Clustering of macroparticles in PWFA simulations and solution to this problem

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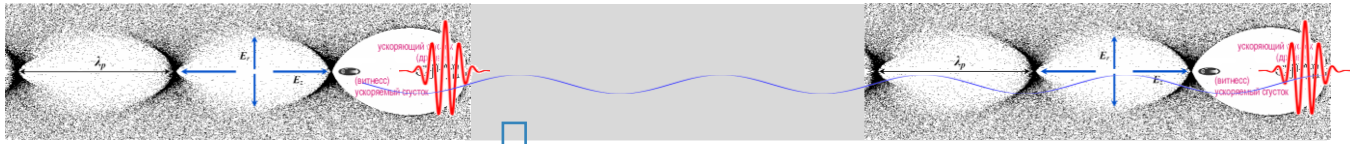
AWAKE Collaboration

Typical problem statements in simulations of plasma wakefield acceleration



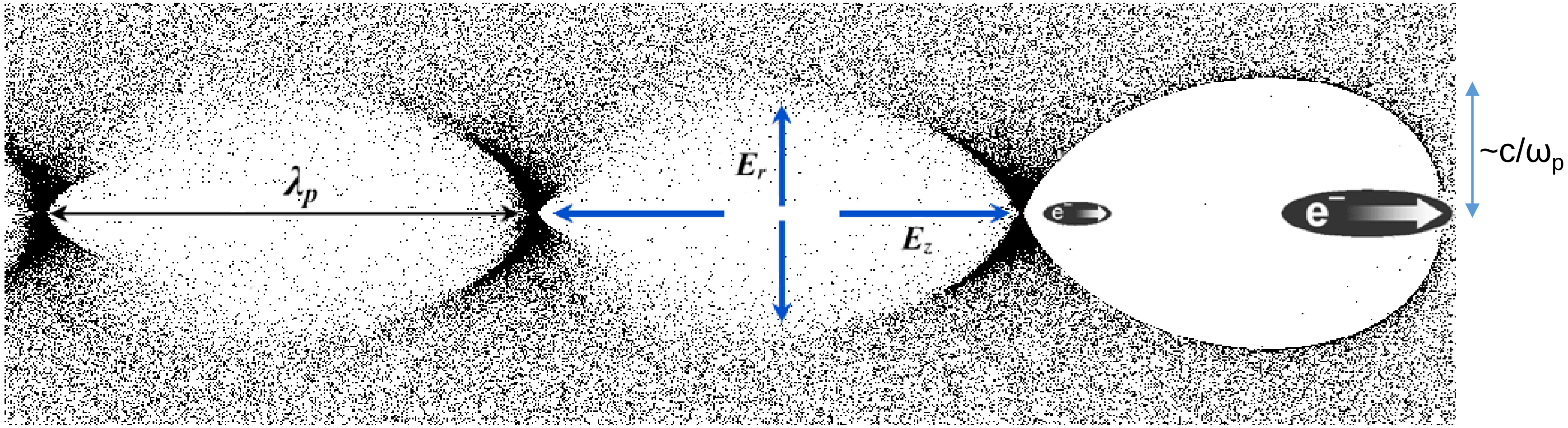
Driver and witness evolution (short beams)

Wakefield evolution

Evolution of long beams (e.g., AWAKE)

We need to simulate the long-term wakefield evolution

Problem: plasma is cold, Debye length is small and cannot be resolved



Electron temperature ~ 5 eV

Electron thermal velocity v_t ~ c/300

Debye length $r_d = v_t/\omega_p \sim (c/\omega_p) / 300$

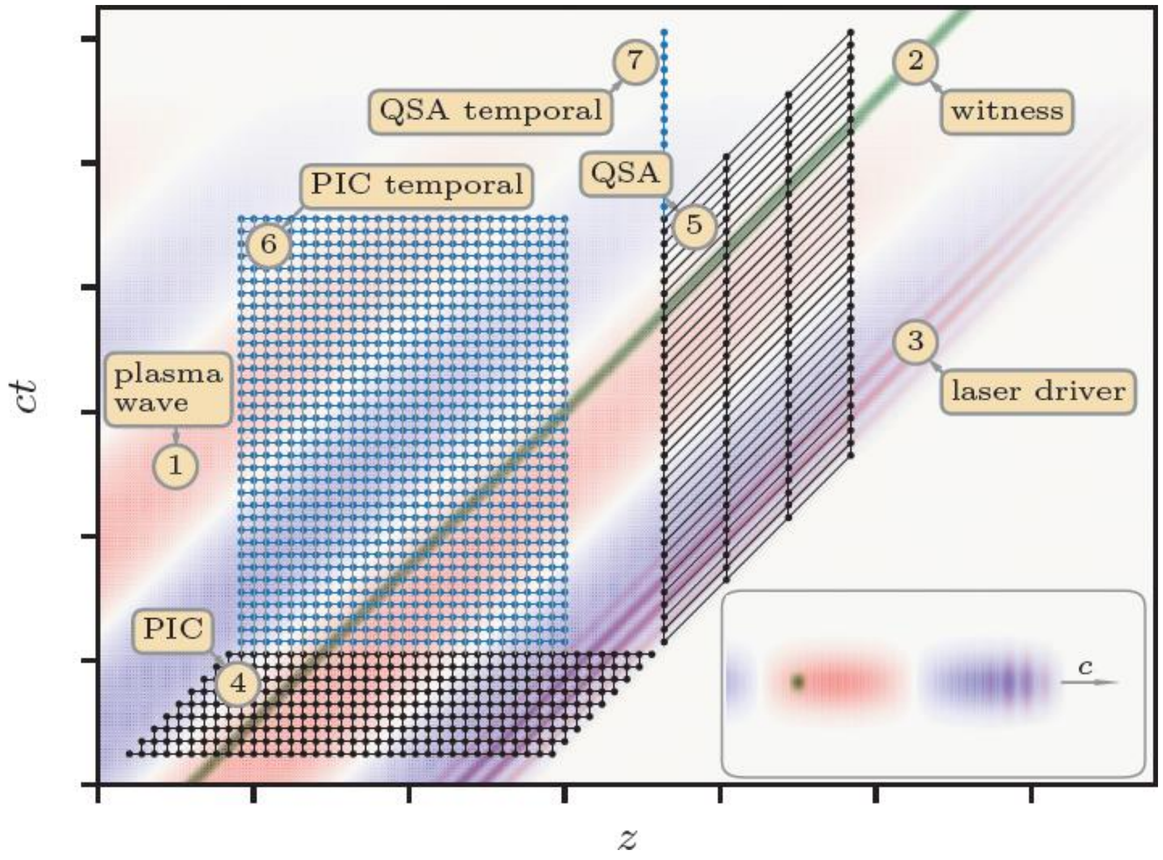
If we resolve r_d, then simulation time increases $300^4 \sim 10^{10}$ times (3d PIC)
or $300^3 \sim 3 \cdot 10^7$ times (3d QSA)

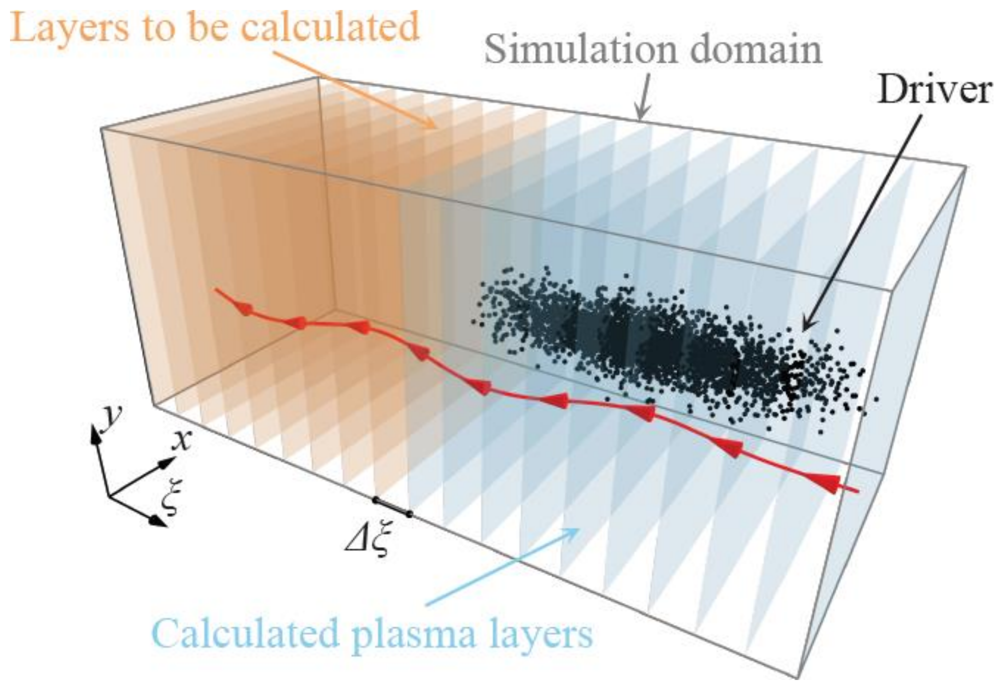
We illustrate the problem and its solutions with quasistatic (QSA) LCODE3D

Based on change of variables $s = z, \qquad \xi = z - ct$

and "diagonal" grid.
We calculate plasma response layer-by-layer
and find fields and particle trajectories as functions of ξ.

+ Speed-up (up to 10^4)
+ Problem dimensionality is reduced by one (when calculating plasma response) because z disappears
+ Efficient modeling of long-term wave evolution
– Limited applicability area





Quasistatic "macroparticle" is a "string" composed of real particles that enter the simulation domain at different times but at the same transverse coordinate and with the same initial momentum

How the problem looks like in QSA code? Test case

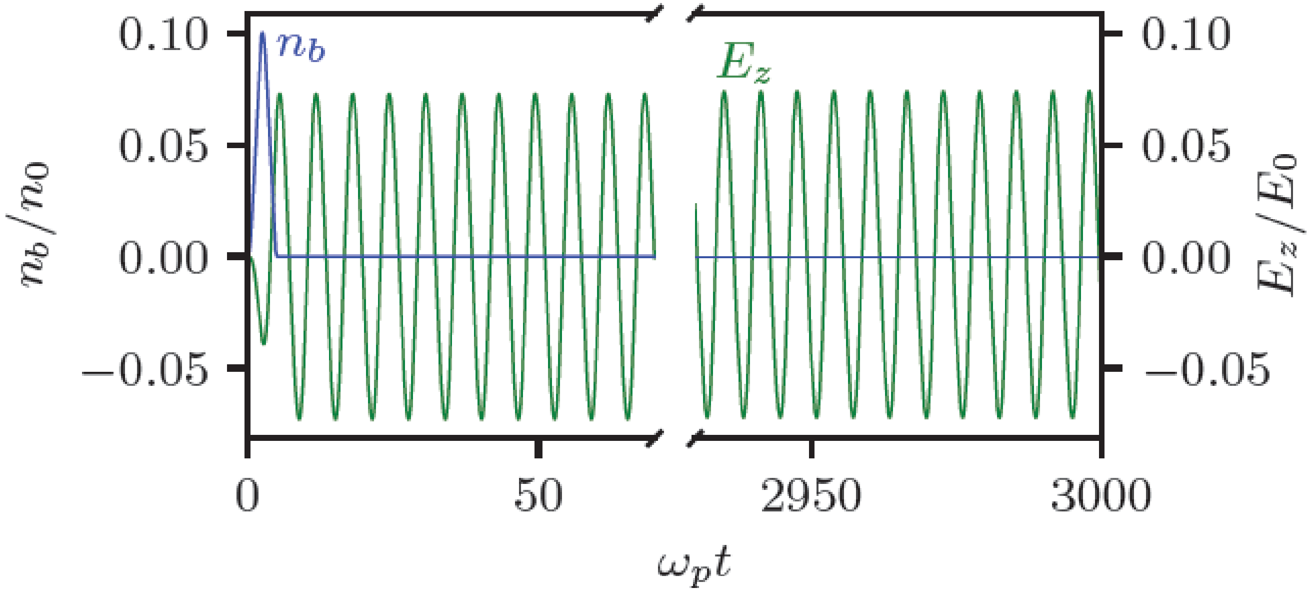
We simulate long-term evolution of a linear wakefield (test1):

$$n_b = \begin{cases} \frac{n_{b0}\, e^{-r^2/(2\sigma_r^2)}}{2}\left[1 - \cos\left(\frac{2\pi\xi}{L}\right)\right], & -L < \xi < 0, \\ 0, & \text{otherwise,} \end{cases}$$

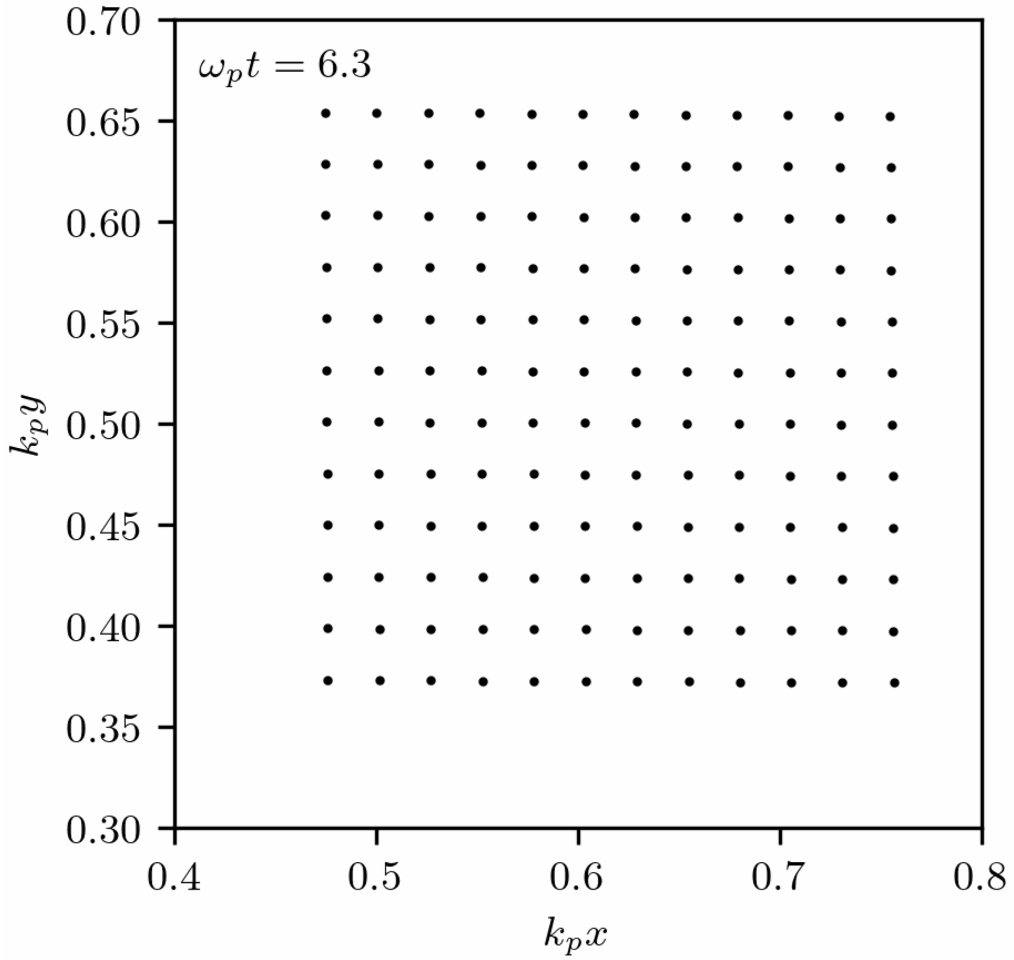
$$n_{b0} = 0.1 n_0, \quad \sigma_r = k_p^{-1}, \quad L = \frac{2\sqrt{2\pi}}{k_p}$$

$h = \Delta\xi = 0.05 k_p^{-1}$ or $h = 0.01 k_p^{-1}, \Delta\xi = 0.005 k_p^{-1}$ (hi-res)

(field damps, but the problem is seen better)

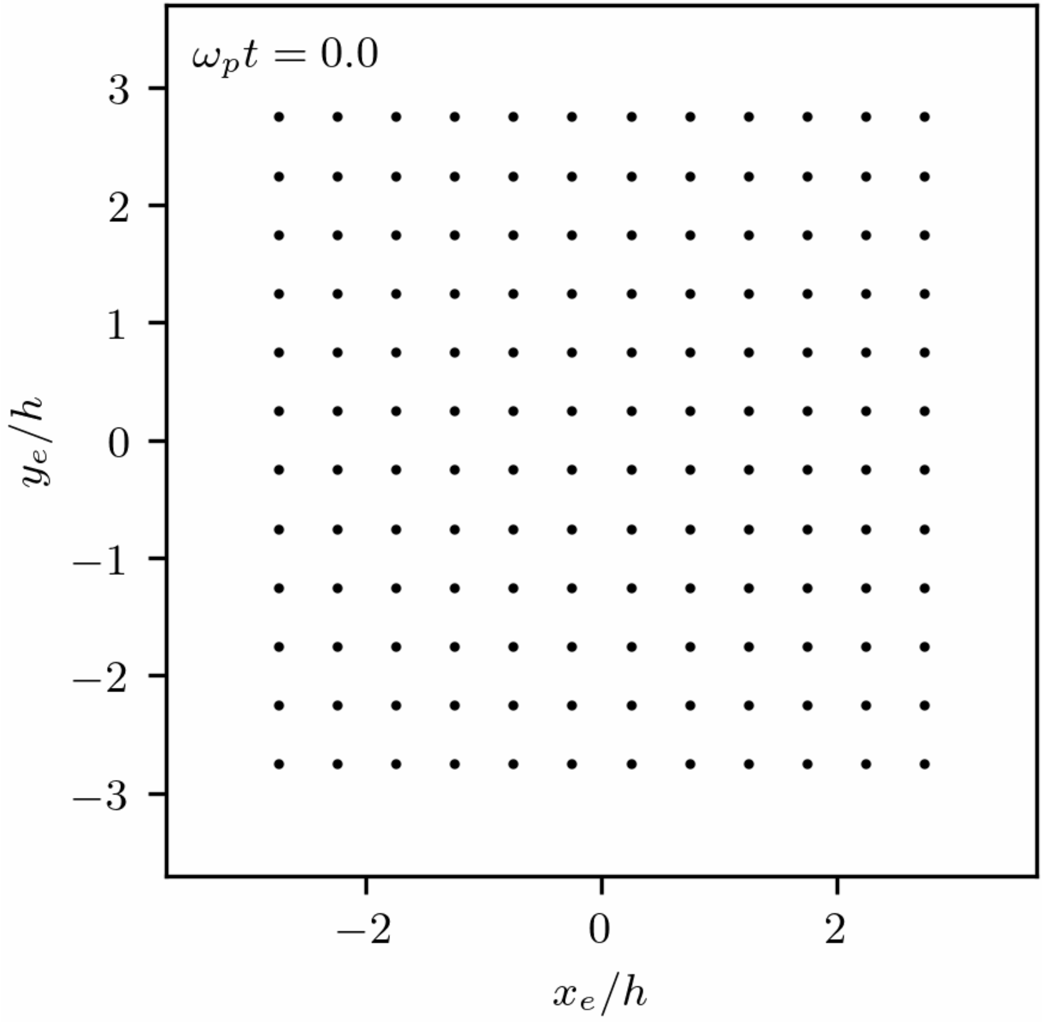


Plasma electrons oscillate in the wave,
it is difficult to see clustering

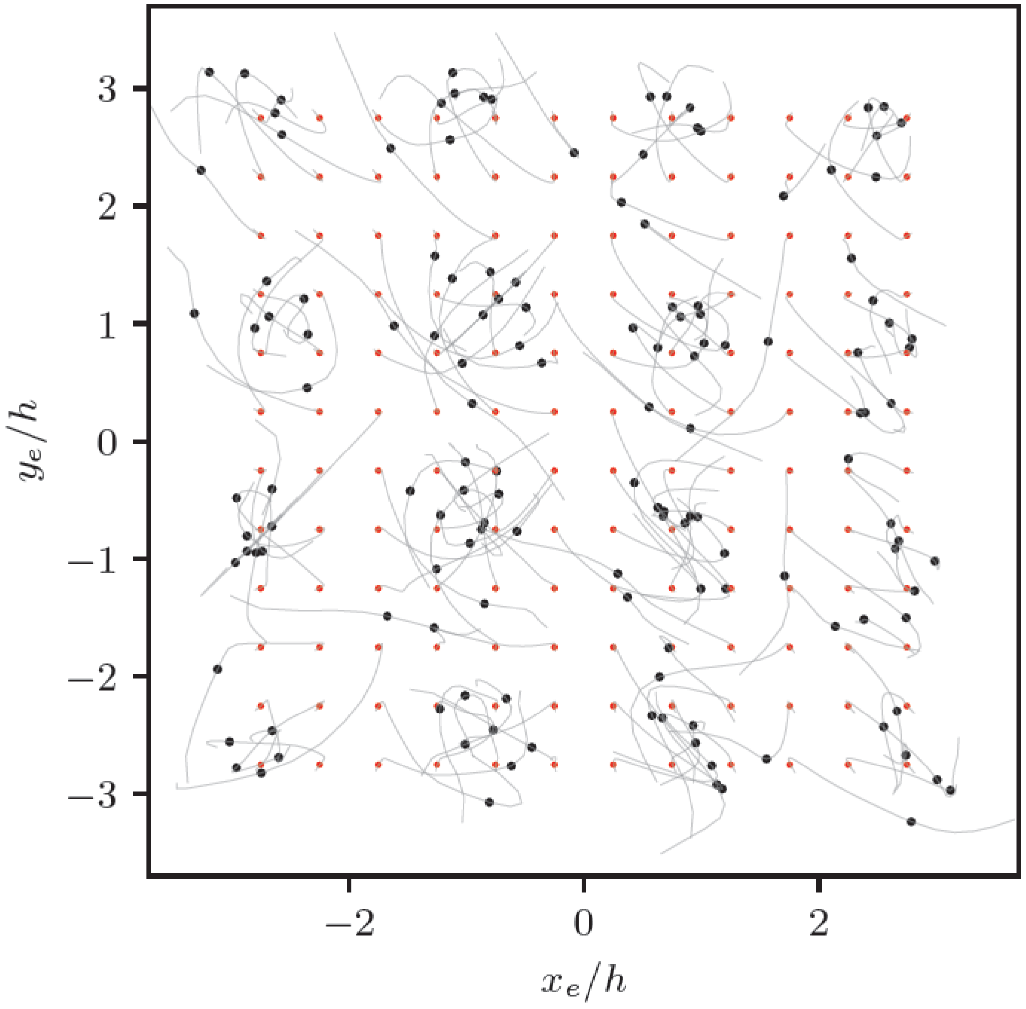


How the problem looks like in QSA code? Clustering and heating

Let us “stop” electron oscillations and look at electron positions with respect to the center of mass of their group:



Red dots are the initial electron locations,
black dots are electron locations at $\omega_p t$=678,
lines are electron trajectories up to time $\omega_p t$=750

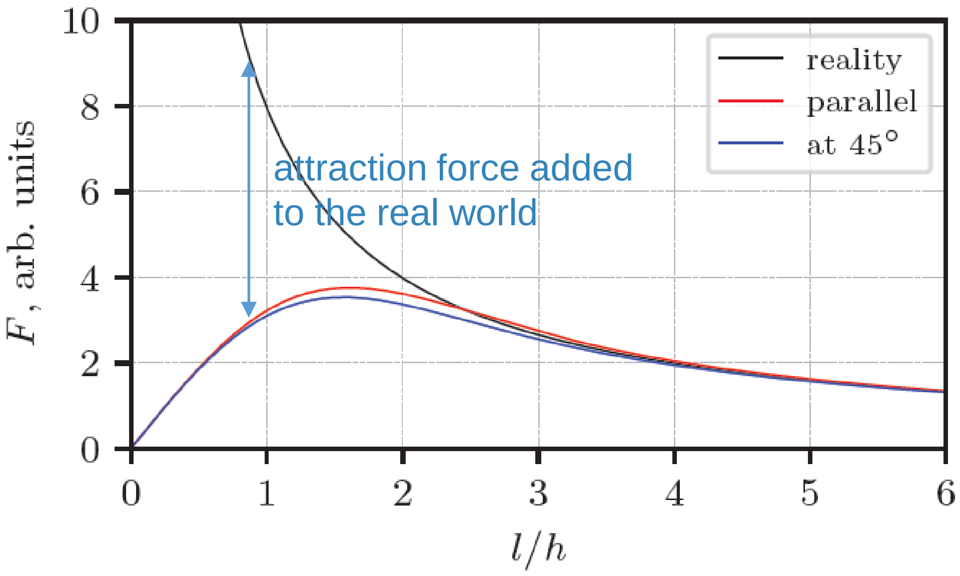


How the problem looks like in QSA code? Cause of clustering

Plasma electrons, while oscillating in the plasma wave, first group together into clusters spaced two grid steps (2h) apart.
Then the electrons continue moving relative to each other and acquire transverse momentum (are heated).

The reason:
Interaction of closely spaced plasma particles is simulated incorrectly, as if there is an additional short-range attraction force between the real electrons.

Real and simulated force between two electrons,
if the line between electrons is parallel or at the angle of 45º to the grid:



Red dots are the initial electron locations,
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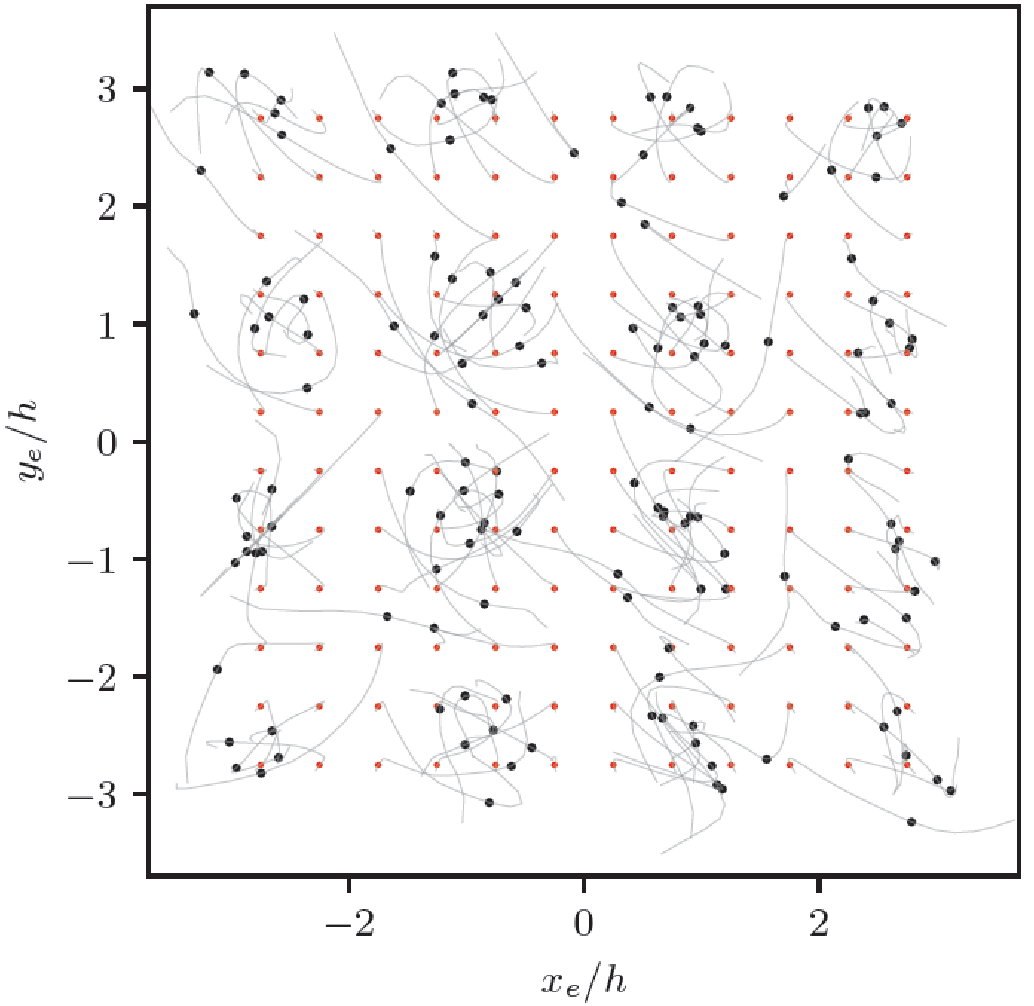
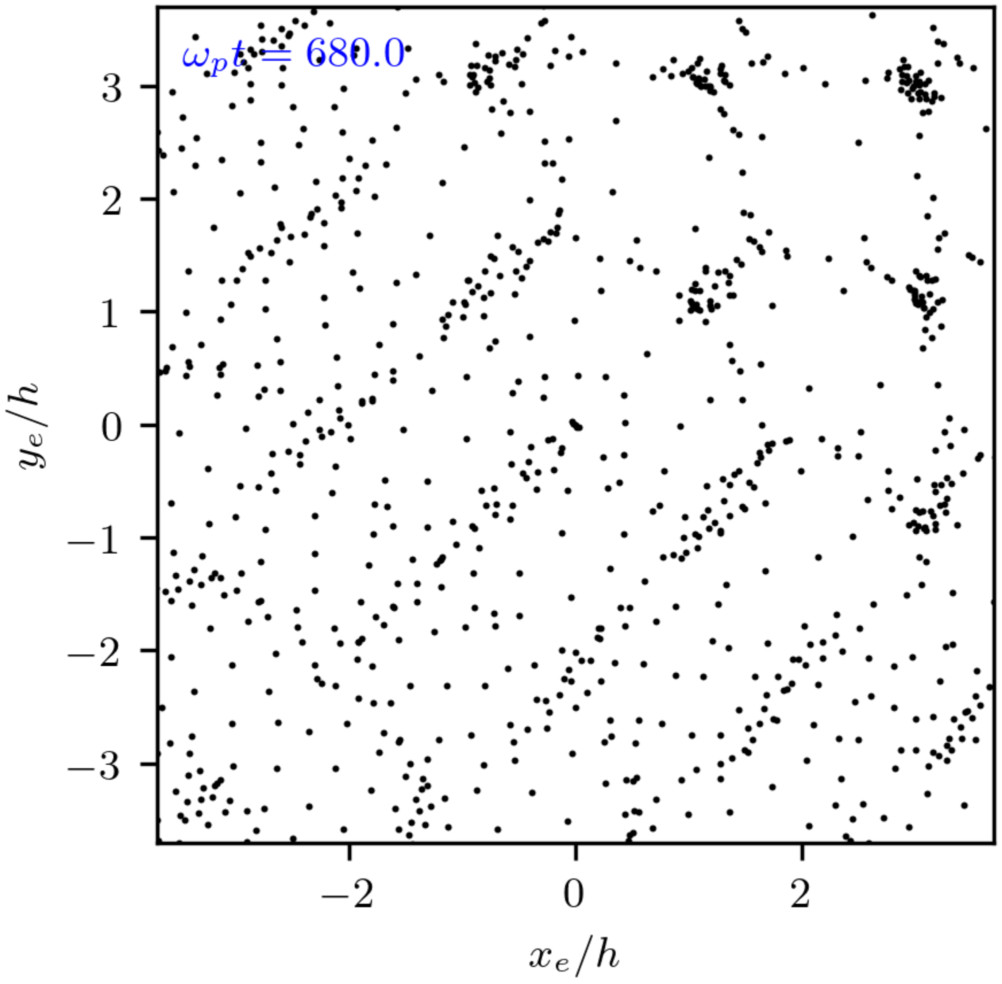
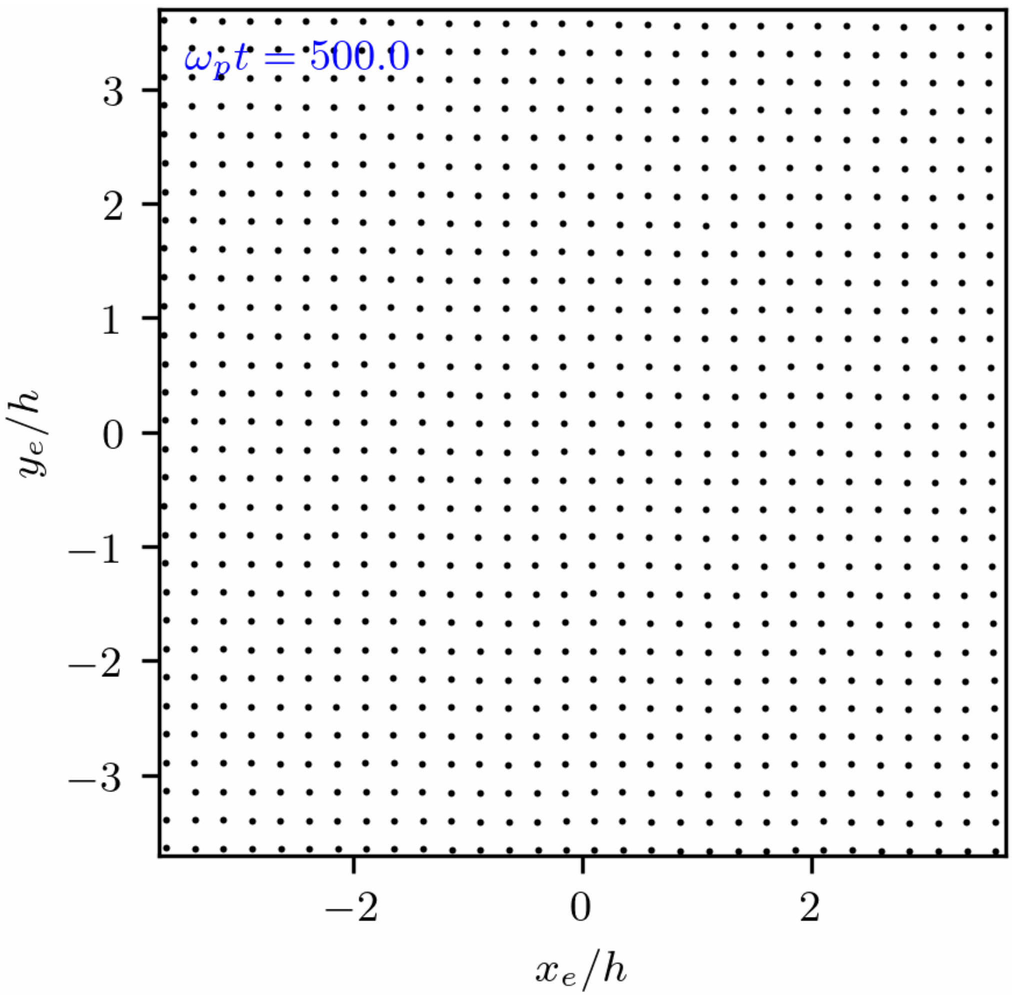


How the problem looks like in QSA code? Variety of clustering

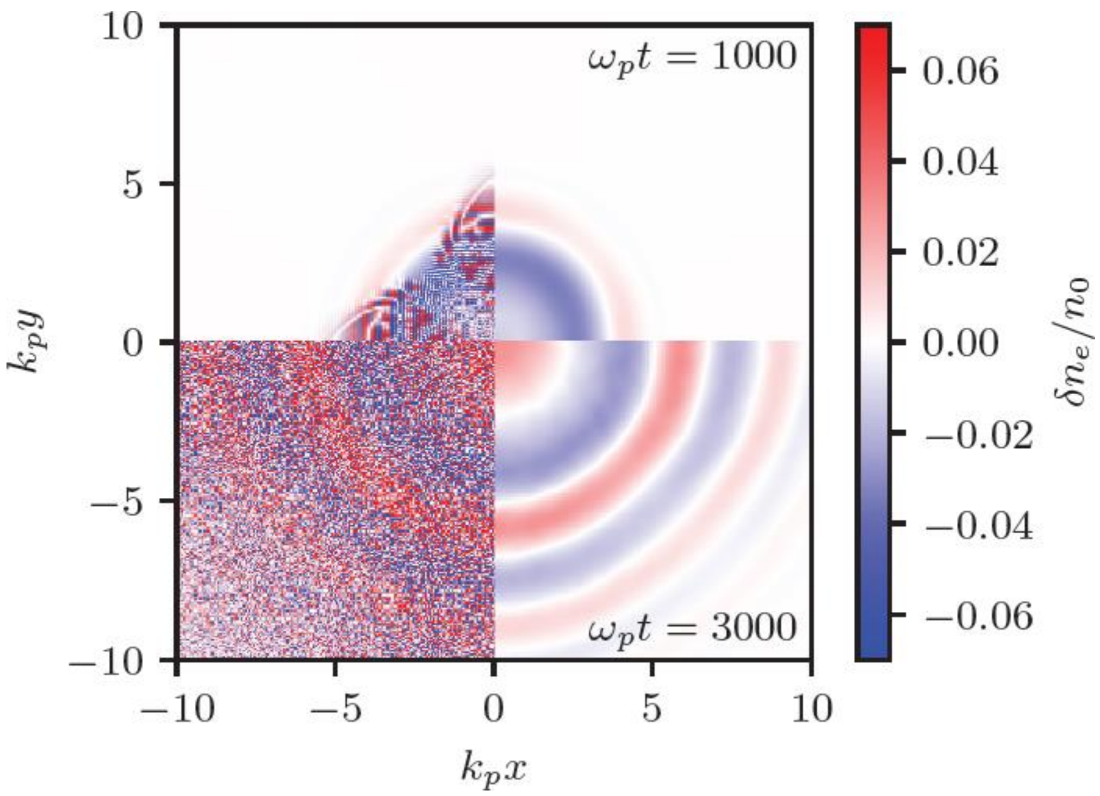
At other simulation parameters, for example, diagonal structures may appear:





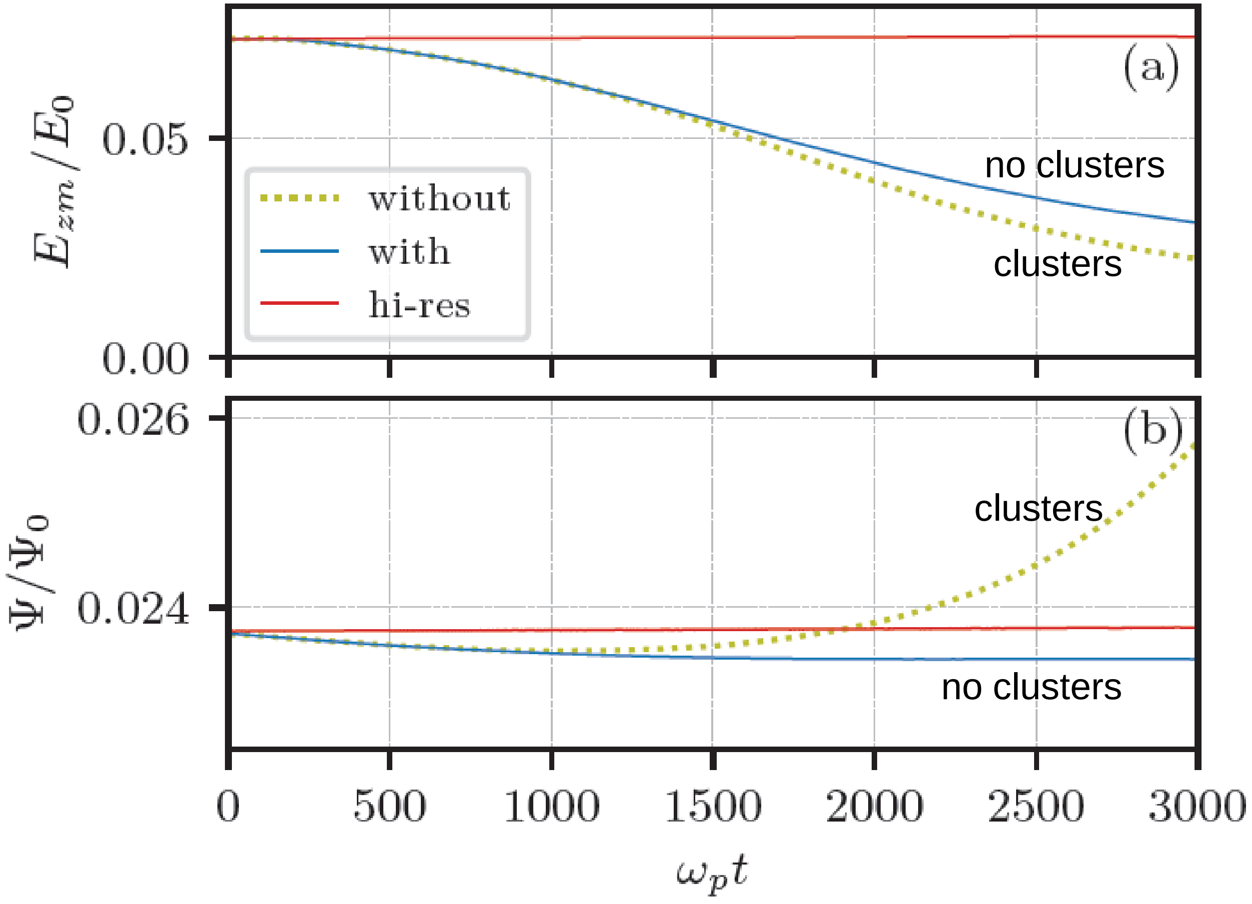
How the problem looks like in QSA code? Plasma electron density

The clusters make the plasma density distribution “noisy”:



However, when averaged over multiple cells, the density becomes regular and smooth

How the problem looks like in QSA code? Fields and energies



(looking ahead, there are already variants with declustering here)

Clustering reduces the amplitude of the wave and (to a lesser extent) increases the energy of the system.

$$\Psi(\xi) = \int \left(\frac{E^2 + B^2}{2} - \left[\vec{E} \times \vec{B} \right]_z \right) dS + \sum_j (\gamma_j - 1)(1 - v_{jz}) M_j,$$

dimensionless energy flux in the comoving window, measure of accuracy

$$\Psi_0 = \frac{m^2 c^5}{4\pi e^2} \approx 2c \, \frac{\mathrm{J}}{\mathrm{m}}$$

How to detect clustering early in its development?

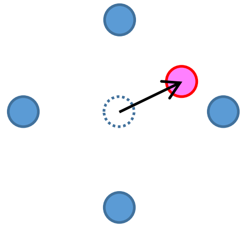
Particle displacements relative to their initial positions:

$$\mathbf{d} = \mathbf{r}_\perp - \mathbf{r}_{0\perp}$$

It is dominated by the particle motion in the plasma wave

Displacement inhomogeneity with respect to neighboring particles:

$$\mathbf{g}_{i,j} = \mathbf{d}_{i,j} - \frac{\mathbf{d}_{i+1,j} + \mathbf{d}_{i-1,j} + \mathbf{d}_{i,j+1} + \mathbf{d}_{i,j-1}}{4}$$



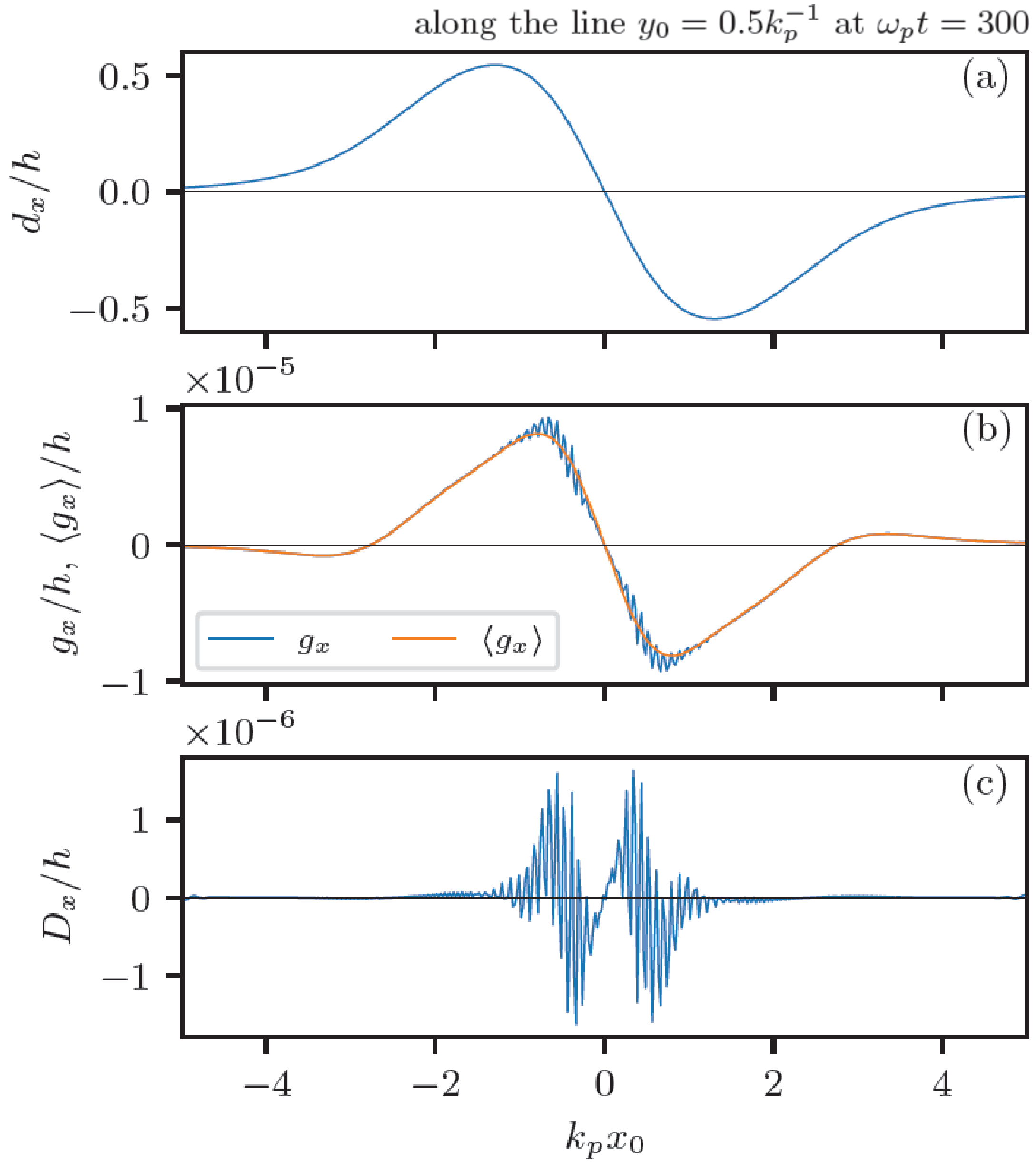
It is still dominated by the plasma wave.

Average and subtract the average: “noise” part of the displacement

$$\mathbf{D} = \mathbf{g} - \langle \mathbf{g} \rangle$$

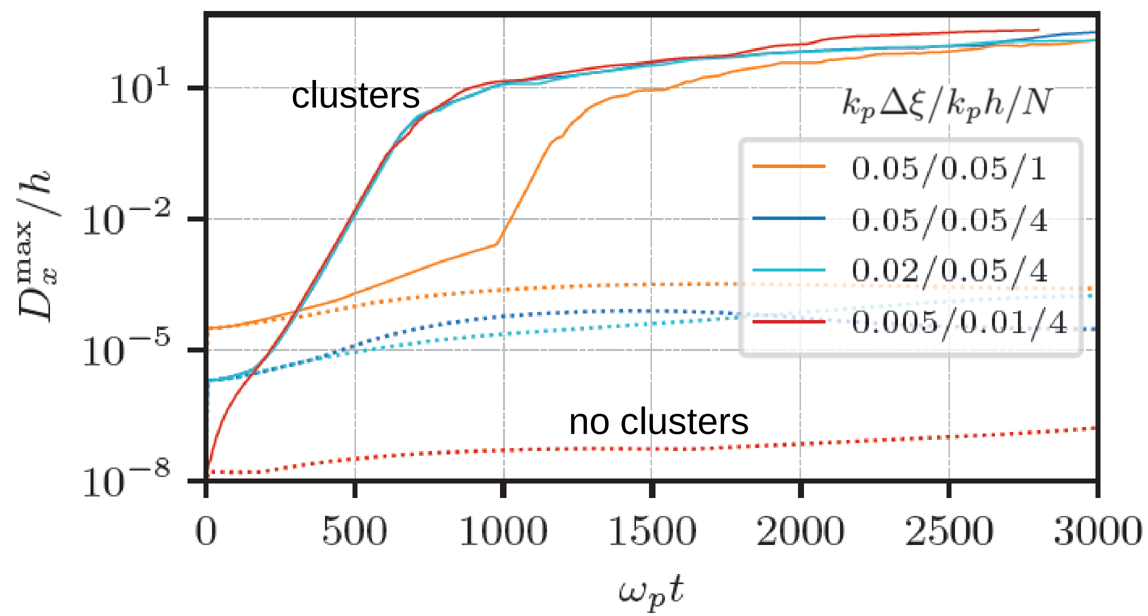
Now we see the displacements leading to clustering

$D_x^{\max}$ – measure of clustering, the maximum noise displacement

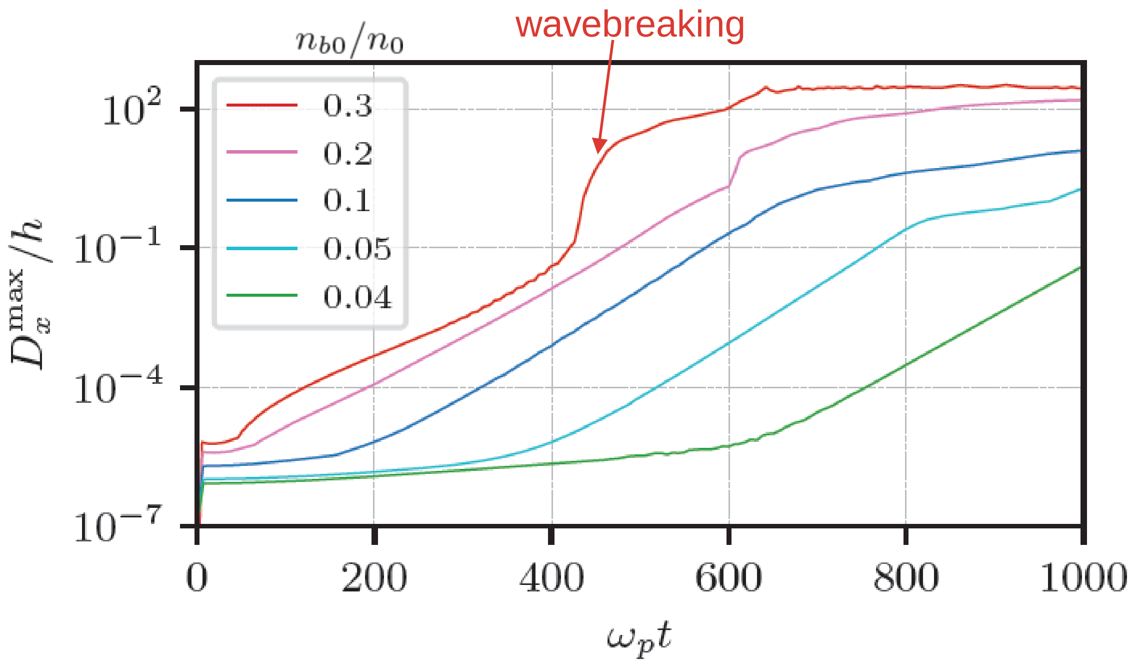


How does clustering grow?

For different simulation parameters (dotted lines – with declustering)



For different wave amplitudes (controlled by varying the driver density)



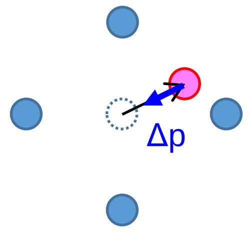
- Grows exponentially (instability)
- The growth rate is independent of grid size and number of electrons per cell N and weakly dependent on the wave amplitude
- The moment (level) of instability onset depends sharply on the parameters of the wave, there is no clustering without the wave
- Typically, the detection level of clustering and the level of transition to the nonlinear regime (when clusters have formed) differ by many orders of magnitude

Declustering

Let us modify the equation of particle motion. We introduce an additional force, i.e. at each ξ-step we push the particle in the direction of decreasing the "noise" displacement:

$$\Delta \mathbf{p}_{i,j} = -K\Delta\xi \left[F_{i,j}\mathbf{D}_{i,j} - \frac{F_{i+1,j}\mathbf{D}_{i+1,j} + F_{i-1,j}\mathbf{D}_{i-1,j}}{4} - \frac{F_{i,j+1}\mathbf{D}_{i,j+1} + F_{i,j-1}\mathbf{D}_{i,j-1}}{4} \right] - \kappa\Delta\xi F_{i,j}\left[\mathbf{D}_{i,j} - \mathbf{D}^{\mathrm{prev}}_{i,j}\right],$$

$$F_{i,j} = \begin{cases} 1 - |\mathbf{D}_{i,j}|^2/D_0^2, & |\mathbf{D}_{i,j}| < D_0, \\ 0, & \text{otherwise}, \end{cases}$$



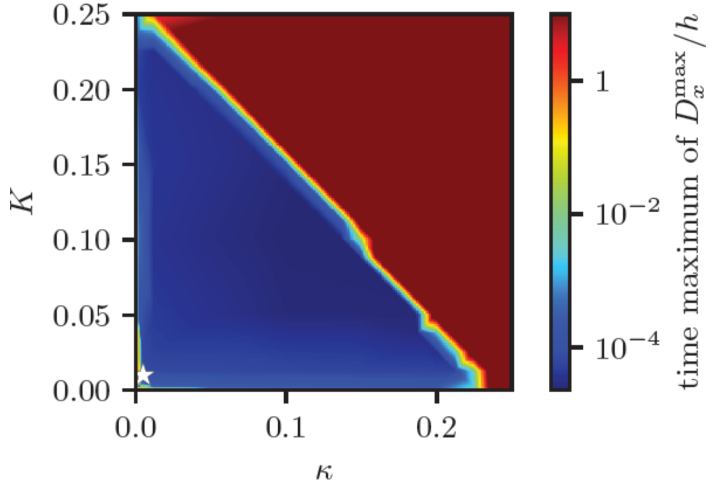
$\mathbf{D}_{i,j}$ is the noise displacement of particle numbered (*i, j*), $\mathbf{D}^{\mathrm{prev}}_{i,j}$ is it at the previous step in ξ

K characterizes the restoring force. We assume that the restoring force is exerted by nearby particles. The fractional terms are responsible for the counterforce (our particle helps neighboring particles to get back in place).

κ controls damping. The restoring force alone cannot suppress the noise, since it is non-dissipative. It forces noise perturbations to propagate with some group velocity. We need dissipation.

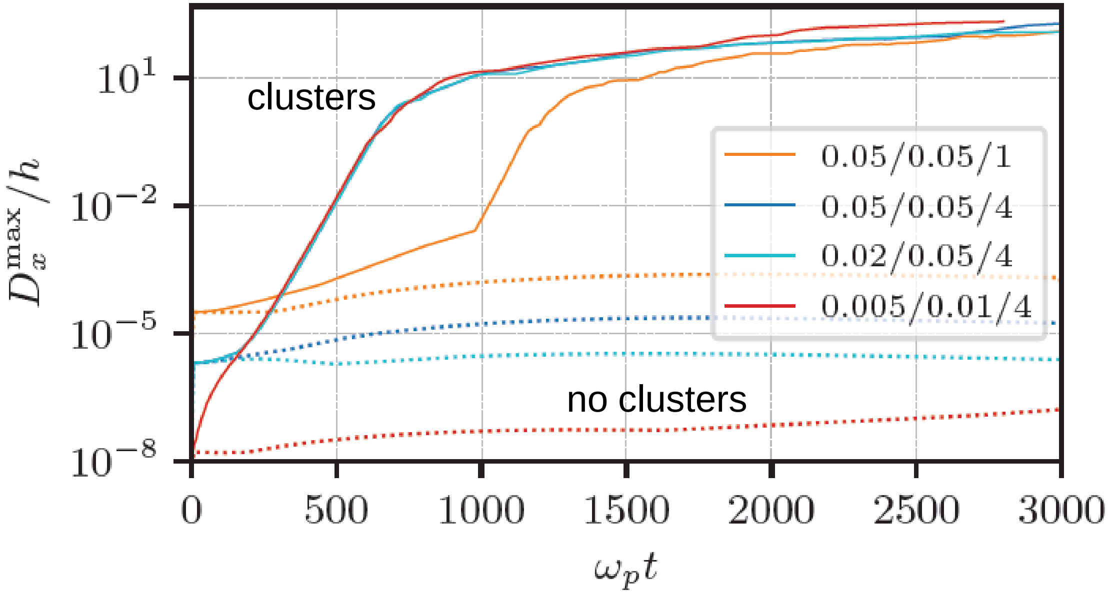
D_0 limits the declustering range. It smoothly reduces the force to zero if the displacement is large (the wave breaks). Is about 10^{-3}h. If the wave breaks, noise displacement of some particles quickly increases, and the force switches off for these particles.

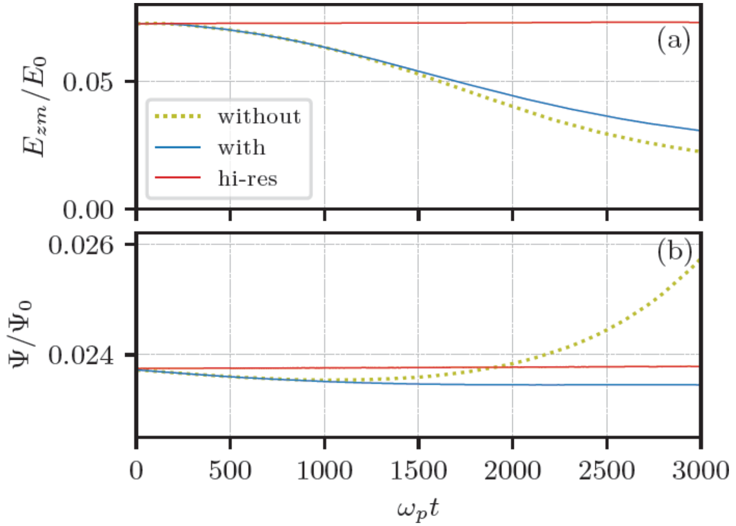
Stability condition: $K + \kappa < \dfrac{h^2}{\Delta\xi^2 N}$



Optimal values of coefficients depend on the problem being solved.

Results of declustering (test problem)





"Noise" does not develop.
Noise displacements remain below 10^{-4}h,
on-axis field is stronger,
the wave energy does not grow,
simulation results change (in some cases).

Declustering in 2d

The declustering implemented in 2d version of LCODE is less efficient than the one described above, but it helped to simulate long wakes for decades, so it deserves one slide.

Suppose that the plasma electron density has a short-scale modulation:

$$\delta n = -A_j \cos(k_h \delta r), \qquad k_h = \pi/h,$$

We can find the modulation amplitude in the vicinity of this node from the density in neighboring nodes:

$$A_j \approx (n_{e,j+1} + n_{e,j-1} - 2n_{e,j})/4.$$

There should appear a radial electric field directed so as to reduce the density perturbations:

$$\frac{1}{r}\frac{\partial}{\partial r} r\delta E_r = 4\pi e A_j \cos(k_h \delta r).$$

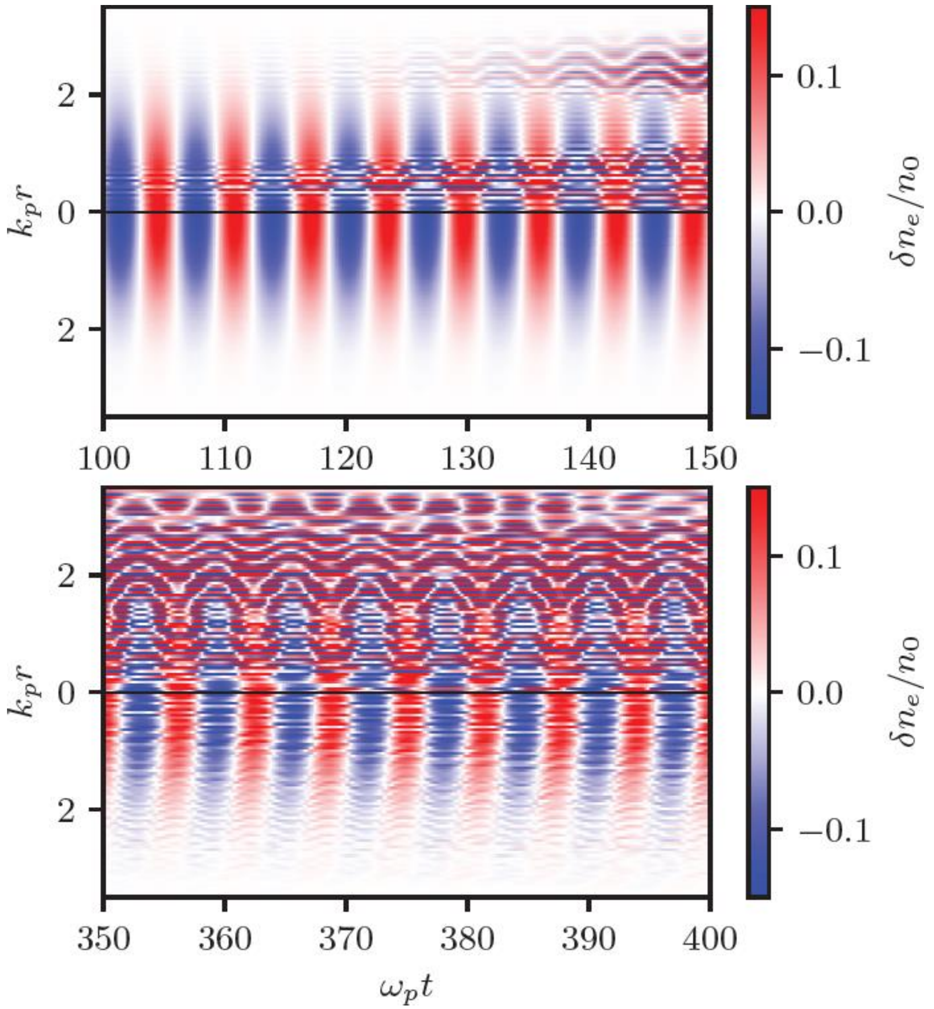
The field amplitude is (so complicated because of cylindrical geometry):

$$\delta E_r = \frac{4\pi^2 e A_j h}{\pi^2 + 1/j^2} \sin(k_h \delta r) + \frac{4\pi e A_j h}{j\pi^2 + 1/j} \cos(k_h \delta r).$$

We cannot resolve this field on a grid, so we add an extra electric force $(-e\delta E_r)$ exerted on particles.

This declustering damps only the fastest instability mode. Other modes still develop (slower). But this is better than nothing.

without / with declustering



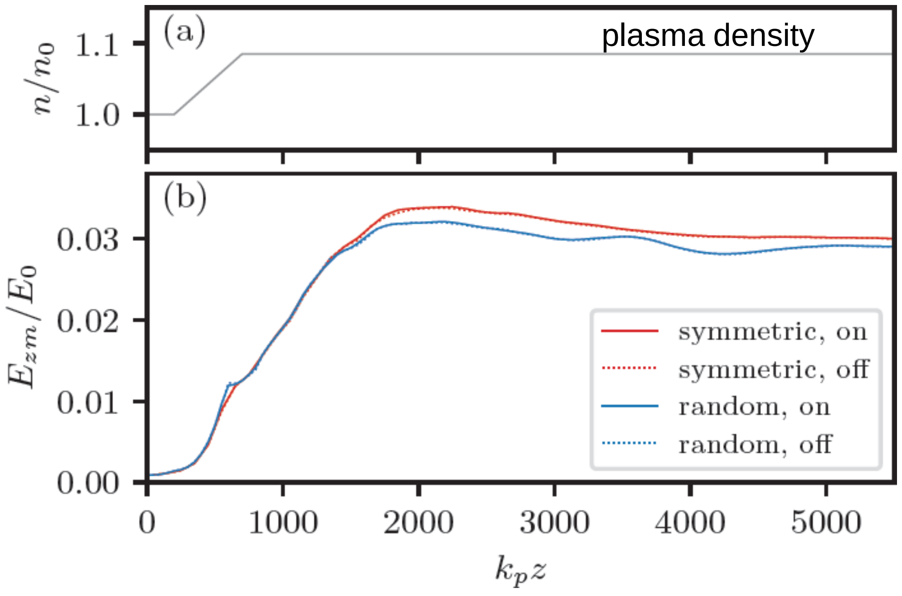
Example where declustering changes the result: self-modulation of a long beam

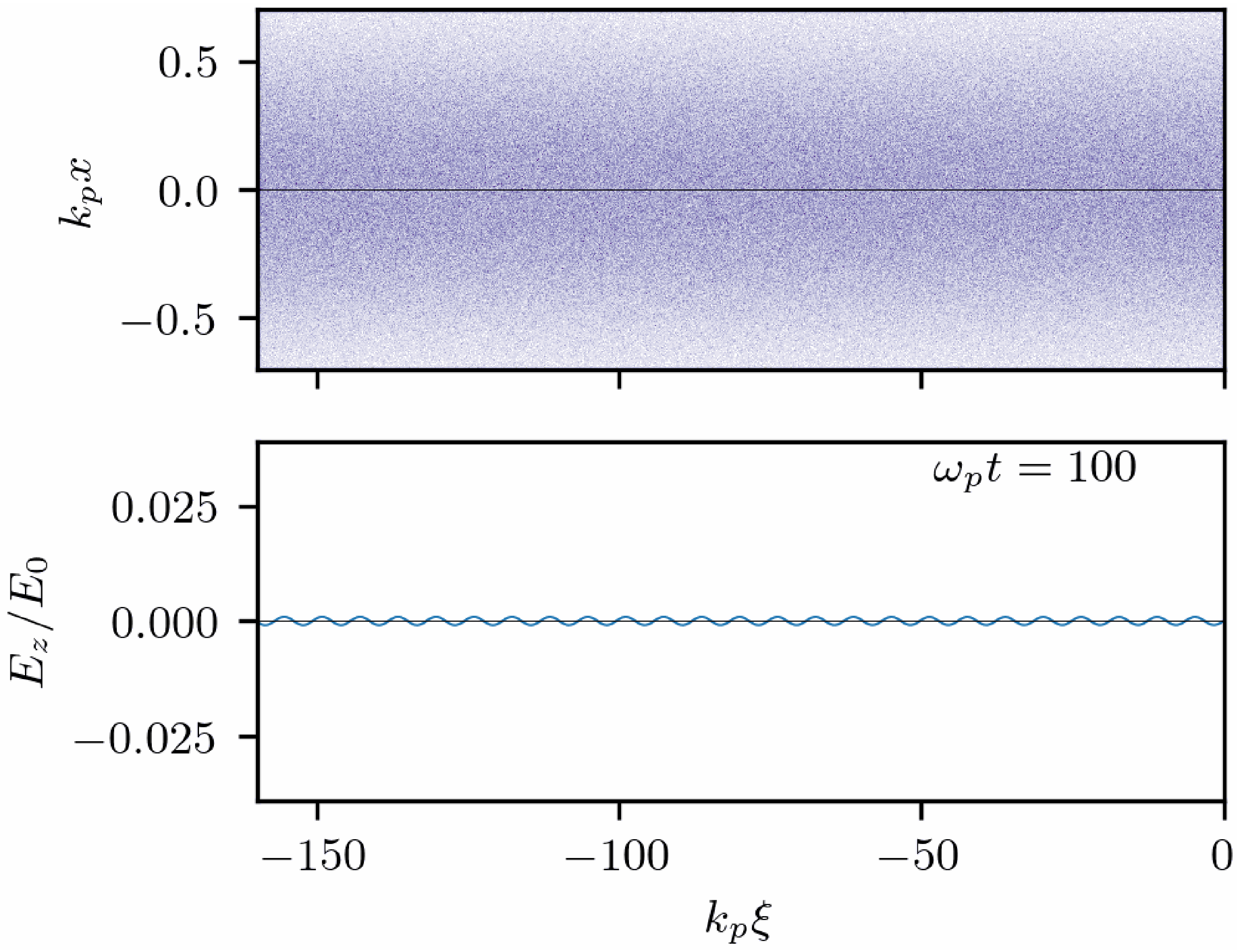
A long beam with a sharp leading edge breaks into microbunches in the plasma

$$n_b = \begin{cases} n_{b0}\, e^{-r^2/(2\sigma_r^2)}, & \xi < 0, \\ 0, & \xi \geq 0, \end{cases}$$

$$n_{b0} = 4 \times 10^{-3} n_0, \qquad \sigma_r = 0.5 k_p^{-1}$$

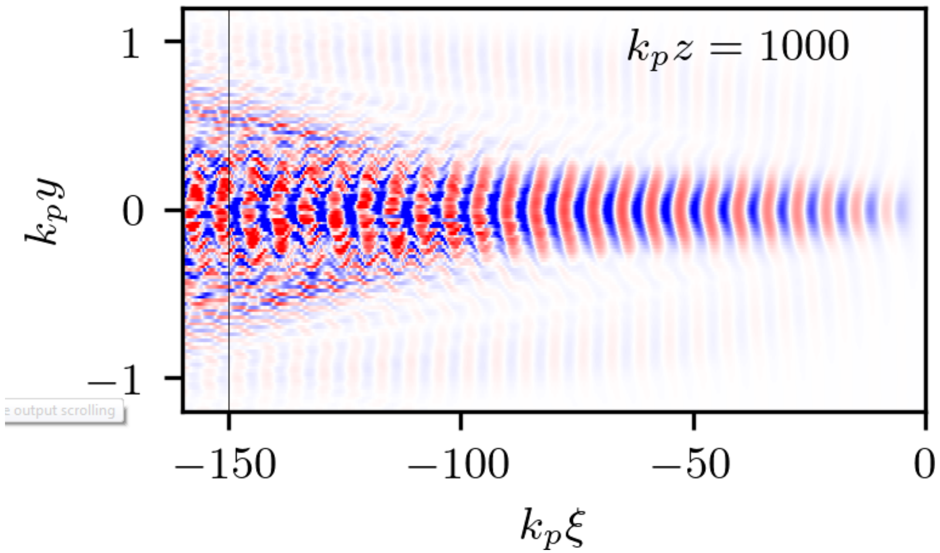
The wakefield grows and remains at a high level.
It does not depend on (de)clustering.

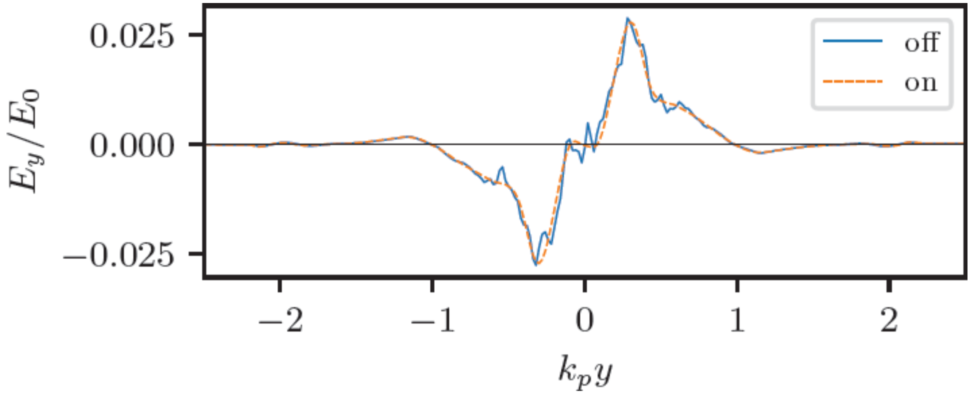


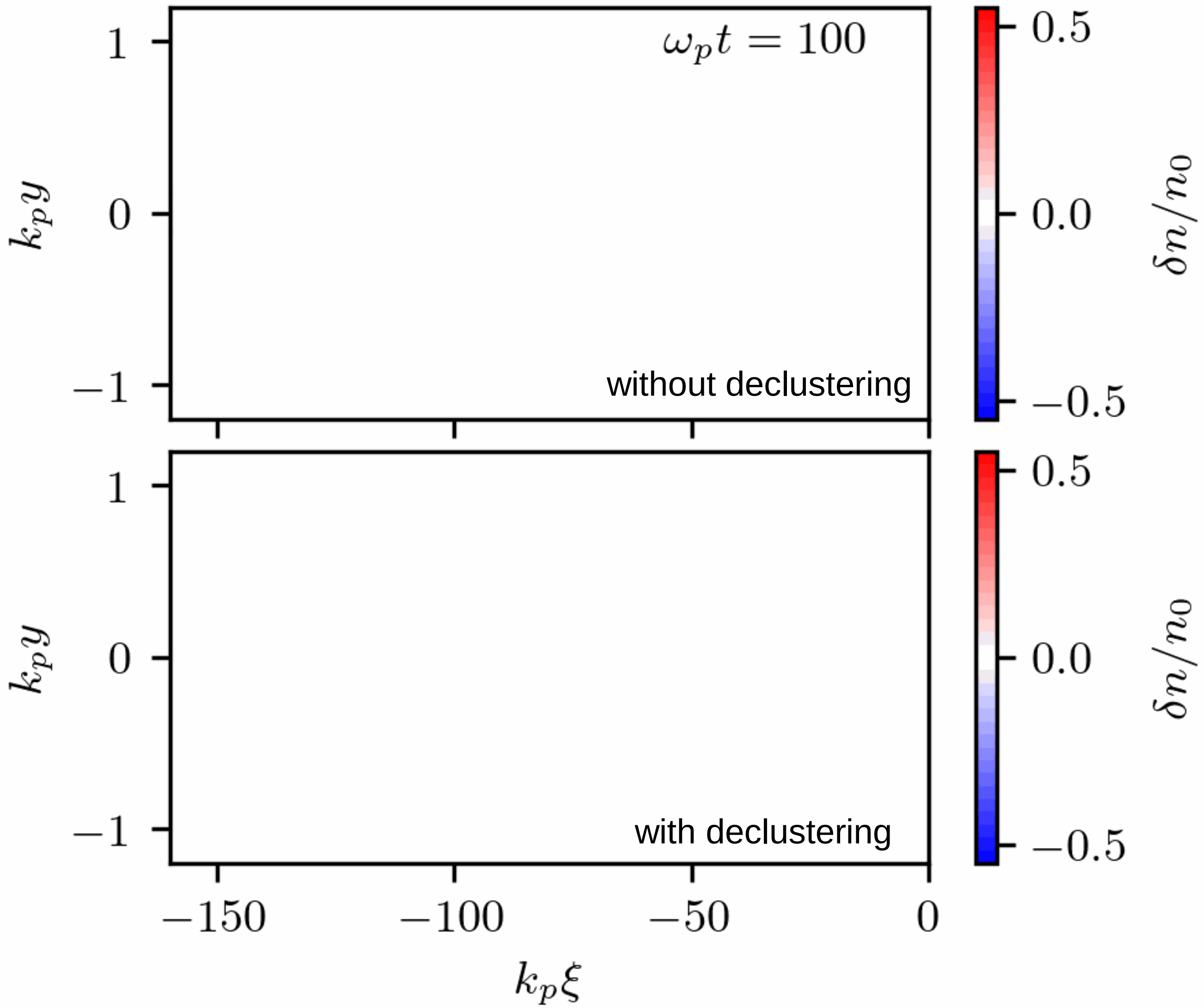


Example where declustering changes the result: self-modulation of a long beam

Clustering affects the electron density profile and the transverse fields. Transverse field noise is generated, which can spoil the emittance of the accelerated beam.







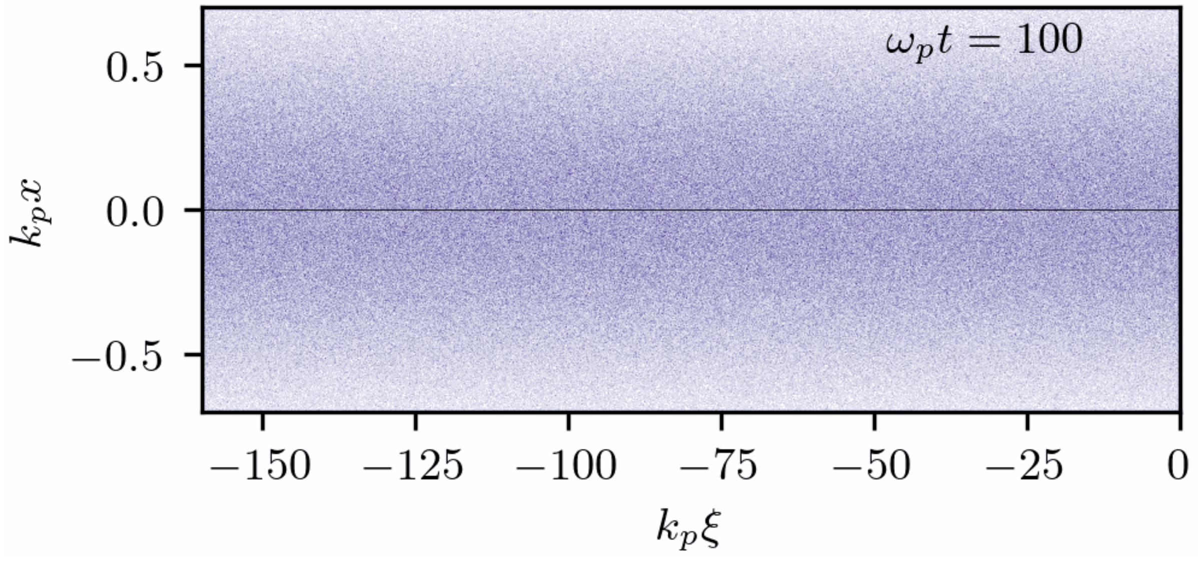
Example where declustering gives confidence in the result: long-wavelength hosing

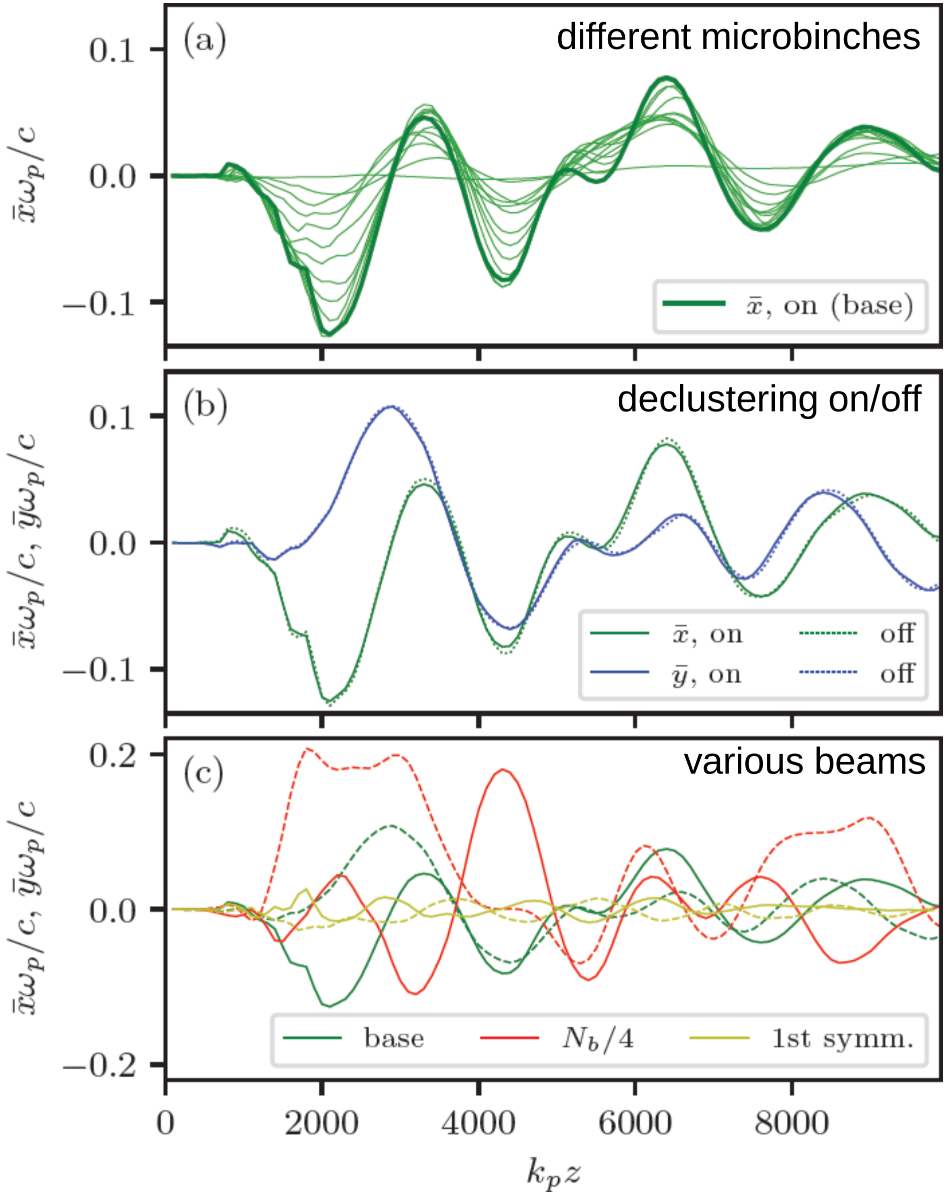
Let us trace transverse displacements of microbunches (centers of mass), and especially of the last one (thick line). We are sure that they are not due to clustering.

Long-wavelength hosing is an instability. It amplifies the displacements along the bunch train: later microbunches are displaced in the same direction as earlier microbunches, but to a greater extent.

Growth of displacements saturates. Starting from some microbunch, the displacement does not increase.

Characteristic time is of the order of the betatron period in the unbunched beam (growth rate is about SSM or usual hosing growth rate). Leading part of the beam plays a dominant role in long-wavelength hosing (it oscillates with this period).





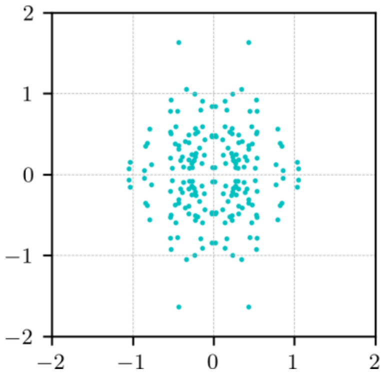
Example where declustering gives confidence in the result: long-wavelength hosing

When the wave has grown, the later microbunches simply copy the oscillations of the previous ones (their betatron frequency is already incomparably larger).

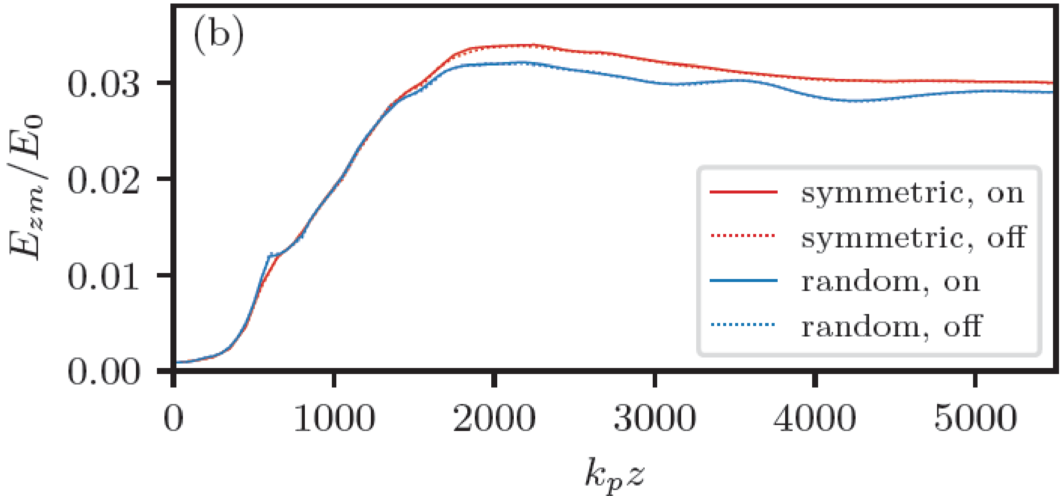
Does not depend on (de)clustering.

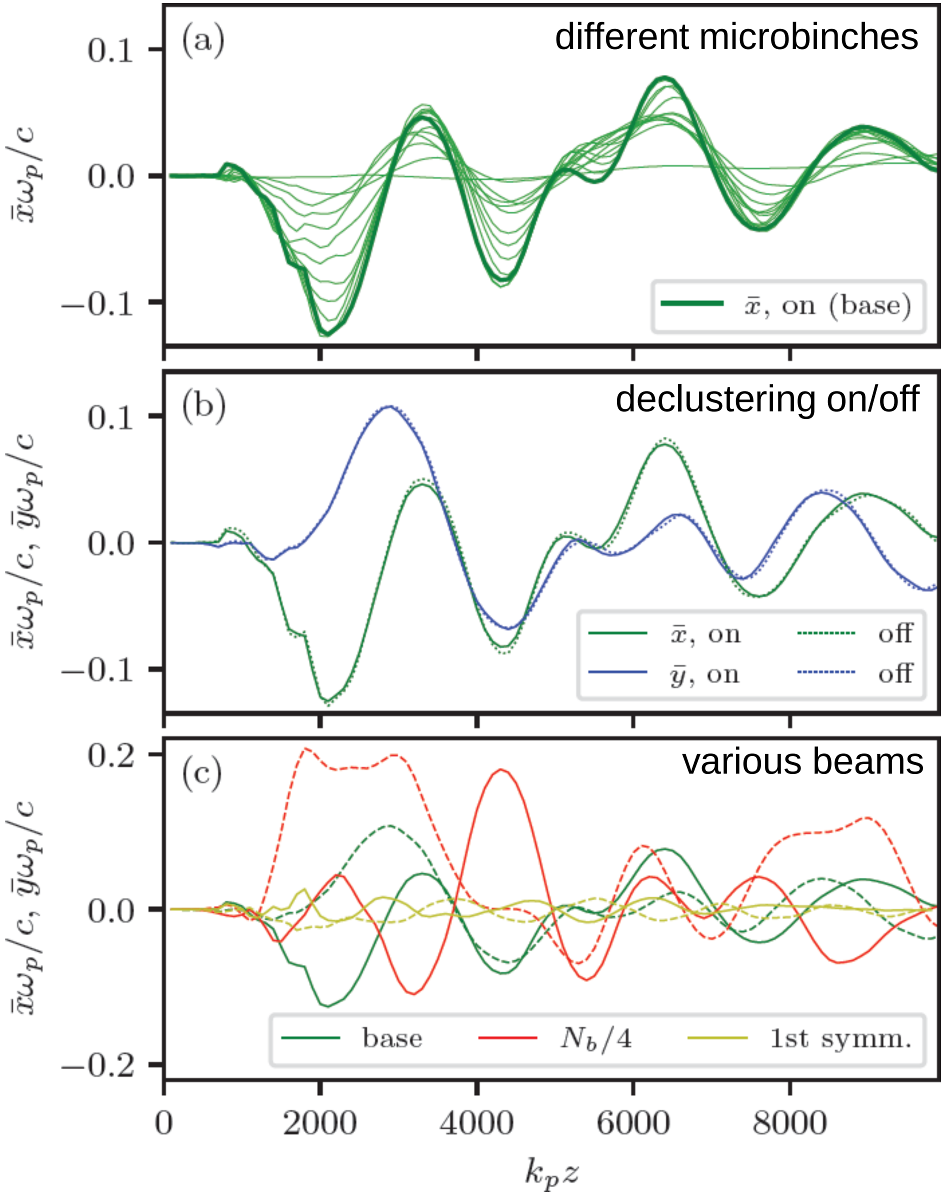
If we decrease the number of macroparticles in the beam, the amplitude increases. Hosing is caused by statistical fluctuations in the first microbunches.

Symmetric particle distribution in the first microbunch: hosing amplitude decreases. Symmetric particle distribution in the beam: no hosing.



In reality, the effect can be weaker (more real particles), or stronger (distorted beam).





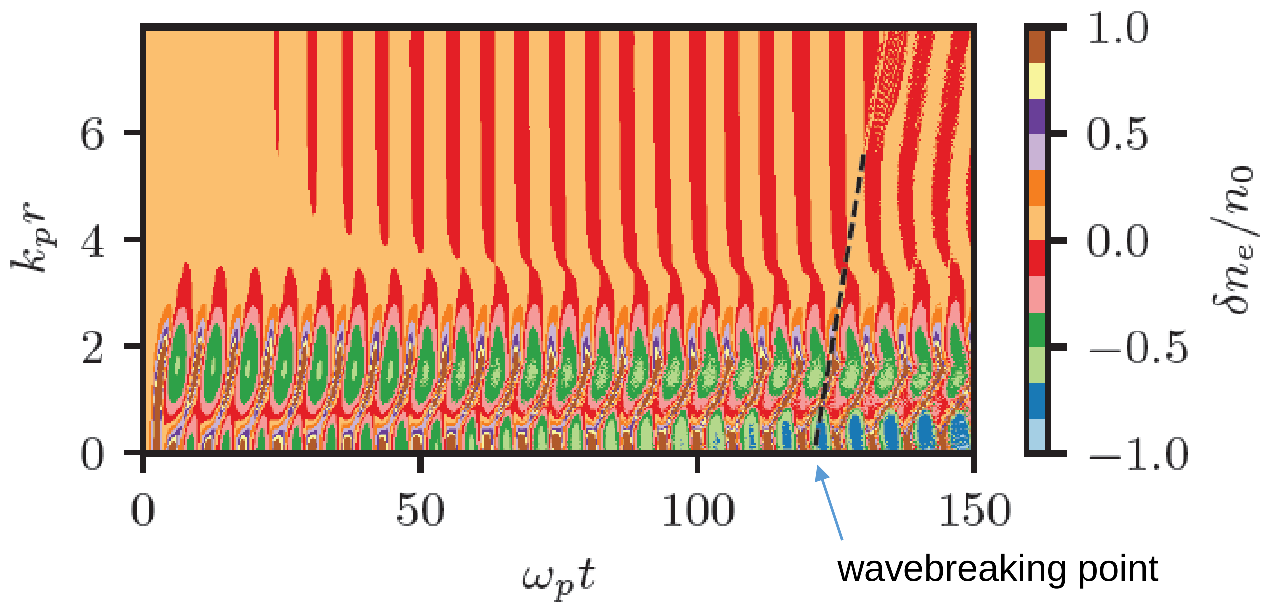
Example where declustering changes the result: transverse wavebreaking

It is an event in which the trajectories of plasma electrons, initially at different radii, intersect, causing one or both electrons to drop out of collective motion in the wave. The wave continues to exist.
TW can lead to electron trapping by the plasma wave, wave dissipation, appearance of radially ejected electrons, and even field growth.

Almost the same test1 variant but $n_{b0} = 2n_0$ $K = 0.3,\ \kappa = 0.1,\ D_0 = 10^{-3}$

$$n_b = \begin{cases} \dfrac{n_{b0}\, e^{-r^2/(2\sigma_r^2)}}{2} \left[1 - \cos\left(\dfrac{2\pi\xi}{L}\right)\right], & -L < \xi < 0, \\ 0, & \text{otherwise,} \end{cases}$$

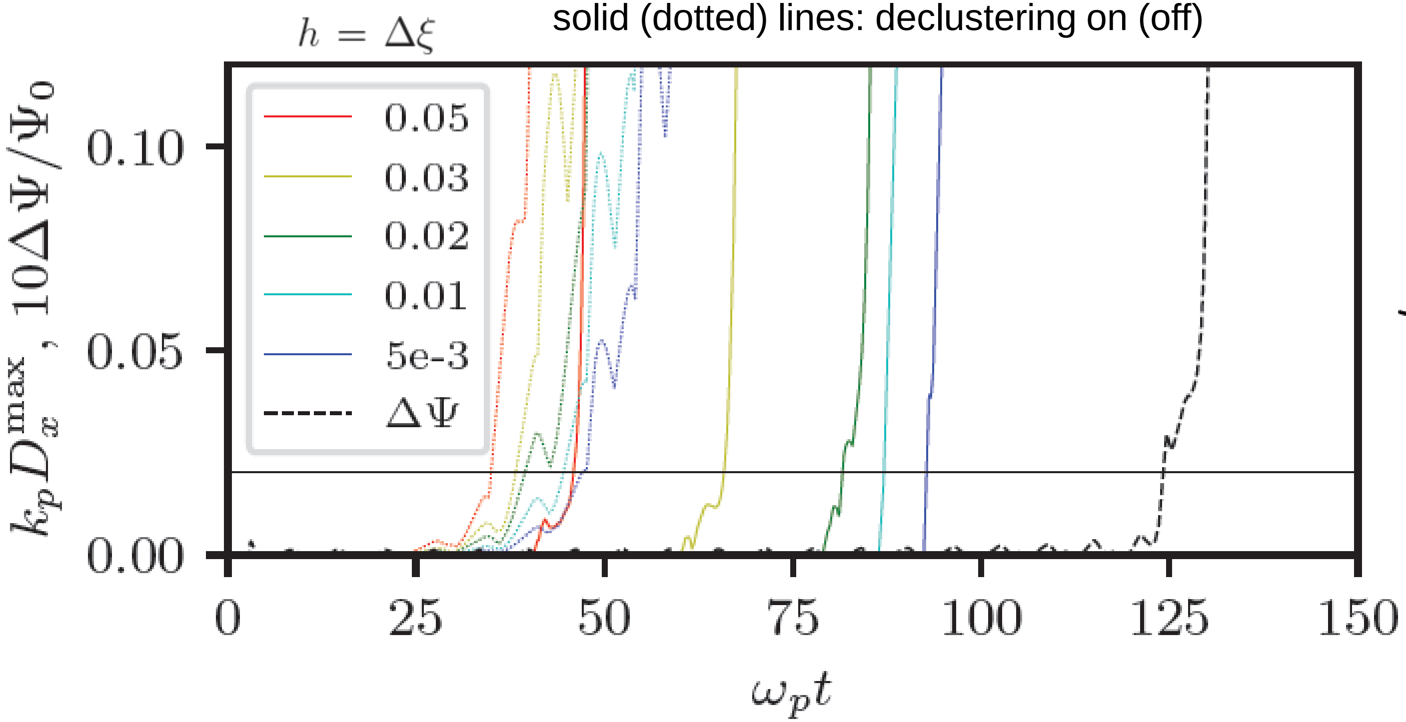
To be compared with hi-res 2d LCODE:

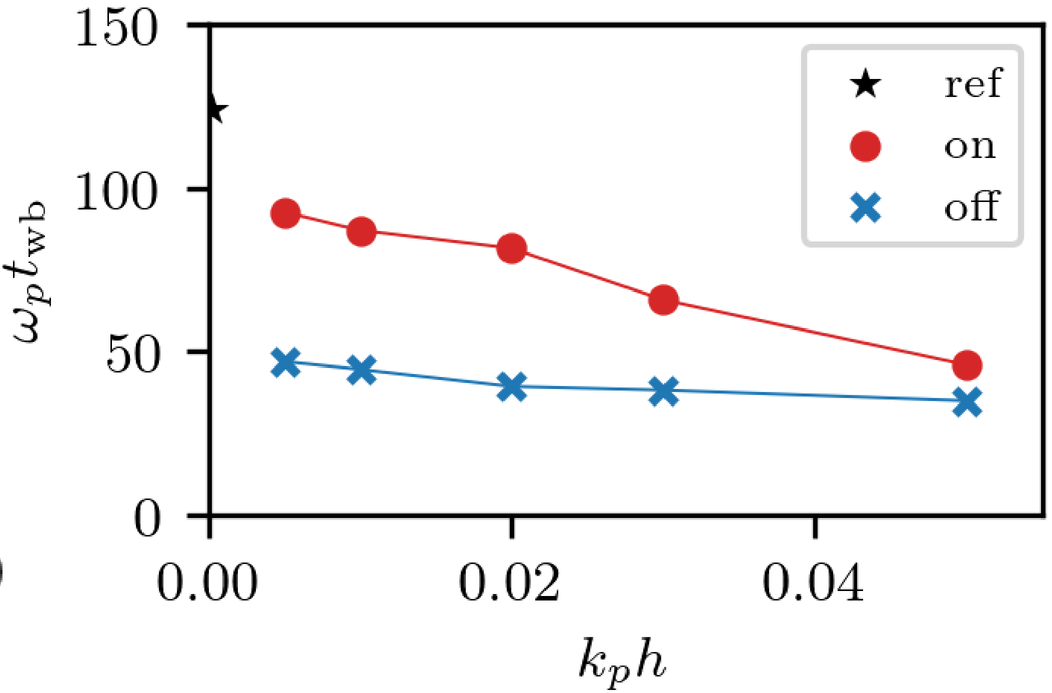


Example where declustering changes the result: transverse wavebreaking

We find the wavebreaking time by looking at the maximum particle displacement $D_x^{\max}$

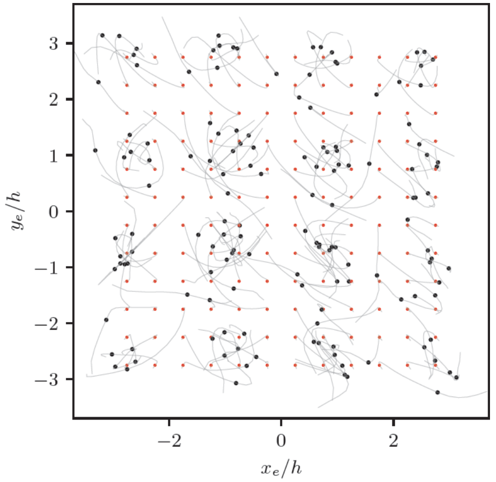
solid (dotted) lines: declustering on (off)



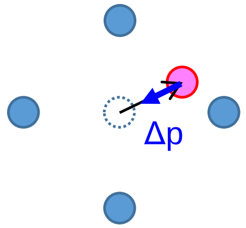


As the grid step decreases, the wavebreaking time approaches that observed in the reference run, but only when the declustering is enabled. If not, then the noise provokes earlier wavebreaking for any resolution.

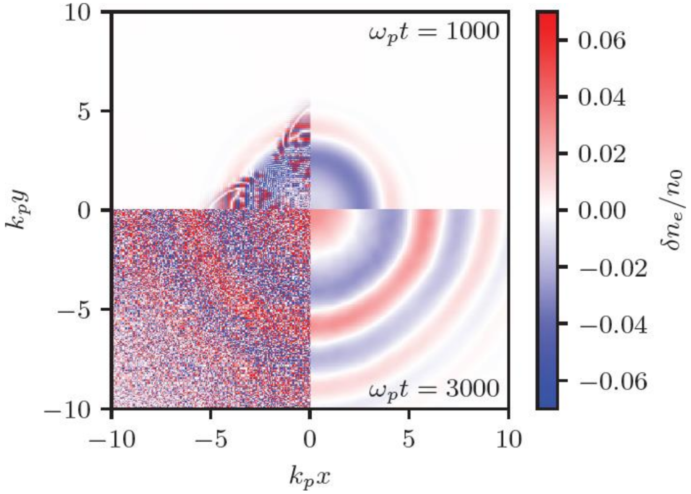
Takeaways:



(Apparently) because we do not resolve the Debye radius in wakefield simulations, the macroparticles are attracted to each other, forming clusters and heating up.

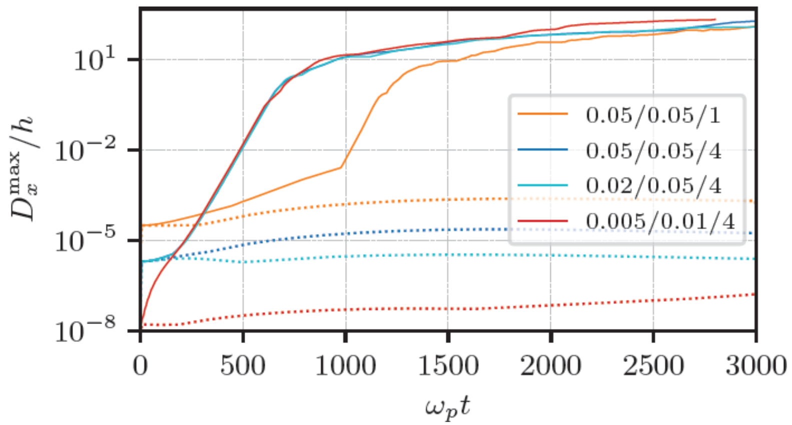


Clustering can be "turned off" by slightly modifying the equations of particle motion. Clustering is suppressed at displacements of the level $<10^{-3}$h.



Clustering leads to small-scale perturbations of plasma density and transverse fields that can spoil the quality of accelerated beams and lead to early breaking and chaotization of the wave.

Clustering must be suppressed (or at least controlled) in simulations of long-term wakefield evolution.



Thank you!