δf Particle-In-Cell simulation.

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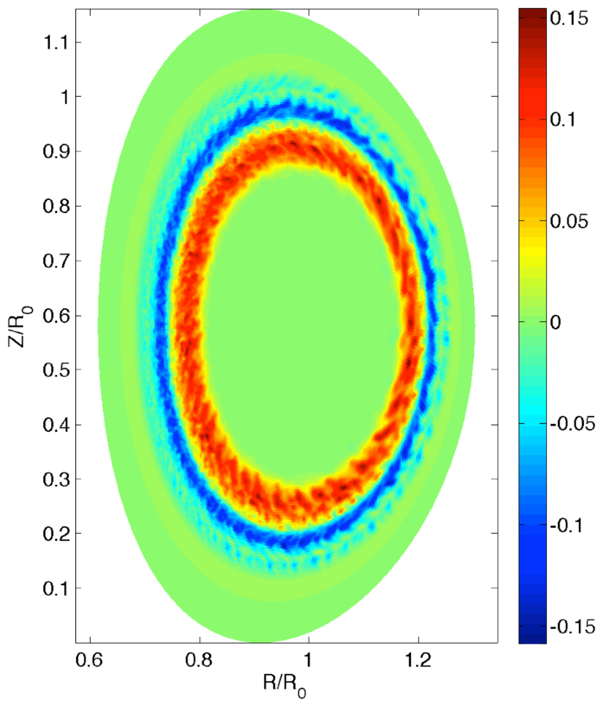
Acknowledgements to the EPOCH team.

Contents

- Numerical simulations for collisionless plasma simulation
- The PIC (Particle in cell) method
  - Noise in the PIC method
- The 'low noise' δf PIC method
  - Formulation
  - Some comparisons with standard PIC

The problem I'm usually solving:



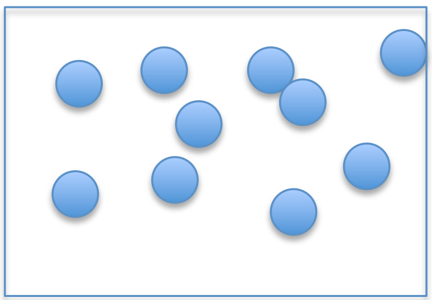
- Simulating turbulence in tokamaks.
- Low–collisionality particles interacting with an electromagnetic field.
- Small fluctuations (1%), large system size to turbulent eddy scale (1000), 5D problem (position and velocity), large range of timescales.

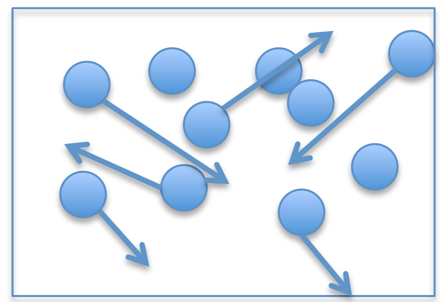
Numerical methods for Vlasov-Maxwell equations.

- Kinetic simulations of plasmas require solution of the Vlasov equation $df(\mathbf{x},\mathbf{v},t)/dt = 0$, with the convective derivative along the particle trajectory.
- Two basic methods:
  1. Fixed discretisation in (x,v) (Eulerian)
  2. Follow characteristics/particle trajectories in (x,v) (Lagrangian/PIC)
- Eulerian generally too hard with 6 phase space directions.

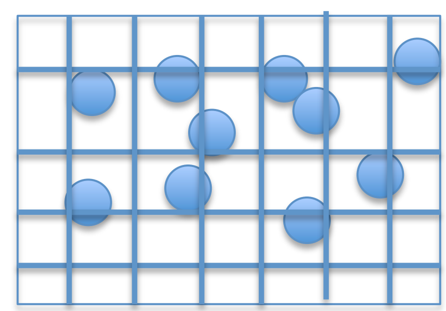
Particle in Cell (PIC) loop

Load particles in a box





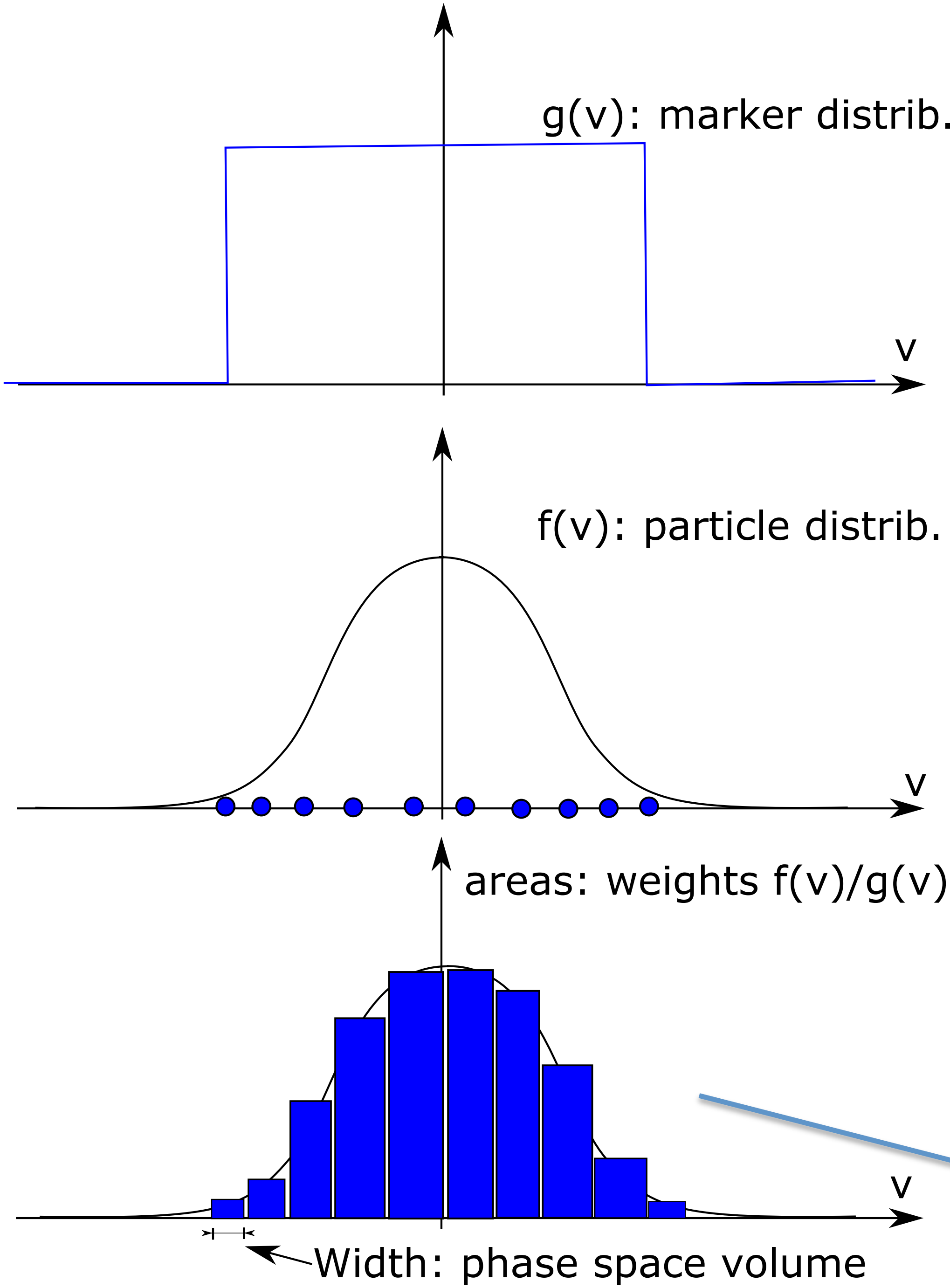
Solve equations of motion for a short time particle $(x_i,v_i)\text{->}(x'_i,v'_i)$ using fields E, B.



Find densities and/or currents on grid associated with particles at (x'_i,v'_i)

Find the new fields E, B.

PIC methods and Monte-Carlo



- The markers in a PIC simulation sample the distribution function: densities/ currents are Monte-Carlo integrals.
- In real simulations, markers are randomly distributed.

Integral->Charge density->Fields

PIC errors.

- Moments have errors scaling like $1/N^{1/2}$
- In a spatial grid cell, usually N=100 for typical simulations.
- Why does this work at all -> 10% density fluctuations are similar/comparable to cases of interest.
  - Fluid properties conserved (roughly). PIC simulations act like a coarse-grained, highly collisional plasma.
  - For some problems, noise mostly at different phase speeds.

Does noise matter?

NOT REALLY?

- Particle simulation can be interpreted as real plasma system with different parameters.
- Simulation results look 'similar' under convergence.
- Can use filtering to remove some of it.

YES?

- Much easier to interpret low-noise simulations.
- Noise introduces unphysical diffusion and unphysical collisions.
- This can prevent the real physics from manifesting.

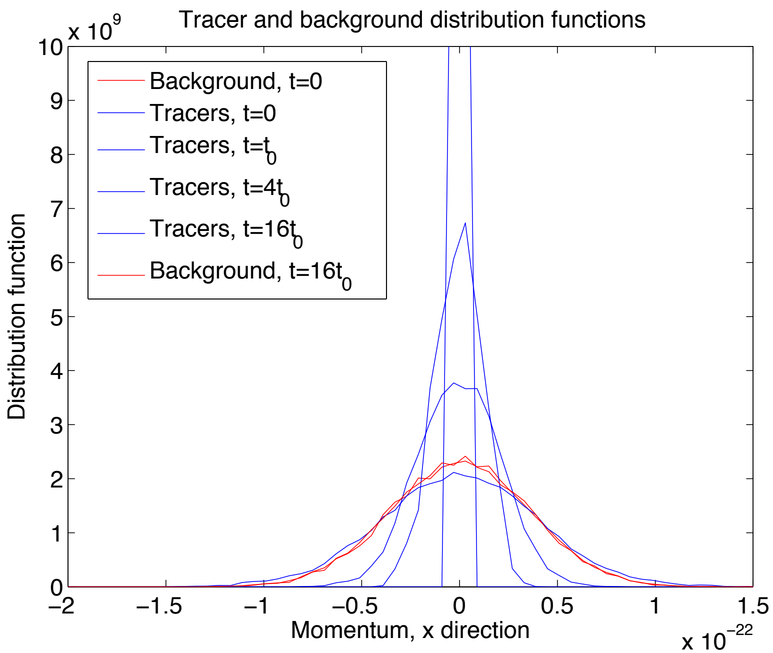
Noise disasters in tokamak simulation.

- PIC simulations predicted lower levels of transport in tokamaks than Eulerian simulations.
- Seemed to be converged with particle number (but weren't!). (See Hammett et. al., 2006)
- It was the diffusion due to noise that killed them.
- Lessons:
  - Understand how much noise is in the system and its effect.
  - Convergence scans necessary but liable to misinterpretation.

Computational noise versus thermal noise.

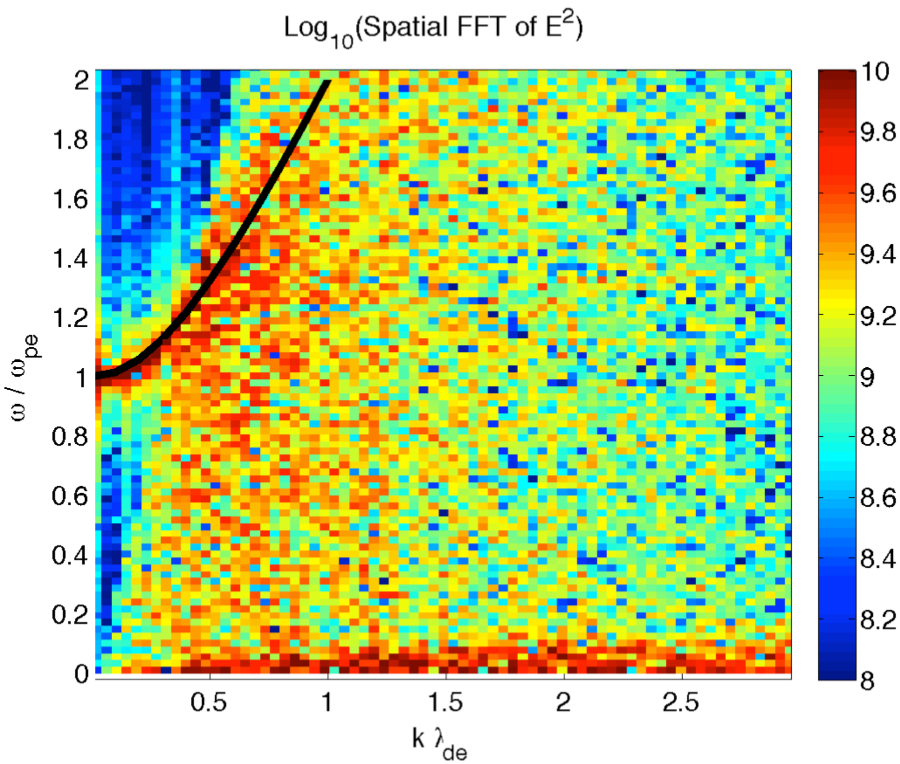
- Point particle versus smoothed ‘cloud’.
- Fluctuation/Dissipation theorem and BBGKY approaches can be used (with reservations) for *computational* gas like a real gas. (A.B.Langdon, Physics of Fluids 22, 163, 1979)
- Very few markers in ‘Debye Sphere’-> numerical collisionality.

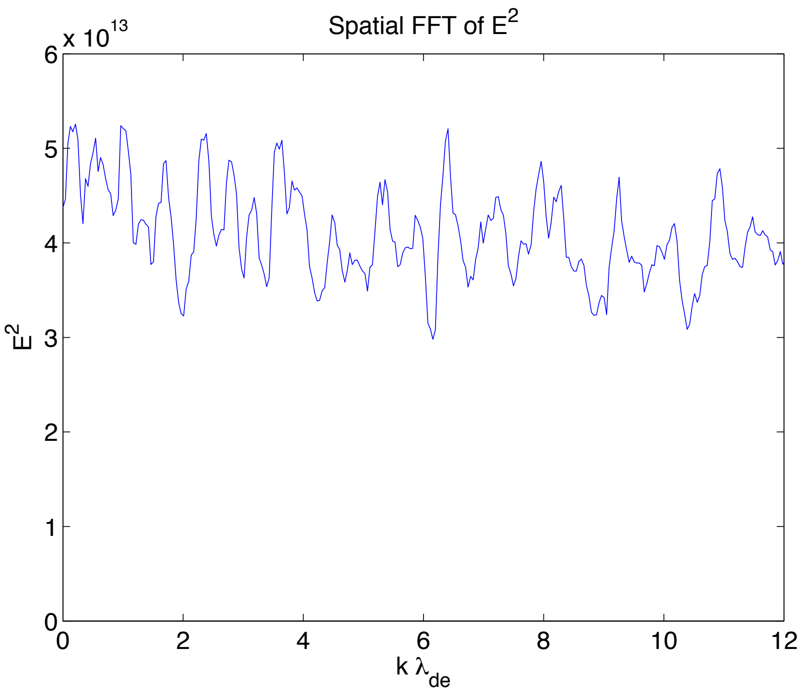
Velocity diffusion.



- Tracers with initially zero velocity in background thermal plasma.
- 300 markers per cell.
- t_0 is $100\omega_{pe}^{-1}$.
- 'Collisional thermalisation' after $\sim 1000\omega_{pe}^{-1}$.

Spectrum of noise.





The δf method

- Noise is mostly a problem when the signal is small: systems close to stability.
- Used widely in gyrokinetics (tokamak turbulence): for standard PIC, see Sydora, JCAM 109, (1999) 243-259.
- Define a 'background function' $f_0(x,v,t)$ which has analytically known moments, and is close to f, and split $f = f_0 + \delta f$.

Choose an f_0 with analytically known moments.

$$f = f_0 + \delta f \tag{1}$$

$$0 = \frac{df}{dt} = \frac{df_0}{dt} + \frac{d\delta f}{dt} \tag{2}$$

As in standard PIC, define N markers which follow particle equations of motion, with phase space position $\mathbf{z} = (\mathbf{x}, \mathbf{v})$. Analogous to standard PIC, the distribution function is written in terms of markers

$$\delta f = \sum w_i(t)\delta(\mathbf{z} - \mathbf{z}_i). \tag{3}$$

The distribution of markers $g(\mathbf{z}, t)$ also satisfies the Vlasov equation.

$$0 = \frac{dg}{dt} \tag{4}$$

Integrate equation 3 over a small volume of phase space to find

$$\delta f =< w_i(t) > g(\mathbf{z}, t) =< w_i(t) > g(\mathbf{z}_0, 0). \tag{5}$$

The marker density at the initial position $g_i = g(\mathbf{z}_{i0}, 0)$ can be interpreted as the inverse of the phase volume represented by each marker.

We solve to find

$$w_i = \frac{1}{g_i}[f(\mathbf{z}_{i0}, 0) - f_0(\mathbf{z}, t)]. \tag{6}$$

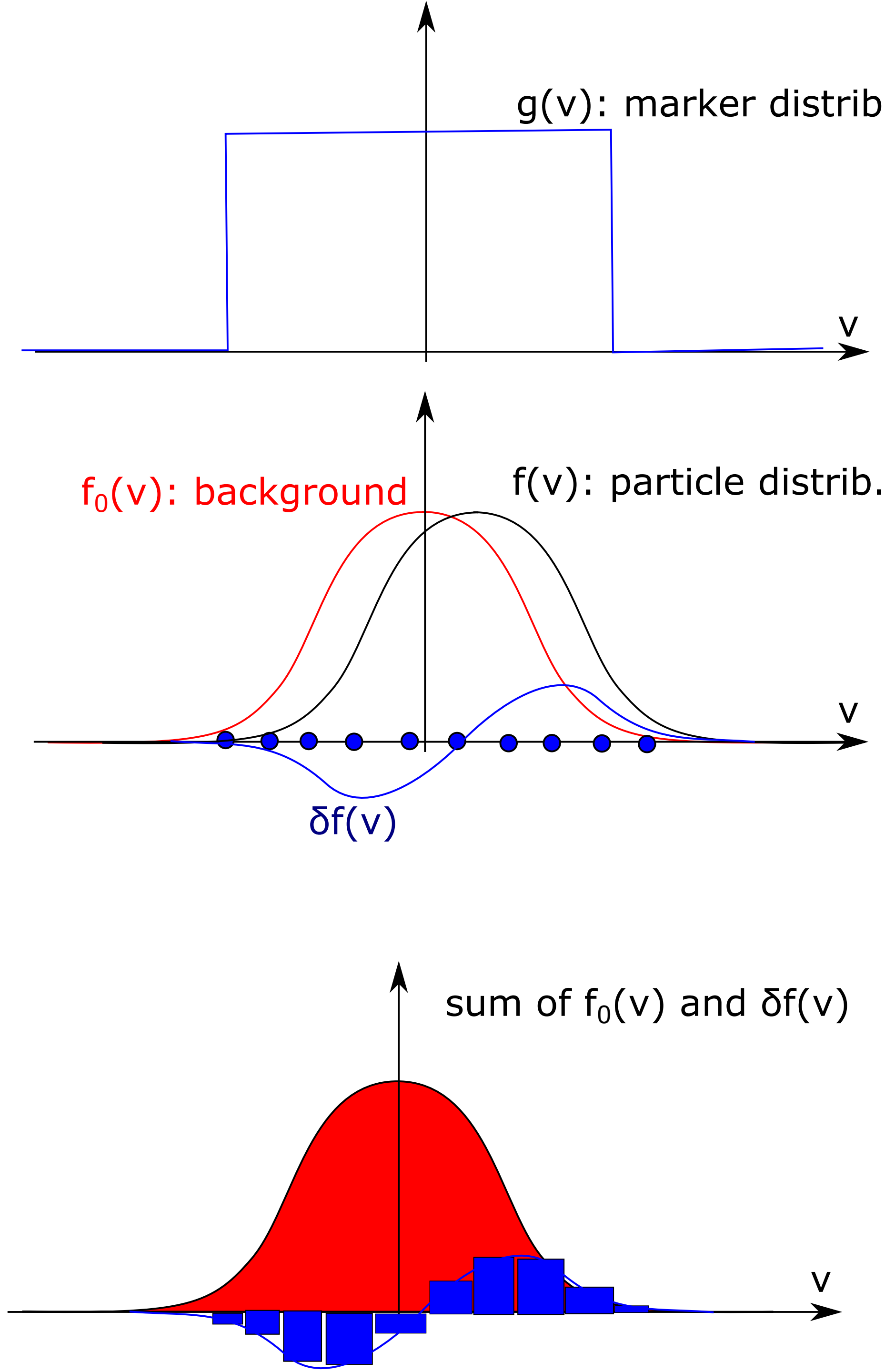
We can also find an equation for the time derivative of $w_i(t)$:

$$\frac{dw_i}{dt} = \frac{1}{g_i}\frac{d\delta f}{dt} = -\frac{1}{g_i}\frac{df_0}{dt} = -\frac{1}{g_i}\left[\frac{\partial f_0}{\partial t} + \dot{\mathbf{z}} \cdot \frac{\partial f_0}{\partial \mathbf{z}}\right]. \tag{7}$$

Currents and densities are defined as

$$\mathbf{J}(\mathbf{x}) = \int d\mathbf{v} f \mathbf{v} = \int d\mathbf{v} f_0 \mathbf{v} + \sum w_i(t)\mathbf{v_i}\delta(\mathbf{x} - \mathbf{x}_i) \tag{8}$$

where the background terms often sum to zero (current-free background).

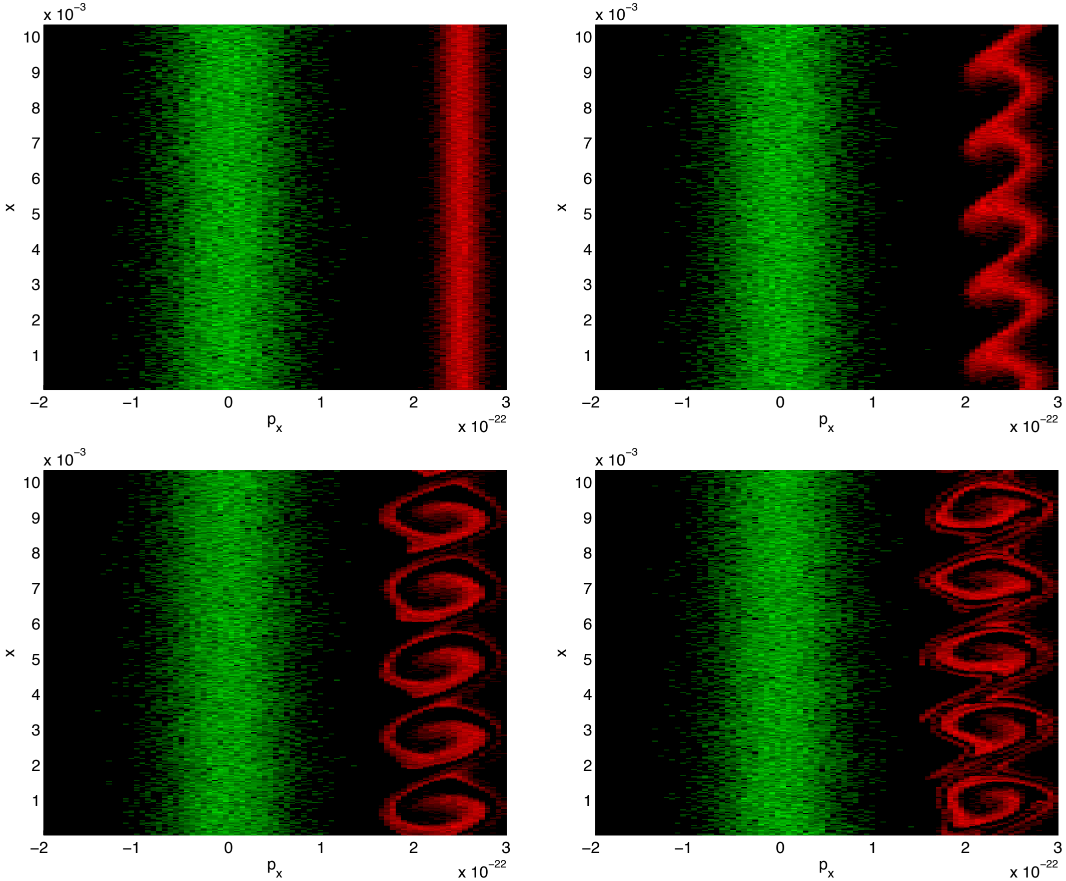


g(v): marker distrib.
v
$f_0(v)$: background
f(v): particle distrib.
v
δf(v)
sum of $f_0(v)$ and δf(v)
v

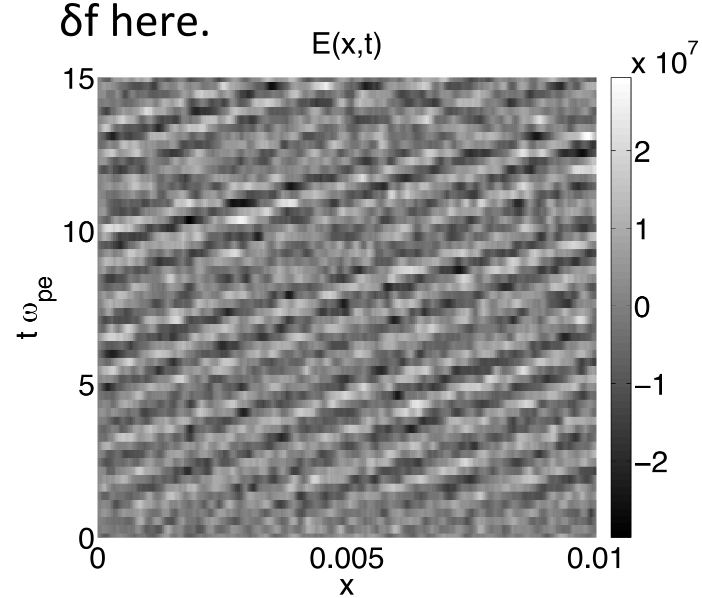
Why does this help?

- Noise in fields/densities lower by factor ($\delta f/f$).
- Moments of distribution have much lower error: diagnostics easier.
- Unphysical numerical collisions much weaker.
- Allows linear simulations:
  - These are pretty difficult/annoying in standard PIC.
  - Much easier to compare with analytic theory.

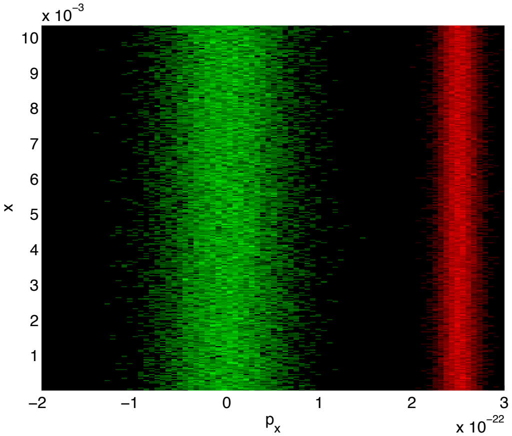
An example: weak beam two stream

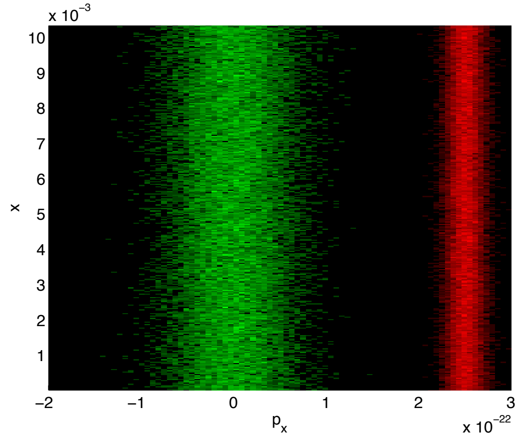


- Background plasma 1000 times the density of beam (red)
- Normal PIC handles this quite well: noise in background doesn't affect the instability.
- Electric field quite noisy (even smoothed).
- Using a δf simulation: the beam is far from Maxwellian so δf not helpful. The background perturbation is small so could use δf here.

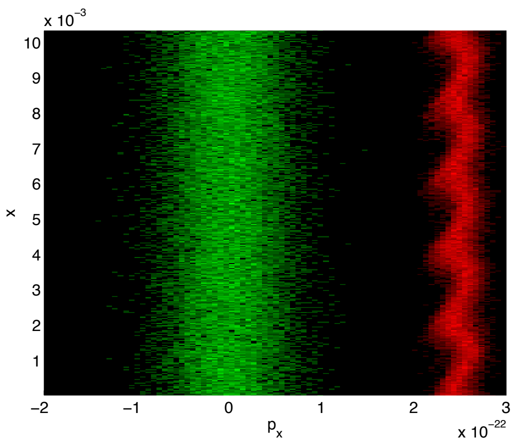


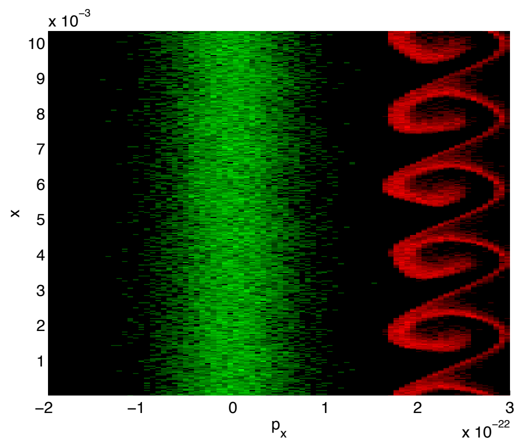
Weak beam, δf

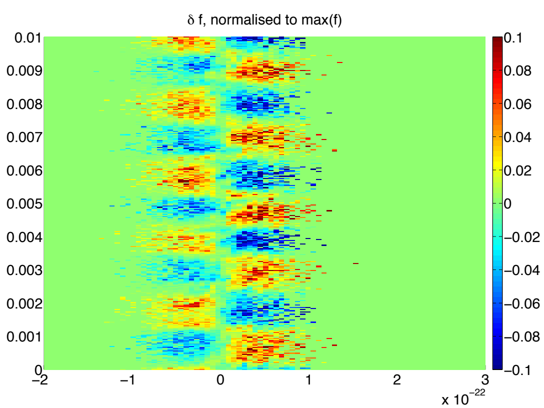




- Instability grows later due to lower initial fluctuations->find growthrate.
- Otherwise similar results for beam distribution.
- Using a δf simulation: much lower noise in electric field. Can see fine structure but care needed in tail of background.
- Can also determine how the background distribution has evolved.

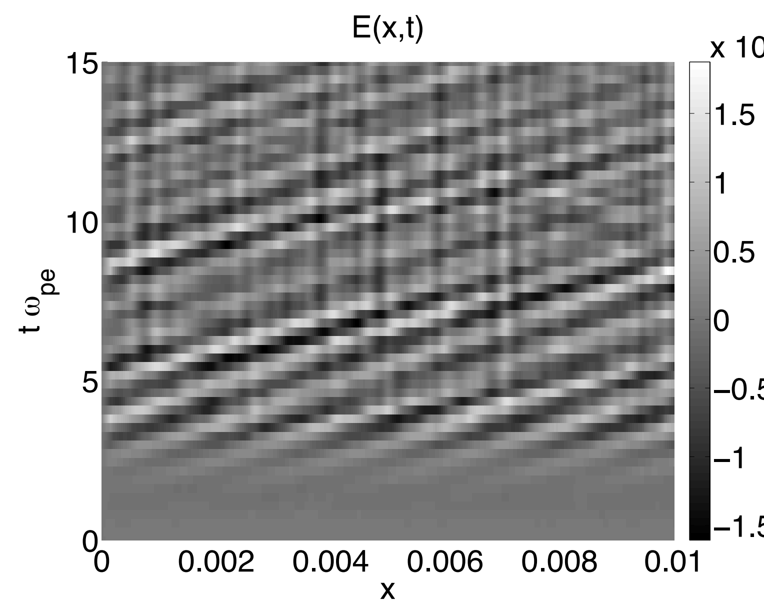




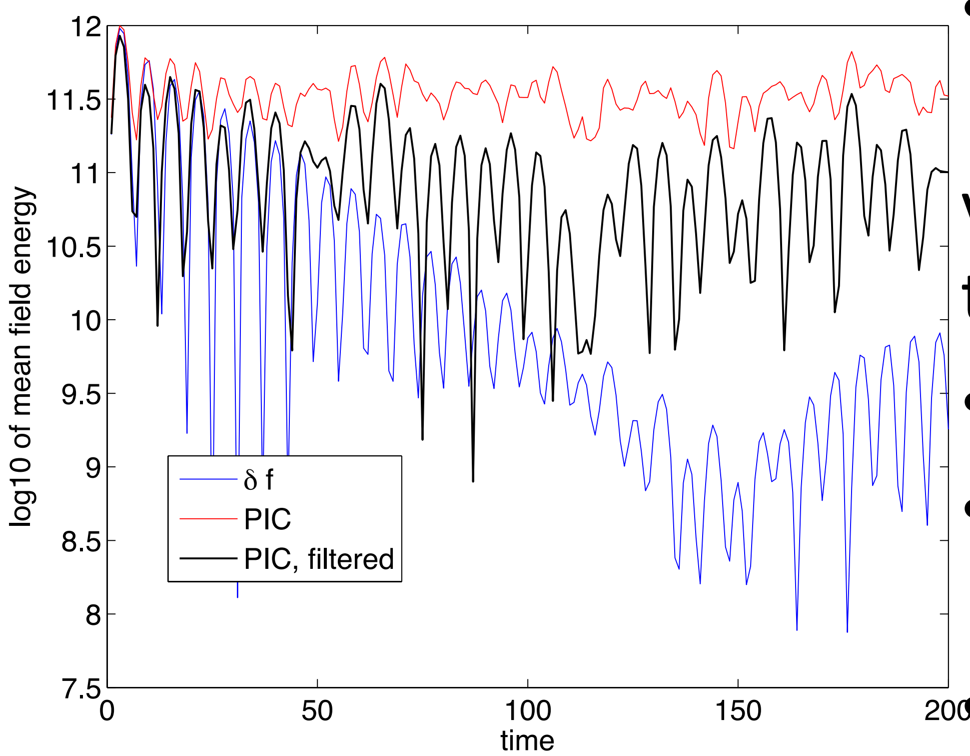


Perturbed distribution function.

Where is sampling important?



Landau damping.



- Initial condition:

  1% sinusouidal variation to velocity of thermal plasma.
- 300 particles per cell
- δf gives clean decay trace.
- Standard PIC needs filtering to see anything.

Conclusions.

- δf PIC used widely in tokamak research.
- Complementary tool to standard PIC simulation.
- Implemented in an EPOCH (Arber, 2015, PPCF) code extension.
- Often very easy to run a δf simulation: change three lines in an EPOCH input file.
- Particularly useful for nearly-linear physics or problems where most particles respond weakly. Waves+beams…
- Needs some real examples.