Vlasov-code simulation

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For decades kinetic space plasma simulation, i.e. the solution of Vlasov-Maxwell equations, has been dominated by PIC (Particle-In-Cell) codes that utilize the motion of the particles along the characteristics of the Vlasov-equation for a Lagrange-Euler approach reducing the solution of the Vlasov - advection type PDE (Partial Differential Equation) to the solution of ODEs (Ordinary Differential Equations) of particle motion. The resulting schemes are simple, robust and easily scalable. Unfortunately, the always limited, finite number of (macro-) particles of PIC-codes introduces shot-noise into the system. Hence, for the investigation of fine resonance and turbulence effects one must directly solve the Vlasov-equation for the evolving distribution function. This means to solve the most complicated fluid dynamics PDE an advection equation. The solution of the dissipationless Vlasov continuity equation leads to a filamentation of the distribution function which causes subgrid structures and nonphysical oscillations resulting in numerical instabilities. Due to these difficulties the application of Vlasov-codes for the last thirty years was restricted to low-dimensional problems. Only the combination of optimum numerical solution schemes modern fast with large memory parallelized computer systems allows the application of Vlasov-codes to multidimensional problems, i.e. a broader class of space plasma problems. We review the state of the art of Vlasov-code simulation and give an outlook to its future application in space physics.

1. Introduction

Many space plasmas are collisionless. Kinetic plasma effects come into play if wavelength or spatial localization, wave frequencies or time scales become comparable with characteristic dispersion scales as there are gyro-radii of particles, inertial or Debye lengths or gyro- and plasma frequencies. In addition nonlinear also interactions between plasma particles and plasma waves have to be described to understand, i.e., kinetic Alfén waves, collisionless shocks, warm beam instabilities, anomalous transport, reconnection. Mathematically the kinetic plasma physics of collisionless plasmas is described by a system of Vlasov- and Maxwell’s equations. Due to their complicated non-linear structure, in most of the cases analytical solutions of these equations cannot be found, their numerical simulation becomes desirable. Most numerical simulations of the Vlasov-Maxwell system of equations have been carried out by Particle-In-Cell- (PIC-) codes (Birdsall and Langdon, 1985). PIC-codes replace the solution of the partial differential Vlasov-equation by the solution of the ODEs (Ordinary Differential Equations) of motion of macro-particles. Each macro-particle represents a large number of the plasma particles. The particle orbits are the characteristics of the Vlasov-equation. This allows a combined Lagrange-Euler method of solution: the phase space density along the trajectories is exactly conserved, i.e. one has just to upgrades charge density and currents by extrapolating them to Eulerian (i.e. fixed in space) grid points. The advantage of PIC codes is their simplicity, robustness and scalability (see Y. Omura’s tutorial). Their disadvantage is the numerical shot-noise, caused by the technically limited number of macro-particles. This particle noise causes numerical collisions and artificial dissipation. A direct solution of the Vlasov-equation avoids the particle noise of PIC codes. However, the numerically complicated solution of the advection-type Vlasov-equation and the filamentation of the phase space have restricted the usage of Vlasov-codes for the last thirty years to the treatment of low-dimensional and electrostatic problems. Electrostatic beam instabilities were considered by electrostatic 1D1V schemes, gradient instabilities already need at least 2D schemes. For the simulation of kinetic reconnection even 3D3V codes are necessary to describe the mode coupling of this essentially three-dimensional process (Büchner, 1999). Most space physics problems are higher-dimensional and, as one the reconnection problem, even up to three-dimensional in the real and three-dimensional in the velocity (3V) or momentum (3P) space, i.e. six-dimensional in the phase space. The solution of the Vlasov-equation for distribution functions in a six-dimensional phase space with a resolution of, say, a hundred grid points in each dimension needs to store a grid of \(10^{12}\) points! High resolution multidimensional Vlasov-code simulations are, therefore, numerically very expensive. They need huge computer resources and parallel computing mandatory as well as the choice of optimum algorithms. At the moment mainly low dimensional electrostatic or simplified Vlasov approaches like gyro-kinetic codes are used, e.g. for strong laser-plasma interactions. The utilization of higher dimensional space physical applications of Vlasov-codes are still in their infancy. At the moment no textbook exists which would cover the major aspects of Vlasov-codes and offer optimum solution schemes like Birdsall and Langdon (1985) for PIC-codes. This tutorial reviews the state of the art of Vlasov coding in order to encourage future developments and the implementation of higher dimensional Vlasov-code simulation into space physics. After introducing the basic equations in an appropriate normalization we discuss the specific problems which appear in any attempt to solve Vlasov-equations and ways to their solution. We cite successful space physics applications of Vlasov-codes and give an outlook toward future research directions.
2. Basic equations

The kinetic physics of collisionless plasmas is well described by the particle distribution function \( f(r, v, t) \), solution of the Vlasov (1938) equation, a Boltzmann equation with a vanishing r.h.s. (no collision term). The Vlasov equation can be formulated either in a advection form, where the velocity is treated as an independent variable

\[
\frac{\partial f_j}{\partial t} + \frac{v_j}{m_j} \frac{\partial f_j}{\partial r} + \frac{e_j}{m_j} (\vec{E} + \vec{v} \times \vec{B}) \cdot \frac{\partial f_j}{\partial \vec{v}} = 0
\]  

(1)

or, mandatory for relativistic applications, in the conservative form

\[
\frac{\partial f_j}{\partial t} + \frac{1}{m_j} \frac{\partial}{\partial r} (\vec{p} f_j) + \frac{\partial}{\partial \vec{p}} \left( F(\vec{E}, \vec{B}, \vec{p} f_j) \right) = 0
\]  

(2)

where the momentum \( \vec{p} \) is a dependent variable. The subscript \( j \) denotes the particle specie, e.g. \( j = e, p \) for electrons and protons, respectively.

3. Filamentation and its numerical treatment

The Vlasov-equation is non-dissipative, entropy conserving, the total derivative of the distribution function vanishes. This means that the consequences of the action of the forces \( \vec{F} = e_j (\vec{E} + \vec{v} \times \vec{B}) \) is neither dissipated nor otherwise removed from the system. The free-streaming evolution of the distribution function causes a finer and finer filamentation of the distribution function in the phase space, down to sub-grid sizes, and, therefore, strong gradients. The physically correct and necessary filamentation can, however, cause non-physical oscillations and numerical instabilities in discrete mathematics. A careful choice of the discretization scheme is, therefore, necessary to avoid the growth of non-physical oscillations out of the filamentation. Lagrange schemes, which are most accurate, cannot be applied due to the increasing with time complication of the phase space structure. Instead, semi-Lagrange schemes were developed. Since they cannot simply be extended to higher-dimensional problems, expansion or transform methods were thought of. The use of higher order schemes might be even counterproductive by the same reason. Perhaps, only improved Euler-grid methods solving conservative Vlasov equations will have to be developed. So far, however, usually, when the filamentation causes non-physical oscillations, artificial dissipation is introduced, or smoothing of gradients or filtration. Artificial dissipation can be introduced, e.g. as \( \partial f/\partial t = \nu \partial^n f/\partial v^n \) with \( n = 4, 6, 8 \). The collision-frequency parameter \( \nu \) should not be chosen too small, neither too large in order not to suppress important physical phenomena. Another possibility is the removal of short wavelength oscillations by Fourier filtering of large-k modes. The latter, and to some extend also the former method pretend what physically happens in the real world: after cascading energy towards smaller and smaller scales microscopic dissipation removes the excess energy avoiding further filamentation. Denavit (1972), e.g., used a scheme of periodic smoothing in the phase space while Klimas and Farrel (1994) implemented filtration. These procedures correspond to the damping of small scale turbulence after its down-cascading. Undamped non-physical oscillations can lead to formally negative values of the newly calculated distribution function, whose positivity has to be maintained. If distribution function values, which turn negative due to numerical inaccuracies, are just put to zero, as often done, the conservation laws of the number of particles and of energy are violated, i.e. the simulation results become unreliable as observed in many unsuccessful attempts to develop a Vlasov-code. The only correct way to maintain positivity is the choice of an appropriately accurate solution scheme.

4. Semi-Lagrange methods

The most accurate way to solve convection (or advection, term \( \nu \partial f/\partial t \)) type of PDE is to use the constancy of the distribution function along the characteristics. Since the Vlasov-equation is a hyperbolic PDE describing a propagation along the characteristics which correspond to the particle orbits in response to the same forces (also used in PIC codes). Also, due to its vanishing r.h.s. the Vlasov equation is a continuity equation. Hence, its solution, the distribution function, stays constant along the characteristics. Although the phase space filamentation (see section 3) inhibits the use of this property to construct a straightforward Lagrange method of solution, semi-Lagrange schemes were successfully implemented to solve low-dimensional problems. In their in two respects pioneering work Cheng and Knorr (1976) utilized a semi-Lagrangian solution of the Vlasov-equation. (Their second ground breaking achievement, time splitting, is discussed below.) The semi-Lagrange approach is most accurate since along the characteristics the distribution function \( f \) stays unchanged. To obtain the solution on a spatial and velocity-space Euler-grid, however, one has to extrapolate the time advanced distribution function onto the neighboring Euler-grid points. This introduces numerical errors (Sonnendrücker et al., 1998). In low-dimensional systems the semi-Lagrange method is very efficient. Applied to higher dimensional problems their efficiency suffers, however, from the difficulties of multidimensional extrapolation. Semi-Lagrange methods are accurate and robust because the use an analytic form of solution. Their disadvantage is the necessity to carry out interpolations back to the Euler grid making semi-Lagrange schemes numerically very expensive and inapplicable for higher dimensional problems.

Fractional Stepping → Time Splitting

The second important step forward in Vlasov coding was another great idea of Cheng and Knorr (1976), the application of the known from the smoothed particle hydrodynamics (SPH) fractional stepping method by splitting the advection-type Vlasov-equation (1) into two advection equations, one in space and one in the velocity space. Both are then solved sequentially by the following stepping algorithm: first evolve \( \delta t f + \nu \delta t f = 0 \) for \( \Delta t/2 \) then solve the field equation, then evolve \( \delta t f + F \delta t f = 0 \) for \( \Delta t \) and, finally, evolve \( \delta t f + \nu \delta t f = 0 \) for \( \Delta t \). Cheng and Knorr (1976) called this fractional stepping "time splitting". As any non-conservative scheme, the stepping algorithm, which calculates function values at different moments of time, introduces numerical
dissipation. Nevertheless, the semi-Lagrangian method with time splitting (see also Cheng, 1977; Gagné and Shoucri, 1977; Shoucri, 1979) is still the most commonly used scheme of space plasma Vlasov simulation and not much attention has been devoted to the development of new types of Vlasov-solvers in its advection form (equation 1) on Eulerian grids. Instead the work has concentrated on improving the accuracy of the advection solvers in the semi-Lagrangian approach, like, e.g., in Horne and Freeman’s (2001) McCormac scheme.

5. Euler methods

Euler schemes omit the extrapolation of the distribution function by directly calculating the function values on the grid. Euler schemes are also more flexible concerning the boundary conditions. A critical comparison of 1D1V Euler schemes for solving the Vlasov equation was carried out by Arber and Vann (2002). Since space physics problems are mostly higher dimensional, perhaps, only accurate conservative schemes, solving the Vlasov-equation (2), bear the potential for efficient future multidimensional Vlasov-codes.

Conservative Vlasov solvers

The conservation form of the Vlasov-equation (2) is of particular interest because for conservation laws very accurate numerical solution methods can be developed. Appropriate algorithms can make the Eulerian solution of Vlasov-equations in their conservation form almost as accurate as semi-Lagrangian algorithms (see, e.g., Filbet et al., 2001). A highly accurate numerical integration method of continuity equations, developed in numerical fluid mechanics, is the flux-corrected transport (FCT) algorithms (e.g., Zalesak, 1979). For 1D1V Vlasov equations Boris and Book (1977) successfully implemented a FCT scheme. For multidimensional problems, however, the FCT schemes become very messy and no good multidimensional scheme has been developed, yet. An unsplit flux-limited transport (FLT) scheme might be the solution (see Elkina and Büchner, 2005).

6. Functional expansion (transform) methods

For special applications transform methods of solving the Vlasov-equation might be useful as discussed, e.g. for 1D1V codes, by Armstrong et al. (1976). A 2D2V Fourier transform solution of the Vlasov-equations was developed by Eliasson (2003). In special applications also other functional expansions like into Hermite polynomials, spherical harmonics, might be appropriate (see, e.g., Shebalin, 2001). Expansion methods are very efficient if they can use specific symmetries. In general, however, expansion methods are not recommendable since they generally cause difficulties in formulating the boundary conditions, the filamentation will call for the introduction of higher and higher order polynomials. Transform methods also do not allow the use of decomposed for the sake of parallelization domains. Also, spectral methods suffer from the same problems as higher (>1st)-order unlimited Eulerian schemes - a monotonicity-preserving spectral scheme has yet to be developed.

7. Boundary conditions

For Vlasov-codes the choice of appropriate boundary conditions (BC) is even more crucial rather than for other codes, since the BC have now to close the equations and to confine the physical processes in a mathematically consistent way not only in the real, but additionally also in the velocity space. The simplest boundary condition for the distribution function in the velocity space is maintaining its initial value. This approach sometimes causes problems because any acceleration (i.e., redistribution toward the boundaries of the velocity space) accumulates plasma near the boundary and increases the gradients. Hence non-physical oscillations due to filamentation often occur first near the boundaries. This is especially true in multidimensional simulations where the velocity space ranges over only a few thermal velocities due to technical (hardware) limits. The introduction of an appropriate artificial dissipation might help here as well, but the better choice are the use of more accurate solvers and larger velocity space ranges are a better choice. Another way is to change the order of the solver from higher, say a fourth order central scheme, to a lower order scheme when approaching the velocity space boundary. If von Neumann boundary conditions are necessary, as, e.g., in flux limiting schemes, for the calculation of the derivatives the introduction ghost grid-cells or ghost zones for the velocity-space boundaries are introduced. Ghost zones are created by surrounding the boundary with additional grid cells used to buffer appropriate neighboring values of data. The ghost boundary might have to have a width greater than 1. If, for example, the computation of new values for a boundary grid point requires values from 2 grid points, then the ghost boundary should have a width 2.

8. Examples and applications

The most common space physics application of Vlasov-codes is the simulation of electrostatic waves. Klimas and Farrel (1994), e.g., used a 1D1V Vlasov-code to simulate the electron acceleration induced by beam instabilities in the Earth’s foreshock region. The anomalous resistivity caused by an ion-acoustic (IA) instability was considered by Watt et al. (2002) using the 1D1V Vlasov-Amperé code of Horne and Freemann (2001). A simulation of this problem was necessary for space physics applications, where the ion temperature is not much less than the electron temperature as required by the usual quasi-linear theory of IA waves due to current driven instabilities. They confirmed the theoretical prediction (see, e.g., Gary, 1993) that similar ion and electron temperatures require higher electron drift velocities $u_{de} > v_{te} = \sqrt{2k_B T_e/m_e}$, most interestingly, Watt et al (2002) obtained a three to five orders larger anomalous resistivity than predicted by the quasi-linear theory. Petkaki et al., 2003 extended this study to investigate the influence of a Lorentzian distribution with small kappa values, i.e., for enhanced above the Maxwellian distribution higher energy parts, on the threshold of an ion-acoustic instability. They confirmed the enhancement, predicted by Meng (1992) and calculated the anomalous resistivity in a non-Maxwellian plasmas. All these calculations were car-
ried out for an artificially low mass ratio of \( M_i/m_e = 25 \). Hellinger et al. (2004) used a 1D1V Vlasov-code with periodic boundary conditions and a Fourier-transform solver of the Poisson equation (Fijalkow, 1999), to verify the results of Watt et al. (2002) and Petkaki (2003) for the realistic mass ratio \( M_i/m_e = 1800 \). They found an enhancement of the anomalous resistivity due to two orders of magnitude above the quasi-linear prediction, i.e. much smaller than the one obtained before for the mass ratio \( M_i/m_e = 25 \) before. Recently, with the availability of modern parallel computer architectures also first multidimensional Vlasov-codes have been implemented to solve space physics problems (Wiegelmann and Büchner, 2001). Using the 2D3V Vlasov version of this code Silin and Büchner (2003) described the nonlinear triggering of bulk kink and sausage instabilities of thin currents by linearly unstable lower hybrid drift waves both in antiparallel and in guided (non-antiparallel sheared) magnetic fields. Using the 3D3V version of the code Silin and Büchner (2005) obtained the triggering of three-dimensional kinetic reconnection by coupling to a lower hybrid drift instability at the edges of a thin current sheet. Based on Vlasov-code results Büchner (2005) discusses the consequences of the anomalous resistivity due to nonlinear lower hybrid drift waves in current sheets, theoretically predicted by Büchner and Daughton (2005).

9. Summary and outlook

Vlasov-codes are advantageous compared to the technically simpler PIC codes due to their noiseless solutions of the evolving with time distribution function and due to the possibility of dissipationless solutions. No, with the evolution of large memory and fast CPU parallel computer architectures the implementation of multidimensional Vlasov-codes, directly solving the kinetic equation of collisionless space plasmas, becomes possible. The main problem is the free-floating advection character of the dissipationless Vlasov-equation and the resulting phase space filamentation in the phase space. Conservative Euler schemes, perhaps, are future of multidimensional Vlasov-simulation, in particular of relativistic Vlasov codes for astrophysical applications. Adaptive grid methods (AGMs) for integrating the Vlasov-Maxwell equations might help to enhance the resolution not just in space, as in fluid and PIC codes, but also in the velocity space, e.g. near resonances or other special sites while saving resources on other parts of the phase space.

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References