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A high-order accurate Particle-In-Cell method for Vlasov-Poisson problems over long time integrations

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https://arxiv.org/abs/1602.00747

Talk Outline

- Background and motivation
- Description of our numerical method
- Implementation using the Chombo framework
- Numerical results
- Summary and future research directions

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The Vlasov-Poisson Equations

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{x}} - \boldsymbol{E} \cdot \frac{\partial f}{\partial \boldsymbol{v}} = 0$$

$$\nabla^2 \phi = -\rho \qquad\qquad \boldsymbol{E} = -\nabla \phi$$

- The Vlasov-Poisson equations describe the evolution of a charged, collisionless fluid in phase space.
- The electric field is obtained by solving Poisson's equation.
- Applicable as a simplified model to plasma physics (space plasmas, accelerator modeling, controlled fusion) and to cosmology.

Eulerian Methods

- Nonlinear advection equation in a high-dimensional space, can be solved by Eulerian techniques.
- Advantages:
  - Strong body of theory on finite volume methods
  - Do not suffer from “noise”
  - High order methods exist (Vogman + 2014)
- Disadvantages:
  - High cost of grids in high-dimensional (4D, 5D, or 6D) spaces

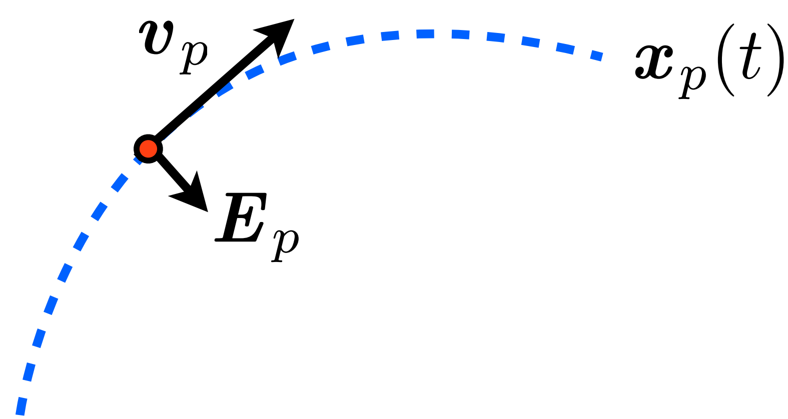
Particle Methods

- Discretize system with set of Lagrangian interpolating points, $\mathbb{P}$

$$f(\boldsymbol{x}, \boldsymbol{v}, t_{\text{ini}}) \approx \sum_{p \in \mathbb{P}} q_p \delta\left(\boldsymbol{x} - \boldsymbol{x}_p^i\right) \delta\left(\boldsymbol{v} - \boldsymbol{v}_p^i\right)$$

- Reduces problem to system of ODEs for particle trajectories:

$$\frac{dq_p}{dt} = 0$$
$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{v}_p$$
$$\frac{d\boldsymbol{v}_p}{dt} = -\boldsymbol{E}_p$$



- Can reconstruct distribution at later times from $(\boldsymbol{x}_p(t), \boldsymbol{v}_p(t))$

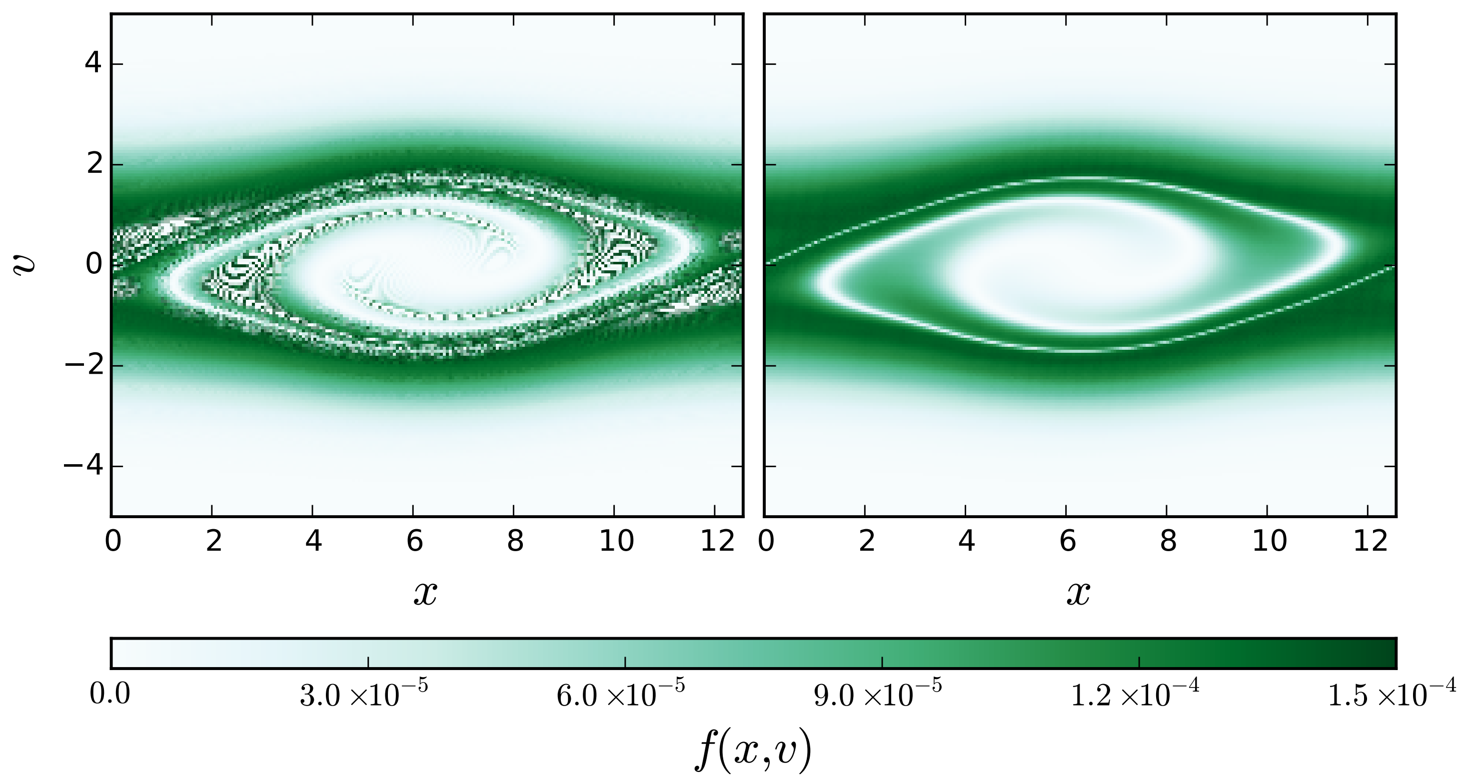
Particle Methods

- Variety of methods - mainly differ in how the force is computed
- PIC methods, in which the force solve is performed on an intermediate grid, are particularly popular.
- Advantages:
  - Mathematically simpler. Reduces a PDE to a set of coupled ODEs.
  - Naturally adaptive - the particles go where more resolution is needed.
  - Usually lower computational cost

Disadvantages of Particle Methods

- Less mathematical guidance
- Particle noise prevents convergence
- Usually limited to 2nd order accuracy

Wang+2011



The goal of this talk

- Describe a particle method (PIC) that attempts to address these downsides.
- Show how to all the PIC stages at 4th-order
  - Heart of this is really the interpolation kernels.
- Describe a high-order remapping procedure to ameliorate particle noise while maintaining 4th order accuracy

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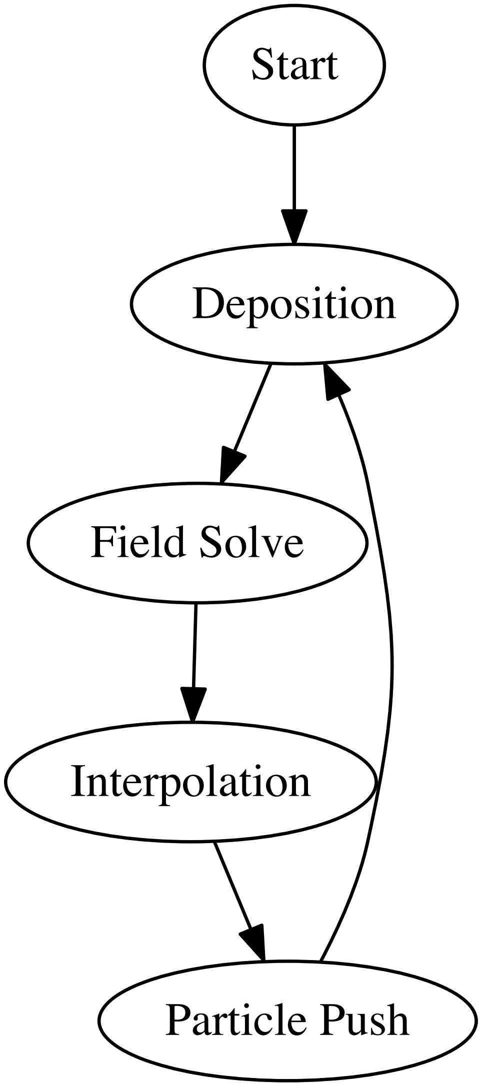
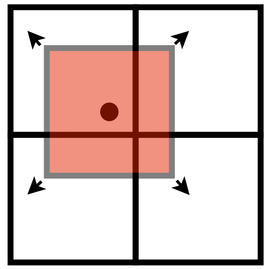
Overview of a Particle-in-Cell time step



- Deposition: Particle charges are deposited onto mesh:



$$\rho_{\boldsymbol{i}}^{n+1} = \sum_p \left(\frac{q_p}{\Delta x}\right) \boldsymbol{W} \left(\frac{\boldsymbol{x}_i - \boldsymbol{x}_p^{n+1}}{\Delta x}\right)$$

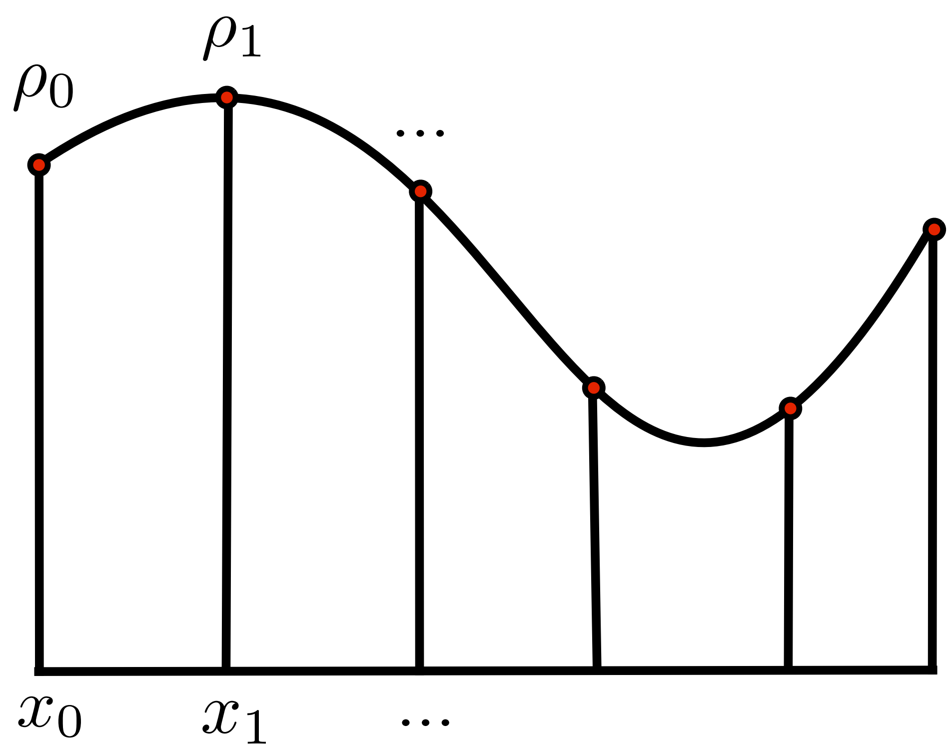
2nd order: Piecewise linear, Cloud-in-Cell interpolation

- Field solve: force is computed on the mesh by e.g. solving Poisson's Equation w/ 2nd order finite differences.
- Interpolation: Force is interpolated back to particle positions using same kernel.
- Particle Push: Particle positions and velocities are updated. 2nd-order leapfrog.

High-order in space (interpolation kernels)

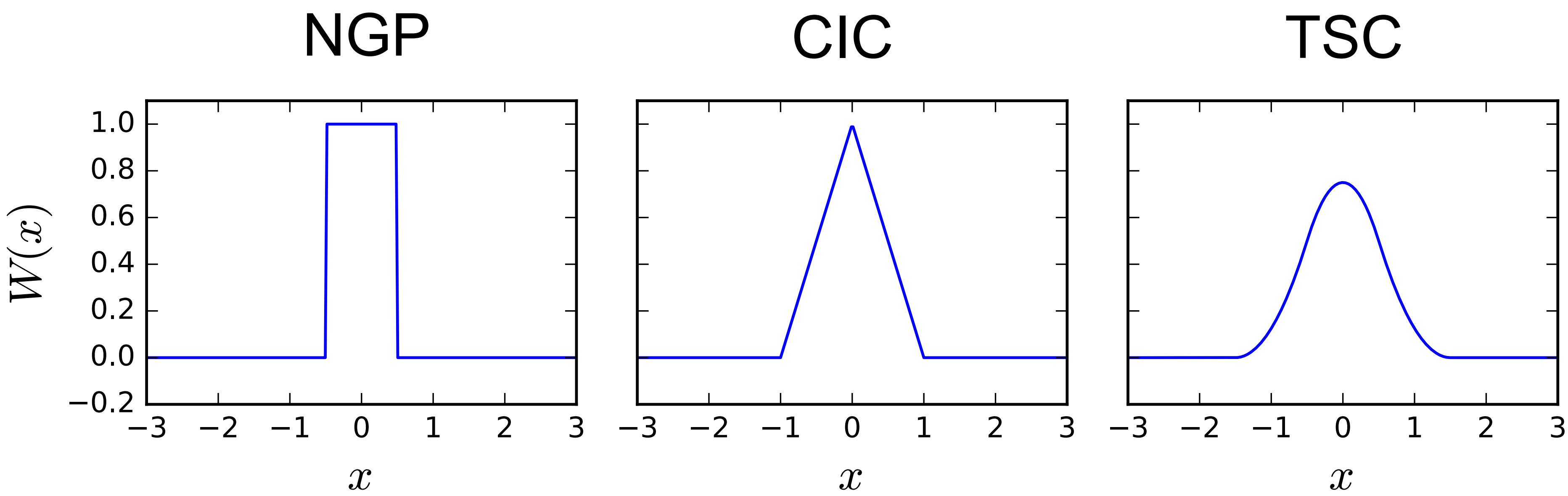
- Given solution at a set of points, reconstruct in between
- Functions W(x) need to be even, normalized, have compact support

$$\rho(x) \approx \sum_j W\left(\frac{x_j - x}{\Delta x}\right)\rho_j$$



High-order in space (interpolation kernels)

- Commonly taken to be one of the B-spline functions. Limited to 2nd Order.



$$M_1(x) = \begin{cases} 1, & 0 \leq |x| \leq 1/2, \\ 0 & \text{otherwise.} \end{cases}$$

$$M_2(x) = \begin{cases} 1 - |x|, & 0 \leq |x| \leq 1, \\ 0 & \text{otherwise.} \end{cases}$$

$$M_3(x) = \begin{cases} \frac{3}{4} - |x|^2, & 0 \leq |x| \leq 1/2, \\ \frac{1}{2}\left(\frac{3}{2} - |x|\right)^2, & 1/2 \leq |x| \leq 3/2, \\ 0 & \text{otherwise.} \end{cases}$$

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High-order in space (interpolation kernels)

- Error analysis involves looking at the Fourier transform of $W(x)$, $\tilde{W}(k)$
- Can show that $\tilde{W}(k) - 1$ must have a zero of order n at $k = 0$ AND $\tilde{W}(k)$ must have zeros of order n at $k = 2\pi, 4\pi, \ldots$ to be O(n).
- For the Basis spline of order n, $\tilde{W}(k) = \left(\frac{\sin(k/2)}{k/2}\right)^n$
- Fulfills the second requirement, but zero at k = 0 is only order 2.
- Hence, all the basis splines interpolate with at best 2nd order accuracy
- They do, however, have increasing degrees of smoothness which may be desirable when the particles are highly disordered.
- See Schoenberg 1975, Monaghan 1985 for more details.

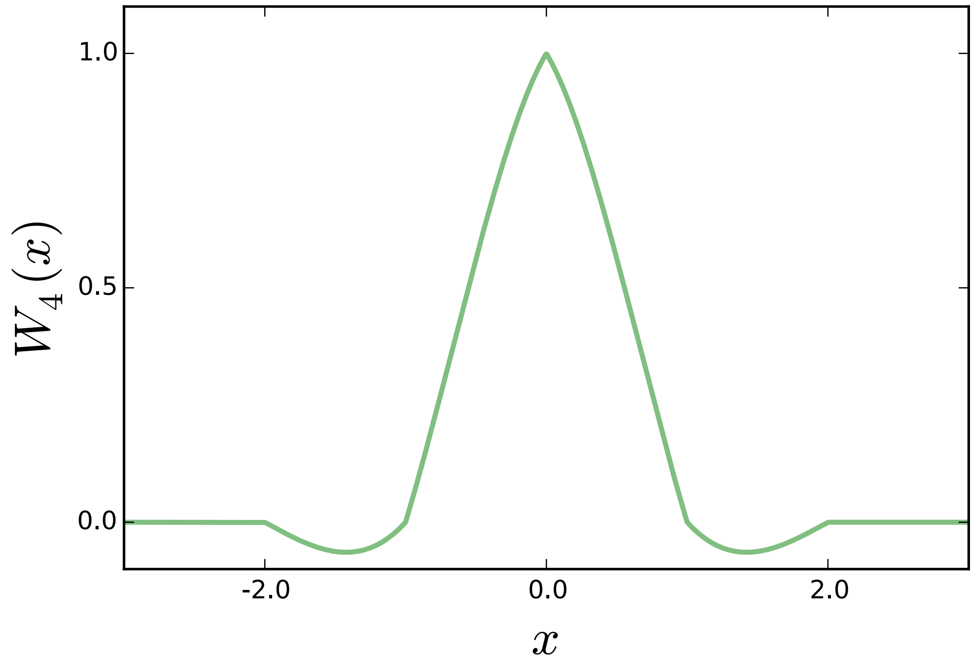
High-order in space (interpolation kernels)

- However, it is possible to design a polynomial with the appropriate zeros in Fourier space and transform back into real space to obtain a $W(x)$ with the desired properties.
- For details, see Lo, Minden, and Colella 2016.

High-order in space (interpolation kernels)

$$W_4(x) = \begin{cases} \frac{|x|^3}{2} - |x|^2 - \frac{|x|}{2} + 1, & |x| \in [0,1], \\ -\frac{|x|^3}{6} + |x|^2 - \frac{11|x|}{6} + 1, & |x| \in [1,2], \\ 0, & \text{else.} \end{cases}$$

- 4-point stencil
- Reproduces cubic functions exactly
- Continuous with discontinuous first derivative



High-order in space (field solve)

- Replace 2nd-order finite difference approximation with 4th-order, centered differences:

$$\nabla^2 \phi = -\rho \quad \rightarrow \quad -\sum_{d=1}^{D} \frac{-\phi_{i+2e^d} + 16\phi_{i+e^d} - 30\phi_i + 16\phi_{i-e^d} - \phi_{i+2e^d}}{12\Delta x^2} = \rho_i$$

$$\boldsymbol{E} = -\nabla\phi \quad \rightarrow \quad \boldsymbol{E}_i^d = -\frac{-\phi_{i+2e^d} + 8\phi_{i+e^d} - 8\phi_{i-e^d} + \phi_{i+2e^d}}{12\Delta x}$$

- Resulting system can be solved with a variety of methods (we used geometric multigrid).

High-order in time (RK4)

- Replace leapfrog with 4th-Order Runge-Kutta method

$$
\begin{aligned}
k_1 &= F\left(t^n, x^n\right) \\
k_2 &= F\left(t^n + \frac{1}{2}\Delta t, x^n + \frac{1}{2}v^n\Delta t + \frac{1}{8}k_1\Delta t^2\right) \\
k_3 &= F\left(t^n + \Delta t, x^n + v^n\Delta t + \frac{1}{2}k_2\Delta t^2\right). \\
x^{n+1} &= x^n + v^n\Delta t + \frac{1}{6}\left(k_1 + 2k_2\right)\Delta t^2 \\
v^{n+1} &= v^n + \frac{1}{6}\left(k_1^n + 4k_2 + k_3\right)\Delta t,
\end{aligned}
$$

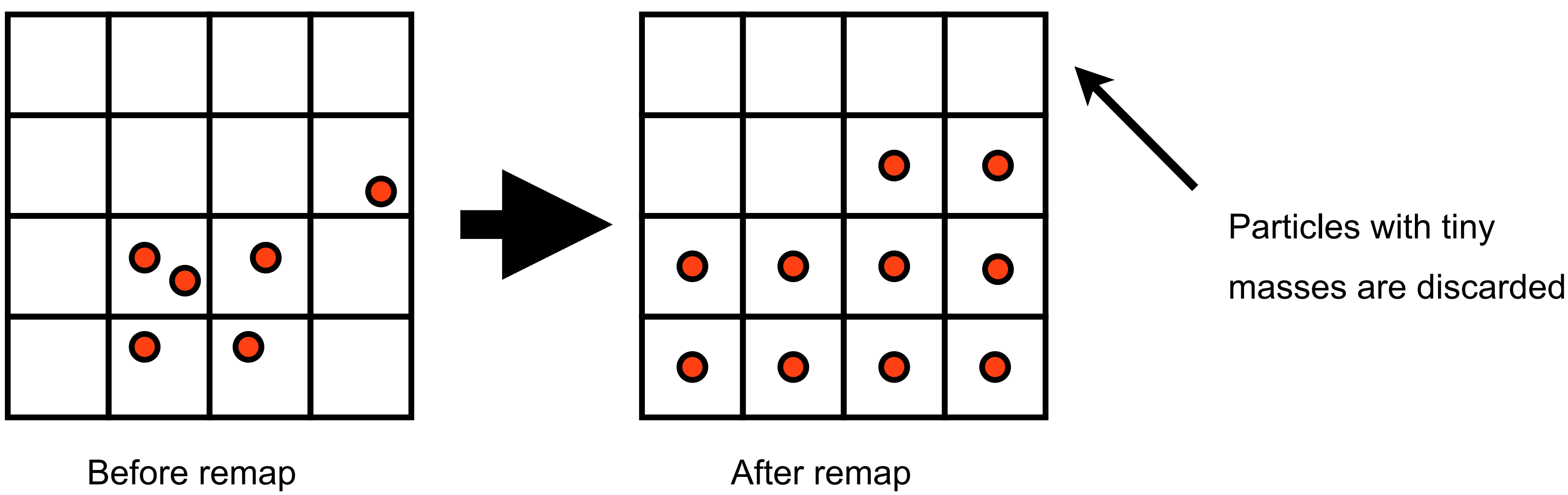
- Requires 3 force solves per time step (velocity independent force), instead of 1
- Self-starting. Gives up on symplectic property.

Particle Remapping

- In PIC convergence theory, stability error for field contains exponential term:

$$e^E(\boldsymbol{x}, t) \propto \exp\left(at\right) \qquad \text{(Wang+2011)}$$

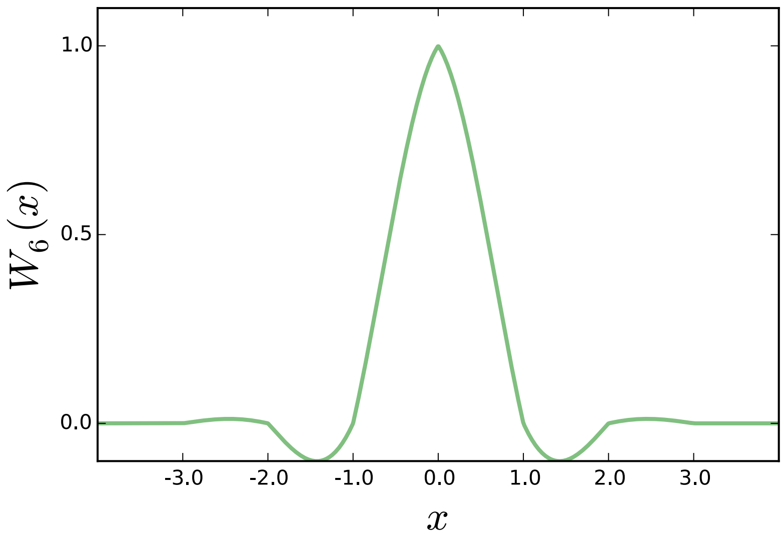
- Periodically restart problem with new particles with interpolated weights



Particle Remapping

$$W_6(x) = \begin{cases} -\frac{|x|^5}{12} + \frac{|x|^4}{4} + \frac{5|x|^3}{12} - \frac{5|x|^2}{4} - \frac{|x|}{3} + 1, & |x| \in [0,1], \\ \frac{|x|^5}{24} - \frac{3|x|^4}{8} + \frac{25|x|^3}{24} - \frac{5|x|^2}{8} - \frac{13|x|}{12} + 1, & |x| \in [1,2], \\ -\frac{|x|^5}{120} + \frac{|x|^4}{8} - \frac{17|x|^3}{24} + \frac{15|x|^2}{8} - \frac{137|x|}{60} + 1, & |x| \in [2,3], \\ 0, & \text{else.} \end{cases}$$

- One order of accuracy is lost during the remap step
- High-order deposition
- 6-point, 6th-order stencil



Particle Remapping

- Particles are laid on at the cell centers of a (possibly AMR) Cartesian grid in phase space. The new weights are then computed as:

$$q_p^* = \sum_p q_p \boldsymbol{W}_6 \left(\frac{\boldsymbol{x}_i - \boldsymbol{x}_p}{h_x} \right) \boldsymbol{W}_6 \left(\frac{\boldsymbol{v}_j - \boldsymbol{v}_p}{h_v} \right)$$

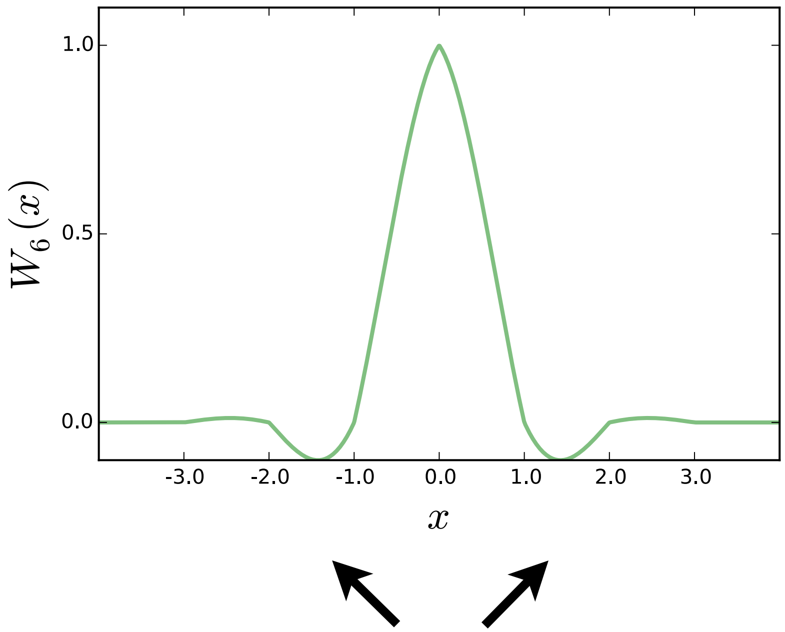
- Particles with small weights are discarded.
- Can be applied every few time steps, or just a few times per calculation
- Can be thought of as Semi-Lagrangian
- Compare the Forward Semi-Lagrangian technique (Crouseilles+2008)

Particle Remapping

- Higher order interpolation functions are not positivity preserving

$$\int_{\mathbb{R}^D} (x-y)^{\ell} W(x-y)\,dy$$

- Can show that the 2nd moment of the interpolating function must vanish for the kernel to have better than 2nd order accuracy.



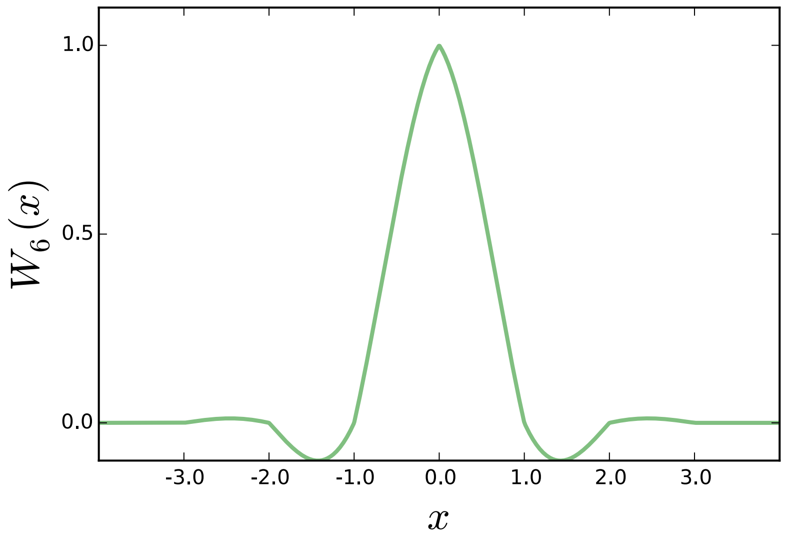
Positivity not guaranteed

Particle Remapping

- Higher order interpolation functions are not positivity preserving

$$\int_{\mathbb{R}^D} (x-y)^{\ell} W(x-y)dy$$

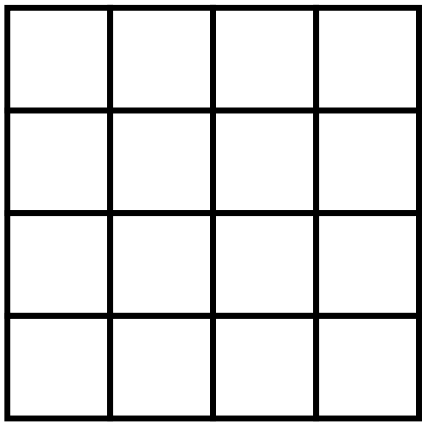
- Use a redistribution procedure to maintain positivity of the distribution function



Positivity not guaranteed

Redistribution procedure

l neighboring cells



$$\delta f_i = \min(0, f_i^n)$$

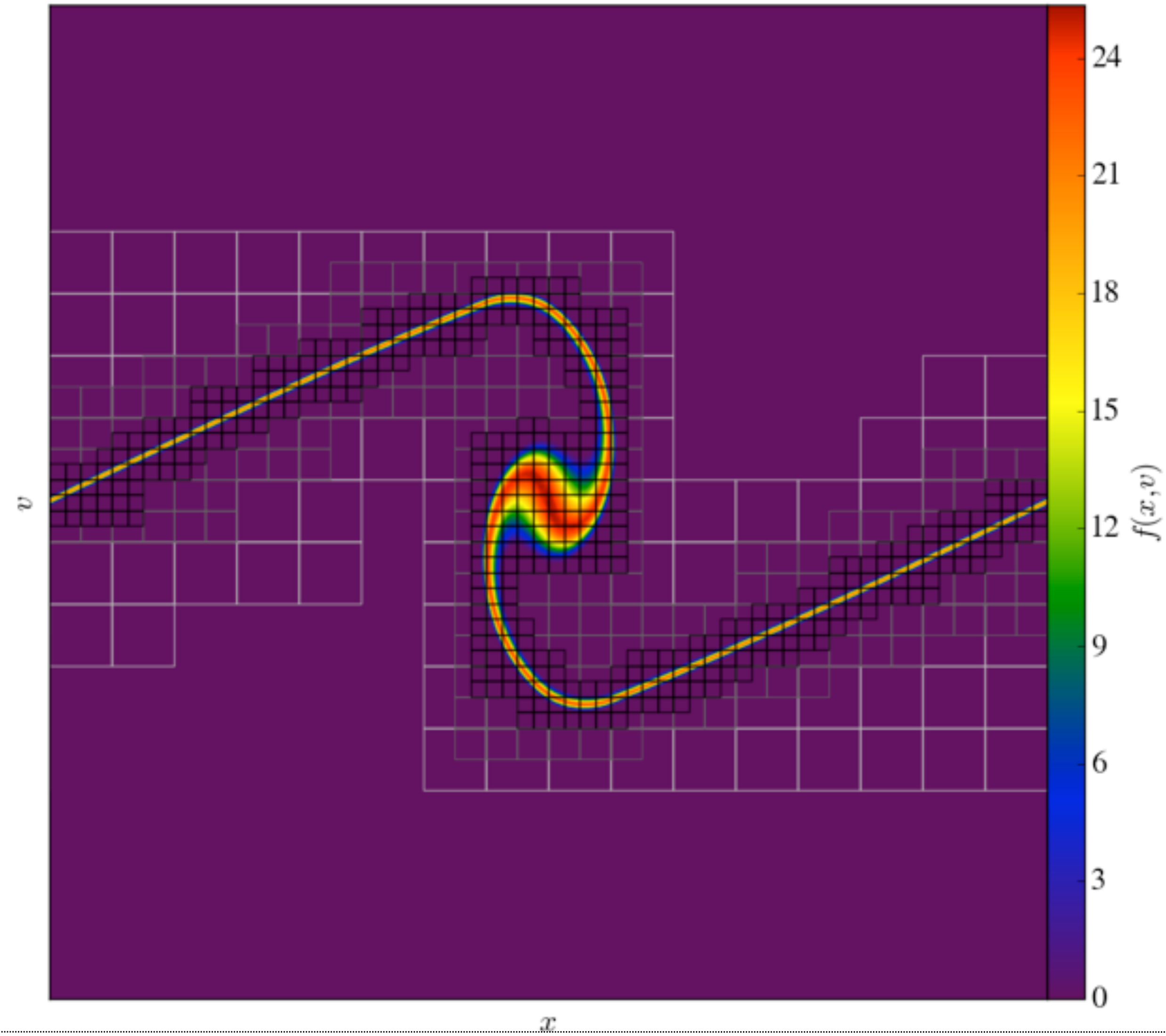
$$\xi_{i+l} = \max(0, f_{i+l}^n)$$

$$f_{i+l}^{n+1} = f_{i+l}^n + \frac{\xi_{i+l}}{\sum_{k \neq 0}^{\text{neighbors}} \xi_{i+k}} \delta f_i$$

- 2 or 3 iterations is usually sufficient

Particle Remapping AMR example

- Example distribution function from a remapping stage, using 4 AMR levels
- Cosmological dark matter test problem (Myers+2015)



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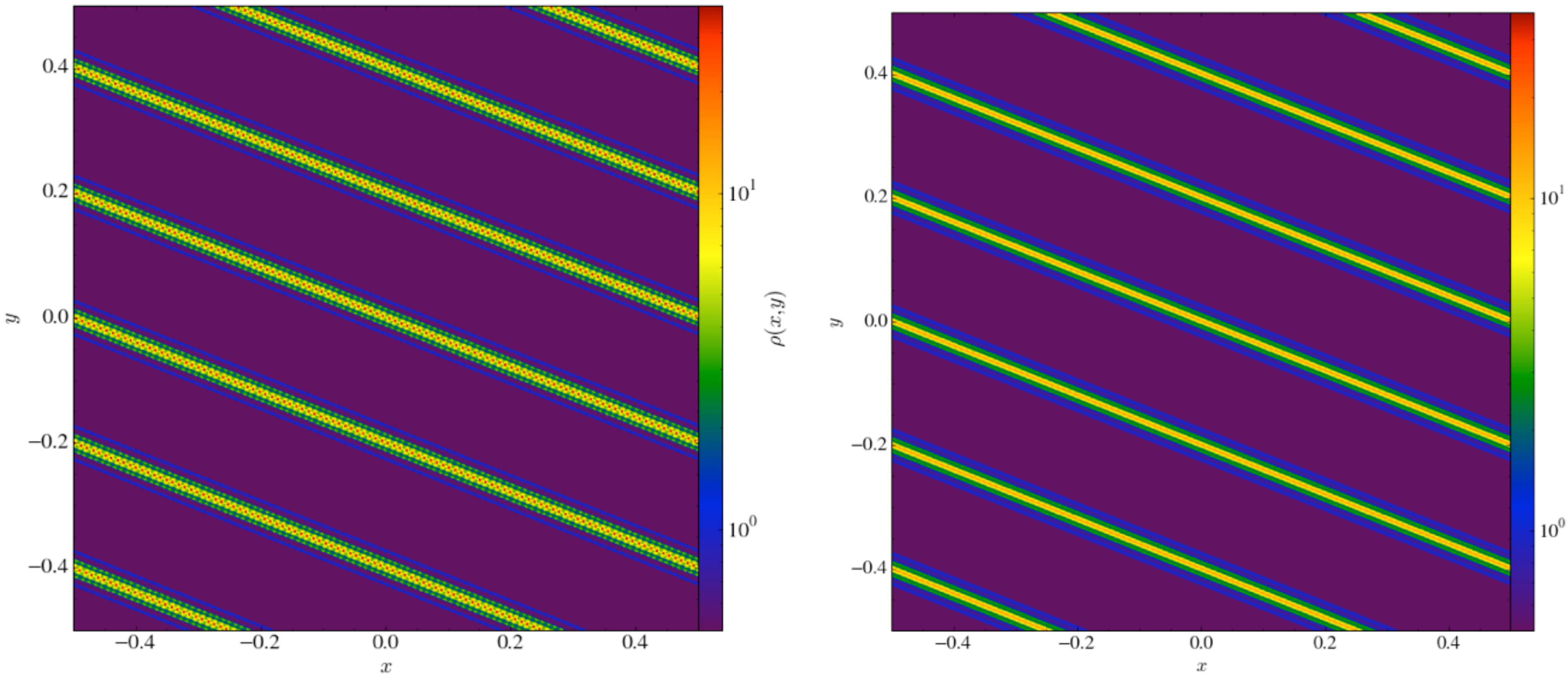
Remapping on Cosmology Calculation

Not remapped | Remapped



http://adsabs.harvard.edu/abs/2016ApJ...816...56M

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Implementation

- Chombo - A set of tools for numerically solving PDEs
- Especially useful for AMR applications
- Mixture of C++ and FORTRAN
- Uses a Box-based, SPMD approach to parallelism
- Provides distributed data containers, including (in the next release) for particle data
- Our method was implemented using these tools, running NERSC's Edison machine + my laptop.
- Code, tests, and analysis scripts are all here:

https://bitbucket.org/atmyers/4thorderpic

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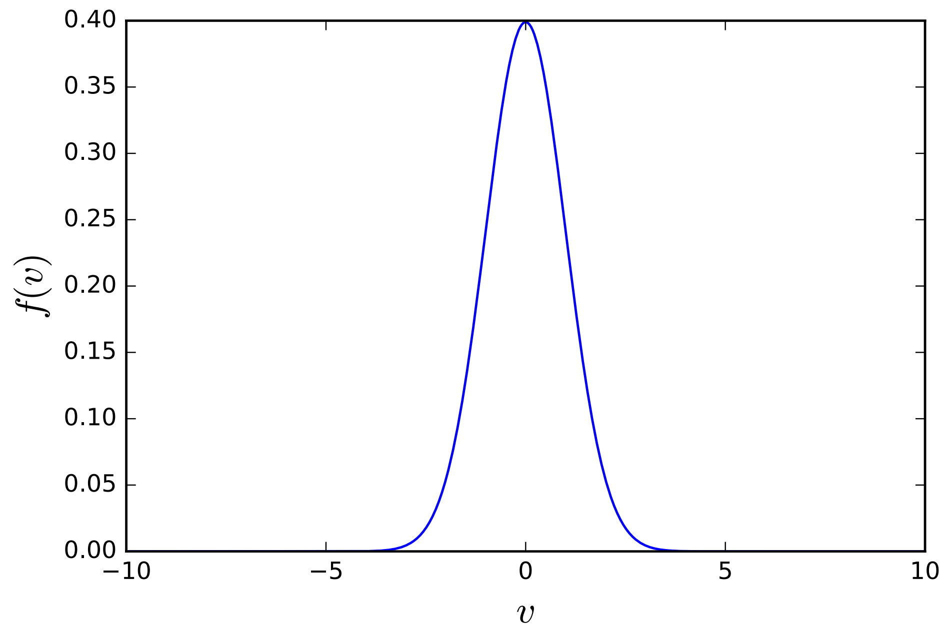
Linear Landau Damping

- Exponentially damped oscillation of a space charge wave
- Wave-particle interactions cause the electric field wave to lose energy to the particles, damping its amplitude
- Very commonly used test problem for PIC codes
  - Analytic solution for the decay rate
  - Long-time evolution is challenging for classical PIC methods

Linear Landau Damping (initial conditions)

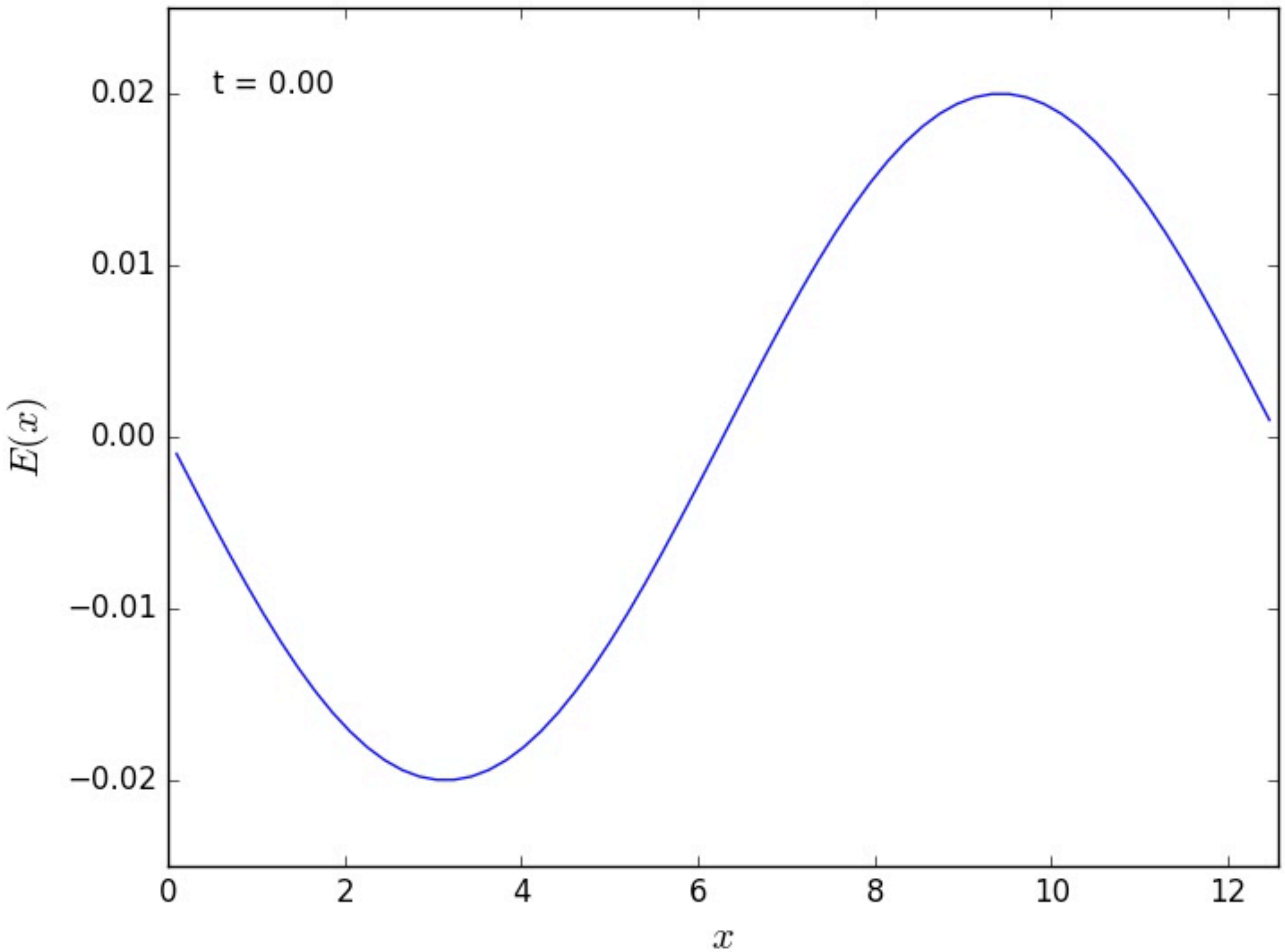
- Gaussian velocity distribution
- Small (linear) perturbation to the charge density (physical space)
- Track the electric field as a function of time



$$f(x, v, t=0) = \frac{1}{\sqrt{2\pi}} \exp\left(-v^2/2\right)\left(1 + \alpha \cos(kx)\right)$$
$$(x, v) = [0, L = 2\pi/k] \times [-v_{\max}, v_{\max}]$$

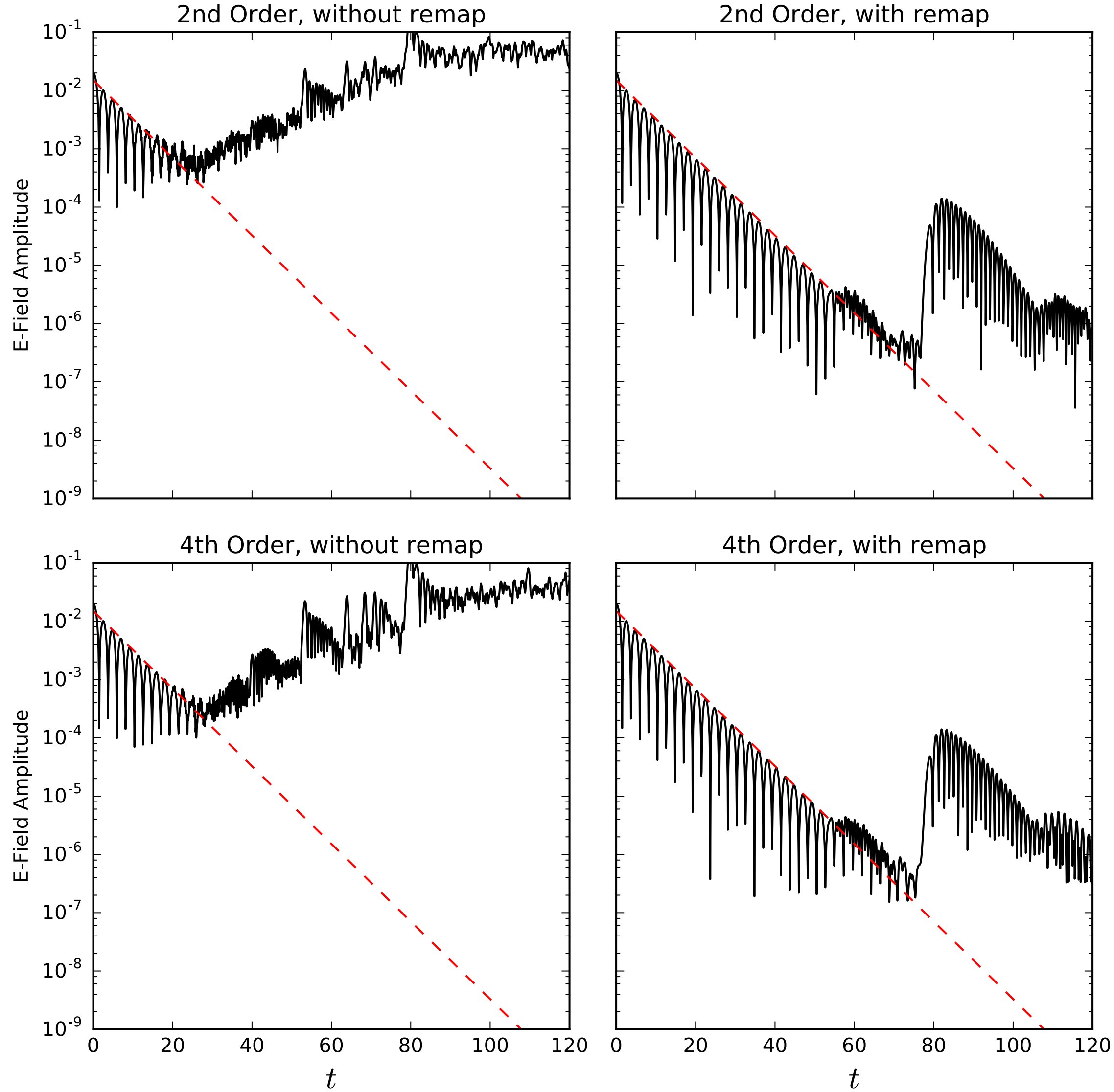
$$k = 0.5$$
$$\alpha = 0.01$$

Linear Landau Damping (movie)



Linear Landau Damping (results)

- Black shows simulation result, red shows damping rate expected from linear theory.
- Remapping is needed to track the analytical damping rate for late times.
- Recurrence effect seen in all simulations past t = 80, a consequence of finite cell spacing in the velocity dimension



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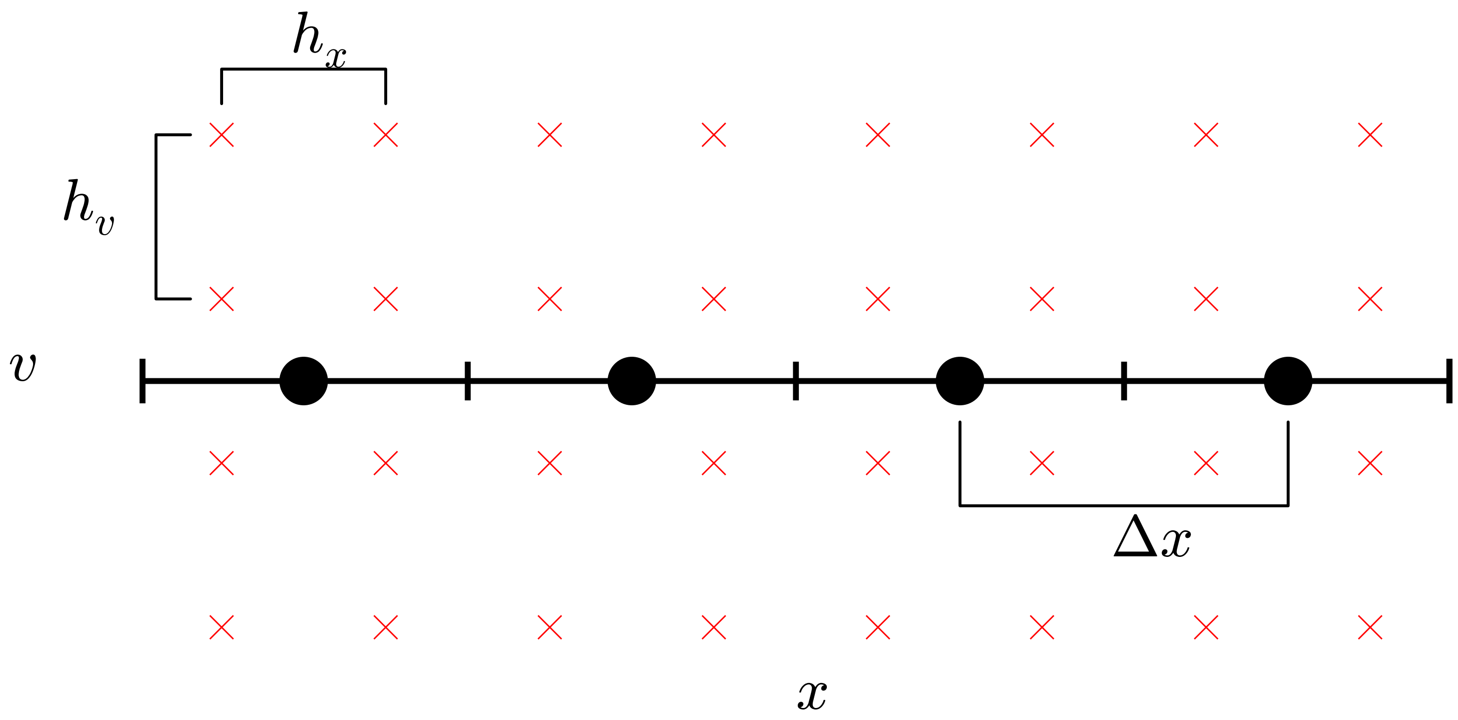
Convergence studies for PIC simulations

- All discrete elements of the problem, including Δt, reduced by factor of 2.
- Ratio of $\Delta x / h_x$ remains fixed.



Convergence studies for PIC simulations

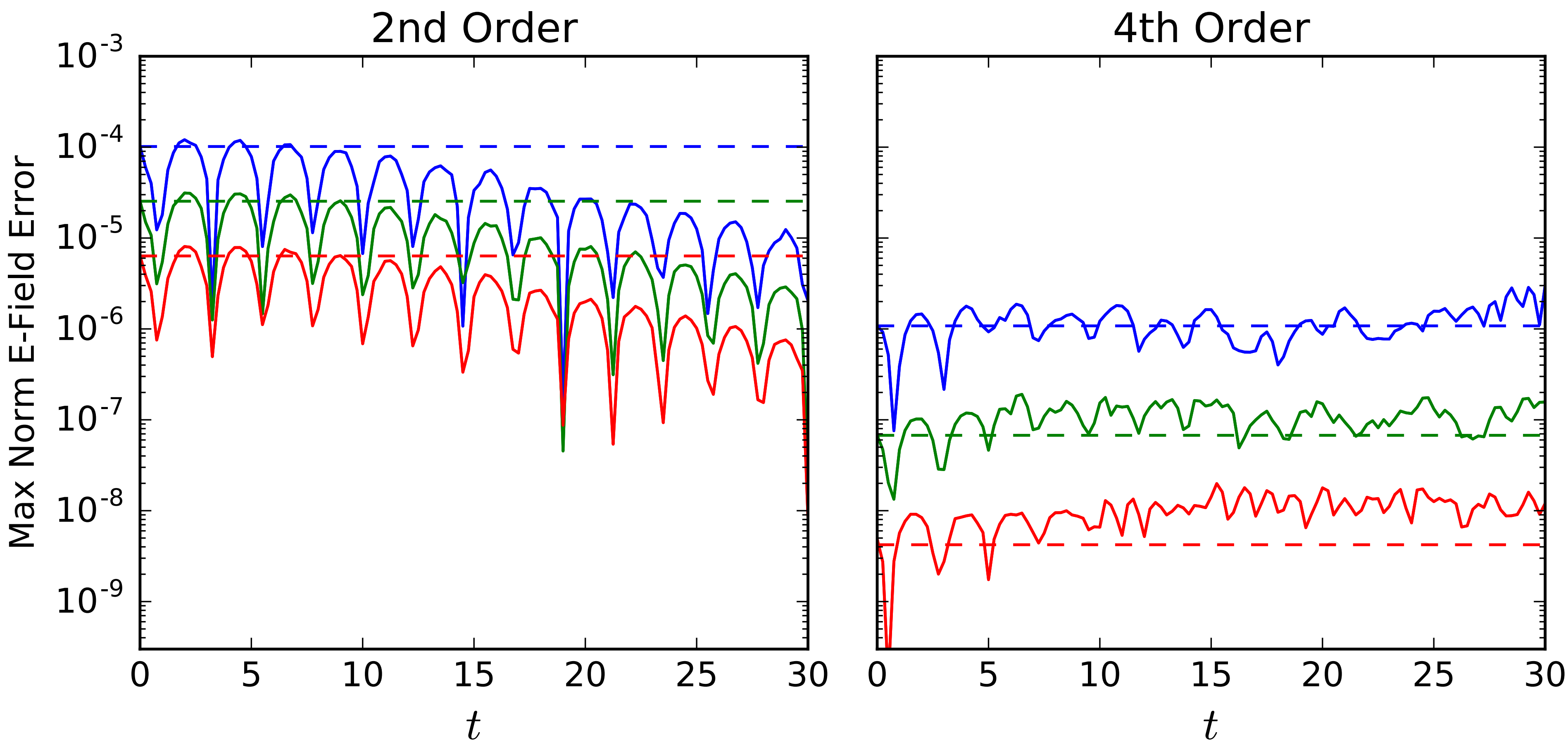
- We then use Richardson extrapolation to compute the error.
- The error in the electric field is then defined as:

$$e^h = |\boldsymbol{E}^h - \boldsymbol{E}^{2h}|$$

- And the order is computed as:

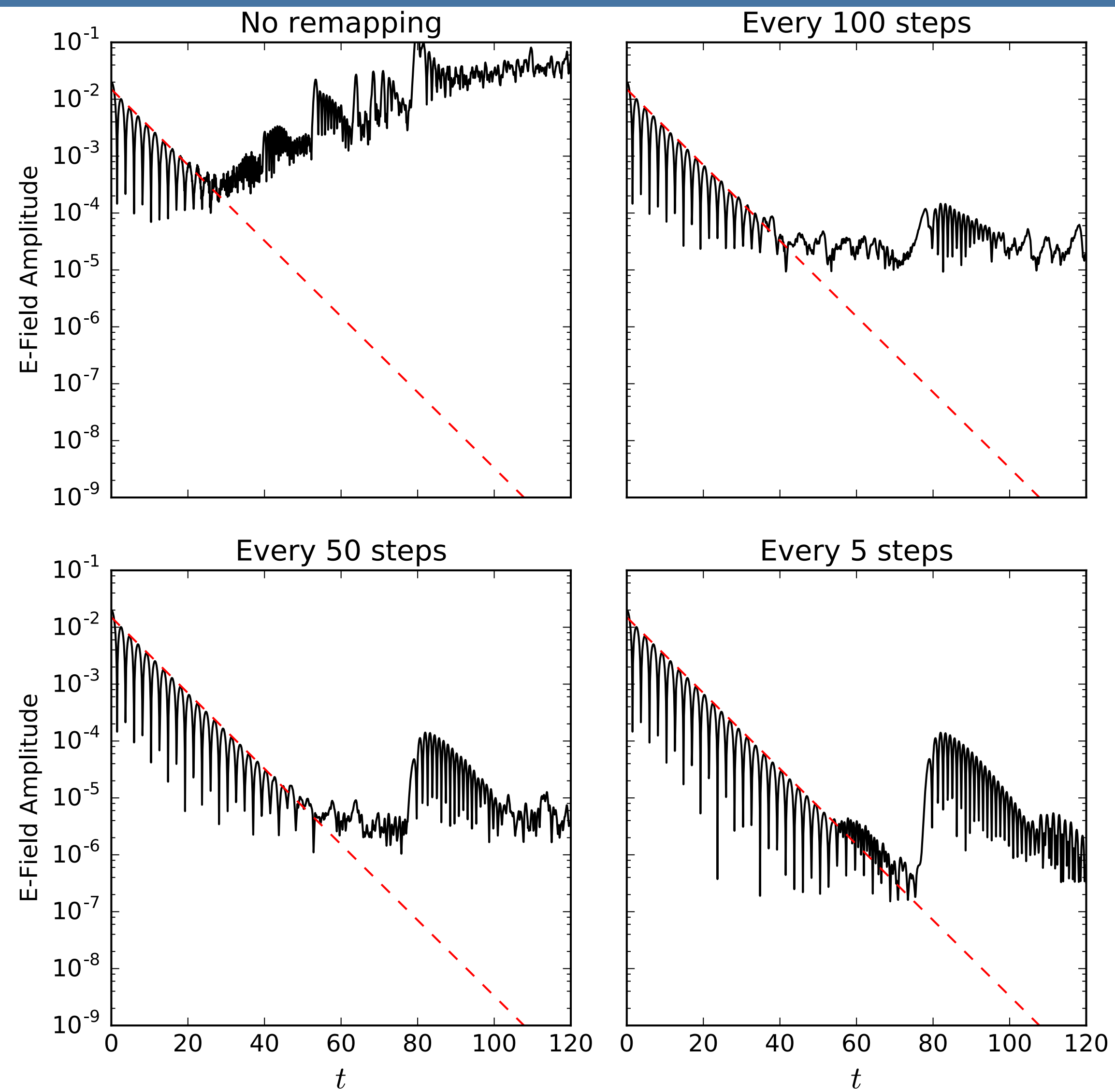
$$q = \log_2\left(\frac{||e^{2h}||}{||e^h||}\right)$$

Linear Landau Damping (convergence results)



Linear Landau Damping (results)

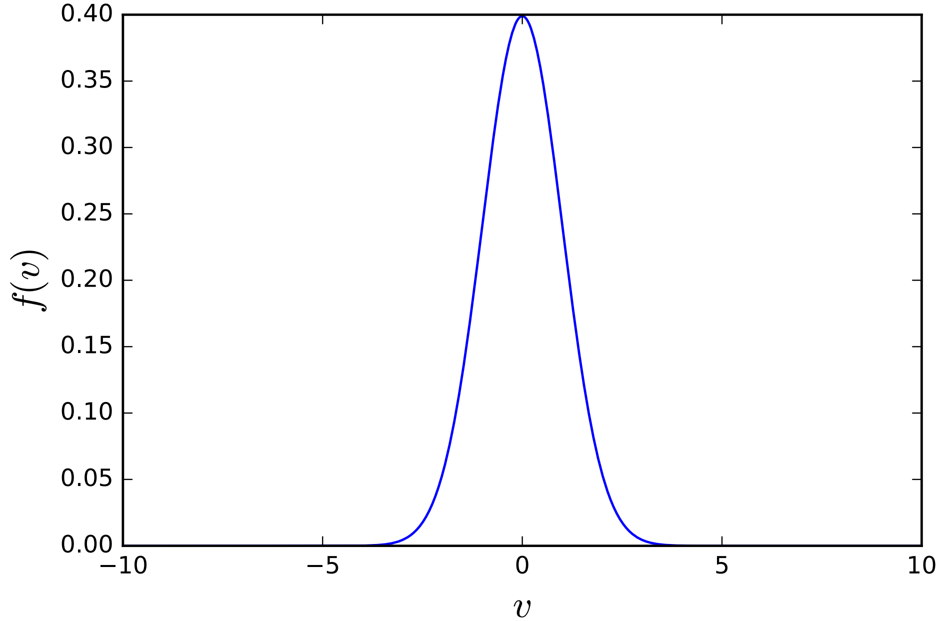
Remapping every 5 steps gives the best results, but even every 100 helps



Nonlinear Landau Damping (initial conditions)

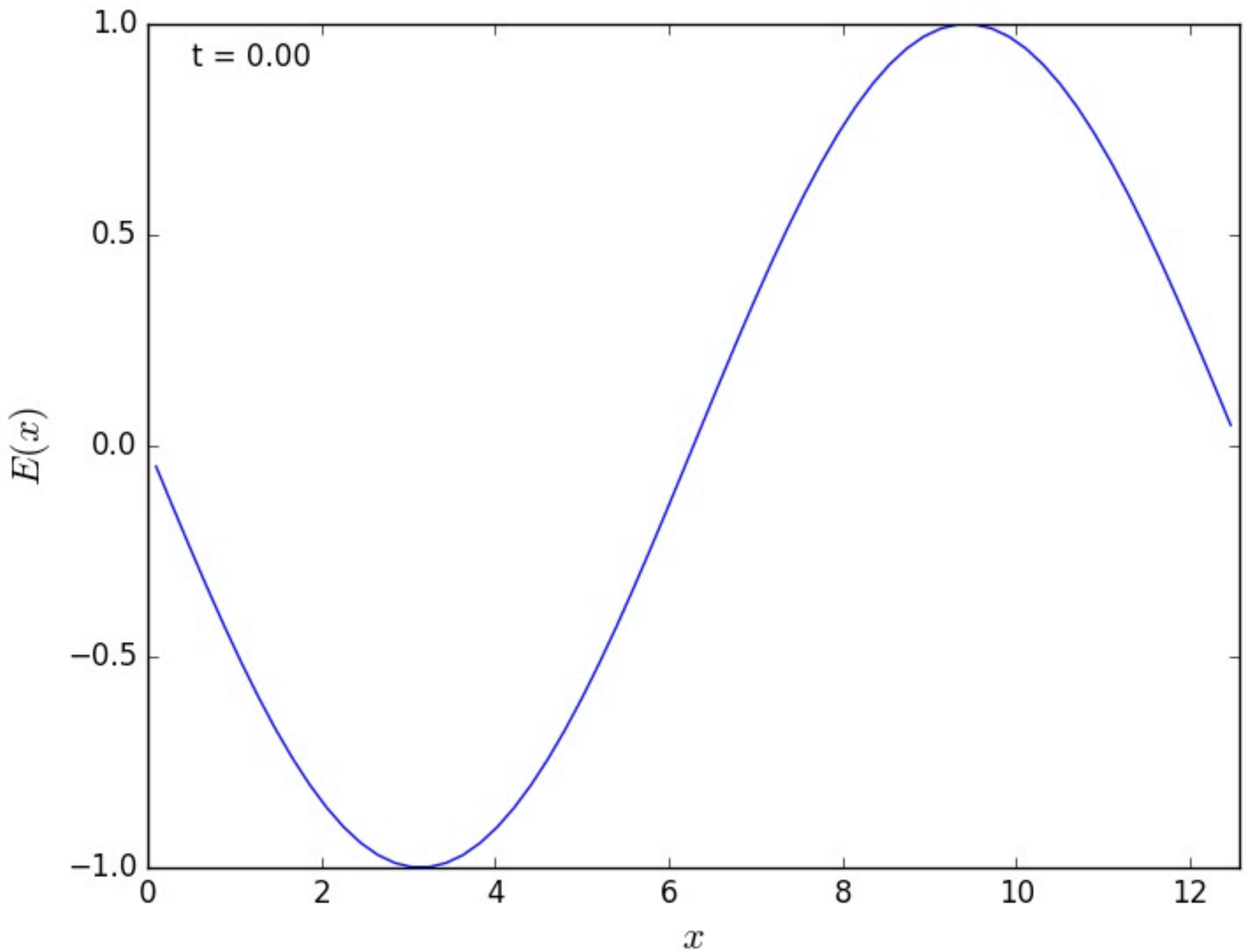
$$f(x, v, t=0) = \frac{1}{\sqrt{2\pi}} \exp\left(-v^2/2\right)\left(1 + \alpha \cos\left(kx\right)\right)$$

$$(x, v) = [0, L = 2\pi/k] \times [-v_{\max}, v_{\max}]$$



$$k = 0.5$$
$$\alpha = 0.5$$

Nonlinear Landau Damping (movie)



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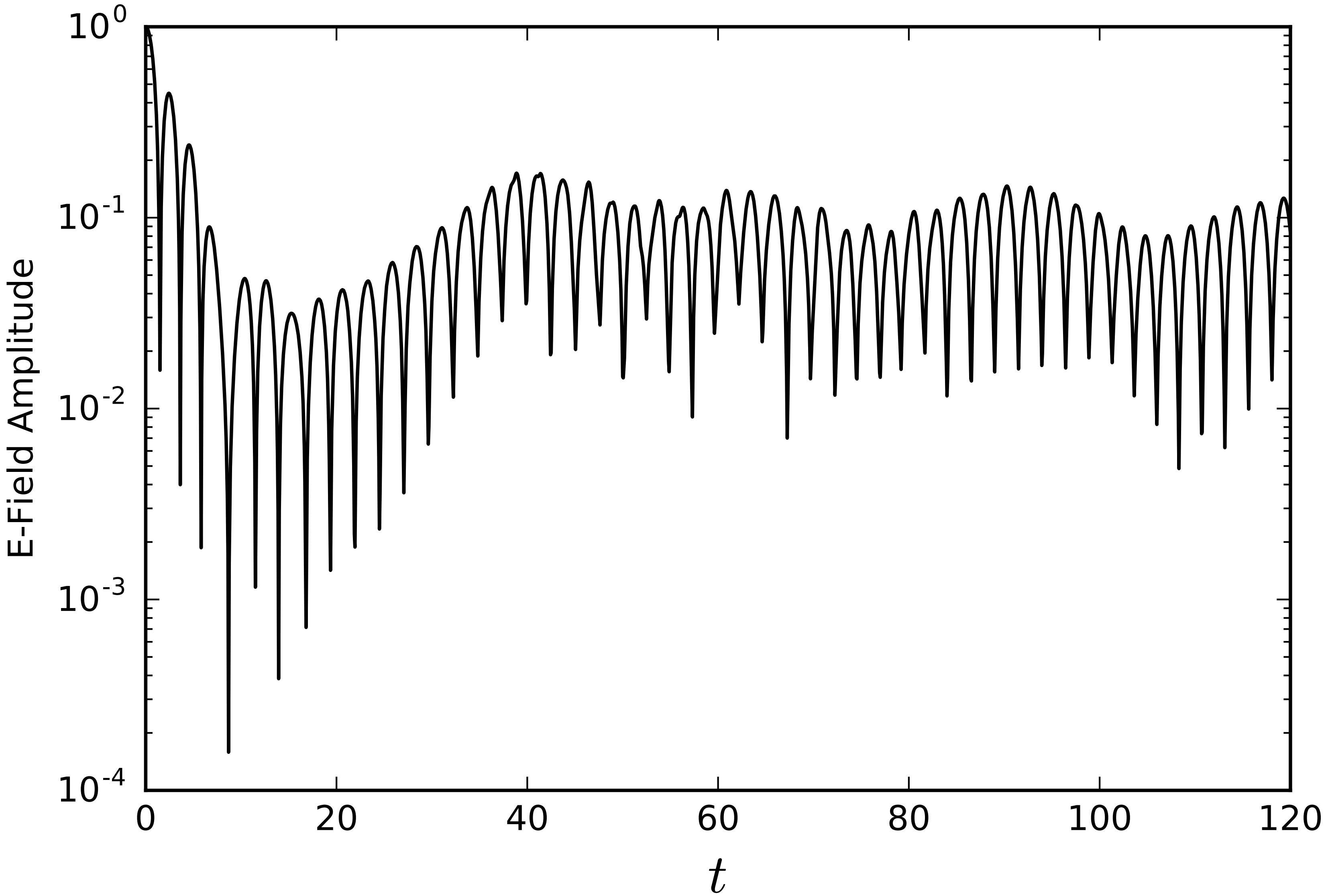
Nonlinear Landau Damping (results)



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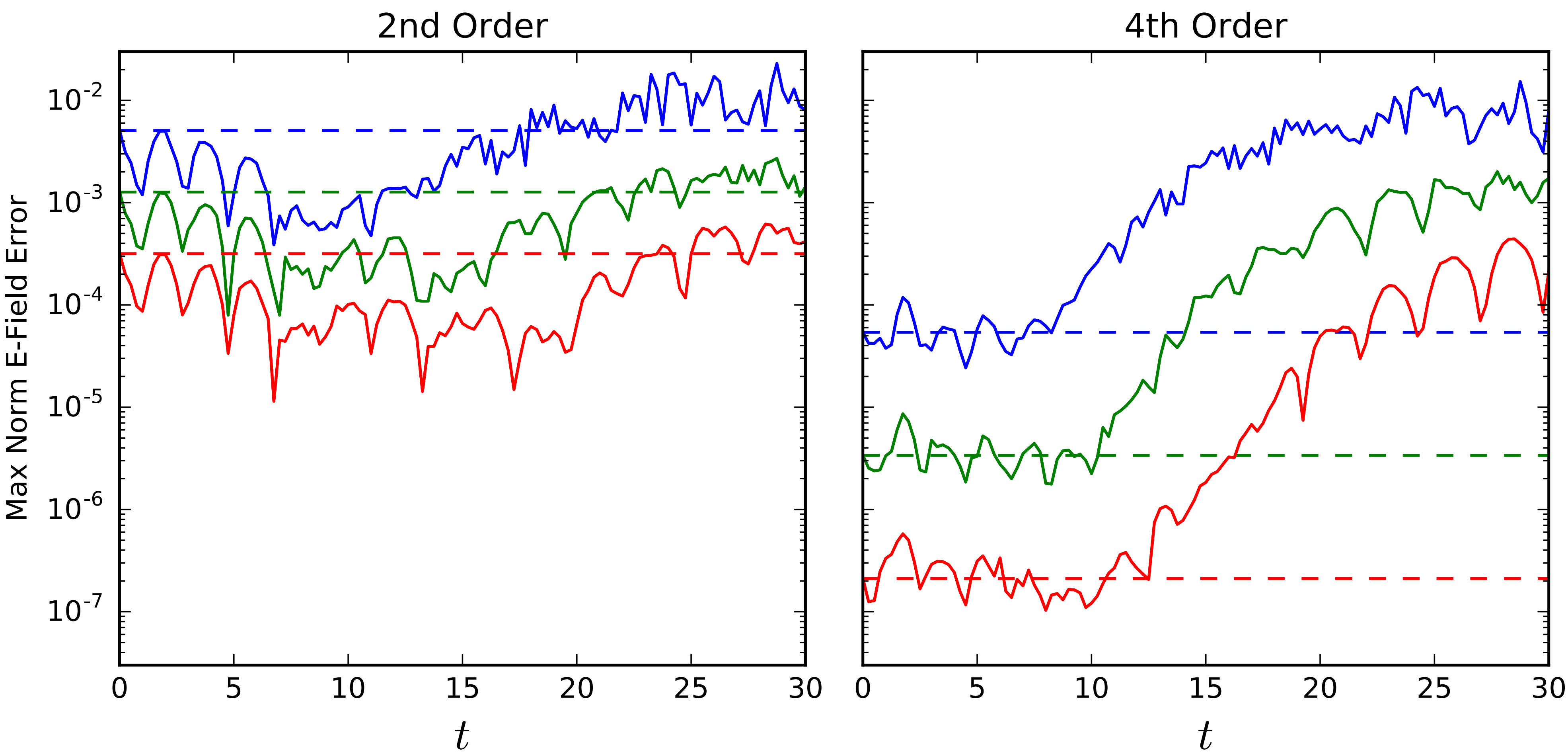
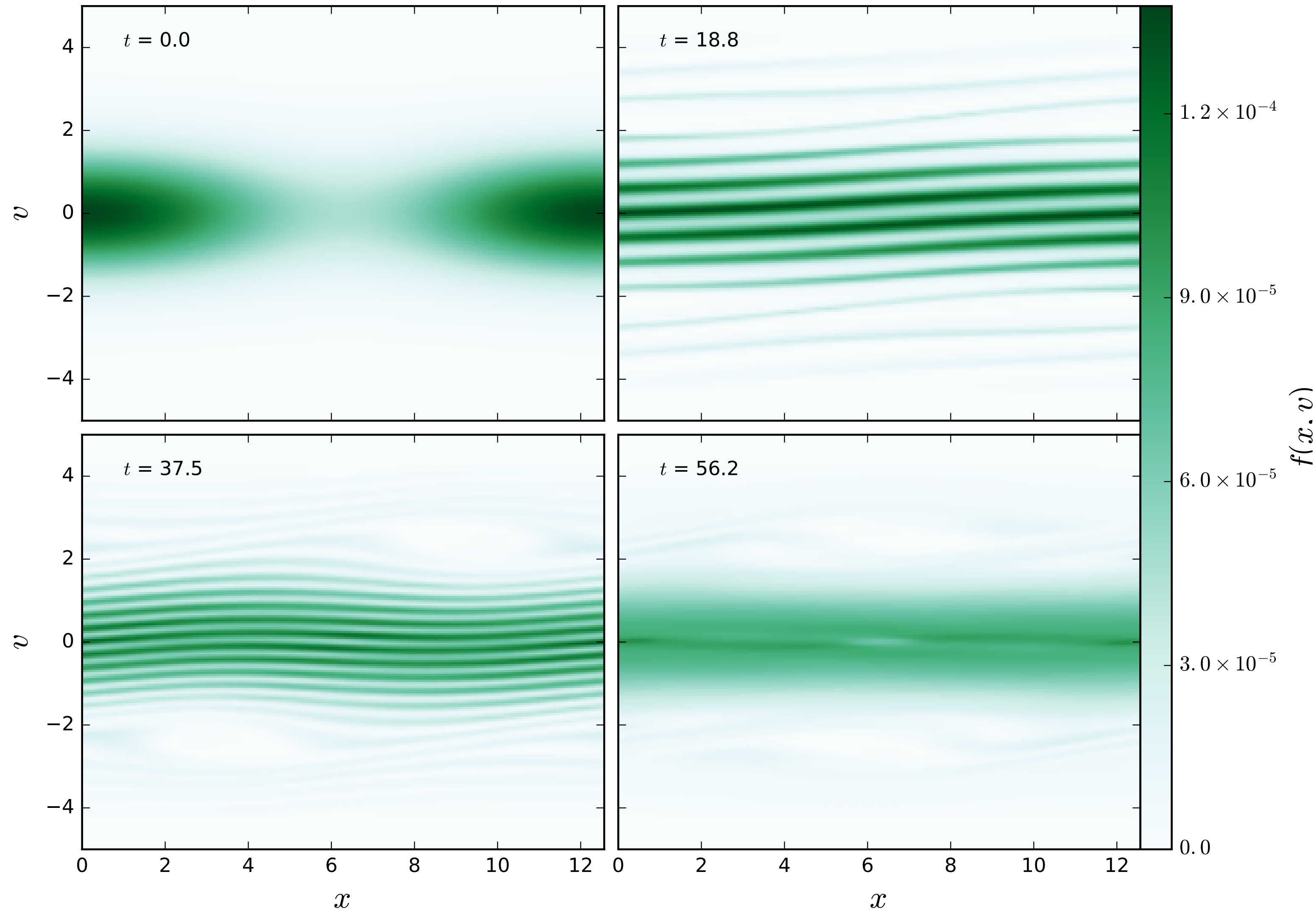
Nonlinear Landau Damping (convergence)



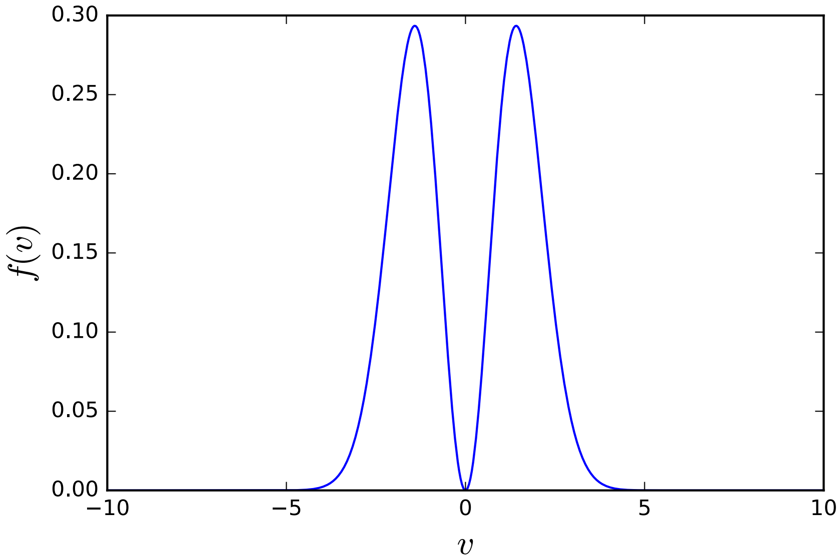
Nonlinear Landau Damping (Phase Diagrams)



Two-Stream Instability

- Initial distribution function corresponds to two particle streams with opposing velocities:

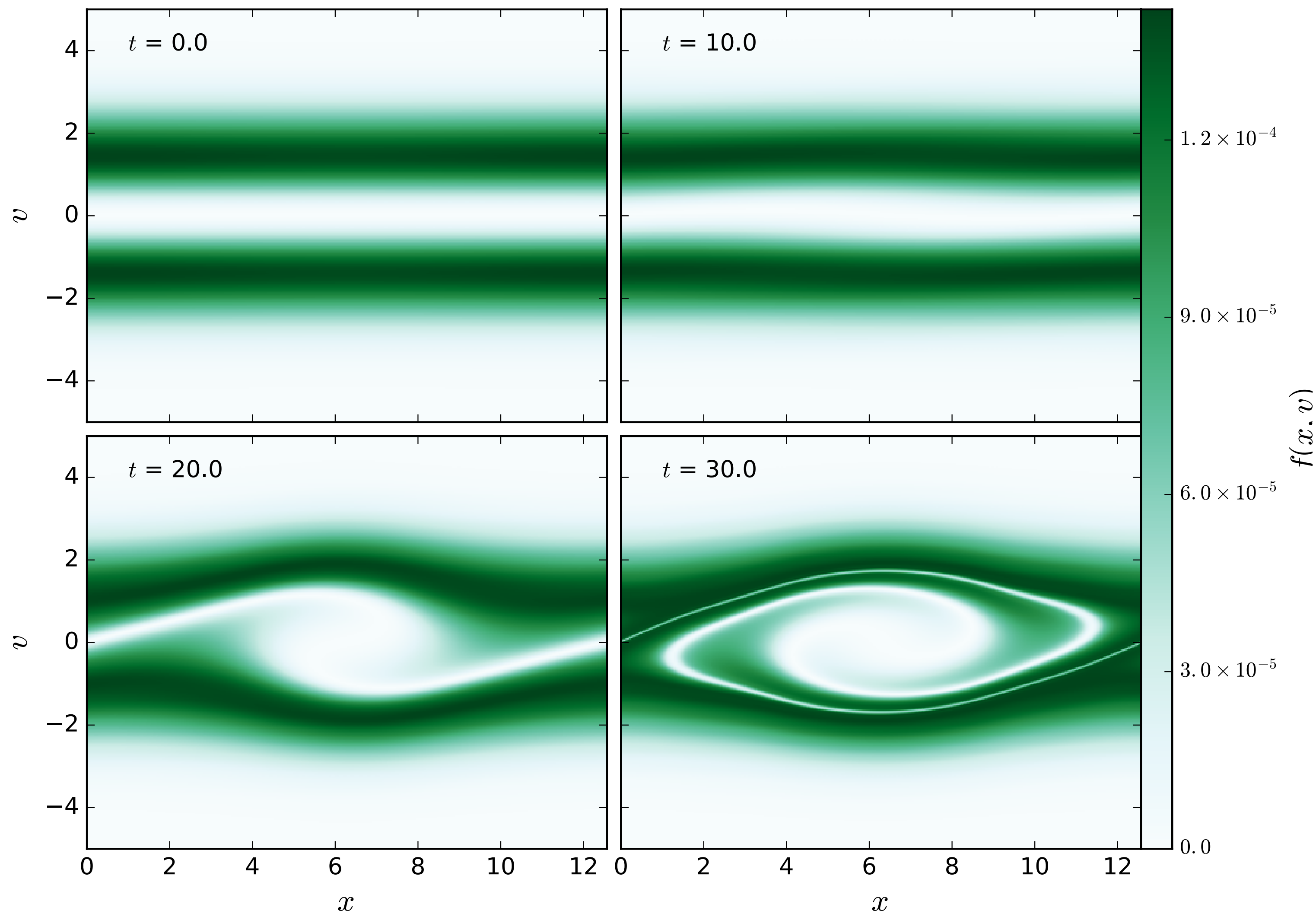
$$f(x,v,t=0) = \frac{1}{\sqrt{2\pi}} v^2 \exp\left(-v^2/2\right)\left(1+\alpha\cos\left(kx\right)\right)$$
$$(x,v) = [0, L=2\pi/k] \times [-v_{\max}, v_{\max}]$$



$$k = 0.5$$
$$\alpha = 0.01$$

"Inverse" of Landau Damping

Two-Stream Instability



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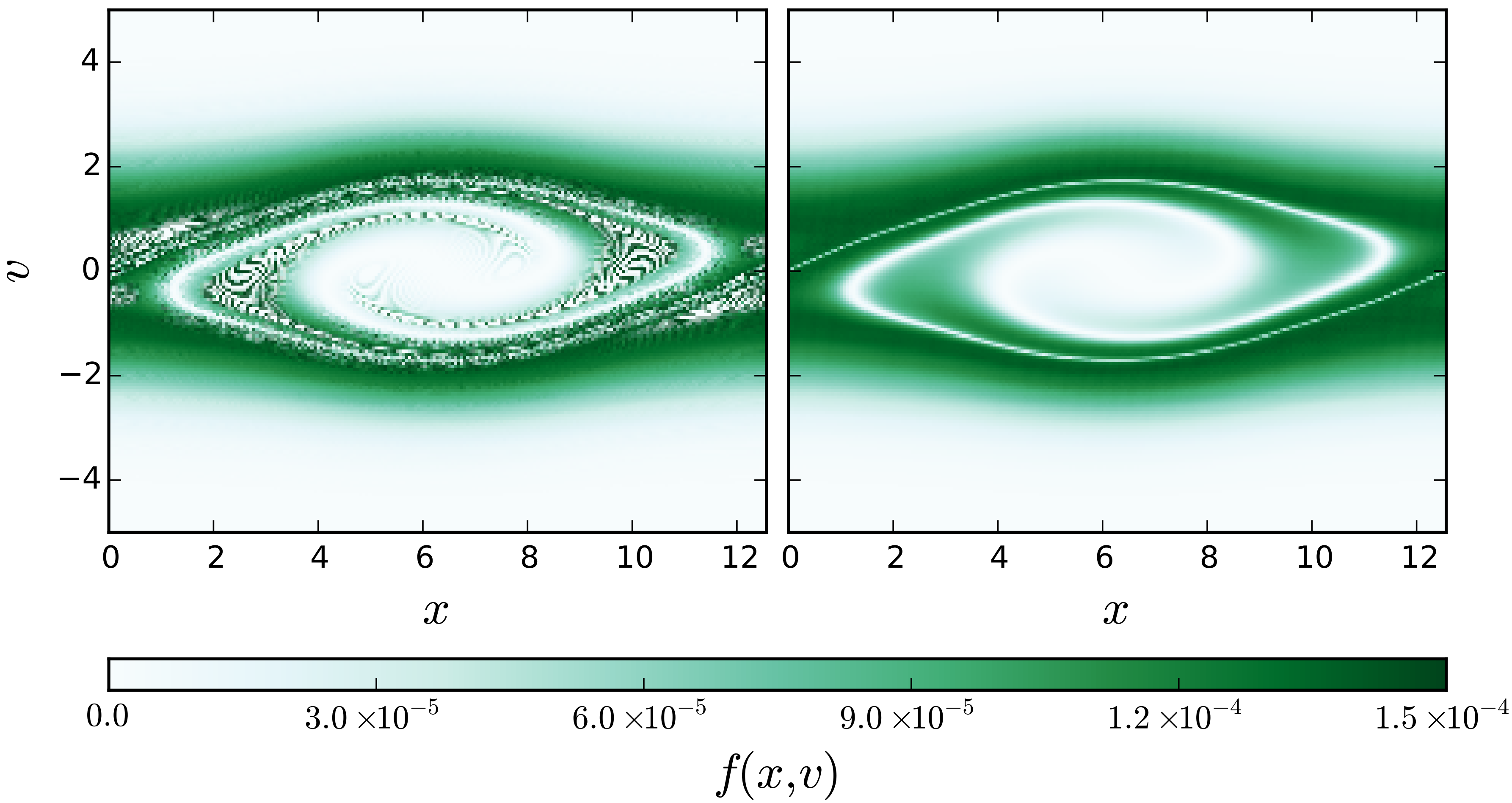
Two-Stream Instability



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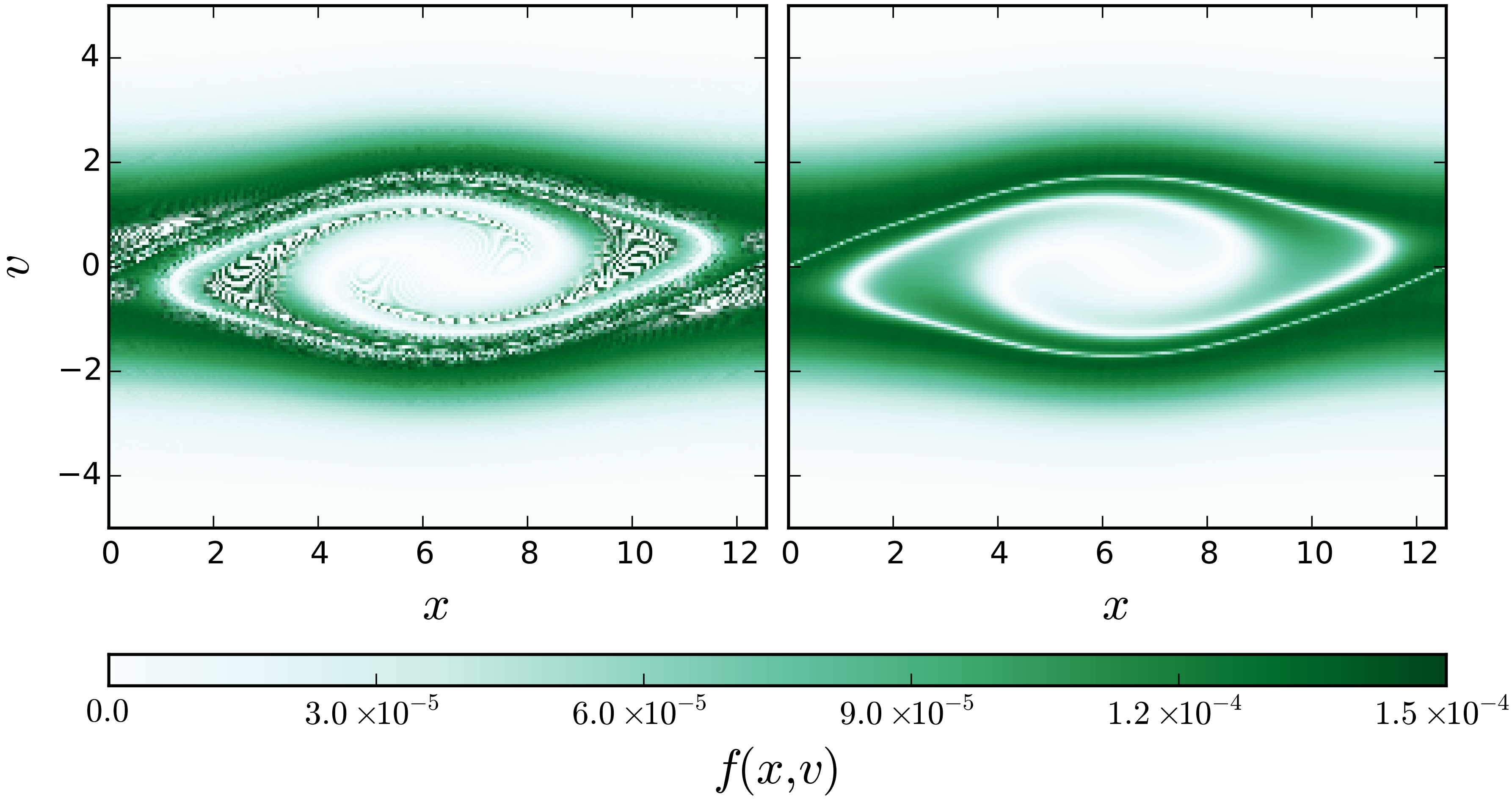
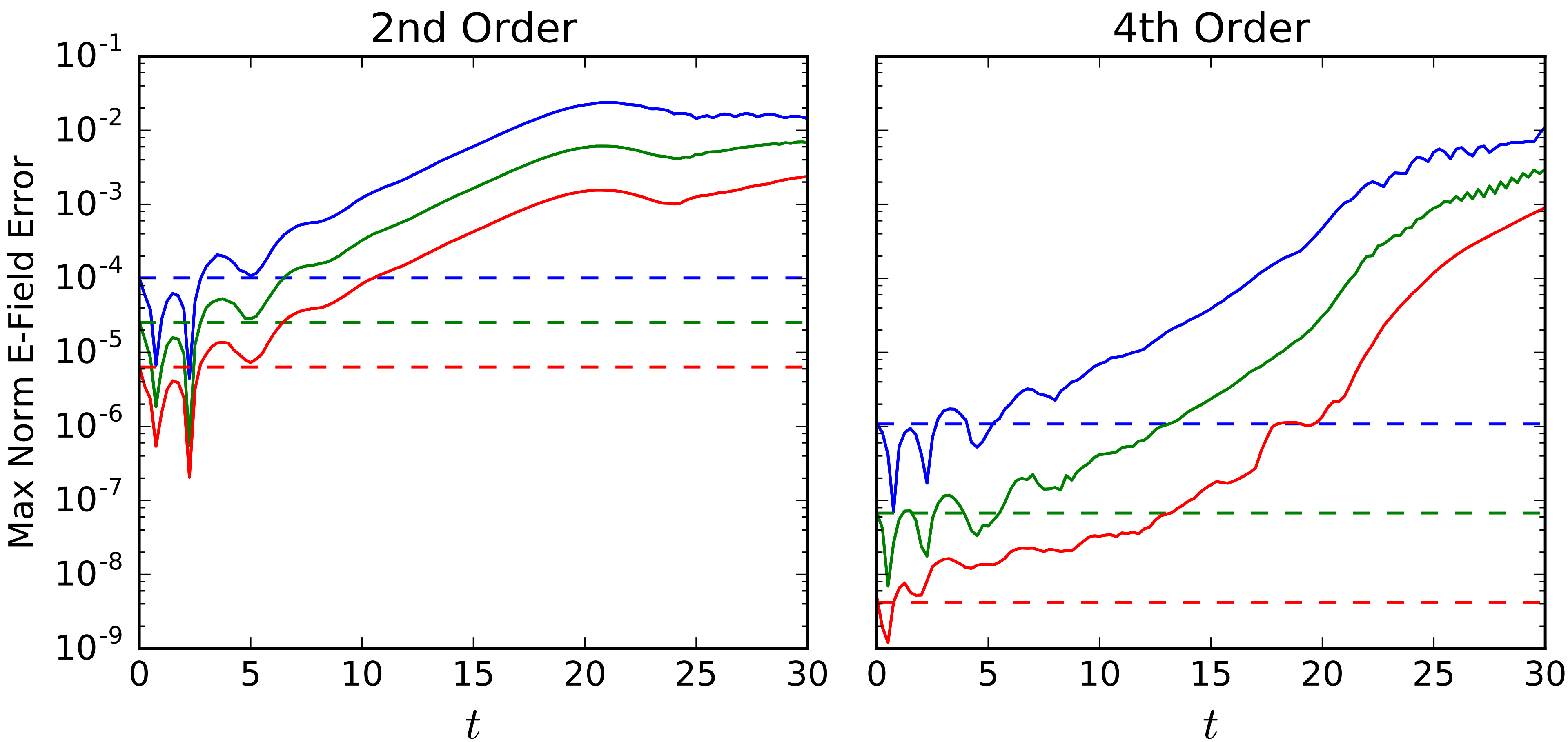
Two-Stream Instability

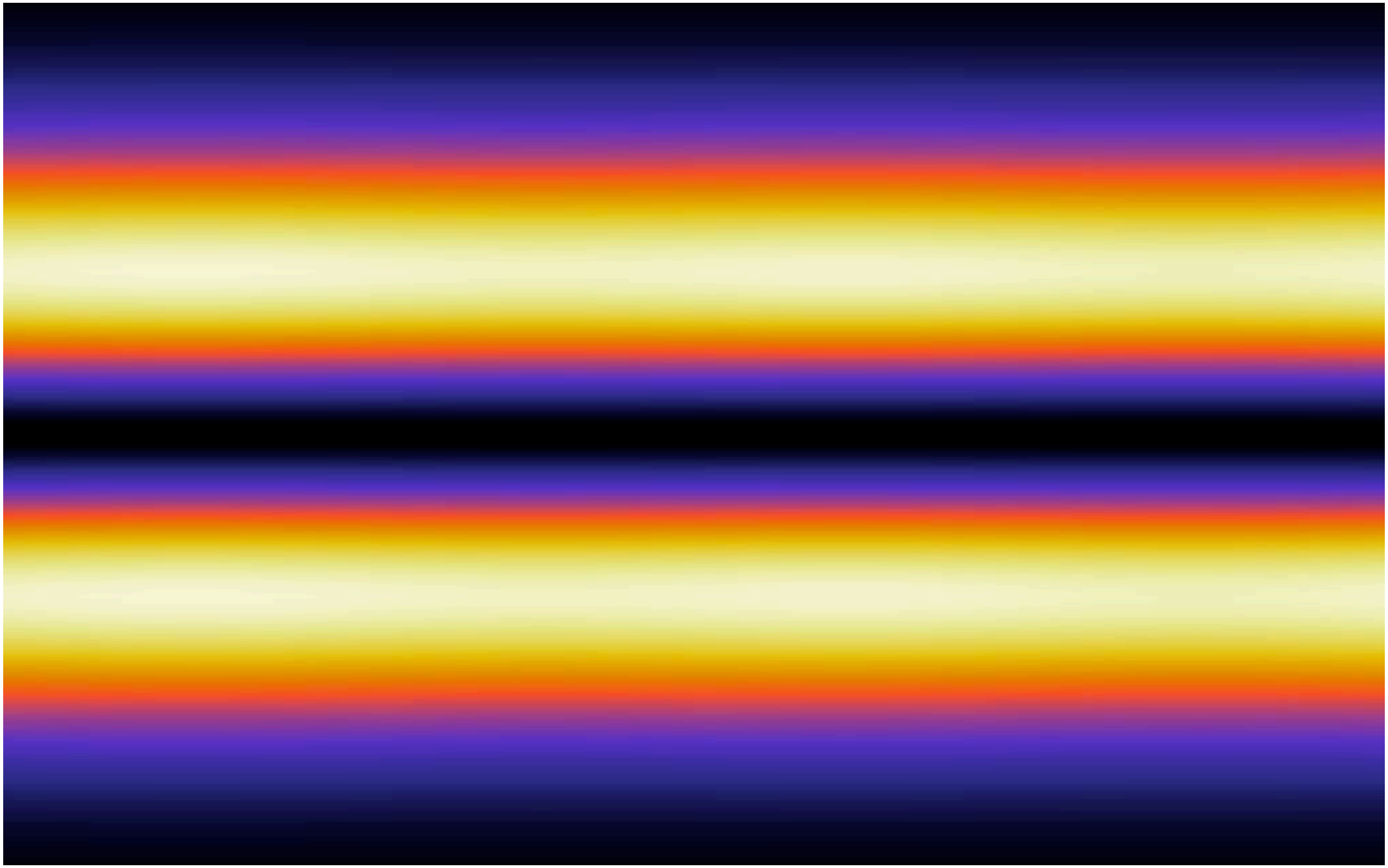
Remapping 10 times (out of ~1000)



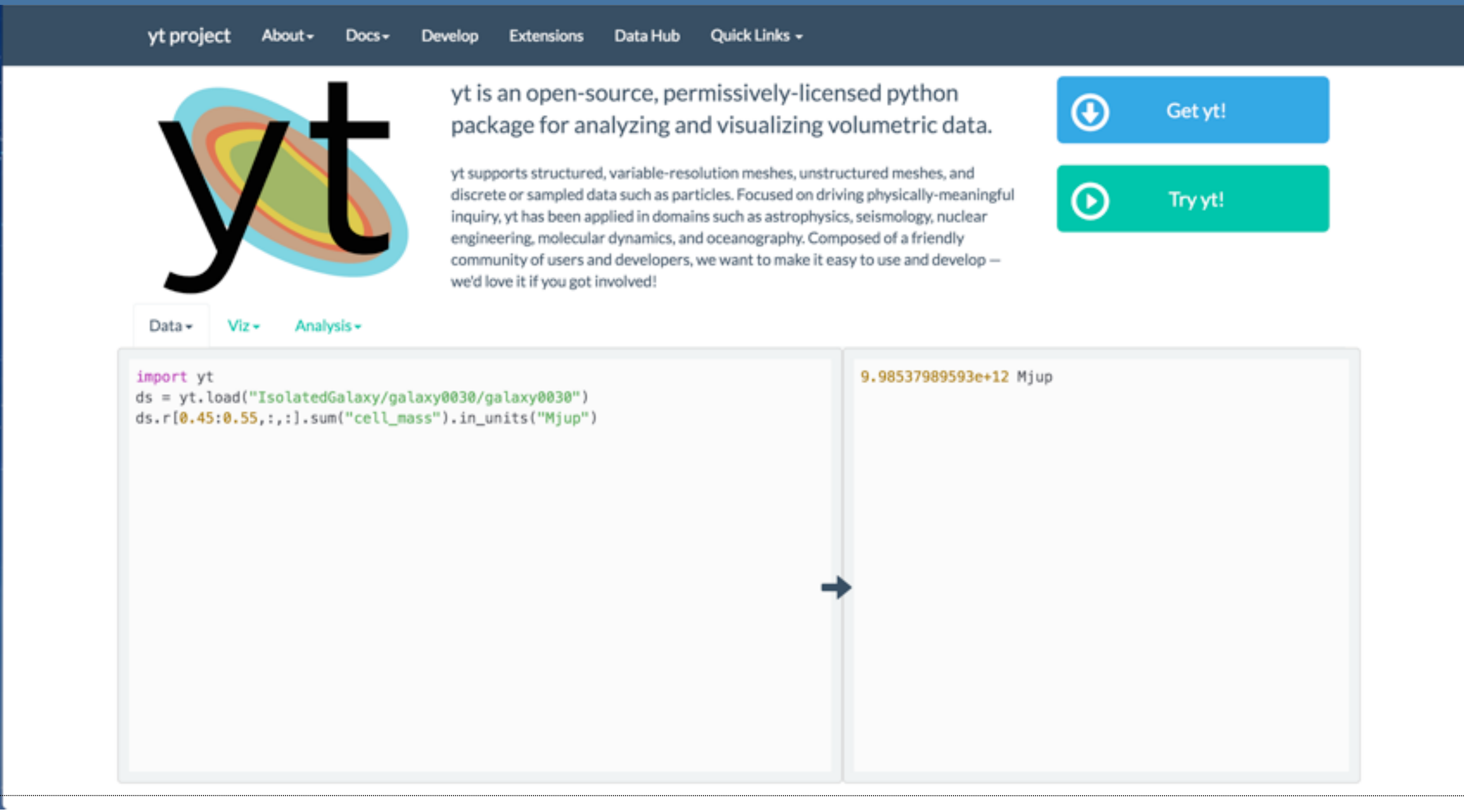
Two-Stream Instability (convergence results)



Two-Stream Instability



http://yt-project.org/



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Summary and Future Research

- High-order method is more accurate in regions where the flow is smooth
- Not more necessarily more accurate for thin or unresolved phase-space features in the nonlinear regime.
- Remapping is necessary to control particle noise over long time evolutions
- Involves some degree of retreat from pure Lagrangian. AMR helps to an extent.Trade-offs need to be explored.
- Future research involves performing the remap selectively rather than globally.
- Coupled with high-order Maxwell solver for electromagnetic PIC (Sven Chilton)

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Thanks for listening!

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with Phillip Colella, Brian Van Straalen, Bei Wang, Boris Lo, Victor Minden

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https://arxiv.org/abs/1602.00747