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A Numerical Method for Solution of the Generalized Liouville Equation

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Abstract

A numerical method for the time evolution of systems described by Liouville-type equations is derived. The algorithm uses a lattice of numerical markers, which follow exactly Hamiltonian trajectories, to represent the operator d/dt in moving (i.e., Lagrangian) coordinates. However, non-conservative effects such as particle drag, creation and annihilation are allowed in the evolution of the physical distribution function, which is itself represented according to a δf decomposition. Further, the method is shown to be ideally suited to the study of a general class of systems involving the resonant interaction of energetic particles with plasma waves. Detailed results are presented for the classic bump-on-tail problem, for which the algorithm yields exceptionally smooth, low-noise evolution of wave energy, especially in the linear regime. Phenomena associated with the nonlinear regime are also described.

1. Introduction and Background

1.1 The Liouville equation

Consider a distribution function f which describes an ensemble of particles (or more generally, an ensemble of system points) following a Hamiltonian flow in the phase space Γ :

$$f = f(\Gamma, t) \quad \text{with} \quad \Gamma \equiv (q_1, \dots, q_N; p_1, \dots, p_N) \quad . \quad (1)$$

The number of system points in the phase volume element $d\Gamma$ at time t is

$$f(\Gamma, t) d\Gamma \quad . \quad (2)$$

So long as points are neither created nor destroyed, the distribution function f is known to satisfy the *Liouville equation*,

$$\frac{df}{dt} = 0 \quad . \quad (3)$$

Thus, the “fluid” of system points in this case moves incompressibly. More generally, because the phase space Γ is by definition Hamiltonian, it will always possess a hierarchy of N integral invariants, the first and N th of which are

$$\int_{\text{proj}\{\Delta\Gamma[t],1\}} dq_1 dp_1 + \dots + \int_{\text{proj}\{\Delta\Gamma[t],N\}} dq_N dp_N = \text{constant} \quad , \quad (4)$$

$$\int_{\Delta\Gamma[t]} dq_1 \dots dq_N dp_1 \dots dp_N = \text{constant} \quad . \quad (5)$$

In the above, $\Delta\Gamma[t]$ refers to any connected, moving collection of phase points. The $N - 2$ intermediate integrals – which we have not included – are written more naturally using differential forms, and we refer the reader to Ref. [1] for a general discussion. These quantities are time (and canonical transformation) invariant.

However, if one wants to model the motion of particles which can be effectively created or destroyed, then the Liouville equation, Eq. (3), is not an appropriate description – even in the case where the particles themselves still follow Hamiltonian trajectories.

1.2 The Generalized Liouville equation

As a simple example, consider the description of a one-dimensional plasma moving in an electrostatic potential field $\varphi(x, t)$. Further, assume that particles are injected into the system at a rate $S(v)$, and effectively removed by charge exchange with background neutrals at a rate $1/\tau_{cx}(v)$. Then, the relevant kinetic equation can be written

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - \frac{\partial \varphi}{\partial x} \frac{\partial f}{\partial v} = -\frac{1}{\tau_{cx}(v)} f \quad . \quad (6)$$

Here, we emphasize that even though the trajectories (or characteristics) in the phase space $\Gamma = (x, v)$ are Hamiltonian, with

$$H(v, q, t) = \frac{v^2}{2} + \varphi(x, t) \quad , \quad (7)$$

the overall motion of the phase fluid is not incompressible. Thus, Eq. (3) is not sufficient to describe the dynamics in this case.

In the general case, one may allow for non-conservative effects – that is, non-conservation along the Hamiltonian flow $\dot{\Gamma}$ – by considering f to satisfy the *generalized Liouville equation*:

$$\dot{f} = \frac{\partial f}{\partial t} + \dot{\Gamma}_i \frac{\partial f}{\partial \Gamma_i} = \Omega(f, \Gamma, t) \quad , \quad (8)$$

Here, the source function Ω simply denotes the rate of change of f along an orbit. Of course, referring back to Eq. (6), it is evident that one must provide a further moment equation for the evolution of φ (i.e., a Poisson-type equation). Despite this complication, we see that the structure of Eq. (6) is nevertheless that of the generalized Liouville equation, Eq. (8).

In all but the simplest of systems, the specification of equations to supplement the set $(\dot{f}, \dot{\Gamma})$ will be required. Specifically, the evolution of the Hamiltonian system may depend on any number of “external” quantities, such as plasma waves, whose evolution is determined self-consistently by the form of the distribution function f (through moment equations, or otherwise). For example, we could close the one-dimensional system described above by specifying a differential equation for the evolution of $\varphi(x, t)$. Regardless of the form of this equation, the motion generated by H in Eq. (7) will by necessity be Hamiltonian.

In Section 2, we describe a general method to solve Eq. (8) by following an ensemble of Hamiltonian trajectories numerically. The method decomposes the distribution f into

continuous and discrete parts according to the low-noise δf scheme². In Section 3, the present method is applied to the classic bump-on-tail problem. Simulation results in both the linear and nonlinear regimes are presented for the case of a single plasma wave, and accurate tracking of wave amplitude is demonstrated in the presence of particle creation, annihilation and wave damping. In Section 4, a discussion of techniques for numerical integration is included. A brief summary is given in Section 5.

2. The Hamiltonian Trajectory Method

The present algorithm was inspired by the work of Parker and Lee³, who outlined a fundamentally similar scheme for the gyrokinetic simulation of drift-waves. In fact, this technique falls into the same general class as any of the so-called δf algorithms², which have found considerable success in the form of low-noise particle codes for the solution of the gyrokinetic equation, and for the study of the nonlinear evolution of toroidicity-induced Alfvén eigenmodes⁴ (TAE). In what follows, we outline a general approach that can be applied to the solution of Liouville-type equations, as outlined in the introduction, including sources, sinks and background wave damping.

2.1. Derivation

For systems of interest in plasma simulation, it is often the case that f will differ only slightly from some known analytic distribution f_0 . In cases where f is only weakly distorted, it is well-established that the δf separation results in a drastic reduction in numerical “noise”. With this in mind, we begin by decomposing $f(\Gamma, t)$ in the following way:

$$f(\Gamma, t) = \underbrace{f_0(\Gamma)}_{\text{analytic}} + \underbrace{\delta f(\Gamma, t)}_{\text{markers}} \quad , \quad (9)$$

where f_0 is a chosen analytic function of coordinates (the generalization to explicit time dependence is trivial), and δf will be represented by a discrete lattice. The evolution of δf , when viewed as a functional $\delta f[\Gamma(t), t]$ on the infinite-dimensional “fluid” phase-space Γ , can then be approximated by the evolution of a finite-dimensional (n_p) set of markers:

$$\delta \dot{f}_i(t) = - \sum_{j=1}^M \dot{\Gamma}_j^{(i)}(t) \left[\frac{\partial f_0}{\partial \Gamma_j} \right]_{\Gamma=\Gamma^{(i)}(t)} \quad ; \quad i = 1, \dots, n_p \quad . \quad (10)$$

Note that we have changed the dimension of the phase space from the even number $2N$, to an arbitrary integer M . We have done so since it is common *not* to have an even dimensional phase space in various cases – such as in a gyro-averaged system, or a beam simulation. We emphasize, however, that the separation into analytic (f_0) and numerical (δf) components in no way presumes that the latter must be much “smaller” than the former. In fact, the

separation is valid in all cases. However, when the condition $\delta f \ll f_0$ is satisfied, the simulation noise is expected to be substantially less than if the entire distribution were represented numerically.

Now, the n_p equations above are supplemented by $M \times n_p$ marker equations

$$\dot{\Gamma}_j^{(i)} = F_j^{(i)}(\Gamma, Z(t)) \quad , \quad (11)$$

where the vector $Z(t)$ is an arbitrary, time-dependent function that appears in the Hamiltonian. The evolution of this vector of *parameters*, Z , need not be Hamiltonian because it does not affect the form of the time derivative operator d/dt which acts on the function $f(\Gamma, t)$ (except to contribute to the explicit time dependence through $\partial/\partial t$). Thus, one can specify an otherwise arbitrary set of equations for Z , such as

$$G(\Gamma(t), Z(t), t, d/dt) = 0 \quad . \quad (12)$$

Moreover, the dimension of Z is in no way connected with the number of markers, and in Section 3 we will show how this parametric representation is a natural means to describe a spectrum of wave amplitudes and phases $\{A_k, \alpha_k\}$ in the bump-on-tail model.

Now, it is convenient to define an arbitrary space $\mathcal{U}$, with $\text{Dim}(\mathcal{U}) = M$, which will be filled with lattice points in an asymptotically *uniform* way. Such a uniform space is related to the original phase space through

$$d\Gamma = \mathcal{J}(\mathcal{U}) d\mathcal{U} \quad , \quad (13)$$

where $\mathcal{J}$ is the determinant of the Jacobian matrix. With these definitions, it follows that integral operators transform as

$$\int f(\Gamma, t) g(\Gamma, t) d\Gamma \longrightarrow \int f_0(\Gamma) g(\Gamma, t) d\Gamma + \sum_{i=1}^{n_p} \delta f_i(t) g(\Gamma_i(t), t) \Delta\Gamma_i \quad . \quad (14)$$

where we have defined the equivalent (time-independent) phase space marker volume

$$\Delta\Gamma_i \equiv \frac{V(\mathcal{U})}{n_p} \mathcal{J}_i \quad \text{with} \quad V(\mathcal{U}) = \int d\mathcal{U} \quad . \quad (15)$$

Of course, $\mathcal{J}_i$ is constant in time as it follows its volume element in $\mathcal{U}$.

In a conventional particle simulation, one represents the entire distribution f as a sum over either δ -function, or shaped, particles. In the present notation, this would imply $f_0 = 0$, and consequently $\delta f = 0$. Thus, each δf_i is constant as it follows the flow in $\mathcal{U}$. Then, a physical quantity is determined from the more familiar association

$$\int f(\Gamma, t) g(\Gamma, t) d\Gamma \longleftrightarrow \sum_{i=1}^{n_p} \delta f_i(0) g(\Gamma_i(t), t) \Delta\Gamma_i \quad . \quad (16)$$

which is equivalent to a sum over weighted particles.

Finally, we mention that the arrow in Eq. (14) has purposely been chosen to point in both directions, as it may be desirable, or conceptually simpler, to formulate a problem initially in terms of *particles* rather than a fluid.

2.2. A nonrandom, low-noise technique to load markers

In this section we indicate a simple procedure for filling the space $\mathcal{U}$ with low-noise point sets. This method and the associated problem of particle loading are described in detail in Ref. [5]. The utility of this method stems from the avoidance of “beaming”-type instabilities which occur when loading on a regular lattice, while still maintaining a higher degree of uniformity than a random population. Such a distribution enables a “quiet-start” to the simulation.

Let $\mathcal{U}$ be the M -cube, and define

$$\mathcal{U}_i \equiv \left\{ \frac{i}{n_p}, \phi_{P(1)}(i), \dots, \phi_{P(M-1)}(i) \right\} \quad . \quad i = 0, \dots, n_p - 1 \quad . \quad (17)$$

as a sequence of n_p points in this cube, where $P(j)$ is the j -th prime ($P(1)=2$, $P(2)=3$, etc.). The function $\phi_b(i)$ is calculated by inverting the base b representation of i in the following manner:

$$\text{if } i = a_0 + a_1 b + a_2 b^2 + \dots \quad , \quad \text{then } \phi_b(i) \equiv \frac{a_0}{b} + \frac{a_1}{b^2} + \dots \quad . \quad (18)$$

Since the sequence defined by Eq. (17) is in general quasi-periodic with period

$$n_0 = P(1) \cdots P(M-1) \quad , \quad (19)$$

we should choose n_p to be an integer multiple of n_0 . An example for $M = 2$ and $n_p = 3000$ is shown in Fig. (1a).

3. Application to Bump-on-tail Instability

We apply the Hamiltonian trajectory algorithm to the classic bump-on-tail (or “warm-beam”) problem, using the Lagrangian formulation developed in Ref. [6]. This model describes the nonlinear interaction of energetic electrons with a spectrum of plasma modes. Since the nonlinearity of the bulk plasma is largely irrelevant for the growth and saturation of the unstable part of the spectrum, it is sufficient to consider the interaction of particles with “fixed” electrostatic modes. In doing so, the need to solve the Poisson equation is eliminated, and replaced by evolution equations for only the amplitude and phase of each discrete mode. Analytic features of this model are also treated in detail in Ref. [7]. In the study of wave-particle interaction, the bump-on-tail problem emerges as an important paradigm, with many features in common with more complicated stability problems, such as that posed by fast-particle-driven modes in tokamaks (i.e., fishbones or TAE modes).

3.1. Formulation in terms of the characteristic method

Throughout this example, we will restrict our discussion to the case of one wave, with amplitude A and phase α described by the natural (suitably normalized) variables $P = A \cos \alpha$ and $Q = A \sin \alpha$. The particle phase space is $\Gamma = (x, v)$. Given an initial distribution $f_0(v)$, particle annihilation rate ν , source $S(v) = \nu f_0(v)$, and background wave damping γ_d , the simulation equations become

$$\dot{x}_i = v_i \quad , \quad (20a)$$

$$\dot{v}_i = Q \cos(x_i - t) - P \sin(x_i - t) \quad , \quad (20b)$$

$$\dot{Q} = -\gamma_d Q - \beta \sum_{i=1}^{n_p} w_i \cos(x_i - t) \quad , \quad (20c)$$

$$\dot{P} = -\gamma_d P + \beta \sum_{i=1}^{n_p} w_i \sin(x_i - t) \quad , \quad (20d)$$

$$\dot{w}_i = -v_i f'_0(v_i) \Delta \Gamma_i - \nu w_i \quad . \quad (20e)$$

In the above, we have introduced the functions $w_i \equiv \delta f_i \Delta \Gamma_i$, with $\Delta \Gamma_i = \mathcal{J}_i / n_p$ (below, $V(\mathcal{U})$ is taken to be unity). Each w_i is analogous to an effective marker “weight”, which

decreases as the number of simulation markers increases, given a fixed value of f_0 . Clearly, if one sets all the w_i equal to unity, the resulting equations will correspond to a traditional particle code. Also, β represents the density of the energetic electron population relative to the fixed background plasma. We have normalized frequency and wavelength so that the resonant velocity is $v = 1$. Note that Eqs. (20a,b) correspond to Eq. (11), Eqs. (20c,d) to Eq. (12), and Eq. (20e) to Eq. (10), in the formulation of Section 2.

For the simulation, we will choose a smooth initial distribution defined over the interval $0 \leq v \leq 2$. This avoids any difficulty with reactive contributions coming from a distribution which goes discontinuously to zero at the endpoints. Choosing $f_0(v)$ to be

$$f_0(v) = \frac{1}{2}v^4(2-v)^2 \quad (21)$$

yields an unstable mode with linear growth rate

$$\gamma_L = \pi^2 \beta \quad . \quad (22)$$

Loading the unit square (y, z) uniformly, and filling the (x, v) space ($0 \leq x \leq 2\pi$ and $0 \leq v \leq 2$) according to

$$x = 2\pi y \quad , \quad (23)$$

$$v = \frac{2z(1 + c(3 - 6z + 4z^2))}{1 + c} \quad , \quad (24)$$

will give a loading preferentially weighted along $v = 1$, in proportion to the value of c (with $c = 0$ uniform, and increasing values more concentrated along $v = 1$). Examples for $c = 2, 4$ are shown in Figs. (1a,b). The Jacobian in this case is simply

$$\mathcal{J} = 4\pi \frac{1 + 3(1 - 2z)^2}{1 + c} \quad . \quad (25)$$

3.2. Linear growth rate and saturation

The first test for the efficiency and accuracy of the algorithm is to reproduce known values for the linear growth rate γ_L , and mode saturation ratio $c_L = \omega_i/\gamma_L$ (with $\omega_i = \sqrt{A}$, and $c_L \sim 3.3$). Fig. (2) shows the results of a 20000 particle simulation. Even for a much smaller number of particles, numerical noise in the linear growth stage is exceptionally low

– much smaller than in conventional simulations⁸ – and the linear growth rate is exactly reproduced. Of course, in this case, deviations from the linear theory are expected due to the finite particle trapping width and variation of the equilibrium distribution; that is to say, the simulation shows the *true* linear evolution. The extent to which the physical distribution is flattened is shown in Fig. (3), which superimposes the distributions corresponding to initial and saturated states. Once the wave has saturated, many more markers are required, in general, to resolve the dynamical evolution; and even as the number of markers is increased indefinitely, convergence is only observed for a finite time, as nearby states will diverge exponentially due to turbulent mixing of phase volume. This phenomenon is illustrated in Fig. (4), where simulations with 20000 and 30000 markers are compared.

3.3. Particle conservation and differential amplitude update

Consider first the special case $\gamma_d = \nu = 0$. Here, we expect the total particle number in the corresponding physical system to be time invariant (since $\nu = 0$). However, this invariance is not exactly realized in the numerical method for a finite number, n_p , of markers due to discretization error. If we begin with $\delta f = 0$ (i.e., all $w_i(0) = 0$), then physical particle numbers are given by:

$$n_0 = \int f_0(v) dx dv \quad (\text{initial number}) \quad , \quad (26a)$$

$$\delta n(t) = \sum_{i=1}^{n_p} w_i(t) \quad (\text{fluctuation}) \quad , \quad (26b)$$

with the total number $n(t) = n_0 + \delta n(t)$. In the limit $n_p \rightarrow \infty$, we expect $\delta n = 0$ to obtain, thus satisfying the requirement of particle conservation. In general, these conclusions indicate that one should consider the size of the relative fluctuation $\delta n/n_0$ as a useful measure of code accuracy and convergence. Fig. (5) shows a plot of this quantity for a simulation with $n_p = 1000$. A general feature, common to this and other models of wave-particle interaction we have studied, is that the simulation noise increases substantially as the mode nears saturation. In the present case, this occurs at roughly $t/2\pi \sim 40$.

A relatively important feature of the algorithm is the differential form of the amplitude update given by Eqns. (20c,d). In fact, this method of update is quite natural in the context of the Lagrangian formulation of Ref. [5]. However, consider the case of a single mode: one can form the following identity directly from the original Lagrangian equations:

$$\left(\frac{P^2}{2} + \frac{Q^2}{2}\right) + \beta \sum_j v_j = \text{constant} \quad . \quad (27)$$

This quantity represents the exact conservation of momentum, where j is simply a physical particle index. In fact, this equation also reflects conservation of system energy, to the extent that

$$\frac{d}{dt} \left(\frac{v^2}{2} \right) = v \dot{v} \simeq \dot{v} \quad (28)$$

for resonant particles. The identity, Eq. (27), represents an algebraic method for the update of the wave amplitude, according to

$$\frac{A(0)^2 - A(t)^2}{2} \longrightarrow \beta \sum_{i=1}^{n_p} w_i v_i \quad (29)$$

However, for a moderate number of particles, the sum over particle momenta is a rapidly oscillating function of time. In practice, an amplitude update based on Eq. (29) yields a much noisier function than the amplitude determined from the differential equations. This contrast is shown clearly in Fig. (6), where the amplitude $A(t)$, calculated according to Eq. (29), is compared with the amplitude computed from the differential forms, Eqs. (20.c,d). The oscillations present in the solid curve of Fig. (5) clearly result from non-resonant particle noise. One must conclude, then, that an extra degree of “smoothing” is obtained from a differential update. Moreover, the wave-particle Lagrangian formulation provides an intrinsic method for the update of wave amplitude in the case of an arbitrary spectrum of waves $\{P_k, Q_k\}$.

3.4. Convergence in the strongly nonlinear regime

The addition of a particle relaxation rate ν and background damping rate γ_d to the model represents a non-conservative generalization to the overall dynamics. When these parameters are finite, two possible wave evolution scenarios are possible. The first is steady-state saturation, and occurs roughly when the relaxation rate exceeds the background damping rate. However, in the opposite limit of strong background damping, “bursting” of the wave amplitude may occur. Both these phenomena occur on time scales much longer than the linear growth phase, and are relatively difficult to resolve numerically. We concentrate on the steady-state regime, for which Ref. [7] gives the following estimate of the ratio of trapping frequency to linear growth rate:

$$\frac{\omega_t}{\gamma_L} = 1.9 \frac{\nu}{\gamma_d} \quad . \quad (30)$$

Comparison of the numerical model with this estimate is illustrated in Fig. (7), where a slow approach to the steady-state value is in fact observed.

4. Choice of Integration Method

The choice of integration method is clearly an important concern for the development of a particle code. Generally, substantial improvements in performance/accuracy over typical adaptive Runge-Kutta or predictor-corrector (PC) methods are achievable. For example, in a traditional particle simulation (i.e., no δf separation or dissipative terms) of the bump-on-tail problem⁸, symplectic integration methods⁹ have been shown to be far superior to Runge-Kutta methods in terms of overall efficiency and accuracy. There are difficulties, however, which arise in the application of symplectic algorithms to the characteristic method of this paper. Most notably, since non-Hamiltonian degrees of freedom are present in the system of equations, one must be content with hybrid symplectic-nonsymplectic algorithms. Moreover, the simplicity of the differential equations describing the bump-on-tail problem makes single-step (i.e., Runge-Kutta) methods somewhat more attractive than for problems for which the time evolution requires comparatively expensive function evaluations.

Our development of the characteristic method was motivated by the study of the non-linear TAE problem^{4,10}, for which the background Hamiltonian orbits are the guiding center motion of fusion-product α -particles. Unfortunately, while the composite wave-particle system in this case is also Hamiltonian (in the absence of sources/sinks), the complicated form of the Hamiltonian function appears to prohibit the construction of an explicit symplectic integrator. Moreover, because of the complexity of function evaluations in the case of general toroidal geometry, we have found that high-order explicit Adams-Bashforth¹¹ methods are particularly efficient. However, for computer systems which have limited amounts of core memory (i.e., < 100 Mb), the order of the algorithm must be decreased to limit storage. Since the dynamics of a particle simulation for $n_p \gg 1$ are expected to be fluid-like – requiring the same temporal resolution throughout the simulation – fixed-time-step algorithms are most appropriate, with the choice of time-step determined by accurate resolution of the motion of resonant particles. Clearly, in this case, selection of a predominantly “resonant” set of particle markers is equally appropriate. We defer a more detailed discussion of these ideas to a subsequent publication.

5. Summary and Conclusions

In this paper we have developed a systematic numerical approach to solve the generalized Liouville equation, which makes use of a numerical grid defined by the Hamiltonian trajectories of the associated conservative system, along with a δf decomposition of the distribution function. The applicability of the method to systems which may have a substantial coupling to non-conservative degrees of freedom (i.e., waves subject to background dissipation) has also been indicated. Various numerical tests have been performed using a discrete particle model of the bump-on-tail problem, and show excellent agreement with existing analytic estimates of wave growth rate and saturation amplitude.

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[1] Marker distributions generated using the sequence defined by Eq. (17). (a) Uniform distribution on the unit square; (b) resonance-loaded distribution, Eqs. (23) and (24), for $c = 2$ and (c) for $c = 4$.

[2] Linear evolution and subsequent nonlinear saturation of a single mode, determined by solving Eqs. (20) for $\beta = 0.002$ and $\gamma_d = \nu = 0$ with 20000 markers. Dashed curves show analytic predictions for linear evolution and saturated amplitude.

[3] Comparison of equilibrium and saturated distributions for simulation of Fig. (2). Flattening at the resonant velocity $v = 1$ is clearly evident.

[4] Close-up of simulation of Fig. (2), including comparison with 30000 marker simulation.

[5] Relative fluctuation in particle number for a simulation with $n_p = 840$ and $\beta = 0.002$. In this case, we expect $\delta n \rightarrow 0$ as $n_p \rightarrow \infty$ to reflect particle conservation in the continuous Liouville system.

[6] Evaluation of $A(t)$ using the energy integral, Eq. (29), (solid curve) compared with differential update, Eqs. (20c,d), (dotted curve) for the simulation of Fig. (5).

[7] Slow relaxation to steady-state wave amplitude in the presence of finite dissipation ($\gamma_d = \nu = 0.001$) for $\beta = 0.004$. Dashed horizontal line shows the analytic estimate, Eq. (30), for the steady-state value.