Numerical challenges in kinetic simulations of three-wave interactions

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Abstract. Generation of radio bursts in CME foreshock regions and turbulent cascades in the solar wind are assumed to be results of three-wave interaction processes of dispersive plasma modes. Using our Particle in Cell code ACRONYM, we have studied the behaviour of kinetic wavemodes in the presence of beamed electron populations, with a focus on type II radio burst emission processes. We discuss the numerical challenges in generating and analyzing self-consistently evolving wave coupling processes with a PiC-Code and present preliminary results of said project.

1. Three wave interaction

Plasma behaviour in general is usually described by a number of nonlinear differential equations. Depending on application, these may be the MHD equations, the Vlasov-Maxwell system or the multifluid equations. Since analytic general solutions to these equations are not available, a typical solution ansatz involves linearized wave solutions which are assumed to be small relative to the fixed background.

In first order, this yields the canonical linear wave solutions of the corresponding system of equations, known as “MHD waves” or “kinetic waves”, for which analytic expressions are well-documented in literature.

However if emission, absorption or interaction processes of these waves are to be investigated, next-higher order terms of the equations need to be taken into account, leading to three wave interaction processes of waves $A$, $B$ and $C$, which may have the forms

$$ A + B \rightarrow C $$

(1)

$$ A \rightarrow B + C, $$

(2)

which are known as wave coalescing- and decay processes, respectively. Analytic derivations of interaction rates for these processes are often quite involved, and only available for limited subsets of certain wave families (Melrose 1986; Spanier & Vainio 2009).

The ability to reproduce the complete nonlinear dynamics of a plasma system, and the possibility to analyze all physical properties of wave-like phenomena within this system make numerical simulations extremely valuable for these studies.
2. Specific Problem: Emission of Type II Radio Bursts

One wave emission process that has been of large importance in this context is the emission of solar radio bursts of type II and III.

These transient radio phenomena from the sun have been observed since the earliest days of solar radio observations in the 1950ies (Wild & McCready 1950). They are characterized by narrowband multi-banded radio emissions, which are rapidly drifting downwards in frequency. In the case of type III bursts, this has been identified with energetic electron acceleration from active regions on the sun, sending strong electron beams along open field lines into the heliosphere.

The case of type II radio bursts is still a subject of active research (Knock et al. 2001; Schmidt & Gopalswamy 2008; Ganse et al. 2010), with models favouring electron drift acceleration on CME shock fronts as the driver behind these events.

Common to both classes of radio bursts is the presence of a beamed electron population in an otherwise quiescent plasma background, which leads to excitation of electrostatic plasma wavemodes (Langmuir waves) through Cerenkov-type instabilities (Pulupa et al. 2010). These electrostatic waves then undergo three wave interaction processes which finally yield transverse electromagnetic waves, which are observed as radio emissions:

\[ L \rightarrow L' + S \]  \hspace{1cm} (3)

\[ L \rightarrow S + T(\omega_{pe}) \]  \hspace{1cm} (4)

\[ L + L' \rightarrow T(2\omega_{pe}) \]  \hspace{1cm} (5)

Where \( L \) denotes Langmuir-, \( S \) sound waves and \( T \) transverse electromagnetic modes at the given frequency (Melrose 1986).

Type II radio bursts are of particular merit for the fundamental study of thee-wave interactions since they are the only naturally occurring three-wave interaction process in which the emitting plasma can be probed in-situ by satellite observations, and high-resolution radio observations of the resulting waves are available.
3. Kinematics of three-wave interaction

Momentum and energy conservation impose certain limits on the waves participating in three-wave interaction processes (Spanier & Vainio 2009), favouring certain wave combinations while entirely forbidding others. In the case of beam-generated Langmuir-wave interaction, the Langmuir waves (L) should primarily be generated parallel to the beam direction, whereas electromagnetic waves are expected to be emitted in quasi-perpendicular directions:

Assuming that

\[ k_L^\parallel = k_T^\parallel + k_S^\parallel \]  \hspace{1cm} (6)
\[ k_L^\perp = k_T^\perp + k_S^\perp \]  \hspace{1cm} (7)
\[ \omega_L = \omega_T + \omega_S \]  \hspace{1cm} (8)

and inserting the dispersion relations for all three waves and neglecting \( k_T^\parallel \) as well as \( k_S^\perp \) due to angular momentum conservation (Spanier & Vainio 2009), we get

\[ 3k_\parallel^2 v_{th}^2 = c^2 k_\perp^2 + k_S^2 v_s^2 + 2k_\parallel v_s \omega_{pe} + k_\parallel v_s c, \]  \hspace{1cm} (9)

(with speed of sound \( v_s \) and electron thermal speed \( v_{th} \)) which results in an expected \( k \)-value for the electromagnetic emission of

\[ k_\perp = -\frac{v_s}{2c} k_\parallel \pm \sqrt{3k_\parallel^2 \left( \frac{v_{th}^2}{c^2} - \frac{v_s^2}{4c^2} \right) - 2\frac{v_s}{c} k_\parallel \omega_{pe}} \]  \hspace{1cm} (10)

4. The ACRONYM PiC-Code

The Particle-in-Cell code ACRONYM (Advanced Code for Relativistic Objects, Now with Yee-Lattice and Macroparticles) is being used in the numerical study of these three wave interaction processes. It is a fully relativistic MPI-parallelized Particle-in-Cell code for 2d3v and 3d3v simulations.

The code is written in fully portable C++ and has successfully been used on different architectures including x86-64, UltraSPARC and PowerPC. The code efficiently scales from single core PCs up to supercomputers with more than 100000 cores.

Development started at the department of astronomy, University of Würzburg in 2007. Since then the code has seen numerous improvements in speed and accuracy. It was used for simulation runs on our local clusters, the NEC Nehalem Cluster at HLRS, the Linux Cluster and the Altix 4700 at LRZ, Louhi at CSC, Mare Nostrum in Barcelona and Europa and Jugene in Jülich.

All important numerical methods used in ACRONYM are accurate to second order. Particles are represented by macroparticles with a triangular shaped cloud (TSC) form factor. The particle motion is propagated using a (second order) Boris push.

ACRONYM has been used for the simulation of a wide range of plasma conditions. It was successfully used in the high-density regime of Laser Wakefield Acceleration with length scales of a few nanometers, up to the case of filamentation simulations where the length scales are hundreds of meters. Large runs of the code regularly contain several billion particles.
5. Numerical Representation of Waves

A Particle-in-Cell code performs completely local calculations within the spatially cell-partitioned simulation domain according to particle kinetics, and as such carries no inherent concept of a wave. The wave behaviour is completely emergent from the large-scale evolution of the simulated Vlasov-Maxwell system.

In order to represent a wave with a certain wave-vector \( \vec{k} \) within the simulation, both sufficient resolution (\( \Delta x < 2\pi|k|^{-1} \)) and sufficient spatial extent (\( \Delta x \cdot n_x > 2\pi|k|^{-1} \)) have to be available. If this is not the case, the normally continuous wave dispersion relation will transform into a set of discrete modes, which form multiples of the inverse spatial length. In simulations with periodic boundaries, these modes will also self-couple across the simulation domain, giving largely unphysical intensities (this is shown in figure 2).

![Figure 2. Wave mode representation in a PIC simulation with insufficient spatial resolution (left) compared to one with sufficient resolution. The physically continuous dispersion relation of an electromagnetic mode decomposes into discrete mode islands.](image)

In the case of a type II radio emission foreshock region, these requirements lead to resolutions of at least 4000 cells in longitudinal and transverse direction to obtain sufficient wave representation. Karlický & Vandas (2007) used a 1d3v code with a resolution of 10000 cells, which recreated all wavemodes with \( \vec{k} \) collinear with the beam direction. In order to represent also waves in oblique and perpendicular directions, an extension to 2d3v has to be performed.

Combining all these numerical constraints, the complete simulation has been shown to require at least \( 8192 \times 4096 \) cells, with a minimum of 200 particles per cell to limit numerical noise. The timescales of the wave coupling processes observed herein demand simulation durations of at least 30000 timesteps, thus leading to a grand total of \( 201 \times 10^{12} \) particle updates, each taking about 8 \( \mu \)s on a modern CPU. The resulting computing time requirements of about 500000 CPU-hours per simulation run (not counting I/O) basically demand large supercomputers to be feasible. If the setup is to be expanded into a third spatial dimension, computation time quickly becomes unmanageable.

Quantitative analysis of wavemodes in the simulation output is performed via temporal and spatial Fourier transforms of the produced, spatially resolved quantities, typically yielding \( \omega - k \) dispersion plots. In these, either intensity or phase of the corresponding waves can be displayed.
Due to the large simulation extents required for sufficient $k$-space resolution, the amounts of data that will be used in these Fourier transforms can be quite massive. In the example of our CME foreshock simulations, total raw data sizes easily exceeded 1 Terabyte. While this can still be handled with a fast Fourier transform in reasonable time, more advanced, less computationally optimized statistical methods quickly become unusable.

Fourier transformation only yields information about the transfer of energy between wavemodes in the simulation, without giving quantitative direct information about the individual wave couplings. Wavelet Bicoherence (Dudok de Wit & Krasnosel’Skikh 1995) would be a suitable method for obtaining these couplings, but can not be used in simulations of this size due to its unfavourable computational scaling behaviour.

6. Results

Figure 3. Dispersion plot of a transverse magnetic field component from a foreshock pic simulation. The electromagnetic mode and nonlinear wave couplings at $\omega_p$ and $2\omega_p$ are visible.

With 2d3v simulation extents of at least $8192 \times 4096$ cells, sufficient resolution for the observation of Langmuir wave coupling to transverse electromagnetic emissions were observed in the foreshock plasma simulations. Figure 3 shows a dispersion diagram of a transverse magnetic field component. The parabola-shaped electromagnetic mode predicted from linear theory is clearly visible, as are low-frequency transverse waves (such as the Alfvén wave), which are not properly resolved.

Additionally two bands of excitation are visible at $\omega = \omega_p$ and $2\omega_p$, which are consistent with the theoretically predicted three wave interaction processes, and couple to the electromagnetic mode at the resonance points.

Note that in this graph, only a small cutout of the complete dispersion plots (in which the relevant physics is happening) is being displayed. Due to kinetic resolution constraints, the much-finer resolved simulation leads to dispersion plots which range to far higher spatial and temporal frequencies.
7. Conclusions and further work

The results presented here show a transfer in energy from beam-driven Langmuir waves into transverse electromagnetic modes at both fundamental and harmonic frequency, consistent with type II radio burst emission models. Since the Fourier method employed for the analysis only yields information about the intensity of the produced waves, quantitative information about the couplings will need to rely on more advanced statistical methods. Effort is currently ongoing to make bicoherence-based algorithms sufficiently scalable for dealing with the data amounts produced in typical PiC simulation runs.

The simulation model will also be extended to compare setups with counterstreaming electron beams (as described here) to single-beam setups, in an attempt to confirm whether a single emission region or multiple beam acceleration sites are necessary for type II radio bursts.

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