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Method- and scheme-independent entropy production in turbulent kinetic simulations

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ABSTRACT

Numerical kinetic models of plasma turbulence require careful treatment of conserved quantities. In the collisionless limit, numerical dissipation can impact entropy in a non-controlled manner. In this paper, the impact of the error in entropy conservation is investigated. In a simulation of ion-acoustic turbulence, a large error (15%) in entropy conservation is found. Surprisingly, this error is independent of the numerical method, scheme, or number of grid points. Adding a collision operator resolves this issue, but only if the collision frequency is large enough that it modifies the qualitative time evolution of observables, such as electric field amplitude, anomalous resistivity, or phase-space structures.

For a wide range of astrophysical and laboratory plasma phenomena, collisions are negligible. Then, the evolution of the particle distribution in phase-space is usually described by the Vlasov equation, which translates the fact that the distribution is constant along particle orbits.

Accurate numerical simulation of collisionless plasmas requires careful treatment of conserved physical quantities, such as total mass, total energy and total entropy. For example, to obtain the turbulent steady-state accurately, spurious heating must be avoided. The numerical treatment of kinetic nonlinearities such as particle trapping is particularly challenging. Indeed, trapping involves the filamentation of phase-space (phase-space mixing), whereby an initially smooth particle distribution is mixed by the particle motion into very fine structures. Phase-space filaments eventually become smaller than the numerical grid size. Then information is inevitably lost, which breaks the conservation of entropy. This problem is well-known for Vlasov codes [1], but the impact on physics of interest, i.e. the evolution of coarse-grained observables, is unknown.

In overcoming the numerical issues associated with phase-space filamentation, one can distinguish three classes of approach. The first approach is to add a collision operator to the model [2], even if the collision frequency has to be artificially increased to overcome the issues. The second approach is to add artificial filters [3] or damping [4] (it can be argued that Fourier codes [5] belong to this class). The third approach is to simply let numerical discretization replace collisions to dissipate the smallest scales and coarse-grain average the distribution function in an uncontrolled manner. For all three classes of approach, however, a concern is that simple models of collisions, numerical filtering, or numerical dissipation, are artificial, and may impact the physics of interest.

In this work, we report a systematic spurious entropy production, of 15% of the initial entropy, when the fully-nonlinear turbulent stage is reached, regardless of the numerical treatment. Indeed, the issue is not limited to Vlasov codes. The same error is found for fundamentally different types of simulation, i.e. Vlasov (semi-Lagrangian) and particle-in-cell (PIC), different schemes and different choices of grid sizes. This is shown in Fig. 1, which is the main figure in this paper, and which is discussed in detail in Section 3. Furthermore, the error is relatively insensitive to parameters of the physical system. As expected, a collision operator with velocity diffusion resolves the issue, but only if the collision frequency is so large that it dominates the long-time evolution.

1. Model

We restrict the analysis to a collisionless, one-dimensional, ion–electron plasma with an initial homogeneous current. We choose physical parameters such that the evolution of the plasma is dominated by ion-acoustic turbulence. Ion-acoustic waves [6,7] are longitudinal electrostatic waves, which are commonly observed in space and laboratory plasmas. The nonlinear saturation

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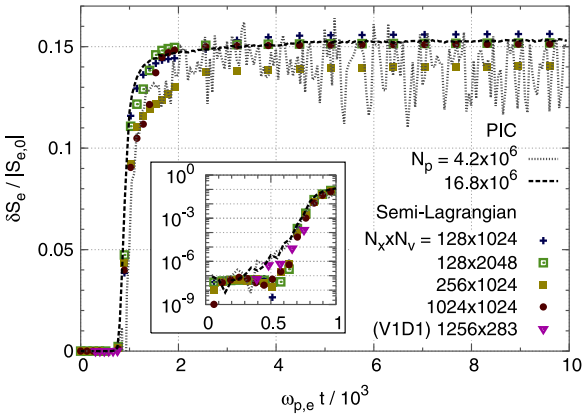

Fig. 1. Time-evolution of the perturbed electron entropy. Inset: zoom on the early stage, in semi-logarithmic scale. The simulation parameters are given in Section 1.4.

Table 1
Normalization.

Physical quantity	Normalization constant
Time	$\omega_{p,e}^{-1}$
Particle charge	e
Mass	m_e
Length	λ_D
Velocity	$v_{T,e}$
Distribution f	$n_0/v_{T,e}$
Electric field	$m_e v_{T,e}^2/(e\lambda_D)$
Energy	$m_e v_{T,e}^2$

has been studied from the early 1960s [8–12]. Theory and experiments indicate that ion-acoustic waves are key agents of magnetic reconnection (via anomalous resistivity) [13–16], turbulent heating [17], particle acceleration [18], and play important roles in the context of laser–plasma interaction [19]. Furthermore, ion-acoustic waves constitute the basis for dominant fluctuations in magnetically confined plasmas. Indeed, drift-waves [20] arise from the ion-acoustic branch, modified by inhomogeneities and geometry effects. Linear instability of ion-acoustic waves requires that the velocity drift exceeds some finite threshold. However, nonlinear theory [21–23] predicts that ion-acoustic turbulence can grow nonlinearly, even for small drifts.

In the present work, we use a model of ion-acoustic turbulence as a paradigm for kinetic models in the presence of strong resonances.

1.1. Normalization

It is appropriate to normalize physical quantities with the constants listed in Table 1, where λ_D is the Debye length, $e = q_i = -q_e$ is the elementary charge, n_0 is the spatially-averaged plasma density, and m_s, $\omega_{p,s}$ and $v_{T,s} = (2T_s/m_s)^{1/2}$ are the mass, plasma frequency and thermal velocity, respectively, of species s ($s = i, e$).

1.2. Model description

The evolution of each particle distribution, $f_s(x, v, t)$ is given by the Vlasov equation,

$$\frac{\partial f_s}{\partial t} + v\,\frac{\partial f_s}{\partial x} + \frac{q_s E}{m_s}\,\frac{\partial f_s}{\partial v} = C(f_s), \tag{1}$$

where $C(f_s)$ is an eventual collision operator.

The evolution of the electric field $E(x, t)$ satisfies a current equation,

$$\frac{\partial E}{\partial t} = -\sum_s \frac{m_s \omega_{p,s}^2}{n_0 q_s} \int v f_s(x, v, t)\, \mathrm{d}v. \tag{2}$$

Table 2
Relative error (order-of-magnitude) in energy and entropy conservation.

	Total energy	Entropy
Dissipative bump-on-tail	10^{-5}	10^{-5}
Ion-acoustic turbulence	10^{-3}	10^{-1}

The initial electric field is obtained by solving Poisson's equation. Analytically, satisfying Eqs. (1)–(2) at all times, if Poisson equation is satisfied at $t = 0$, is equivalent to satisfying Eq. (1) and Poisson equation at all times (given that the collision operator conserves particle number and momentum). Numerically, we have thoroughly checked that there is no significant discrepancy in the results between the method chosen in this work (solving Poisson at $t = 0$ and solving Eq. (2) at each time step), and a method that can seem more natural (i.e. solving Poisson at each time step).

The model is applicable as a statistical description of a plasma when electromagnetic perturbations are dominated by electrostatic waves in one direction. This is relevant for plasma immersed in a strong, relatively homogeneous magnetic field [24].

1.3. Numerical codes

To investigate the impact of the numerical method, and of the numerical scheme, we perform the same simulation with three different kinetic codes.

The first code is the semi-Lagrangian code COBBLES, which is based on the splitting method [3], and on the Constrained-Interpolation-Profile, Conservative Semi-Lagrangian (CIP–CSL) scheme [25]. In the CIP–CSL scheme, the evolution of space- and velocity-integrals of the distribution function is computed from separate kinetic equations, along with the evolution of the distribution function itself, in a way that keeps a flux balance between neighboring grids. The implementation guarantees the local conservation of density, up to the machine precision. COBBLES was described, verified, validated and benchmarked in Ref. [26] for a dissipative bump-on-tail (single species) model. COBBLES is capable of accurate long-time simulations, in various regimes, including chaotic ones [27,28], of the bump-on-tail instability in a one-species, 1D plasma. COBBLES was recently extended to treat two species kinetically. The extended code and its diagnostics are verified and benchmarked in the Appendix, by recovering several results of Ref. [12], including statistical properties of anomalous resistivity.

As a side note, and a general message in computational science, let us emphasize that the conservation properties strongly depend on the simulated physics. With the same COBBLES code, for two-species ion-acoustic turbulence, compared to one-species simulations of the dissipative bump-on-tail instability [29], the conservation of entropy and total energy is degraded by several orders of magnitude. Table 2 shows the order-of-magnitude of relative error in energy and entropy conservation for these two models for the same code (COBBLES).

The second code is the semi-Lagrangian code V1D1, which was developed at the British Antarctic Survey in Cambridge, originally by R.B. Horne and M.P. Freeman, and then further by C.E.J. Watt. V1D1 is based on the MacCormack method, which is an explicit finite difference method with predictor–corrector algorithm. It was used in many works, e.g. Refs. [30,12].

The third code is a simple PIC code, PICKLES (Particle-In-Cell Kinetic Lazy Electrostatic Solver), which is based on a fourth-order Runge–Kutta method. PICKLES can handle both full-f and δf treatments [23]. In this paper we use the δf version only. We denote the number of marker-particles per species as N_p.

1.4. Numerical simulations

Unless stated otherwise, and except in the appendix, we analyze a single physical system. The mass ratio is $m_i/m_e = 4$. The system