierarchical expression

- A piecewise affine approximation of f can be expressed equivalently:
  - Using uniform expression:

$$f(x) = \sum_i c_i S_h(x - x_i) \quad \text{with } c_i = f(x_i).$$

  - Using hierarchical expression:

$$f(x) = \sum_i c_{2i} S_{2h}(x - x_{2i}) + \sum_i d_{2i+1} S_h(x - x_{2i+1})$$

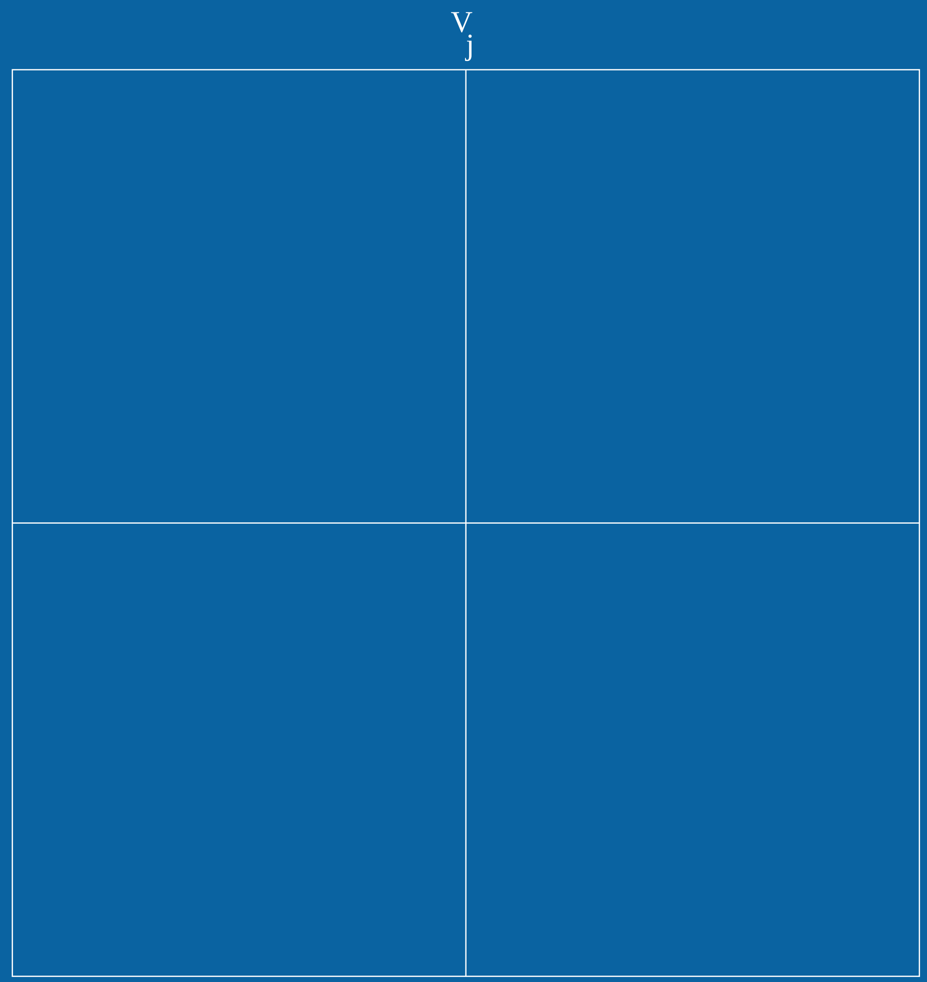
with $c_{2i} = f(x_{2i})$ and $d_{2i+1} = f(x_{2i+1}) - \frac{1}{2}(c_{2i} + c_{2i+2})$.

Nonlinear approximation

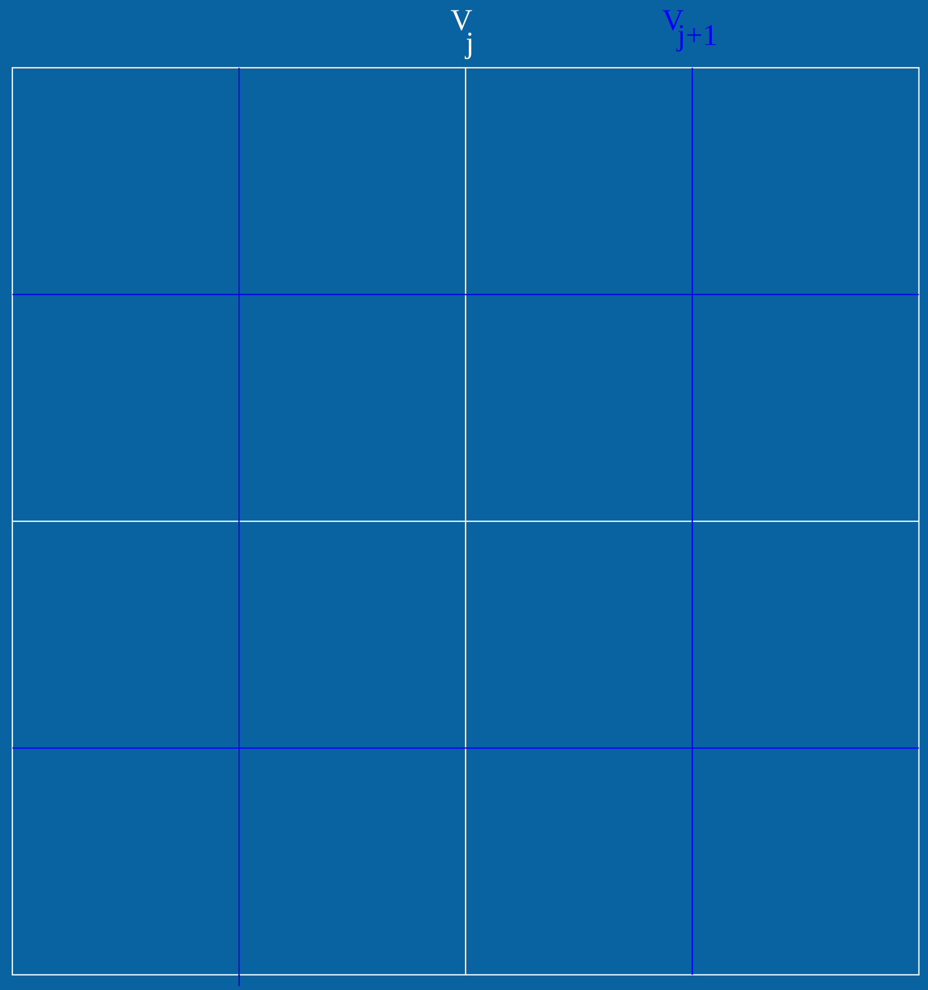
- In hierarchical decomposition coefficients d_{2i+1} at fine scale are small if f is close to affine in $[x_{2i}, x_{2i+2}]$.
- Linear (uniform) approximation consists in using a given number of basis functions independently of approximated function f.
- Nonlinear approximation consists in keeping the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

Adaptive semi-Lagrangian method

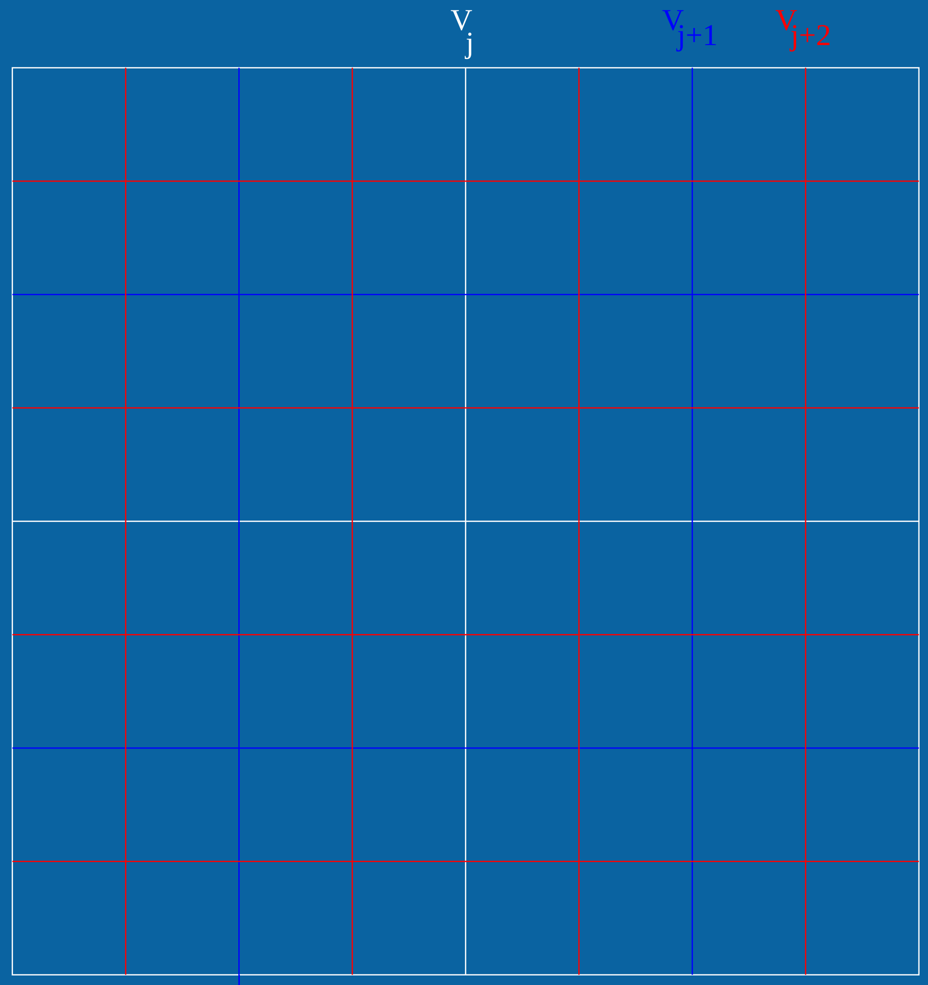
- Semi-Lagrangian method consists of two stages : advection and interpolation
- Interpolation can be made adaptive : approximate f^n with as few points as possible for a given numerical error using non linear approximation.
- Construct approximation layer by layer, starting from coarse approximation 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.



Grid G_j, grid points $x_k^j = k\,2^j$, level j



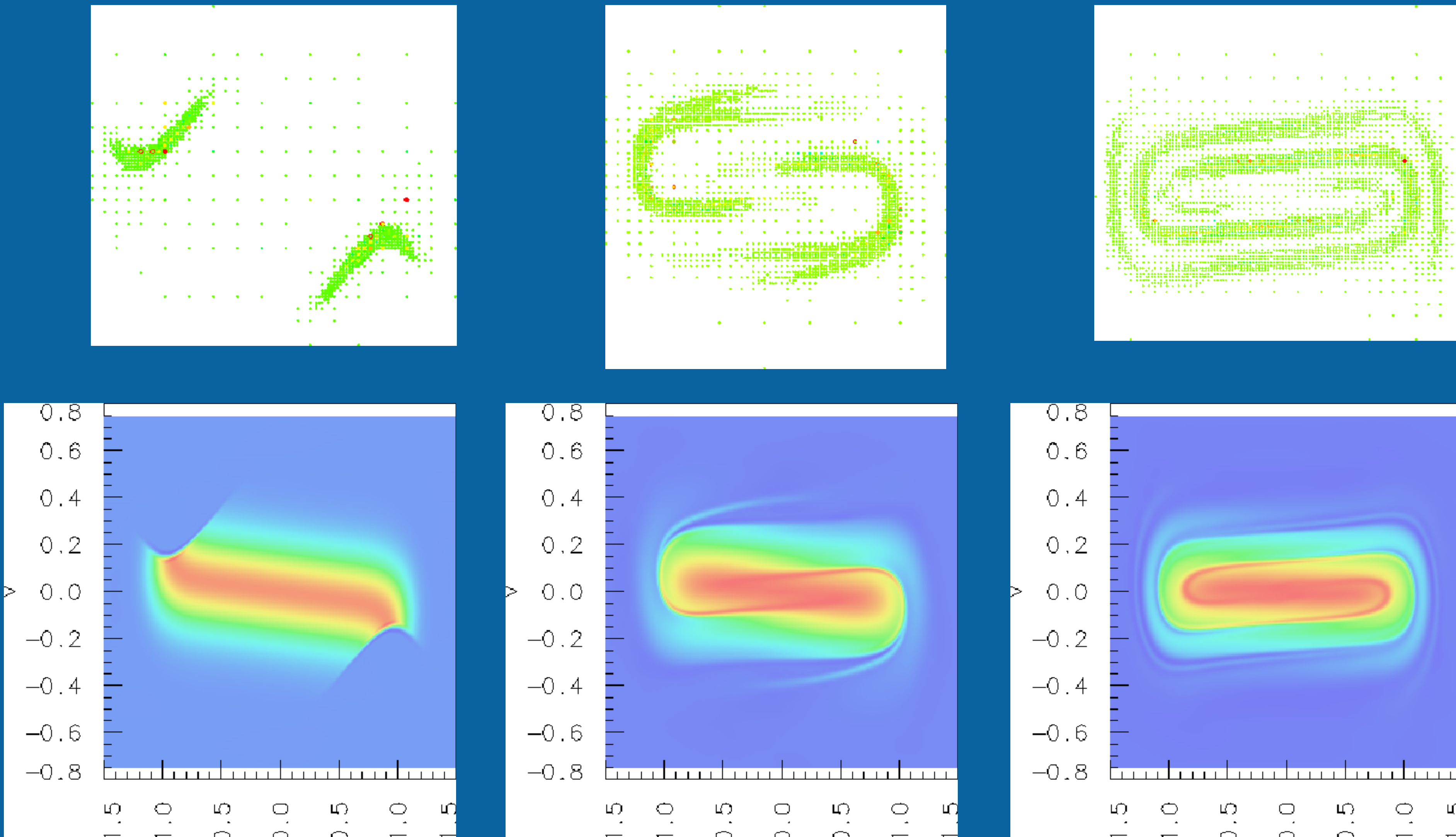
Grid G_{j+1}, grid points $x_k^{j+1} = k\,2^{j+1}$, level $j+1$



Grid G_{j+2}, grid points $x_k^{j+2} = k\,2^{j+2}$, level $j+2$

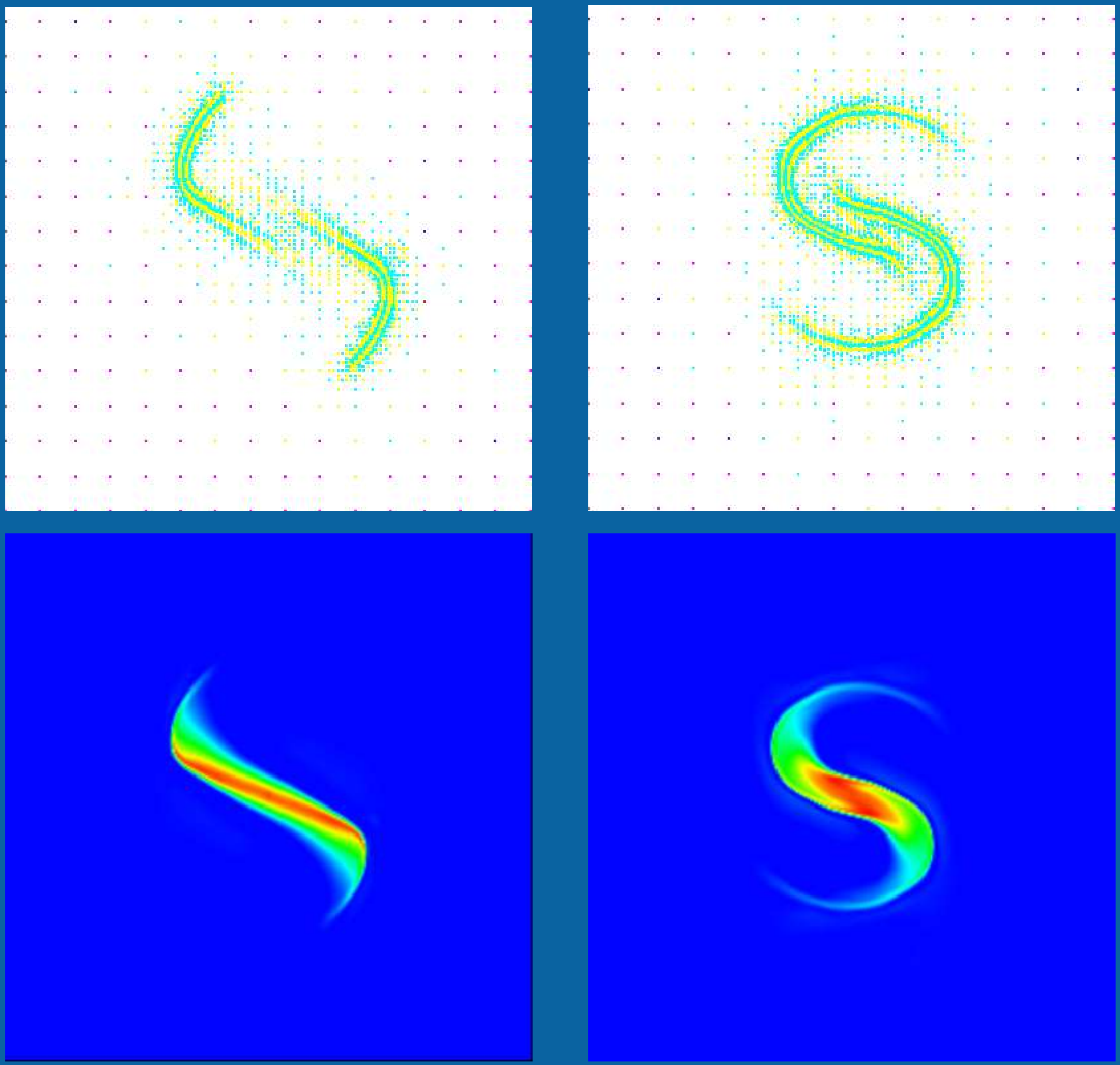
Semi-Gaussian beam evolution in uniform focusing channel

- Potassium ions
- Beam energy 80 keV
- Uniform focusing
- Tune depression 0.25


0.8
0.6
0.4
0.2
v
0.0
−0.2
−0.4
−0.6
−0.8
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5

Semi-Gaussian beam evolution in periodic focusing channel

- Potassium ions
- Beam energy 80 keV
- Periodic focusing field of the form $\alpha(1 + \cos 2\pi z/S)$.
- Tune depression 0.17



Conclusions

- Thanks to adaptive method computational complexity of grid based methods becomes comparable to PIC method.
- 1D and 2D adaptive codes are running
- Likely that such methods can be applied even to $2D\frac{1}{2}$ and $3D$ in the future.
- **However**
  - Coding become a lot more complex.
  - Appropriate efficient data structure needs to be used.

- Moving grid semi-Lagrangian method feasible and easy to implement.
- Interesting for beam simulations where computing box can be easily determined from envelope motion.
- Needs to be implemented for realistic 2D simulations.
- Other kinds of transforms enabling to follow more closely the particle trajectories should be tried.