Adaptive Dynamical Approximations with tensors

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- Motivation
  - Solving high-dimensional PDEs
  - Equations in Kinetic Theory
- The Vlasov-Poisson system
  - Hamiltonian formulation and symplectic integration
  - Dynamical Tensor decomposition
- Improving the representation
  - Hierarchical local sub-tensor approximations
- Conclusions and Perspectives

Motivation

- High-dimensional Partial Differential Equations
  - Kinetic Theory: $\Omega = \Omega_x \times \Omega_v \times \mathbb{R}^+$
  - Optimal Transport: $\Omega = \Omega_1 \times \ldots \times \Omega_k, \quad \Omega_i \subseteq \mathbb{R}^d$
  - Uncertainty Quantification: $\Omega = \Omega_x \times \Omega_\vartheta \times \mathbb{R}^+$
  - …

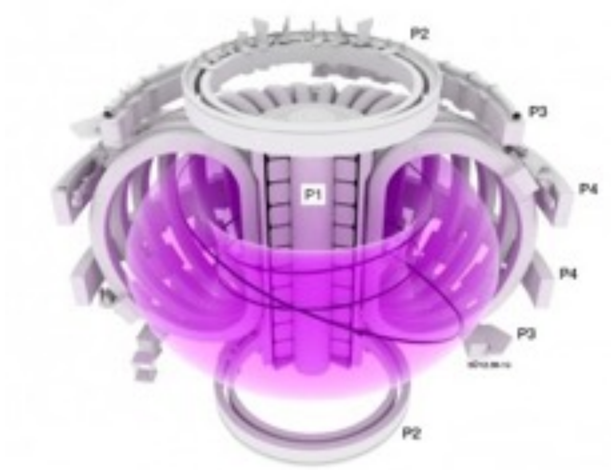
- Solution approximation
  - Curse of dimensionality: $\mathcal{N} \propto C^d$
  - Numerical approximation by standard methods is unfeasible

The Vlasov-Poisson system

Kinetic Theory:

- The purpose of Kinetic Theory is the description of dilute particle gases at an intermediate scale between the microscopic scale and the hydrodynamic scale*
- Domain: $\Omega = \Omega_x \times \Omega_v \times \mathbb{R}^+$
- The unknown is the distribution of particles in the phase space (position and velocity), as function of time.

  $f(t,x,v) : \Omega \to \mathbb{R}^+$



- Normalization: $$\int_{\Omega_x} \int_{\Omega_v} f(t,x,v)\ dv\ dx = 1$$
- Density: $$\varrho(t,x) = \int_{\Omega_v} f(t,x,v)\ dv$$
- No collision: the value of the particle distribution is constant along the characteristics in the phase space.

* J. Dolbeault, *An introduction to kinetic equations: the Vlasov-Poisson system and the Boltzmann equation*, Discrete and continuous dynamical systems, Volume 8, Number 2, 2002.

The Vlasov-Poisson system

- Vlasov-Poisson: mean-field approximation of electrically charged particles (electrons in this work), with no collisions, in the electro-static approximation

$$\partial_t f + v \cdot \nabla_x f + a \cdot \nabla_v f = 0$$
$$a(t,x) = -\nabla_x U(t,x)$$
$$\Delta U = 1 - \varrho(t,x)$$
$$f(0,x,v) = f_0(x,v)$$

- Theorem:*

If $f_0 \in L^1(\mathbb{R}^3 \times \mathbb{R}^3) \times L^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ satisfies the following condition:

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} |v|^m f_0(x,v)\, dx\, dv < +\infty \qquad \text{for some } m > 3,$$

then, there exists a global strong non-negative solution f to the Vlasov-Poisson system so that

$$f \in \mathcal{C}(\mathbb{R}^+; L^1(\mathbb{R}^3 \times \mathbb{R}^3)) \cap L^\infty(\mathbb{R}^+ \times \mathbb{R}^3 \times \mathbb{R}^3).$$

* P.L.Lions, B.Perthame, *Propagation of moments and regularity for the 3-dimensional Vlasov-Poisson system.*, Inventiones mathema (1991), Volume: 105, Issue: 2, page 415-430.

The Vlasov-Poisson system

Numerical Methods:

- Particle in Cell: stochastic particle methods (subject to statistical noise)
- Semi-lagrangian methods and Discontinuous Galerkin (few 3D-3D)
- Full Eulerian (few 3D-3D)

Tensor Methods:

- Semi-lagrangian method and Tensor-Train format*

Main goal:

- Full-Eulerian approach taking generic geometries in x (and possibly v) into account
- Parsimonious discretisation

* K. Kormann, *A semi-lagrangian Vlasov solver in tensor train format*, SIAM Journal on Scientic Computing, 37(4):B613-B632, 2015.

Notation:

- Tensor = separate discretisation for x and v

$$g(x,v) = \sum_{k=1}^{n} r_k(x) s_k(v)$$

n is the tensor rank

- For any functions $r : \Omega_x \to \mathbb{R}$ and $s : \Omega_v \to \mathbb{R}$, we use the notation

$$r \otimes s : \begin{cases} \Omega_x \times \Omega_v & \to & \mathbb{R} \\ (x,v) & \mapsto & r(x)s(v). \end{cases}$$

- For any linear operator A acting on real valued functions defined over Ω_x, and for any B acting on real valued functions defined over Ω_v

$$(A \otimes B)(r \otimes s) = (Ar) \otimes (Bs), \quad \text{for all } r : \Omega_x \to \mathbb{R}, \quad s : \Omega_v \to \mathbb{R}.$$

- Two main points:
  - Respect the Hamiltonian nature of the Vlasov-Poisson system
  - Use tensor methods to build a parsimonious discretisation starting from arbitrary a priori chosen separate discretisations for x and v

$$\mathcal{H} = \int_{\Omega_x} \int_{\Omega_v} \frac{1}{2}|v|^2 f(t,x,v)\, dxdv + \int_{x\in\Omega_x} \varrho(t,x) U(t,x)\, dx.$$

$$\{a,b\} := \nabla_x a \nabla_v b - \nabla_v a \nabla_x b$$ Poisson bracket

$$h = \frac{1}{2}|v|^2 + U$$ reduced Hamiltonian

$$\partial_t f + \{f,h\} = 0$$

- The main idea:

$$f(t,x,v) \approx \sum_{k=1}^{n_t} r_k(x,t) s_k(v,t)$$

$\propto t$

$\propto t$

- <u>At each time step</u>, the solution is decomposed into a sum of pure product tensor functions

$$\partial_t f + \{f,h\} = \partial_t f + \left(\sum_{i=1}^{d} \partial_{x_i} \otimes v_i + \sum_{i=1}^{d} a_i(x,t) \otimes \partial_{v_i}\right) f = 0.$$

tensorised operator:

$$\sum_{k=1}^{n_t} \left(\sum_{i=1}^{d} \partial_{x_i} r_k \otimes v_i s_k + \sum_{i=1}^{d} a_i(x,t) r_k \otimes \partial_{v_i} s_k\right)$$

The Method

- Second order in time symplectic integrator:

  - Let $\Delta t > 0$, $m \in \mathbb{N}^*$, $t_m := m\Delta t$, we denote:

$$f^{(m)}(x,v) \approx f(t_m,x,v)$$

  - Three step scheme:

$$\begin{cases} \left(I + \frac{\Delta t}{2} a^{(m)}(x) \cdot \nabla_v\right) f^{(m+1/3)} & = \left(I - \frac{\Delta t}{2} v \cdot \nabla_x\right) f^{(m)}, \\ \left(I + \frac{\Delta t}{2} v \cdot \nabla_x\right) f^{(m+2/3)} & = f^{(m+1/3)}, \\ f^{(m+1)} & = \left(I - \frac{\Delta t}{2} a^{(m+2/3)}(x) \cdot \nabla_v\right) f^{(m+2/3)}, \end{cases}$$

  - Elementary step structure:

$$(I + \Delta t P) f^{\frac{i+1}{3}} = (I + \Delta t Q) f^{\frac{i}{3}}$$

The Method

- Elementary step: $\delta f := f^{\frac{i+1}{3}} - f^{\frac{i}{3}} \Rightarrow (I + \Delta t P)\delta f = g$
  - Idea: fix point $\delta f^{(l+1)} = g - \Delta t P \delta f^{(l)}$

- Fix point POD/PGD
  - Hypotheses and notation:
    - Let H_x, H_v be two Hilbert spaces
    - $I = I_x \otimes I_v$, where I_x (I_v) bounded, self-adjoint coercive operator acting on H_x (H_v)
    - $P = \sum_{q=1}^{N} P_x^{(q)} \otimes P_v^{(q)}$, where $P_x^{(q)} \in \mathcal{L}(H_x)$ and $P_v^{(q)} \in \mathcal{L}(H_v)$
    - $g \in H_x \otimes H_v$

- The algorithm:

1. initial guess: $\delta f^{(0)} = 0$.
2. For $l \in \mathbb{N}^*$, compute $(r_l, s_l) \in H_x \times H_v$ such that:

$$(r_l, s_l) = \arg\min_{r,s} \|g - \Delta t P \delta f^{(n-1)} - I r \otimes s\|_{H_x \times H_v}$$

3. Set: $\delta f^{(l)} = \delta f^{(l-1)} + r_l \otimes s_l$

- Proposition (Ehrlacher, L. 2016):

Let $\kappa := \max_{1 \leq q \leq N} \|I_x^{-1} P_x^{(q)} \otimes I_v^{-1} P_v^{(q)}\|_{H_x \times H_v}$.
Then, the algorithm converges provided that:

$$3 N \Delta t \kappa < 1.$$

The Method

- Recompression step:

$$f^{\frac{i}{3}} \approx \sum_{k=1}^{n} \tilde{r}_k \otimes \tilde{s_k}$$

$$\tilde{f}^{\frac{i+1}{3}} \approx \sum_{k=1}^{n} \tilde{r}_k \otimes \tilde{s_k} + \sum_{k=1}^{n_1} r_k \otimes s_k$$

$$f^{\frac{i+1}{3}} = POD(\tilde{f}^{\frac{i+1}{3}}, \eta)$$

<u>Computational Complexity</u>:

- Modified PGD step: solved by Alternated Least Square

  at iteration $l = K$ of the fixed-point PGD: $\mathcal{O}((N_x + N_v)(n + K)(d + 1))$

- POD step, solved by QR+SVD

  recompression step: $\mathcal{O}(n^3 + n^2(N_x + N_v))$

The Method

- Back to Vlasov-Poisson:
  - Solve by PGD/POD step:

$$\left(I + \frac{\Delta t}{2} a^{(m)}(x) \cdot \nabla_v\right) f^{(m+1/3)} = \left(I - \frac{\Delta t}{2} v \cdot \nabla_x\right) f^{(m)}$$

  - Solve by PGD/POD step:

$$\left(I + \frac{\Delta t}{2} v \cdot \nabla_x\right) f^{(m+2/3)} = f^{(m+1/3)}$$

  - Compute: $a^{m+2/3}(x)$
  - Solve by PGD/POD step

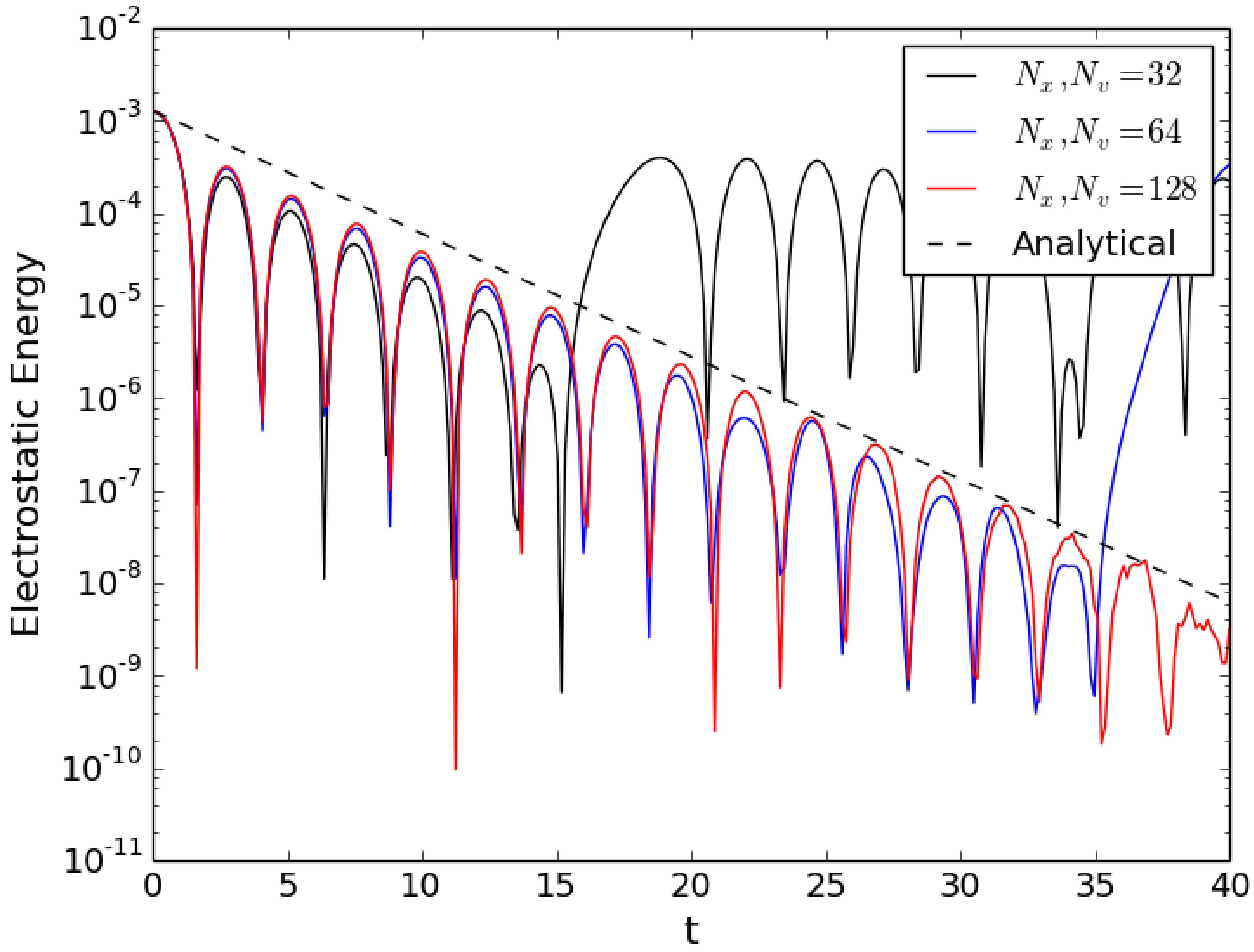
$$f^{(m+1)} = \left(I - \frac{\Delta t}{2} a^{(m+2/3)}(x) \cdot \nabla_v\right) f^{(m+2/3)}$$

  - Compute: $a^{m+1}(x)$

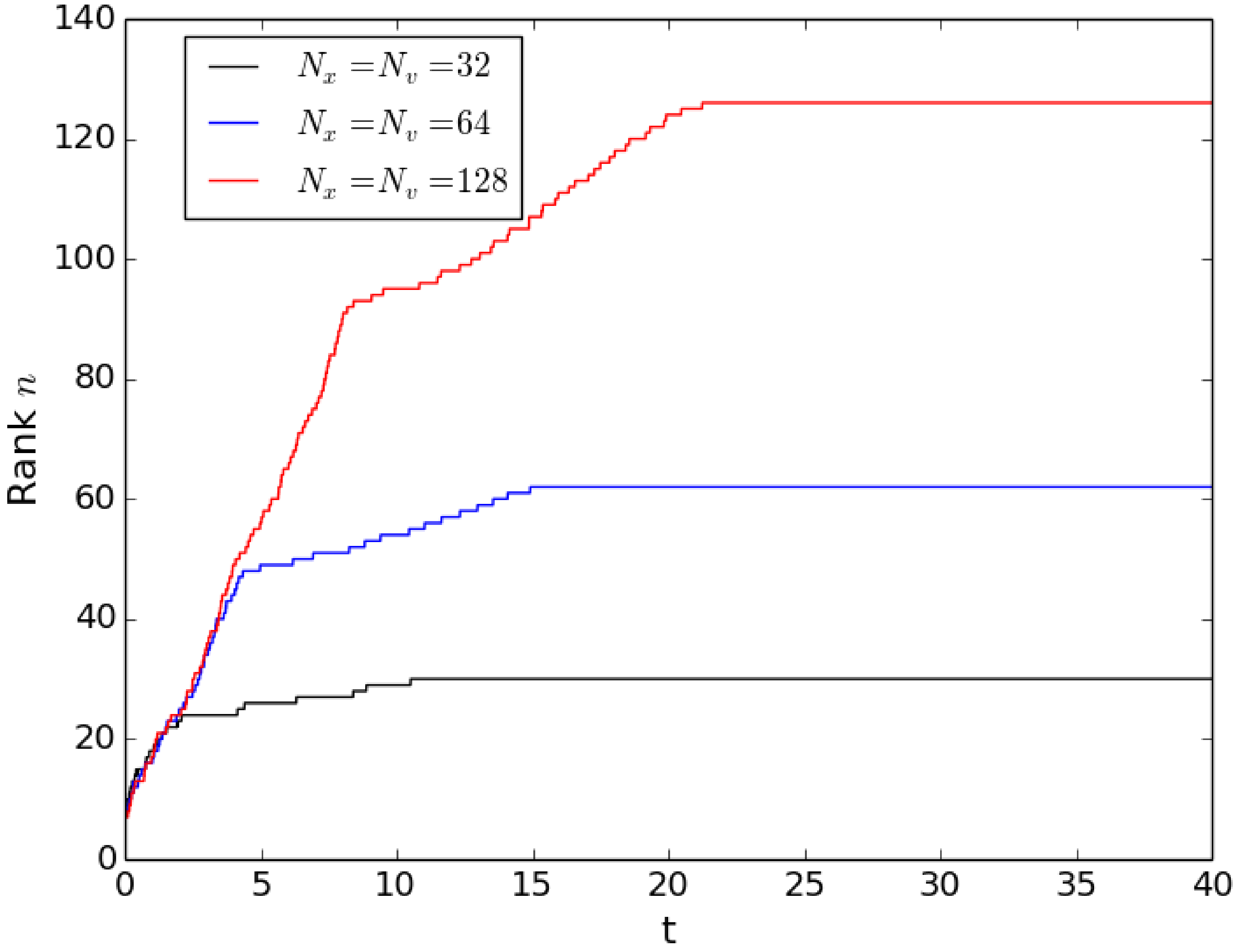
Landau Damping 1D:

- $$f(x,v;t=0) = F(x)G(v),$$
  $$F(x) = 1 + \beta\cos(kx),$$
  $$G(v) = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{v^2}{2}\right),$$
- $k = 0.5, \quad \beta = 0.01$
- $\Omega_x = [0, 4\pi], \quad \Omega_v = [-10, 10]$
- Space discretisation: spectral collocation in x (Fourier), finite differences in v
  $N_x = N_v = [32, 64, 128]$
- $\Delta t \approx 6.25\ 10^{-4}$

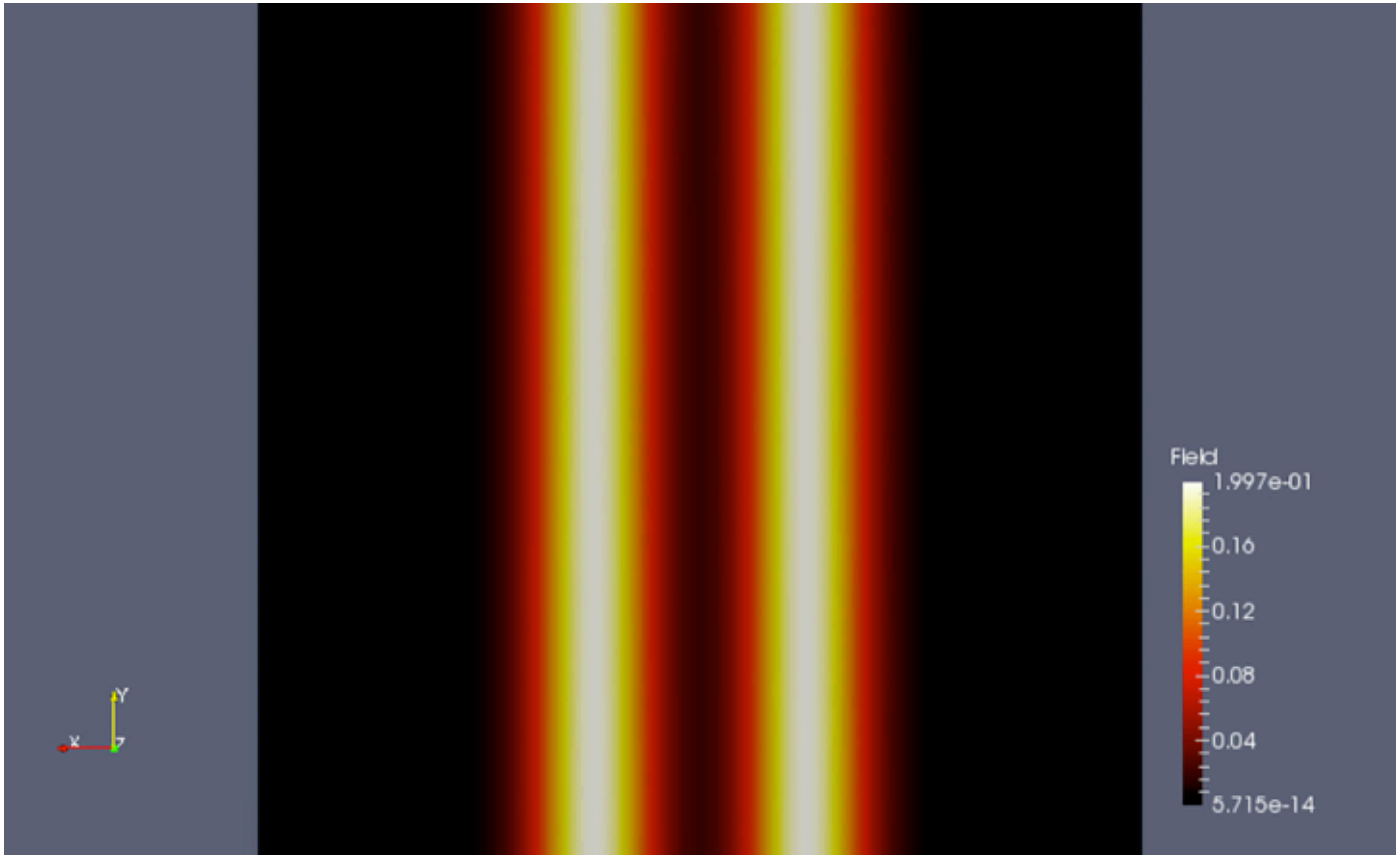
Numerical Experiments



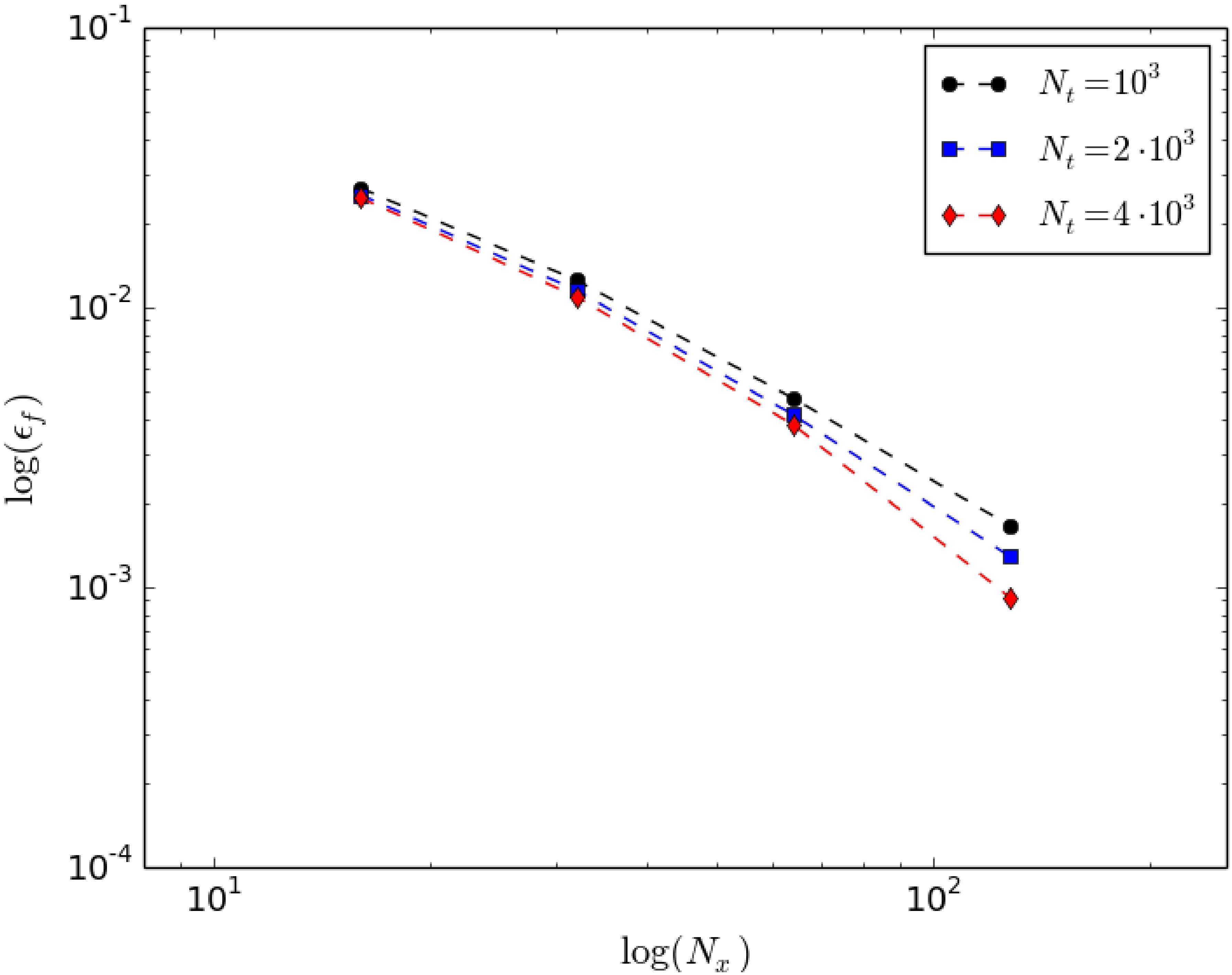
Numerical Experiments



- Two stream instability 1D:

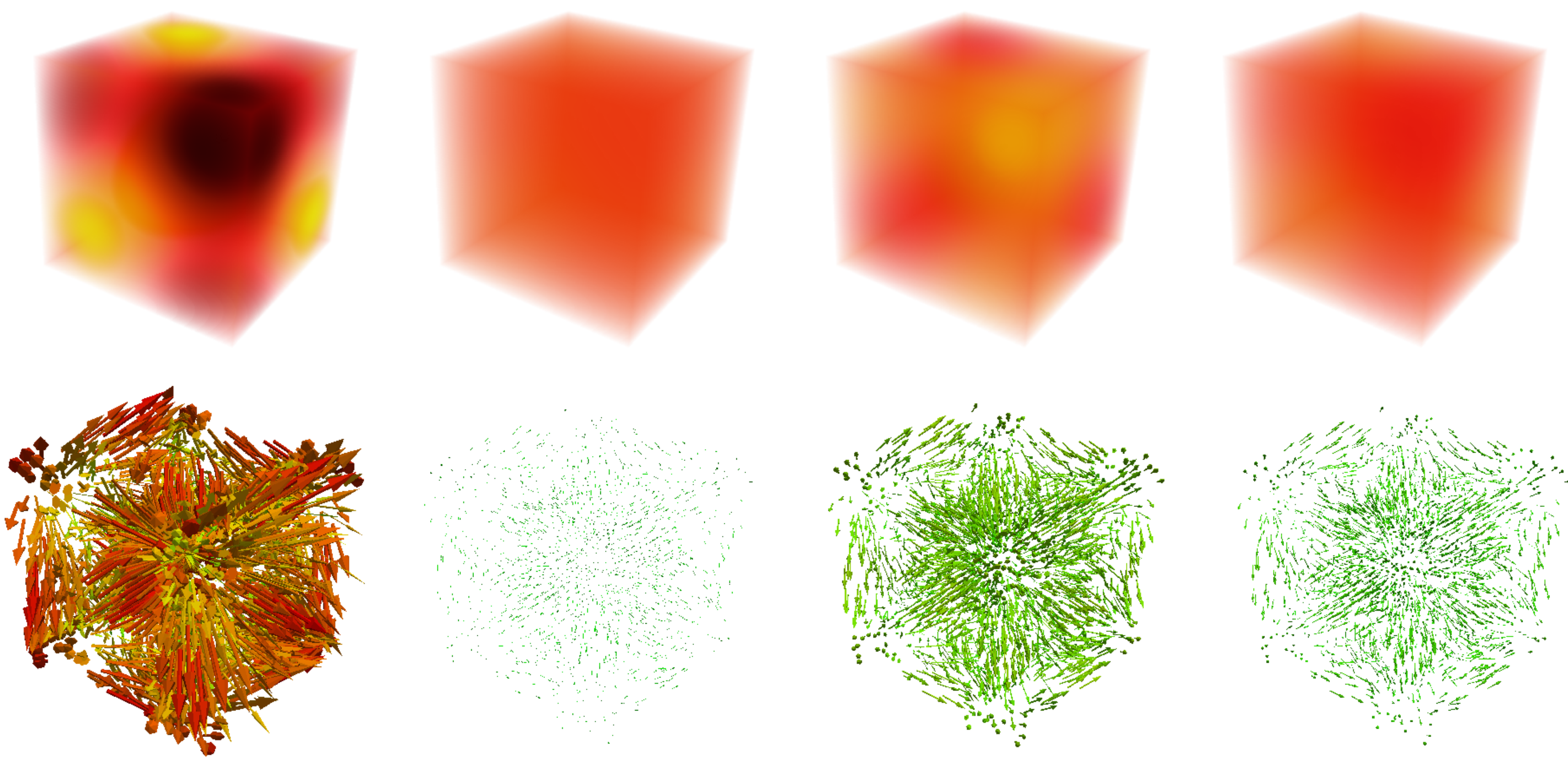


Numerical Experiments



Numerical Experiments

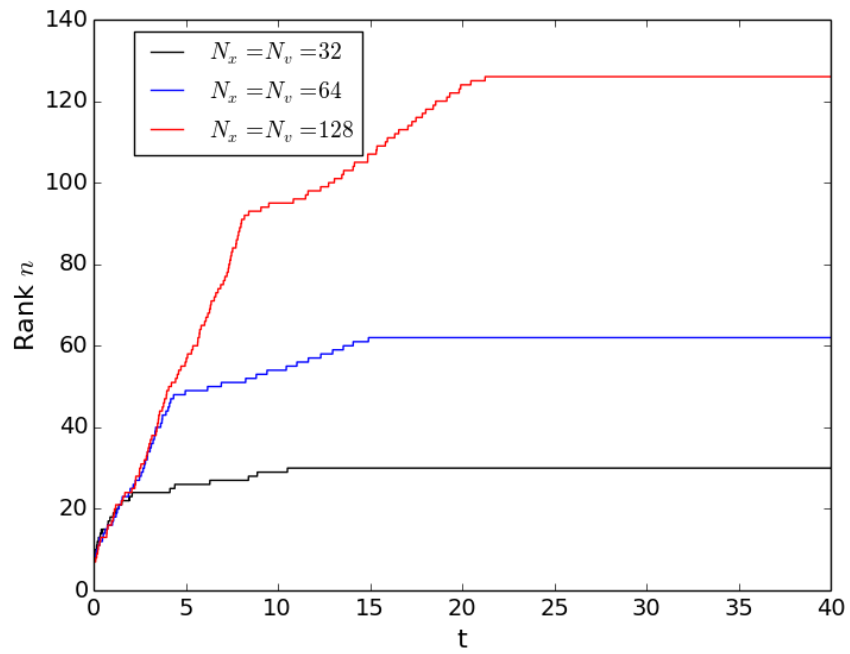
- Landau Damping 3D:
  - $N_x = N_v = 64^3$ $\mathcal{N} \approx 6.9\ 10^{10}$
  - $c = \mathcal{N}/(\max_t n_t(N_x + Nv)) \approx 1100$



$1 - \varrho$

$-\nabla_x U$

- The rank increase (too much?):
  - The solution cannot be well represented **globally** by tensor approximation



- Idea:
  - On smaller sub-domains the solution can be represented by a small rank tensor, even if globally it cannot
  - Subdivide the domain, build a local tensor approximation

Hierarchical sub-tensors

- When a local sub-tensor partition is effective?

1. *Proposition: Let the domain be* $Q \in \mathbb{R}^d$ *and the function to be approximated be* $u \in W^{k,p}(Q)$*, with* $\|u\|_{W^{k,p}(Q)} \leq 1$*. Let* $1 \leq p \leq q \leq \infty$ *and* $\lambda = \frac{k}{d} - \frac{1}{p} + \frac{1}{q} > 0$*. Then, let* $\varepsilon > 0$*, there exist a congruent partition in* 2^{dN} *sub-domains such that a piece-wise finite rank (*$R \leq \frac{(k-1+d)!}{(k-1)!d!}$*) tensor approximation of* u *achieves:*

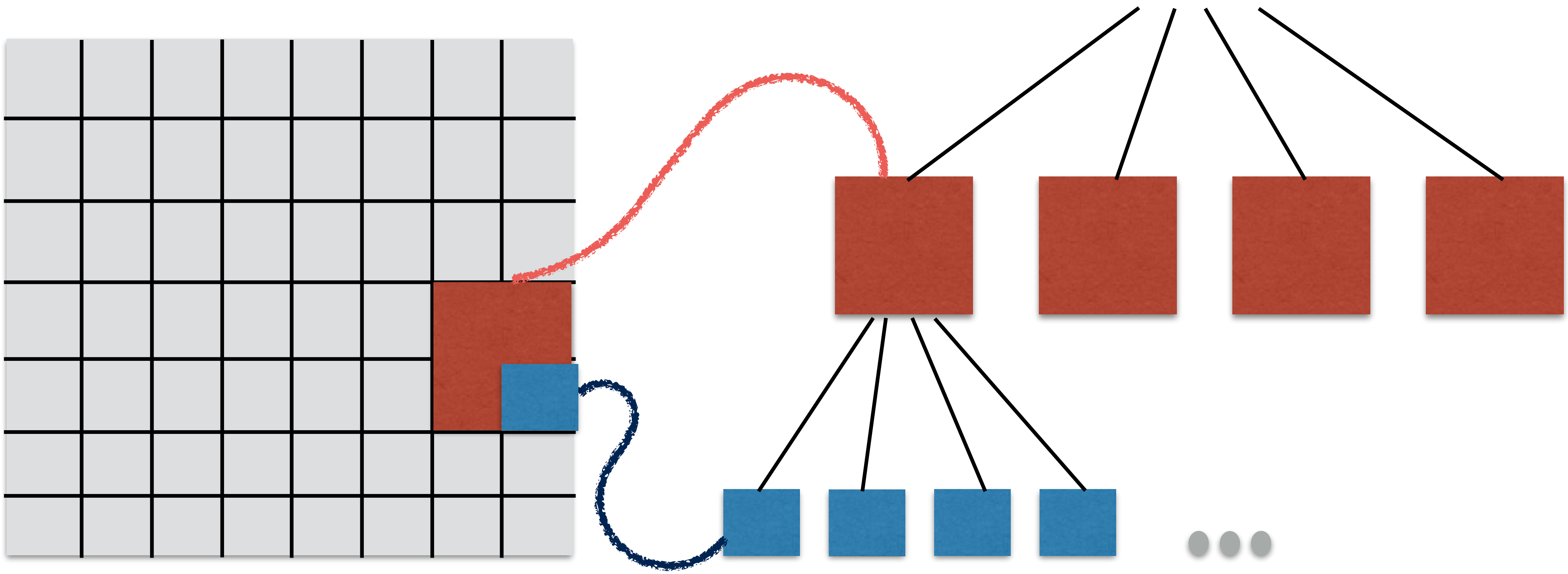
$$\|u - \sum_{j=1}^{2^{dN}} T_j\|_{L^q(Q)} \leq \varepsilon. \qquad (2)$$

A fact:

- If the embedding is compact, there exist a partition such that an error on the piece-wise tensor approximation can be guaranteed

Hierarchical sub-tensors

- The method:
  - Sub-divide the tensor into sub-tensors
  - Greedy algorithm to **distribute the error** of the approximation (HOSVD)
  - Optimise the partition to **minimise the storage**

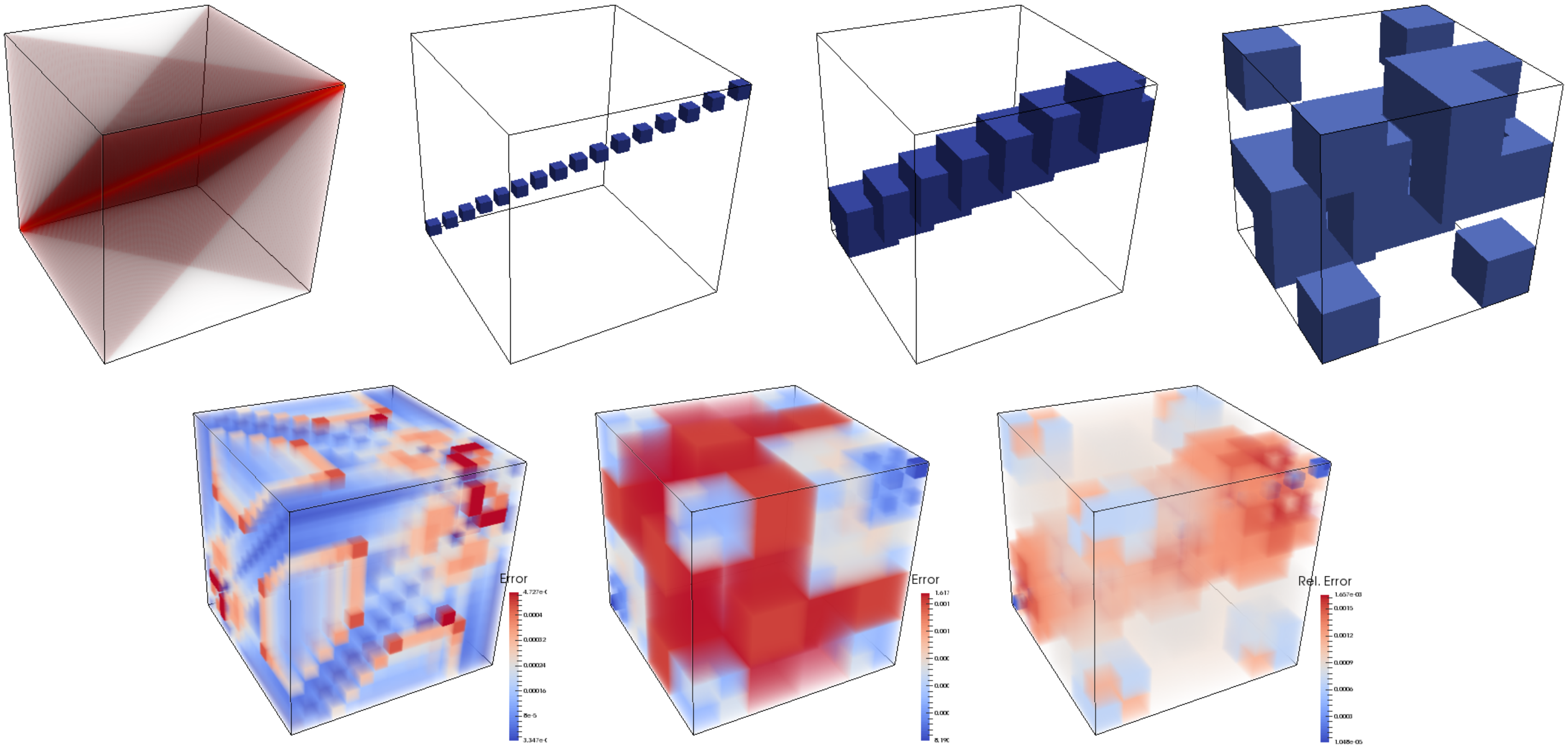


Hierarchical sub-tensors

- Methods characteristics:
  - Well adapted to **moderate dimension** tensors (partition is subjected to *curse of dimensionality*)
  - It is easily **parallelisable** (!), contrary to classical HOSVD, better suited for large number of degrees of freedom
  - The error is **distributed automatically** and guaranteed throughout the whole approximation
  - Memory gain is significant with respect to classical HOSVD format for a wide class of functions of interest

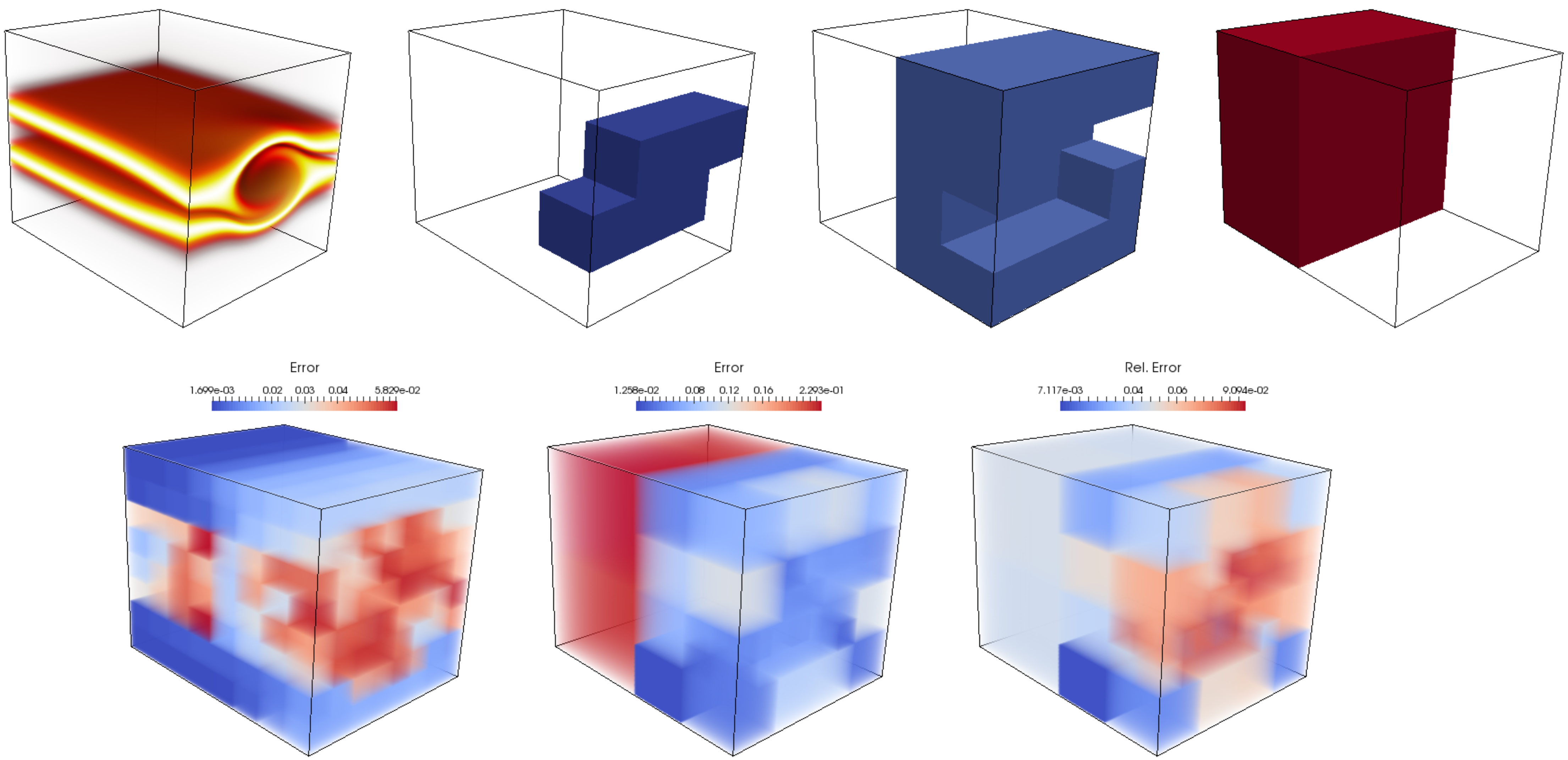
- Coulomb potential:

$$V(x_1, \ldots, x_d) = \sum_{1 \le i < j \le d} \frac{1}{|x_i - x_j|}.$$



Hierarchical sub-tensors

- Vlasov Poisson: double stream instability



- Compression factor in phase-space time: 250

Conclusions

- **Tensor method for the Vlasov-Poisson system:**
  - Build a discretisation starting from a priori chosen separate discretisations in x and v
  - The number of terms is adapted dynamically, depending on a chosen error threshold
  - At each sub-step solve only linear problems in the separate spaces
  - For short time simulations it allows for a significant memory compression and speed-up

- **Drawbacks:**
  - The rank increases with time: the compression rate decreases
  - Simulations are still long in realistic 3D-3D settings

Perspectives

- Parallelised Hierarchical local approximation:
  - Improve the compression via a better function adapted representation
  - Error can be guaranteed and distributed
- Solve in this compress format
  - Solve linear system in this adaptive format
- Boltzmann:
  - Collision term might be beneficial for the proposed approach, if it drives the dynamics towards a tensorised equilibrium solution. (in preparation)

Thank you!