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H. Sigurgeirsson and A.M. Stuart,

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Appears in *Foundations of Computational Mathematics*, *LMS Lecture Note Series 284,*

editors R.A. DeVore, A. Iserles and E. Suli.

Cambridge University Press (2001).

London Mathematical Society
Lecture Note Series 284

Foundations of Computational Mathematics

Edited by
Ronald A. DeVore, Arieh Iserles & Endre Süli

CAMBRIDGE
UNIVERSITY PRESS

Statistics From Computations

Hersir Sigurgeirsson
Scientific Computing and Computational Mathematics Program
Gates 288, Stanford University
Stanford CA94305-4040, USA
Email: hersir@stanford.edu

A. M. Stuart
Mathematical Institute
Warwick University
Coventry CV4 7AL, UK
Email: stuart@maths.warwick.ac.uk

Abstract

The study of numerical methods for initial value problems by considering their approximation properties from a dynamical systems viewpoint is now a well-established field; a substantial body of knowledge, developed over the past two decades, can be found in the literature. Nonetheless many open questions remain concerning the meaning of long-time simulations performed by approximating dynamical systems. In recent years various attempts to analyse the statistical content of these long-time simulations have emerged, and the purpose of this article is to review some of that work. The subject area is far from complete; nonetheless a certain unity can be seen in what has been achieved to date and it is therefore of value to give an overview of the field.

Some mathematical background concerning the propagation of probability measures by discrete and continuous time dynamical systems or Markov chains will be given. In particular the Frobenius-Perron and Fokker-Planck operators will be described. Using the notion of ergodicity two different approaches, *direct* and *indirect*, will be outlined. The majority of the review is concerned with indirect methods, where the initial value problem is simulated from a single initial condition and the statistical content of this trajectory studied. Three classes of problems will be studied: deterministic problems in fixed finite dimension, stochastic problems in fixed finite dimension, and deterministic problems with random data in dimension $n \to \infty$; in the latter case ideas from

statistical mechanics can be exploited to analyse or interpret numerical schemes.

Throughout, the ideas are illustrated by simple numerical experiments. The emphasis is on understanding underlying concepts at a high level and mathematical detail will not be given a high priority in this review.

1 Introduction

It is well-known that, in general, individual trajectories of dynamical systems cannot be well approximated over long time-intervals, since well-posed initial-value problems admit exponentially divergent trajectories.† However, experimental evidence strongly suggests that often statistics can be robustly computed even when trajectories cannot. The aim of the paper is to survey various avenues of investigation which attempt to justify this observation. Definitive results are few and far between and the overall picture is far from complete. However a general framework is starting to emerge and it is therefore useful to set it out here. Ultimately, study of the robustness of statistics generated through computations of dynamical systems will both add significantly to the body of existing theoretical results concerning the approximation of dynamical systems [30, 34] and lend weight to the large number of initial-value calculations routinely performed in the sciences and engineering where statistical information is extracted from the data. Our presentation is informal and is intended to be suggestive of the important ideas, rather than being precise and detailed.

We will study both the effect of rounding error on maps and of time-discretization on (ordinary and stochastic) differential equations. To illustrate the kinds of issues to be discussed consider the following

Example – The Hénon map Figure 1.1 shows some results from computer simulation of the map

$$\begin{aligned} x_{n+1} &= 1 - 1.4x_n^2 + 0.3y_n, & x(0) &= 0, \\ y_{n+1} &= x_n, & y(0) &= 0. \end{aligned} \tag{1.1}$$

Figure 1.1 top left shows the attractor for this map, generated by a double-precision arithmetic simulation. Figure 1.1 top right shows the difference between the two trajectories, one with single precision arithmetic, the other with double. Since these trajectories are so different

† In the special case of hyperbolic systems shadowing ideas can be applied to give long-time approximation for problems with divergent trajectories.

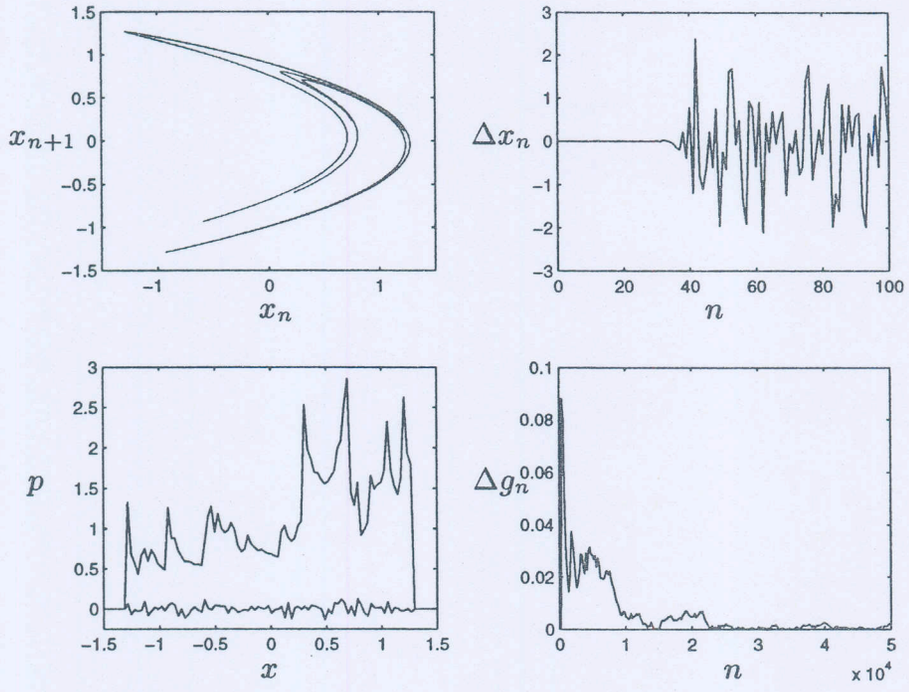

Fig. 1.1. The Hénon map. Upper left: Attractor, generated by a double-precision arithmetic simulation. Upper right: The difference between two trajectories, one computed with single precision arithmetic, the other with double. Lower left: Histogram of the empirical probability density for the x variable, computed from very long-time simulations in single precision, and the difference between the histogram computed in single and double precision. Lower right: Difference in the time averages $\frac{1}{n+1}\sum_{k=0}^{n} g(x_k)$ with $g(x) = \left(\frac{x+1.5}{3}\right)^2$.

it is natural to question whether they contain any meaningful information about (1.1). In this paper we will concentrate on the statistical properties of such simulations. To this end it is natural to compare the empirical probability densities generated by the single and double precision calculations. Histograms for the x variable, computed from very long-time simulations in both single and double precision, and their difference are shown in Figure 1.1 bottom left, and the difference in the time averages $\frac{1}{n+1}\sum_{k=0}^{n} g(x_k)$ with $g(x) = \left(\frac{x+1.5}{3}\right)^2$ in Figure 1.1 bottom right. The closeness of the single and double precision calculations in Figures 1.1 (bottom) is remarkable and suggests that, even when the trajectories themselves are unreliable, the statistics contained within them may be meaningful. ■

In many of the examples that follow we show figures similar to Figure 1.1. In each case we perform two computer simulations of the same

trajectory using single and double precision in the case of maps, and two different time steps in the case of differential equations. The upper left corner shows a single trajectory or its projection onto some two dimensional space, the upper right the difference between the x coordinates of the two trajectories, the lower left corner shows the densities of the x coordinate and their difference, and the lower right figure shows the difference between some time averages.

In section 2 we outline some mathematical background which will suggest what is required to substantiate observations about the robustness of statistics such as those exemplified by the Hénon map. We will introduce the Frobenius-Perron operator and the Fokker-Planck or Liouville equations which describe the propagation of measures by deterministic or random dynamical systems. Using this mathematical background we will distinguish between direct and indirect approaches to the problem of approximating statistics and we will highlight three important classes of problem:

A) deterministic problems in $\mathbb{R}^n$ with n fixed;
B) stochastic problems in $\mathbb{R}^n$ with n fixed;
C) deterministic problems in dimension $n \to \infty$ with random initial data.

In sections 3,4 and 5 we will discuss problems from categories A), B) and C) respectively.

2 Mathematical Background

We start by outlining how probability measures are propagated by a variety of deterministic and random dynamical systems. For simplicity we first consider deterministic maps. Imagine that

$$x_{n+1} = G(x_n), \tag{2.1}$$

where x_0 is a random variable with density p_0. If we define the *Frobenius-Perron* operator

$$(\mathcal{L}p)(x) = \sum_{y \in G^{-1}(x)} \frac{p(y)}{|\det\, dG(y)|},$$

and provided sufficient smoothness allows us to construct a density p_n for x_n, then this density satisfies

$$p_{n+1} = \mathcal{L}p_n.$$

A smooth *invariant measure* has density p:

$$p = \mathcal{L}p.$$

In both cases suitable decay of the densities at infinity is required.

It is interesting to note that, in general, this iteration may admit quite non-smooth densities. The following example shows this.

Example – The Tent Map If

$$G(x) = \begin{cases} 2x, & x \in [0, \frac{1}{2}), \\ 2 - 2x, & x \in [\frac{1}{2}, 1], \end{cases} \tag{2.2}$$

then

$$G^{-1}(x) = \left\{ \frac{x}{2}, \frac{2-x}{2} \right\}.$$

Thus

$$p_{n+1}(x) = \frac{1}{2}\left[p_n\left(\frac{x}{2}\right) + p_n\left(\frac{2-x}{2}\right) \right], \quad x \in [0,1].$$

Thus any singularity in p_n will produce a singularity in p_{n+1}. However, some limited smoothing is present due to the repeated scaling by a factor of 2 and a smooth invariant measure is

$$p(x) \equiv 1, \quad x \in [0,1].$$

In fact this invariant measure is unique within a sufficiently smooth class of functions and $p_n \to p$ in this class – see [42]. ■

We now randomise (2.1) to get the Markov chain (θ_n i.i.d. ν)

$$x_{n+1} = G_{\theta_n}(x_n) \tag{2.3}$$

where x_0 is distributed as before. For simplicity we assume that $G_\theta(\cdot)$ is invertible for all θ. We define the Frobenius-Perron operator

$$(\mathcal{L}p)(x) = \int \frac{p(G_\theta^{-1}(x))}{|\det\, dG_\theta(G_\theta^{-1}(x)|} \nu(d\theta).$$

Then, if it exists, the probability density for x_n satisfies

$$p_{n+1}(x) = (\mathcal{L}p_n)(x).$$

Again a smooth invariant measure has density p:

$$p = \mathcal{L}p.$$

Often the randomisation smoothes through the averaging process though

this need not necessarily happen. The following example illustrates such smoothing.

Example –AR(1) Process Consider the following random map, which arises in autoregressive time series analysis:

$$G_\theta(x) = \frac{1}{2}x + \theta$$

with θ picked from the standard normal distribution $\mathcal{N}(0,1)$. Thus

$$G_\theta^{-1}(x) = 2(x-\theta)$$

so that

$$p_{n+1}(x) = \int \frac{\exp(-\theta^2/2)}{\sqrt{2\pi}} 2p_n(2x-2\theta)d\theta.$$

The invariant measure is given by the law of the random variable

$$y := \lim_{n\to\infty} \sum_{j=0}^{n} \frac{1}{2^j}\theta_j.$$

See [7] for further examples of this type. ■

Now we move to continuous time where the issues are similar: in the absence of randomness, non-smoothness in probability densities abounds; randomness can often act to introduce smoothing.

Consider the Itó stochastic differential equation

$$dx = f(x)dt + \sigma(x)dW, \tag{2.4}$$

with $x \in \mathbb{R}^m, W \in \mathbb{R}^d$ being standard d-dimensional Brownian motion and $f : \mathbb{R}^m \to \mathbb{R}^m$, $\sigma : \mathbb{R}^m \to \mathbb{R}^{m\times d}$ and $B : \mathbb{R}^m \to \mathbb{R}^{m\times m}$ defined by $B(u) = \sigma(u)\sigma(u)^T$, where $m \geq d$. Again we assume that $x(0)$ is distributed randomly with density p_0.

If we define the *Fokker-Planck* operator† by

$$\mathcal{A}p = -\nabla\cdot(fp) + \frac{1}{2}\nabla\cdot\nabla\cdot(Bp) \tag{2.5}$$

then $x(t)$ generates a probability measure with density satisfying

$$\frac{\partial p}{\partial t} = \mathcal{A}p, \quad p(x,0) = p_0(x),$$

together with suitable decay conditions as $|x| \to \infty$. A smooth invariant measure has density p:

$$0 = \mathcal{A}p,$$

† The divergence of a matrix A is here defined in the fashion standard in the continuum mechanics literature, that is $(\nabla\cdot A)_i = A_{ij,j}$, see [11].

again together with decay conditions at infinity.

In the absence of noise, highly non-smooth p is possible, as the following example shows.

Example – Linear Decay If

$$f(x) = -x, \quad \sigma(x) \equiv 0$$

then

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\{-xp\}$$

with solution

$$p(x,t) = e^t p_0(xe^t),$$

where $p_0(x)$ is the initial density, assumed to have compact support. Then, as $t \to \infty$, the density approaches a point mass at the origin – the invariant measure for this problem.

However, if

$$f(x) = -x, \quad \sigma(x) = \epsilon$$

then

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\{-xp\} + \frac{\epsilon^2}{2}\frac{\partial^2 p}{\partial x^2}.$$

The addition of the noise, however small, gives parabolic smoothing for p and the unique invariant measure is now a Gaussian with density

$$p(x) \propto \exp(-x^2/\epsilon^2). \quad \blacksquare$$

Invariant measures play a fundamental role, not only over many realizations of the noise and/or random data, but also for individual realizations. This is because of *ergodicity*. Roughly, the map (2.1) ergodic. if for some class of real valued functions g

$$\frac{1}{n}\sum_{j=0}^{n-1} g(x_j) \to \int g(x)p(x)dx \tag{2.6}$$

or, for continuous time (2.4),

$$\frac{1}{t}\int_0^t g(x(s))ds \to \int g(x)p(x)dx, \tag{2.7}$$

together with some assumptions on the set of initial conditions for which this holds.

Birkhoff's ergodic theorem states that the limit in (2.6) exists for almost every point with respect to any invariant measure for the map, with

similar results in continuous time [42]. If for some x_0 this limit exists for every continuous bounded function g, it defines a linear functional and can hence be viewed as a Borel measure. If

$$\frac{1}{n}\sum_{j=0}^{n-1}\delta_{x_j} \Rightarrow \mu$$

(with $\Rightarrow$ denoting weak convergence) and the limit is independent of the initial point x_0 when it is taken in some set of positive Lebesgue measure, then the resulting measure is called a physical measure, or SRB (for Sinai-Ruelle-Bowen) measure, since it can then be physically observed, see [42].

To compute time averages in general we may either:

directly: calculate p and hence the right hand side in (2.6) or (2.7);
indirectly: calculate a trajectory and sum/integrate to get the left hand side of (2.6) or (2.7).

For a general discussion of the direct and indirect methodologies for the calculation of invariants of dynamical systems see the preface in [34]. Direct methods are not the subject of this review, but we give a brief bibliography before moving to the subject of indirect methods. In [40] the idea of discretising $\mathbb{R}^n$ to obtain a finite state space Markov chain approximation to (2.3) was introduced. Subsequent analysis of this approach was given in [22] and [19]. More recent theoretical work, and numerical experiments, includes [18, 17] and [16]. In the last few years these ideas have been employed as an effective computational tool, in particular by use of adaptive choice of the spatial discretization – see [4, 3, 5] for example, together with [15] and [31] where applications to molecular dynamics are described. A recent overview of the subject may be found in [9].

We will concentrate here on indirect methods and split our study into the three classes of problems described at the end of the last section. The most satisfactory theory is for problems in Category B) where, for example, the parabolic smoothing of probability densities for (2.4) is exploited. A coherent theory of ergodicity for Category A) is very hard, and hence so is any perturbation theory; much of what is currently known is limited to expansive maps and certain hyperbolic maps – see [42], [43], [23] for more details. Category C) is, somewhat surprisingly at first glance, more tractable than A) in some instances. This is because ideas from statistical mechanics allow certain problems in Category C)

to be approximated by Markov processes; their stochastic stability is a strong property with implications for the robustness of statistics generated by approximation schemes.

3 Deterministic Problems

Problems in Category A) are the hardest in which to treat the effect of any approximation, including numerical. For the Hénon map SRB measures are known to exist [43] and it is reasonable to conjecture that the robust statistics observed in numerical simulations such as those shown in section 1 are due to robust calculation of an SRB measure. However, although the example of the Henon map is very suggestive that strong results might be provable in the deterministic case, the following example should strike a note of caution.

Example – The Tent Map Consider again the map (2.1), (2.2). If the initial condition x_0 is irrational the resulting trajectory is chaotic, and hence the problem is chaotic for a.e. initial condition. However, if x_0 is of the form $u/2^p$, where u is an odd integer, then $x_n = 0$ for $n \geq p+1$ and thus any computer simulation of this map (using floating point arithmetic) will have trivial dynamics. To create the effect of the irrational initial conditions which lead to chaos one can add random noise slightly larger than machine precision at each step, and Figure 1.2 shows results from two such simulations using single and double precision. Consistent statistics are observed at the two levels of precision and the empirical density is close to the true (Lebesgue) density generated by chaotic solutions of the original map. No rigourous justification of this is known as yet, but work of Kifer [20] comes close. He shows that replacing (2.1) by its restriction to a uniform lattice of scale δ, and adding noise with scale ϵ, yields a Markov chain with invariant measure close to an invariant measure of the original map (2.1), provided that $\delta = \mathcal{O}(\epsilon^{1+c}), c > 0$. Further study of the effect of rounding error on iterated maps, concentrating on attractors, may be found in [6]. ■

However, despite this cautionary example, the numerical evidence for many deterministic problems is similar to that seen for the Henon map in the introduction - namely that statistics are well-reproduced, even when trajectories are not. To illustrate this we give a simple example from ODEs:

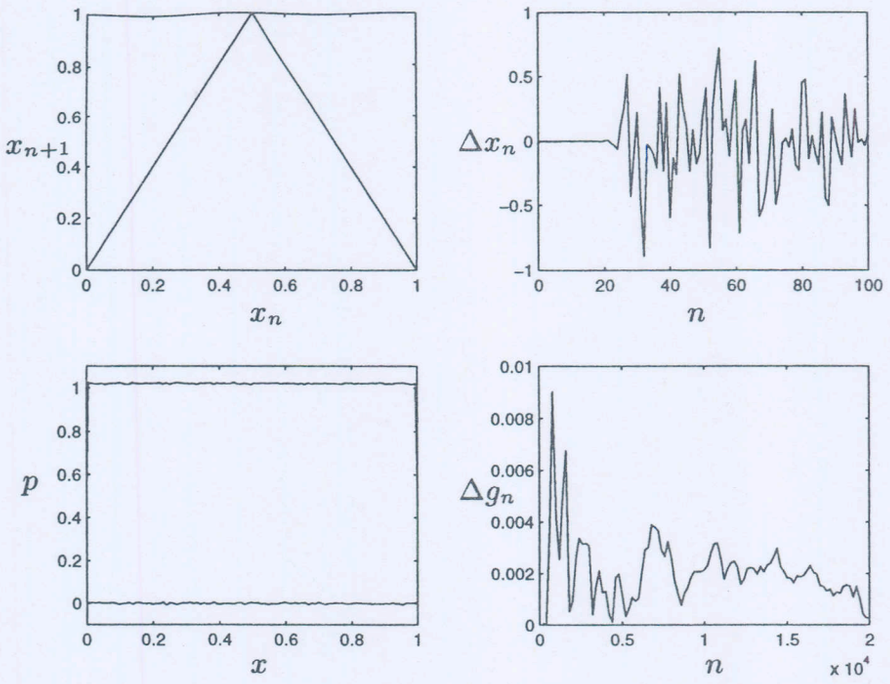

Fig. 1.2. The tent map. Upper left: x_{n+1} vs. x_n, generated by a double-precision arithmetic simulation. Upper right: The difference between two trajectories, one computed with single precision arithmetic, the other with double. Lower left: Histogram of the probability density for x, computed from very long-time simulations in single precision, and the difference between the histogram computed in single and double precision. Lower right: Difference in the time averages $\frac{1}{n+1}\sum_{k=0}^{n} g(x_k)$ with $g(x) = x^2$.

Example – Lorenz Equations Consider the equations

$$\begin{aligned} \dot{x} &= 10(y-x) \\ \dot{y} &= 28x - y - xz \\ \dot{z} &= xy - \tfrac{8}{3}z \end{aligned}$$

Figure 1.3 shows two calculations using the Euler method, one with time-step twice the other. It is clear that the method reproduces statistics well even though trajectories are completely wrong. There is no satisfactory theory to rigourously justify this observation at present but the recent work of Tucker [39] may facilitate rigourous justification. ■

The previous problem is dissipative with a global attractor, but the observation about robustness of statistics extends to some Hamiltonian problems also†. The following example illustrates this:

† Note that, in a generic sense, such problems are not ergodic on every energy shell [24].

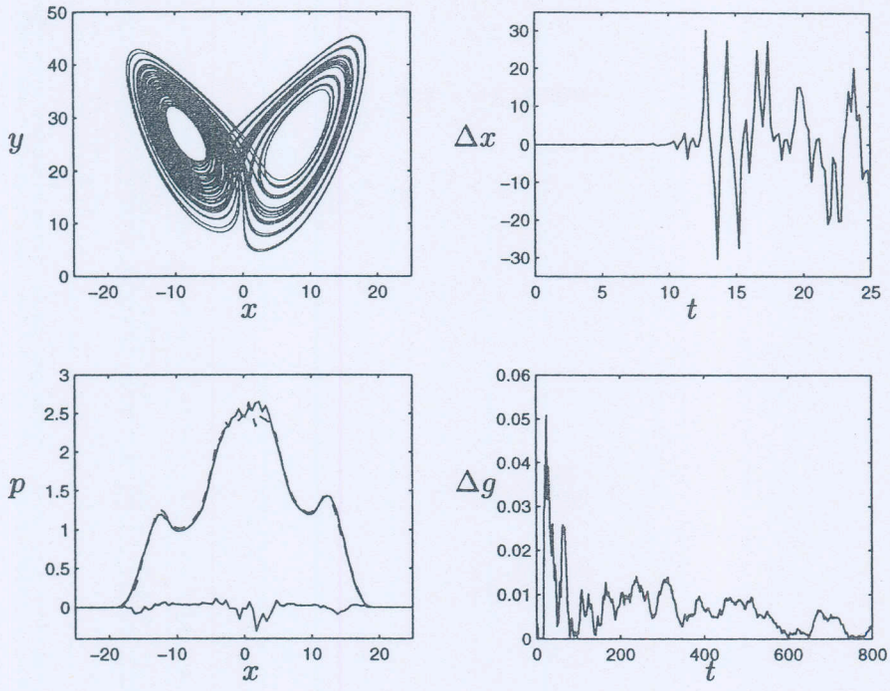

Fig. 1.3. The Lorenz equations. Upper left: The attractor computed using Euler's method. Upper right: The difference between two trajectories, one computed with time step twice the other. Lower left: Histogram of the probability density for x, computed from very long-time simulations, and the difference between the histogram computed with two different time steps, one twice the other. Lower right: Difference in the time averages $\frac{1}{n+1}\sum_{k=0}^{n} g(x_k)$ with $g(x) = \left(\frac{x+25}{50}\right)^2$.

Example – Three Interacting Particles Consider a system of three particles with pairwise interaction potential $U_i(r) = 1/r$, where $r > 0$ is the distance between the two particles, and potential energy

$$U_b(q_x, q_y) = e^{(q_x/4)^2} + e^{(q_y/4)^2} - 2e$$

added to keep the particles in a finite area [27].

Figure 1.4 shows calculations with two different time-steps (related by a factor of two) using the Verlet method [41]. Once again it is clear that the method reproduces statistics even though trajectories are completely wrong. Reich [27] has an explanation for why symplectic methods reproduce time-averages well which, in outline, goes like this: hypothesise that some Poincaré suspension of the flow satisfies the conditions developed by, for example Young and Liverani (see [43, 23, 42]) which yield decay of correlations, the law of large numbers or the central limit theorem. Note that, for times of order $\exp(-1/\Delta t)$, a symplectic method approximates a nearby Hamiltonian problem [30]; then use stochastic stability

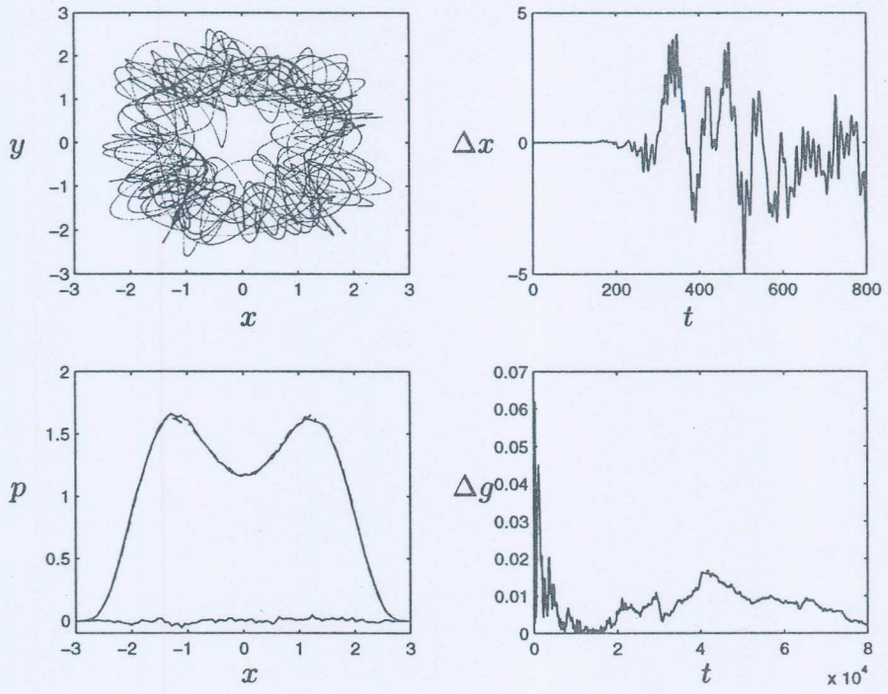

Fig. 1.4. Particle system. Upper left: Trajectories of the particles computed using the Verlet method. Upper right: The difference between two trajectories of a single particle, one computed with time step twice the other. Lower left: Histogram of the probability density for x, computed from very long-time simulations, and the difference between the histogram computed with two different time steps, one twice the other. Lower right: Difference in the time averages $\frac{1}{n+1}\sum_{k=0}^{n} g(x_k)$ with $g(x) = \left(\frac{x+3}{6}\right)^2$.

of the original Hamiltonian problem, which follows from the assumptions on the flow, to study time averages for the perturbed Hamiltonian problem. The conclusion is that time averages are well approximated for times exponentially long in Δt^{-1}. (Standard convergence theory would give times only logarithmic in Δt^{-1}.) Note however that Reich's assumptions appear very hard to verify on any concrete examples and so his ideas, whilst very suggestive, fall short of a completely satisfactory explanation. ■

4 Stochastic Problems

Because of the parabolic smoothing induced by white noise (see (2.5)) the picture here is fairly well-developed from a theoretical standpoint. The simplest examples are of the following type:

Example – Lorenz with Noise Consider the Lorenz equations with

additional white noise:

$$\begin{aligned} dx &= 10(y-x)dt &+ dW_1 \\ dy &= (28x - y - xz)dt &+ dW_2 \\ dz &= \left(xy - \tfrac{8}{3}z\right)dt &+ dW_3 \end{aligned}$$

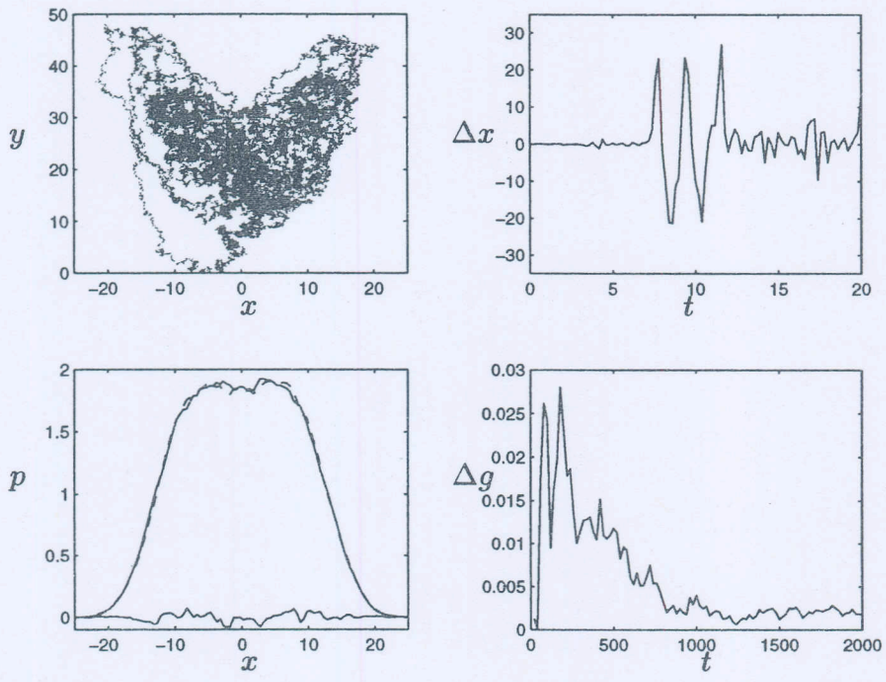

Fig. 1.5. The Lorenz equations with white noise. Upper left: A trajectory computed using Euler's method. Upper right: The difference between two trajectories, one computed with time step twice the other. Lower left: Histogram of the probability density for x, computed from very long-time simulations, and the difference between the histogram computed with two different time steps, one twice the other. Lower right: Difference in the time averages $\frac{1}{n+1}\sum_{k=0}^{n} g(x_k)$ with $g(x) = \left(\frac{x+25}{50}\right)^2$.

Figure 1.5 shows simulations, for a single realization of the noise, using the Euler-Maryuma method [21]. Once again we see that the method appears to reproduces statistics well even though trajectories are completely wrong. However, in contrast to the deterministic case, for this problem there is a very well-developed and satisfactory theory. Since $B = I$ the Fokker-Planck equation with generator $\mathcal{A}$ is uniformly parabolic; this fact, combined with dissipativity of the deterministic vector field, gives ergodicity [13]. Exploiting this structure, Talay [36, 37, 10] proves theorems which show that the densities and time averages

shown in Figure 1.5 are indeed accurate approximations of their true counterparts in the SDE.†

We now modify the previous problem so that noise is only present in the x and y equations

$$\begin{aligned} dx &= 10(y-x)dt &+ dW_1, \\ dy &= (28x - y - xz)dt &+ dW_2, \\ dz &= \left(xy - \tfrac{8}{3}z\right)dt. \end{aligned}$$

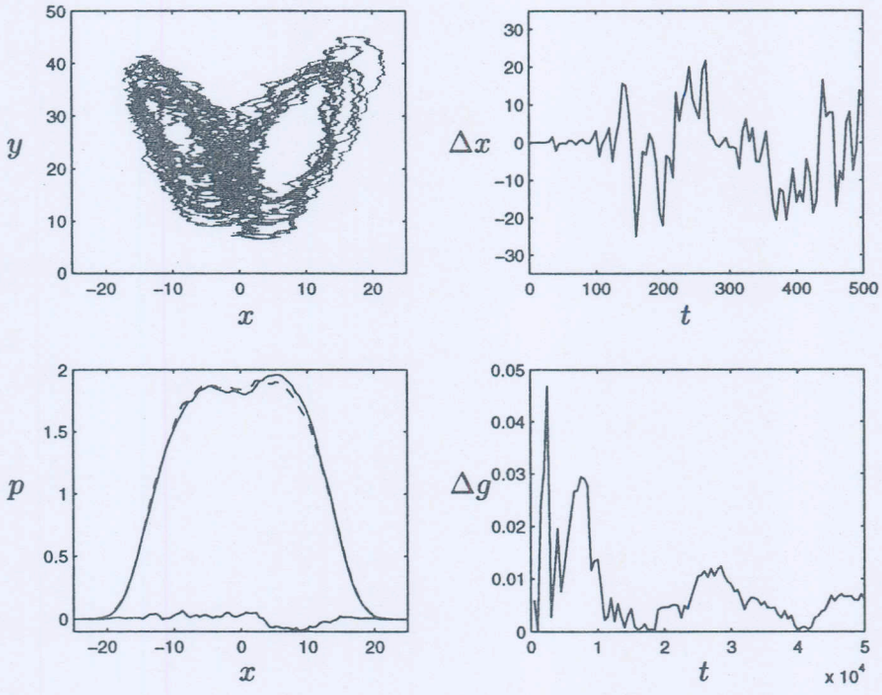

Fig. 1.6. The Lorenz equations with white noise in two components. Upper left: A trajectory computed using Euler's method. Upper right: The difference between two trajectories, one computed with time step twice the other. Lower left: Histogram of the probability density for x, computed from very long-time simulations, and the difference between the histogram computed with two different time steps, one twice the other. Lower right: Difference in the time averages $\frac{1}{n+1}\sum_{k=0}^{n} g(x_k)$ with $g(x) = \left(\frac{x+25}{50}\right)^2$.

The theory of Talay in [36, 37, 10] no longer applies since B is now singular so that the Fokker-Planck equation with generator $\mathcal{A}$ is not uniformly parabolic. Nonetheless the SDE itself is provably geometrically ergodic (see [25]) and the numerical evidence in Figure 1.6 suggests that the Euler-Maryuma method reproduces statistics well even though

† Note that this theory requires globally Lipschitz vector fields. Recent work by Talay [38] is aimed at removing this restriction.

trajectories are completely wrong. A theory for the approximation of such degenerate diffusions is being developed in [32] and [14], using the approach to Markov chains described in [26], and by [38] using Malliavin calculus. ■

5 Statistical Mechanics

We have seen that for stochastic problems study of the statistics of trajectories is made simpler than for deterministic problems, essentially because of smoothing in the propagation of probability densities. This smoothing in Markov chains/processes can, in some cases, be exploited to study deterministic problems with random data. In particular such problems often simplify, as the dimension $n \to \infty$, to yield the Markov property; random noise in the initial data becomes near memoryless noise when only a subset of the variables is observed. We now exploit this basic idea from statistical mechanics to study numerical schemes.

The general picture here is to consider ODEs partitioned in the form

$$\begin{aligned} \dot{x} &= f(x,y), \quad x(0) = x_0 \\ \dot{y} &= g(x,y), \quad y(0) = y_0 \end{aligned} \tag{5.1}$$

with (x_0, y_0) a random variable distributed according to some measure ν.

Thus

$$y(t) = \mathcal{G}(y_0, \{x(s)\}_{0 \le s \le t})$$

and so

$$\dot{x} = f(x, \mathcal{G}(y_0, \{x(s)\}_{0 \le s \le t})), \quad x(0) = x_0. \tag{5.2}$$

In previous sections we have concentrated on whether we can calculate statistics accurately over long times, where trajectories are not accurate. Here we shift emphasis slightly and ask whether we can accurately compute the statistics of the x variable without accurately computing y. There are many problems where only a subset of the variables is of interest so that this question is natural – it may be be desirable to under-resolve y for reasons of computational efficiency.

A recent approach to this problem by Chorin *et al* [2] (1998) is to develop an equation for $X(t) = \mathbb{E}x(t)$, where expectation is with respect to ν on (x_0, y_0). Assuming stationarity leads to the approximate equations

$$\dot{X} = F(X), \quad X(0) = x_0,$$

where

$$F(X) = \mathbb{E}\{f(x,y)|x = X\},$$

and now expectation is with respect to ν on (x,y) There is strong experimental evidence to show that this gives good approximations for some problems, but no substantial theory as yet. Some preliminary theoretical investigations may be found in [12]. Another approach is to try and identify low-dimensional stochastic models from numerical simulation of the full problem, without explicit *a priori* knowledge of which variables will comprise the low-dimensional approximation. This work may be found in [15] and [31].

We will consider a less ambitious approach where the complete system for x, y is still integrated, but methods used which are cheap and formally inaccurate trajectory-wise in the y component. The reason to expect that we might still accurately compute x, or at least its statistics, is that, often, for dimension $n \to \infty$, one obtains from (5.2) a Markov process or chain such as

$$dx = f_0(x)dt + \sigma_0(x)dW.$$

This can be accurately approximated without approximating y accurately. We look at three examples which illustrate this idea.

Example – Construction of an SDE [1] Consider the equations, $j = 0, \ldots, N$

$$\ddot{u}_j + j^2 u_j = 0,$$

$$\dot{z}_N = f(z_N) + \sum_{j=0}^{N} u_j(t),$$

$$u_j(0) = \sqrt{\frac{2}{\pi}}\eta_j, \quad \dot{u}_j(0) = 0, \quad z_N(0) = z_0$$

where the η_j are i.i.d. $\mathcal{N}(0,1)$. Thus $x = z_N$ and $y = \{(u_j, \dot{u}_j\}_{j=0}^{N}$.

For large N, z_N approximates the solution of the SDE

$$dz = f(z)dt + dW, \quad z(0) = z_0,$$

where W is standard Brownian motion. Precisely we have that, for $T \in [0, \pi]$,

$$\mathbb{E}\|z(T) - z_N(T)\|^2 \leq \frac{C(T)}{N}.$$

Let $z^n = z(n\Delta t)$ and let $Z^n \approx z_N(n\Delta t)$ be our numerical approximation. In order to make precise the notion of computing inaccurately with respect to the y variable we take the limit

$$N \to \infty, \quad \Delta t \to 0, \quad N\Delta t = \zeta. \tag{5.3}$$

Under this limit process the oscillators u_j are not well resolved for large j. We apply Leap-Frog to the oscillators with $\zeta \leq 2\dagger$ and the theta-method to the z equation. Then, for $n\Delta t \in [0, \pi]$,

$$\mathbb{E}\|z^n - Z^n\|^2 \leq C(n\Delta t)\Delta t^{2/3}.$$

For sufficiently smooth g and for linear f

$$|\mathbb{E}g(z^n) - \mathbb{E}g(Z^n)| \leq C(n\Delta t)\Delta t^{2/3}.$$

Precise statements of these theorems, together with numerical results illustrating them, can be found in [1]. ■

A more physically realistic model – based on a mechanical description of a *heat bath* due to Ford and Kac [8] – is the following:

Example – Heat Bath [35] Consider the equations, for $j = 1, \ldots, N$

$$\ddot{u}_j + j^2(u_j - q) = 0,$$

$$\ddot{q} + V'(q) = \sum_{j=1}^{N} \gamma^2(u_j - q)$$

$$u_j(0) = \sqrt{\frac{2}{\pi}}\eta_j, \ \dot{u}_j(0) = 0, \ q(0) = q_0, \ \dot{q}(0) = p_0$$

where $x = \{p, q\}$ and $y = \{\{v_j, u_j\}_{j=1}^N, p, q\}$, and the η_j are as before.

When N is large the motion of q is governed by an SDE:‡

$$\ddot{Q} + V'(Q) - \frac{\gamma^2}{2}Q + \frac{\gamma^2\pi}{2}\dot{Q} = \dot{B}$$

$$Q(0) = q_0, \quad \dot{Q}(0) = p_0 - \frac{\gamma^2\pi}{2}q_0,$$

$$B(t) = \gamma\sqrt{\frac{\pi}{2\beta}}[W(t) - \frac{t}{\pi}W(\pi)].$$

Here $W(t)$ is as before. In fact, for any $T \in [0, \pi]$,

$$\mathbb{E}\{\|q - Q\|^2_{L^\infty(0,T)} + \|\dot{q} - \dot{Q}\|^2_{L^2(0,T)}\} \leq C(T)\frac{\ln(N)^2}{N}.$$

† The method then gives exact solutions to a nearby linear oscillator problem; see [28]

‡ This formal equation can be put in first order form and cast as an Itó SDE.

Again we compute q numerically by solving the large system in the limi (5.3). Precise statement of results, together with numerical experiment showing that under-resolved simulations can produce accurate (i.e. clos to Q) simulations of q, can be found in [35]. ■

Example – Billiards [33] Small particles suspended in a fluid with velocity field v can be modelled by having the particles obey Stokes' law between elastic collisions. Briefly we have

$$m\ddot{z}_i = \alpha[v(z_i,t) - \dot{z}_i], \quad i = 1,\dots,N,$$
$$+\text{ELASTIC COLLISIONS},$$
$$z_i(0) \sim U([0,1]\times[0,1]), \quad \dot{z}_i(0) \sim \mathcal{N}(0,I).$$

We may think of $x = (z_1, \dot{z}_1)$; y comprises the positions and velocities of the remaining particles.

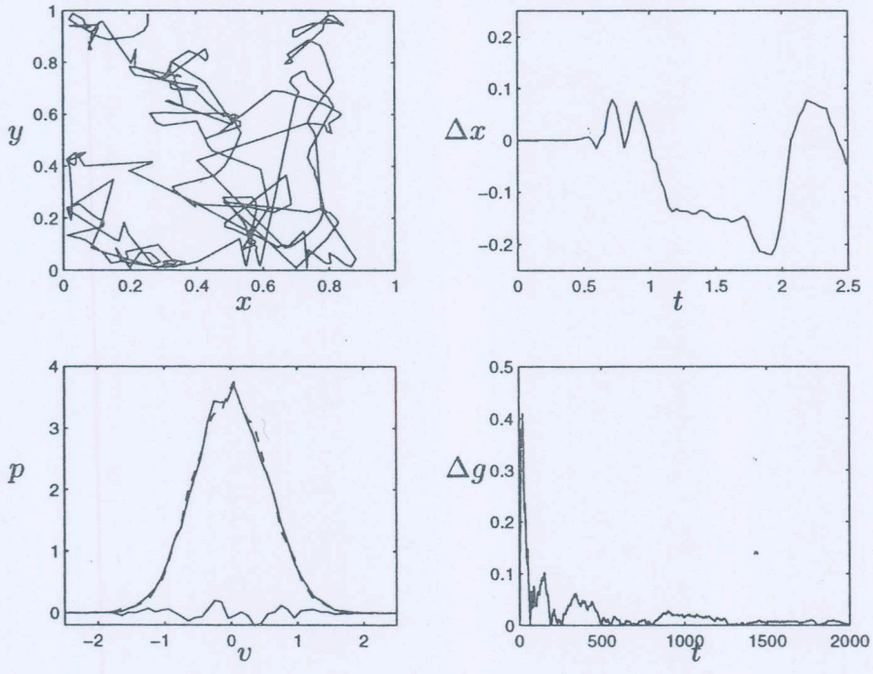

Fig. 1.7. The Billiards Problem. Upper left: A trajectory of a single particle, computed in double precision. Upper right: The difference between two trajectories, one computed with single precision arithmetic, the other with double. Lower left: Histogram of the probability density for the velocity of a single particle, computed from very long-time simulations in single precision, and the difference between the histogram computed in single and double precision. Lower right: Difference in the time averages $\frac{1}{n+1}\sum_{k=0}^{n} g(x_k)$ with $g(x) = \left(\frac{x+3}{6}\right)^2$.

Figure 1.7 shows data generated from a simulation of this problem

with 210 particles and $\alpha = 0$. All data is generated by considering one particle. Figure 1.7 top left shows the particle trajectory, generated by a double-precision arithmetic simulation. Figure 1.7 top right shows the difference between two trajectories, in double and single precision; as is to be expected the trajectories rapidly diverge. However, once again, the statistics are well-reproduced: Figure 1.7 bottom left shows for that the empirical density is close in both precisions and that hence time-averages are insensitive to precision – see Figure 1.7 bottom right.

There is no rigourous explanation for the observation. However, it is believed that, for $N \gg 1$ $z_1, \dot{z}_1$ can in some situations be modelled by a Markov stochastic process of the form:

$$m\ddot{Z}_1 = \alpha[v(Z_1, t) - \dot{Z}_1] + \sum_{j=1}^{\infty} \delta(t - t_j)\mathcal{F}_j,$$

Here $\{t_j, \mathcal{F}_j)\}_{j\geq 1}$ form a family of i.i.d. random variables. Their joint distribution is calculated by arguments similar to those Boltzmann used to derive his equation. Assuming that this equation has a unique exponentially attracting invariant measure then its statistics are likely to be insensitive to perturbation; arguments showing the effect of rounding error on invariant measures of Markov chains may be found in [29] and the effect of time-discretization on time-continuous Markov chains may be found in [32]. ■

6 Conclusions

The numerical experiments and accompanying mathematical discussion in this paper have illustrated the following main points concerning the statistical content in numerical simulations of initial value problems:

- Experimental evidence strongly suggests that, often, statistics are robust under time-discretization and round-off error even when trajectories are not.
- Substantiating this is typically far harder for deterministic problems than for stochastic ones.
- Large deterministic problems with random data fall somewhere in between deterministic and stochastic problems; some progress has been made using ideas from statistical mechanics, but this work is in its infancy.
- Much remains to be done.

Acknowledgement

We are grateful to Michael Dellnitz, Gary Froyland, Oliver Jünge and Sebastian Reich for helpful readings of drafts of this manuscript.

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