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Can Computer Simulation Predict the Real Behavior of Turbulence?

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Abstract

Most of laws of physics have the form of ordinary or partial differential equations, amenable to various numerical approaches. If the number of absolute degrees of freedom, unconstrained by conservation laws, is three or more, the dynamics are generally chaotic. The chaos primarily manifests itself in the sensitive dependence on the initial conditions (the Lyapunov exponentiation of phase-space orbits). As any initial inaccuracy, which may be due to finite space grid, time step, or roundoff error, is exponentially enhanced by the dynamics, there is no chance, whatever the available computer power, to have quantitatively accurate predictions in terms of *individual orbits*, as far as many Lyapunov time scales are concerned. In terms of *average quantities*, however, numerical predictions can be satisfactory and correct. This is the case, when the original system and its finite-difference model, both chaotic, are characterized by (almost) the same statistical properties. We discuss the conditions under which this requirement of *statistical consistency* can be fulfilled. We arrive at the conclusion that there is a wide class of turbulent systems, for which this question remains completely unanswered, namely those where turbulence is non-Gaussian. Plasma turbulence in tokamaks and weather prediction are practically important examples of such systems. For these kinds of turbulence, the predictions of high-resolution computation may have nothing to do with real dynamics. The reason for this difficulty is that finite-dimensional discretizations, used to cast partial differential equations into a form understood by computer, do not generally converge to what we expect in the high-resolution limit.

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1 Introduction

With the advent of supercomputers and fast workstations, theoretical physicists have got a powerful extention of their traditional tools: brain, pen, and paper. Many people now think that, given the exact mathematical formulation of the physical laws appropriate for the given problem, plus sufficient computer power, one can make an accurate prediction of the system behavior. In this way, we are supposed to find out, for example, what the energy life time of fusion plasma in a tokamak reactor [1], or the weather and climate [2] are going to be.

The job of making numerical predictions about natural or artificial dynamical systems involves several steps.

1. Mathematical formulation of the problem. That is, writing down a closed system of equations for appropriate variables. Typically, these equations can be cast in the form of ordinary (ODE) or partial (PDE) differential equations with possible integral closures.

2. Identifying appropriate initial and boundary conditions.

3. Choosing a numerical algorithm which fits best the underlying system. Digital computers cannot manage continuous space and time, and therefore one has to model the original differential system by a finite-difference scheme. For ODE this implies a discrete-time mapping. For PDE, a discretization should be done first, whereby the PDE is replaced by a sufficiently large number of ODE's. The representation of the discretized system may vary from fixed or adjustable grids in real or Fourier space to singular (point) vortices. Then a time-advance mapping for these discrete variables should be worked out.

4. Coding the algorithm and running the code.

One can encounter difficulties, including fundamental ones, on any step of the above program. The purpose of this note is to emphasize the fundamental problems which are found on step 3 and which appear to be not appreciated by computer-using communities. Specifically, we will discuss the problem of the discretization of PDE for the purpose of computation. We restrict this discussion to the case of Hamiltonian, or weakly dissipative, continuum systems exhibiting turbulent behavior. To the surprise of this author, the procedure of PDE discretization is found to be inherently ambiguous for many systems of interest. Because of this ambiguity, the predictions of many contemporary high-resolution turbulence computations may only by a lucky chance resemble the behavior of real systems they model. So far, this chance is out of our understanding and control.

2 Computing ODE's beyond the Lyapunov time

The phase space of an ODE system is finite-dimensional. Understanding the structure of phase space helps understanding the dynamics, often in a very nice way such as in the problem about two wide wagons trying to pass each other on a narrow road [3, p. 2].

Conservations laws, if any, project the entire N-dimensional phase space onto an $(N-N_I)$-dimensional manifold, where N_I is the number of the invariants of motion. When $N-N_I \leq 2$, the system is integrable, because we do not expect anything bad of a field of non-self-intersecting 1D orbits constrained to lie on a 2D surface (the existence and the unicity of the solution is assumed). However, when the dimension of the conservative manifold is three or more, phase-space orbits can, and generally will (unless we overlook another conservation law), perform chaotically. The trajectories can remain perfectly smooth, but, when the dynamics are chaotic, they become *sensitive to the initial conditions.* Mathematically, this means that two infinitesimally close trajectories diverge *exponentially* from each other. The characteristic time of e-folding of the distance between the two trajectories, called the Lyapunov time t_L, is of order the nonlinear interacton time in the system, such as the collision time for particles. The situation can be more complicated for systems close to integrable [4, 5, 6], which we do not discuss here.

The exponential $\exp(t/t_L)$ is not just a function of time; it is such a thing that any realistic initial or roundoff error will lead to a hopelessly invalid solution in just a few Lyapunov times. Even setting aside the problem of the accuracy of the initial data, we dare to say that computers will never become "exponentially accurate," and therefore a satisfactory computation of *individual orbits* over many Lyapunov times is, and will be, out of question.

So what, one may say, chaos is reality and the computer complies with this reality. Absolutely! But the meaning of "complies" should be defined more precisely. Namely, when the dynamics are chaotic, we must use a statistical description, whereby various observable averages are to be predicted. So we arrive at the principal requirement imposed on our finite-difference algorithm:

> The statistics of the original system and those of the numerical algorithm must be the same, at least in the limit of "high resolution" (small time step, fine space grid, many Fourier modes, etc.).

This requirement, which we will refer to as the *statistical consistency* of the numerical algorithm, seems to be hard to fulfil, because, known the exact statistics of the original system, why should the computation at all be necessary? It appears, fortunately, that one can compare statistics of two different systems without the knowledge of what these statistics exactly are.

Consider the case of a Hamiltonian system, where the Hamiltonianity is important only in as much as the Liouville theorem holds. The Liouville theorem says that there are variables (not necessarily canonical) such that the motion in the corresponding phase space is incompressible. This makes the trajectories uniformly (at least in the limit of the large dimension $N - N_I \gg 1$) cover the conservative manifold, thereby leading to the microcanonical Gibbs statistics, whose predictions for "usual" thermodynamical systems are found to be in a remarkable agreement with experiment.

Hence the statistical properties of an ODE system are completely determined by the geometry of the phase space, including the dimension and the shape of the conservative manifold and the Liouvillianity of motion on this manifold. Then the statistical consistency means the following:

1. The finite-difference scheme should conserve the same (and as many) integrals of motion, as the original system. This conservation may be exact or approximate; in the latter case the error in invariants should be small over many Lyapunov times. This requirement is relatively easy to fulfil by taking sufficiently small time step and/or smart integrator.

2. For a Hamiltonian system, it is best to use a symplectic integrator [7, 8, 9], which is an incompressible time-advance mapping respecting the Liouville theorem. This requirement may also be relaxed, but to a lesser degree than the exact conservativity of the mapping: If the stepper is compressible, then the phase volume tends to shrink/expand exponentially with the number of steps. In this case one must not believe the numerical results obtained by integration over time longer than the stepper's phase volume e-folding time. (Has anyone been concerned with measuring this time?)

By and large, the satisfactory (i.e., statistically consistent) computation of not too many Hamiltonian ODE's over many Lyapunov times is feasible, provided that the symplecticity of the integrator is ensured, or the small non-symplecticity is duly controlled.

When the number of degrees of freedom goes beyond reasonable limits, physicists switch to the description in terms of continuous media. The corresponding PDE systems have an infinite-dimensional phase space, where real computational problems start.

3 Discretization of PDE systems and statistical consistency

The message of this section is that all Hamiltonian PDE systems can be divided into two categories: (1) those which can be modelled numerically in a statistically consistent way and (2) those which cannot, at least at the present level of understanding of turbulence.

Under "turbulence" we broadly understand chaos in PDE's. The infinite-dimensionality of the functional phase space requires the standard definitions of chaos and statistical averages, borrowed from finite-dimensional phase spaces, be carefully reconsidered.

There appears to be no major problem with the concept of norm, or distance, in the functional space. The norm, defined as the square integral of a function over the domain of interest, satisfies all usual properties (like the inequality of triangle) and can be used to define the Lyapunov exponent as a measure of chaos. One must be warned, however, that chaotic properties are no longer invariant with respect to the variables used to describe the system. For example, the magnetic field $\mathbf{B} = \boldsymbol{\nabla} a(x, y, t) \times \hat{\mathbf{z}}$ and the fluid velocity $\mathbf{v} = \boldsymbol{\nabla}\psi(x, y, t) \times \hat{\mathbf{z}}$ in two-dimensional MHD turbulence behave chaotically, in the sense of the exponentiation of the square distance $\int[(\mathbf{B}_1 - \mathbf{B}_2)^2 + (\mathbf{v}_1 - \mathbf{v}_2)^2]d^2\mathbf{x}$ between the two infinitesimally close solutions, but the magnetic flux a and the fluid stream function ψ do not [10].

What is more important, the statistical description of turbulence necessarily requires taking averages, or *integrating in a functional space.* One should not think that, once the concept of *distance*, or *norm* is easily extended to the functional space, we can go ahead and do the same for *volume*, or *measure.* Not at all! Attempts to integrate functionals with respect to functions have been around for many years [11, 12, 13, 14], and it was found that these integrals make sense (i.e., converge to something unique under reasonable limits) only when the integrand involves the exponential of square highest-order derivative, which is characteristic of Gaussian functionals. Such functional (path) integrals are known as Wiener or Feynman integrals for the case of real or imaginary exponential, respectively. This kind of integrals do exist, if a proper care of normalization is taken, regardless of the way the system is discretized before passing to the continuum (infinite-dimensional) limit [12].

The simplest example of Wiener's integral for functions of one variable is due to Wiener himself. Consider a particle performing a continuous-time Brownian motion along the x axis, starting from $x = 0$, with the diffusion coefficient D. Then the probability density of the particle position at time t is a function of x:

$$p(x) \propto \exp\left(-\frac{x^2}{4Dt}\right) . \tag{1}$$

If one is interested in the probablity density of the entire history $x(t)$, $0 < t < T$, then the functional

$$P[x(t)] \propto \exp\left(-\int_0^T \frac{\dot{x}^2(t)}{4D} dt\right) \tag{2}$$

should be used.

The average over the distribution (1) in the 1D space of x,

$$\langle f(x) \rangle = \frac{\int f(x) p(x) dx}{\int p(x) dx} , \tag{3}$$

is a well defined quantity. The functional-space average,

$$\langle F[x(t)] \rangle = \frac{\int F[x(t)] P[x(t)] \mathcal{D}x(t)}{\int P[x(t)] \mathcal{D}x(t)} , \tag{4}$$

on the contrary, may or may not exist even for "well-behaved" functionals $F[x(t)]$. Unlike the existence of the usual average (3), this is a very nontrivial fact that quantity (4) may be *sometimes* well defined. The latter means that the result of averaging is independent of the way the functional space of $x(t)$ is discretized. Specifically, if we choose to parametrize the function $x(t)$ by its values $x_1, x_2, \ldots, x_N$ at times $t_1, t_2, \ldots, t_N = T$, respectively, and thereby replace $\mathcal{D}x(t) \to dx_1 dx_2 \dots dx_N$, we must require that the result be independent of the lengths of the time intervals $t_i - t_{i-1}$, in the limit when the longest of them goes to zero. It can be shown [12] that this is true for functionals $F[x(t)]$, which do not depend on the derivatives of x, such as for $F[x] = \int_0^T f(x(t))dt$.

The existence of certain averages can also be ensured for probability functionals different from (2), but only if P is Gaussian (that is, proportional to the exponential of a negative definite quadratic form) in the highest-order derivative of x. The Gaussian path integrals can be solved using various discrete variables, such as truncated Fourier, or other eidenmodes; the result will be the same. On the contrary, non-Gaussian path integrals have no definite value. For example, for $P \propto \exp\left(-\int_0^T \dot{x}^4(t)dt\right)$, the result of the averaging (4) will essentially depend on the ratio of the time intervals used to discretize the function $x(t)$.

What is the relation between the Gaussian and non-Gaussian functional integrals and the numerical solution of chaotic PDE's? As disscussed in Sec. 2, the statistical properties of the computer code must be identical, or converge in the high-resolution limit, to those of the original system. In order to impose this requirement, we must understand the general statistical properties of the system.

For a conservative Hamiltonian system evolving over many Lyapunov times, the probability functional is usually given by the Boltzmann-Gibbs distribution

$$P[\psi(\mathbf{x})] \propto \exp\left(-\sum_{i=1}^{N_I} \alpha_i I_i[\psi]\right) , \tag{5}$$

where $\psi(\mathbf{x}, t)$ denotes the field variables, the summation in the exponential is taken over all isolating invariants I_i, and α_i are the reciprocal temperatures corresponding to each invariant. The temperatures are to be found from the initial state by requiring the average values of the invariants, $\langle I_i \rangle$, be equal to their initial values. As discussed in Ref. [10], this results in a Gaussian probability functional only when *all invariants are not more than quadratic in the highest-order-derivative variable.* Consider three examples.

Reduced magnetohydrodynamics [15] describe the slow plasma motions across a strong magnetic field in terms of the perturbed magnetic flux function $a(x, y, z, t)$ and the fluid stream function $\psi(x, y, z, t)$:

$$\partial_t a - \partial_z \psi = \{\psi, a\} , \tag{6}$$

$$\nabla_\perp^2 (\partial_t \psi - \partial_z a) = \{\psi, \nabla_\perp^2 \psi\} - \{a, \nabla_\perp^2 a\} , \tag{7}$$

where $\{\ldots, \ldots\}$ denotes the Jacobian and $\nabla_\perp^2$ the Laplacian in the (x, y) plane, and non-dimensional variables are used. The invariants of energy

$$E = (1/2) \int [(\nabla_\perp a)^2 + (\nabla_\perp \psi)^2] \, d^3\mathbf{x} , \tag{8}$$

magnetic topology

$$I_n = \int a^n \, d^3\mathbf{x} , \tag{9}$$

and cross topology [16]

$$J_n = \int a^n \, \nabla_\perp a \cdot \nabla_\perp \psi \, d^3\mathbf{x} \tag{10}$$

involve the highest-order-derivative variables, ∇a and $\nabla \psi$, not more than quadratically. Therefore the Gibbs ensemble (5) of ideal RMHD turbulence is Gaussian, and averages taken with the help of any convenient set of variables have a uniqie meaning in the high-resolution limit.

The Charney-Hasegawa-Mima equation [17] describes two-dimensional nonlinear drift waves in a magnetized plasma or Rossby waves in a rotating atmosphere or ocean:

$$\partial_t \omega = \{\psi, \omega\} , \quad \omega = \psi - R^2 \nabla^2 \psi + h(x, y) , \tag{11}$$

where R is the ion Larmor radius or the Rossby radius and $h(x, y)$ models possible inhomogeneity. In the limiting case of $R \to \infty$ and $h(x, y) \equiv 0$, Eq. (11) becomes the Euler equation describing two-dimensional incompressible inviscid liquid, of which several high-resolution computations have been reported recently [18, 19, 20, 21, 22]. The invariants of

Eq. (11) are the energy

$$E = (1/2) \int [\psi^2 + R^2 (\nabla\psi)^2] \, dxdy \tag{12}$$

and the topological (frozen-in) invariants

$$I_n = \int \omega^n \, dxdy \; . \tag{13}$$

As the generalized vorticity ω involves second derivatives of the stream function ψ, the topological invariants are non-quadratic in the highest derivative of ψ, and the Gibbs ensemble (5) is non-Gaussian. Hence the statistics computed using different sets of discrete variables will be different. For example, one can model the continuum vorticity field by a large number of point vortices with the strengths q_i:

$$\omega(\mathbf{x}, t) = \sum_{i=1}^{N} q_i \delta(\mathbf{x} - \mathbf{x}_i(t)) \; . \tag{14}$$

The given field of ω can be approached by (14), as $N \to \infty$, for different choices of q_i/q_j. The corresponding Gibbs statistics in this limit happen to be also different [23, 24], which is due to the non-Gaussianity of the Gibbs distribution (5). This raises doubts in the applicability of the canonical Gibbs statistics to 2D fluid turbulence [10].

The Vlasov-Poisson system describing the collisionless stellar dynamics, is as follows:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} - \frac{\partial \phi}{\partial \mathbf{x}} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0 \; , \tag{15}$$

$$\frac{\partial^2 \phi}{\partial \mathbf{x}^2} = -4\pi G \int f \, d^3\mathbf{v} \; , \tag{16}$$

where $f(\mathbf{x}, \mathbf{v}, t)$ is the (6D) phase-space density of stellar matter, $\phi(\mathbf{x}, t)$ the gravitational potential, and G the gravity constant. Various modifications to Eqs. (15)-(16) can be done in order to describe a plasma with different particle species, where the effects of magnetic field should be included. In addition to momentum and angular momentum, which are linear in f, the Vlasov-Poisson system conserves the energy

$$E = (1/2) \int f \mathbf{v}^2 \, d^3\mathbf{x} \, d^3\mathbf{v} + (G/2) \int f\phi \, d^3\mathbf{x} \, d^3\mathbf{v} \; , \tag{17}$$

and the topological invariants (Casimirs)

$$I_n = \int f^n \, d^3\mathbf{x} \, d^3\mathbf{v} \ . \tag{18}$$

As the potential ϕ involves an integration of the density f [by virtue of solving the Poisson equation (16)], the quantity f appears as the highest-order-derivative quantity. Then the arbitrary-power topological invariants (18) kill the Gaussianity of the Gibbs distribution. The non-uniqueness of the most probable state, which was discovered by Lynden-Bell [25], is due to this non-Gaussianity.

Thus, if the canonical ensemble (5), where all invariants of motion are incorporated, applies to stellar relaxation [25] or 2D fluid turbulence [26, 27, 28], these kinds of turbulence are non-Gaussian. Then there is no way to compute averages in a manner independent of the choice of discretization, and statistics become pointless.

We do believe, however, that these, non-Gaussian systems have unique and predictable statistics of non-Gibbsian nature. It is quite possible that the correct averages can be obtained by formally using the Gibbs probability functional (5); however, for this purpose the discretization, on which the averages depend significantly, must be *appropriately chosen.* These special, but perhaps non-unique, discrete variables are most appropriate for the numerical algorithm to be used for the considered system.

A similar conclusion has been reached by J. B. Taylor [24] who pointed out the necessity of an appropriate choice of the strengths of point vortices, which are another kind of discretization of two-dimensional Euler fluid. In Ref. [24] it was suggested that this choice be made on the basis of the vortices' response to small viscosity.

4 Remarks on dissipative systems

Dissipation, which is always present both in nature and in computer algorithms, acts so as to make the effective dimension of the phase space finite-dimensional. More precisely, a driven dissipative PDE system has an attractor, whose dimension N is bounded [29].

This may be of no help for the computation of fluid turbulence at high Reynolds number $\mathcal{R}$, because $N(\mathcal{R})$ increases without limit as $\mathcal{R} \to \infty$. When the number of variables N, necessary to resolve the motion on the atractor, goes beyond the numerical feasibility, one has to solve a PDE system, with the entailed discretization problems. Even low-dimensional attractors have a sophisticated fractal geometry, which has complicated the development of the statistical ("ergodic") theory of motion in such systems [30].

It therefore appears very difficult to address the *a priori* statistical consistency of codes used to compute the high-Reynolds-number fluid turbulence, and one has to rely upon empirical comparisons of various codes [22].

5 Conclusion

We can summarize as follows. In order to carry out the numerical solution of an intrinsically chaotic system for many Lyapunov times, one must design a computer code which will reproduce the statistical behavior of the system. This requirement is stringent, but controllable for a small number of ODE.

For PDE describing Hamiltonian turbulence, the situation depends drastically on the structure of the integrals of motion. If all these integrals are not more than quadratic in the highest-order-derivative variable, then increasing the resolution of any reasonable algorithm means increasing the accuracy of computation in the statistical sense. This is only a general property of convergence in such PDE systems which does not address the important practical issues of the code efficiency.

For Hamiltonian systems, having invariants non-quadratic in the highest-order derivatives, the situation is more complicated. These systems include the practically important examples of geophysical fluid dynamics and collisionless plasma kinetics. For these systems, increasing the resolution may not lead to desired results, unless the discretization of the PDE is appropriately chosen. It appears that to make this choice is not much easier than solving the underlying problem of turbulence.

This principal conclusion is somewhat negative, and more conceptual work is needed to understand the statistics of non-Gaussian turbulence and thereby the appropriate choice of computer algorithms, by which this kind of turbulence may be satisfactorily modelled.

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