CFHall Code Validation with 3D3V Weibel Instability Simulation

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Abstract. Despite the existence of massively parallel codes and their application to plasma simulation, in the field of computer simulations the unsolved problems still remain. The necessity of various approximations in practical problems, for example, decreasing of the simulation dimension and physical parameter calibrations, arises, but such approximations can make the simulation results questionable.

While aiming for the maximal efficiency of computational algorithms it is possible to manage without the majority of popular approximations and to broaden the applicability limits of the numerical research. Such possibility arises with the use of the Locally Recursive non-locally Asynchronous (LRnLA) algorithms as the base for a program code. This was used as a basis for CFHall plasma simulation code development. CFHall is presented in this work along with the brief description of the underlying algorithms. The applicability of the CFHall to plasma instability simulation is demonstrated on the example of weibel instability simulation.

1. Introduction
During the years of the existence of the numerical experiment in plasma physics it has shown its benefits in theoretical research for the verification of the arising hypotheses, as well as for the development of plasma technologies. Plasma simulation is used to obtain information which is impossible to get in the laboratory experiments, for simulation of stars and galaxies scale, or for small scale simulations, for which the probing devices are inefficient, or for simulation of the systems, where the presence of the probing devices distorts the plasma properties. While aiming for the advance of plasma technologies numerical experiment allows to observe the system changes caused by calibration of control parameters. Such calculation enables to save on the production of various devices to achieve the best device construction.

Fully kinetic codes are chosen for the simulation in the systems where the plasma distribution function cannot be approximated by its equilibrium state. Since the early 1980s a variety of plasma simulation codes has been developed, and the development of computer systems has always been accompanied by program code enhancements. However, despite the appearance of the massively parallel codes and their use on supercomputers, problems unsolved by numerical experiments still remain.

To overcome one of such problems, namely, to investigate the anomalous electron transport in Hall Effect thruster [1], the fully kinetic 3D3V code for plasma simulation CFHall has been developed.

The essence of the problem is in the fact that electron transport to anode in the Hall effect plasma thrusters is not explained within the theoretical approach. Plasma instabilities are...
considered the main reason of the process. However due to a large parameter range in the Hall thruster system (the ratio of plasma frequency to ion travel time, Debye radii to channel size) the necessary mesh size and time steps quantity becomes too large for a simulation with the existing simulation codes on the existing systems, including supercomputers. Therefore to obtain the estimates of Hall thruster parameters various approximations are commonly used. For example, lower dimensions, physical parameter calibration, hydrodynamic approach. One important drawback of the use of above approximations is the inability of adequate description of plasma instabilities while the instabilities play a decisive role. So such codes cannot be used for investigation of anomalous transport.

By improving the efficiency of the computational algorithms at the code’s base it is possible to overcome the arising limits of the given computer systems. This had become the main idea in the development of the CFHall code. While aiming for the maximal efficiency of computational algorithms it is possible to manage without the majority of popular approximations and to broaden the applicability limits of the numerical research. The use of Locally Recursive non-Locally Asynchronous algorithms (LRnLA) [3] enables such possibility.

At the same time the code in question isn’t limited by the above problem. It may be used for plasma research problems in various fields of plasma theory and technology, including the whole range of numerical experiment application in problems where the kinetic plasma description is necessary. Among the problems for which the code has been tested there are simple study problems such as Langmuir oscillations, Larmor circumrotation, skin effect, as well as numerical experiments for specific applications, such as laser interaction with sub-critical plasma layer, wake-field plasma acceleration, plasma transport through the crossed electric and magnetic fields fields.

In this work we demonstrate the CFHall code along with the basic algorithms in its base, and its applicability to plasma instability simulation is demonstrated on the example of the Weibel instability.

2. Code features

We use Vlasov equation for collisionless plasma dynamics and Maxwell equations for fields evolution. The numerical methods in use are PIC (Particle-in-Cell) [4] and FDTD (Finite Difference Time Domain). The main idea of the project is to maximize the efficiency of the computational algorithms.

For the numerical schemes with local dependencies the common way of data storage in multidimensional arrays require excessive time expenses for data access operations. Recursive data storage as in a Morton Z-curve [5] provide a solution to this problem. The Z-curve was implemented as a “cubeLR” data structure. In CFHall code we utilize Z-curve storage along 2 of the 3 spatial dimensions. In each cell of a 3D cubeLR structure a one cell wide column of field values along Z axis is stored.

LRnLA algorithms provide the superior dependency graph traversal rules by taking advantage of memory subsystem hierarchy, from on-chip CPU cash and up to disk and network memory. The benefits of the algorithms may be explained by the locality of the sequentially processed data. While providing a noticeable acceleration for sequential calculations, it is also optimized for distributed computations and is adaptable to parallel computations on any levels. In the CFHall code the LRnLA algorithm family ConeFold is utilized. Similarly to Z-curve storage, it may be considered as a recursively divided blocks, but in operation space (fig. 1).

CFHall also utilizes AVX/SSE vectorization for further acceleration. The component values along z axis are stored in a vectorized array. Array elements are stored in 4-element vectors. Operations on such vectors take the same amount of time as operations on scalars (double or float). Therefore it is possible make the calculation up to 4 times faster. The actual acceleration is slightly less due to costs of vector formation.
Figure 1. cubeLR visualization in data space and ConeFold visualization in operation space (left). ConeFold is recursively divided similarly to cubeLR (right).

3. Weibel instability

In the current study the Weibel instability is chosen to demonstrate the ability of plasma instability simulation, as well as computing time. The instability is named after E. Weibel who described it in 1959 [6] and arises in plasmas with anisotropic velocity distribution. Its mechanism has been explained on a simple model of two counterstreaming plasmas [7]. According to it one should take into account 2 cold charged particle streams flowing in opposite directions and a small magnetic field perturbation $B_x e^{iky}$ had appeared (see fig. 2). The Larmor rotation of plasma particles causes the periodical ($\sim e^{iky}$) unbalancing of the currents, which in turn adds to magnetic field growth due to Amper law. Thus the further exponential growth of the perturbation is explained. Since the wavelength of the most unstable modes are comparatively small, the filamentary structure is expected in the resulting oscillations.

Such magnetic field formation had become of interest as a possible reason of a stable magnetic field generation in plasmas, containing anisotropic velocity distribution.

Figure 2. Weibel instability growth illustration. Initially there are two counterstreaming plasmas along $z$ axis and a small perturbation $B_x e^{iky}$.

Figure 3. 3D distribution of the $B_x(x, y, z)$ field. $t = 11.52, B_x \sim 0.1$. As expected from theory, filaments along $z$ axis are observed.

4. Problem statement and simulation results

In the current study the rise of the instability is observed in a system of the two colliding plasma streams. Plasma distribution function is written as

$$f(\vec{v}) = f_m(v_x)f_m(v_y)f_m(v_z - 0.5) + f_m(v_x)f_m(v_y)f_m(v_z + 0.5),$$

(1)
where $f_m$ is a Maxwell distribution function with temperature equal to 0.005. We use the
dimensionless units. Electron masses $m_e$ for mass, electron charges $e$ for charge, light speed $c$
for velocities. From these the units for distances $c/\omega_p$ and for fields $m_e\omega_p c/e$ follow. All initial
field values are zero. For the estimate of the maximal instability increment on the linear stage
the formula from [8] was used. For the chosen parameters the most unstable mode has the
wavenumber $k \sim 35$ ($\vec{k} \perp \vec{B}$), and its increment is $\gamma \sim 0.592$. The mesh size and time and space
steps were varied. Following variants are of note to the current paper.

The first one included $128 \times 128 \times 120$ mesh size, 10 electrons from each stream in each cell,
time steps equal to $dx = dy = dz = 0.01$, $dt = 0.0025$. The simulation domain is too small
to show the 3D instability structure, so only the Weibel instability is visible and the result is
two-dimensional. It allows to perform a 2D Fourier analysis along $x$ and $y$ axes, by averaging
on the $z$ axis. The result of such analysis for $B_z$ field component is shown on fig. 3. The
simulation process shows the filament formation on the linear stage of the instability growth,
and their merging into a large-scale stable magnetic structure at later stages.

To observe the 3D nature of the instability a greater mesh has been chosen for further
simulations, namely $512 \times 512 \times 240$ mesh size, mesh steps $dx = dy = 0.02$, $dz = 0.05$, time step
$dt = 0.005$. The simulation has been performed on the Intel core i5-2400 @ 3.1GHz desktop
computer, 1 time iteration step takes approximately 8 seconds.

The result for energy dependency on time are shown on fig. 4. To show the correspondence
with the theoretical estimate of the increment, Fourier analysis had been carried out (fig. 5).

![Energy dependency on time](image4.png)

**Figure 4.** Energy dependency on time. Energy of the $E_z$ field component which grows
due to beam plasma instability, and weibel instability induced $B_x$ and $B_y$ component
energy are shown. Full energy of fields and particles are also present on the figure. Their
sum is conserved with 1.2% accuracy by the end of calculation.

![Fourier mode amplitude time dependency](image5.png)

**Figure 5.** Fourier mode amplitude time dependency. Modes which were dominant on
some time step were chosen for the plot. The straight curve shows theoretical estimate.

### 5. Results

We have developed a 3D3V kinetic code for plasma particle-in-cell simulation. The code is
optimal for plasma instability simulations since it doesn’t contain most common approximations:
a full self-consistent Vlasov-Maxwell system is solved, the second-order numerical scheme is used
both for field and PIC calculations, multiscale simulations are possible, parameter calibrations
are not present. The focus of the development is on the most effective computational algorithms:
the LRnLA algorithms and vectorization are implemented.
For the demonstration of the code possible applications the Weibel instability study has been performed. The instability growth on a linear stage shows good correspondence with analytical estimations, and the stable magnetic field structure at later stages agrees with theoretical expectations. High computational effectiveness allows the simulation to be performed in a reasonable time even on a desktop computer.

The combination of the high effectiveness and numerical scheme accuracy becomes a key benefit of the CFHall code. With it it becomes possible to perform numerical experiments in the problems which were not solved before.

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