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Influences of artificial numerical noise on statistics and qualitative properties of chaotic system

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ABSTRACT

Taking the nonlinear Schrödinger equation (NLSE) as an example, we provide from a mathematical viewpoint, rigorous evidence that numerical noise of a chaotic system as tiny artificial stochastic disturbances can increase exponentially to a macro-level. As a result, numerical simulations given by traditional algorithms in double precision may rapidly become badly polluted leading to huge deviations from the 'true' solution not only in trajectory but also, sometimes, even in statistics and/or some qualitative properties. Small physical disturbances in time and space are unavoidable in practice, which are often much larger than artificial numerical noise. So, from a physical viewpoint, it is wrong to neglect small spatio-temporal disturbances of a chaotic system: chaos should not be described by deterministic equations.

1. Introduction

Chaos theory [1–7] has been regarded as one of the three greatest theories of physics in 20th century, compared to quantum mechanics and Einstein's relativity. The sensitivity dependence on initial condition of chaotic systems was first discovered by Poincaré [8] and then rediscovered by Lorenz [9] in 1963. It has been popularized through its colloquial name 'butterfly effect', whereby a hurricane in North America might be created by flapping of the wings of a distant butterfly in South America several weeks earlier. Later, Lorenz [10,11] further discovered that numerical simulations of chaotic trajectories are sensitive not only to the initial condition, which has physical meaning, but also to the choice of numerical algorithm, which is purely artificial, being subjective and thus without physical meaning. This is easy to understand: all numerical algorithms involve numerical noise, i.e. truncation error and round-off error, which lead to small disturbances at each time-step that become exponentially enlarged in chaotic systems due to the so-called 'butterfly-effect'. As a result, any numerical simulation s of chaos is a mixture of the 'true' solution p and false numerical noise δ, which are mostly at the same order of magnitude, i.e. $p \sim \delta$. In other words, a numerical simulation of chaotic systems given by traditional algorithms (in double precision) is quickly polluted, say, $s = p + \delta$ with $p \sim \delta$. This fact leads to some misunderstanding and confusion concerning chaotic systems [12].

For example, the nonlinear Schrödinger equation (NLSE) is a classical and significant research topic in quantum mechanics [13,14], nonlinear optics [15,16], plasma physics [17,18], hydrodynamics [19,20], as well as many other fields of nonlinear mechanics [21,22]. Note that the forced and damped NLSE is a prototypical model of spatio-temporal chaos [23,24]. It is well-known that the mode number of its attractor increases with the dimension of the spatial domain L. In theory, if the attractor has more than two linearly unstable modes (LUMs), i.e. $L > L_c$, where L_c is a critical length scale, spatio-temporal chaos should appear in the forced and damped case [24]. But, only temporal chaos should be observed when $L < L_c$. For details, please refer to Cai et al. [24]. However, Shlizerman & Rom-Kedar [25] numerically solved a one-dimensional (1D) conservative ac-driven periodic NLSE (without damping) [26,27] and found that spatio-temporal chaos sometimes might appear even when $L < L_c$. This is contrary to the finding by Cai et al. [24]. Certainly, these two opposite conclusions lead to confusion: which one should we believe?

The key of answering the above-mentioned question is to obtain a sufficiently accurate numerical simulation s of the chaotic trajectory over a prescribed, long interval of time during which the numerical noise δ is negligible compared to the true solution p, i.e. $|\delta| \ll |p|$, so that the numerical simulation s is very close to the true solution p. This is now possible by means of Clean Numerical Simulation (CNS) developed by Liao [28,29]. The basic idea behind CNS is to reduce the background numerical noise, i.e. truncation error and round-off error, to such a tiny level that the influence of numerical noise can be neglected compared to the 'true' solution over a time interval $0 \le t \le T_c$ that is long enough for calculating statistics, where T_c is called the

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critical predictable time. Unlike most traditional algorithms that use double precision, CNS adopts multiple-precision [30] so as to maintain the round-off error below a required level. Thus, the CNS result can be used as a benchmark solution for comparison purposes. Then, the influence of numerical noise on chaotic systems can be investigated by comparing the CNS benchmark solutions with those given by traditional algorithms.

To date, CNS has been successfully applied to many chaotic dynamical systems, such as Lorenz system [31], three-body problem [32,33], complex Ginzburg–Landau equation [34], and the Lagrangian chaotic property of the Arnold–Beltrami–Childress (ABC) flow [35]. It has been found that tiny amounts of numerical noise can lead to huge deviations in prediction of Rayleigh–Bénard turbulent convection [36], and turbulent Kolmogorov flow [37], not only in terms of temporal–spatial trajectories but also even in statistics.

As mentioned above, due to the well-known butterfly effect, the numerical simulation using traditional algorithm of a chaotic system quickly becomes a mixture of the 'true' solution p and false numerical noise δ, which are mostly at the same order of magnitude (i.e. $p \sim \delta$). Any statistics, which are calculated using such kind of mixture, are based on a hypothesis that the statistics are stable to numerical noise. In other words, the statistics based on this kind of mixture (i.e. $p+\delta$) are the same as those based on the 'true' physical solution p, say,

$$\langle p+\delta \rangle = \langle p \rangle \tag{1}$$

must hold, where $\langle\ \rangle$ is a statistical operator. Unfortunately, there exists no theoretical proof of this hypothesis, even though it is widely utilized. Is the hypothesis (1) true for all chaotic systems? With the help of CNS, a sufficiently accurate numerical simulation s can be obtained, where the numerical noise δ is negligible so that the numerical simulation s is very close to the true solution p. Hence, in this paper we can investigate the hypothesis (1), say, investigate the influence of artificial numerical noise on statistics and qualitative properties of a chaotic system, by comparing the CNS benchmark solution (i.e. $s \approx p$) with the result given by a traditional algorithm (i.e. $p+\delta$).

2. Governing equation and numerical implementation

Without loss of generality, we follow Shlizerman & Rom-Kedar [25] to consider the focusing periodic 1D NLSE perturbed by an ac-driver $\epsilon e^{i\Omega^2 t}$ of frequency Ω^2 and amplitude ϵ, which is conservative and can be transformed to the following autonomous NLSE having a constant potential [25–27]:

$$i\Psi_t - \Psi_{xx} - (g|\Psi|^2 - \Omega^2)\Psi = \epsilon \tag{2}$$

with a periodic boundary condition

$$\Psi(x,t) = \Psi(x+L,t) \tag{3}$$

and the initial condition

$$\Psi(x,0) = \Psi_0(x), \tag{4}$$

where $i = \sqrt{-1}$ is the imaginary unit, Ψ is an unknown complex function, t and x are temporal and spatial variables, the subscript denotes the partial derivative, g is a constant and e is the natural constant. For the unperturbed system ($\epsilon = 0$), its simplest solutions are plane waves: $\Psi_{\rm PW}(t; M_{\rm PW}, E_0) = \sqrt{M_{\rm PW}}\exp[i(\Omega^2 - gM_{\rm PW})t - iE_0]$ with the mass $M_{\rm PW}$. Noth that these plane waves are called resonant with the frequency $\Omega^2 - gM_{\rm PW} = 0$. According to the linear stability analysis, the solution is stable (elliptic) when $M_{\rm PW} < M_1$, neutral (parabolic) when $M_{\rm PW} = M_1$, and unstable (hyperbolic) when $M_1 < M_{\rm PW} < M_2$, with $M_j = \frac{1}{2g}(\frac{2\pi}{L})^2 j^2$ [25,27]. For the conservative periodic case investigated in this paper, it was observed that when the corresponding parabolic plane wave is resonant, say, $M_{\rm PW} = M_1 = \frac{1}{2g}(\frac{2\pi}{L})^2 = \frac{\Omega^2}{g}$, thus, $\Omega^2 = \frac{1}{2}(\frac{2\pi}{L})^2$, some initial distributions near this plane wave exhibit the development of spatio-temporal chaos [25].

Following Shlizerman & Rom-Kedar [25] again, we use the same initial distribution

$$\Psi_0(x) = \sqrt{0.15}e^{i\frac{5\pi}{9}} + 10^{-3}e^{i\frac{2\pi}{L}x}, \tag{5}$$

and the same parameters, $g = 2$, $\Omega^2 = 0.45$, $\epsilon = 5\times 10^{-2}$ and $L = 2\pi/0.9$. In short, we adopt the same mathematical model (i.e. the same governing equations with the same parameter values) as used by Shlizerman & Rom-Kedar [25], who reported that, when $\Omega^2 = 0.45$ and $L = 2\pi/0.9 < L_c = 2\sqrt{2}\pi/\Omega$, the corresponding system was found to exhibit spatio-temporal chaos.

In this investigation, we applied a traditional numerical algorithm (i.e. the 4th-order Runge–Kutta method with double precision, denoted RKwD) [25,27,38] to solve Eqs. (2)–(5) and found that spatio-temporal chaos appeared when $t > 800$, confirming the conclusion by Shlizerman & Rom-Kedar [25]. However, using CNS to solve the same equations, we found that in the time interval $t \in [0, 1500]$ only temporal chaos exits and spatio-temporal chaos hardly appears, as described below in detail. Note that our result is contrary to the numerical simulation of Shlizerman & Rom-Kedar [25] but supports the theoretical analysis given by Cai et al. [24].

By means of CNS, we first gain a reliable simulation of Eqs. (2)–(5) over a sufficiently long interval of time $t \in [0, 1500]$ by means of a rather small temporal allowed tolerance $tol = 10^{-120}$ for the high-order Taylor expansion in time, a mode number $N = 512$ for the spatial Fourier expansion in the spatial interval $x \in [-L/2, L/2]$, and a significant number of digits $N_s = 120$ in multiple precision for all variables and parameters. Then, in order to verify the reliability of this result, we compare it with another CNS result with even smaller numerical noise, which is obtained by means of the same mode number $N = 512$ in space, but smaller temporal allowed tolerance $tol = 10^{-130}$ and higher multiple precision with $N_s = 130$. Comparing the two CNS results, we find they have no distinct differences in the time interval $0 \le t \le 1500$, which is long enough for calculating statistics. This verifies the convergence and reliability of our CNS result in $t \in [0, 1500]$ given as $tol = 10^{-120}$, $N = 512$ and $N_s = 120$, which is used hereon as the 'clean' benchmark solution for comparison purposes. For details about the CNS algorithm of the NLSE under consideration, please refer to Supplementary Material.

Besides, the same Eqs. (2)–(5) with the same physical parameters as mentioned above are solved by means of a traditional algorithm [25,27,38] using the same mode number $N = 512$ of the spatial Fourier expansion in the spatial interval $x \in [-L/2, L/2]$ and the 4th-order Runge–Kutta method with double precision (marked by RKwD) and time step $\Delta t = 2.5\times 10^{-5}$. Here, the numerical noise increases exponentially (and quickly) until to the same level of the 'true' physical solution and thus the RKwD result becomes badly polluted by numerical noise (see Supplementary Material).

3. Influence of numerical noise

Fig. 1 compares the CNS benchmark solution and the RKwD result for $|\Psi(x,t)|$ in the spatial interval $x \in [-L/2, L/2]$ and time interval $t \in [0, 1500]$. On the whole, $|\Psi(x,t)|$ given by the RKwD agrees well with the case of the so-called parabolic resonance as reported in [25], noting that spatio-temporal chaos indeed appears when $t > 800$. However, the CNS benchmark solution provides a closer match to elliptic one (see [25]) because spatio-temporal chaos never appears, say, only temporal chaos remains, in the interval of time $0 \le t \le 1500$. This qualitative deviation between the CNS benchmark solution and the RKwD result is triggered solely by the artificial numerical noise infecting the RKwD result.

Fig. 2 compares the total spectrum energy

$$E_s(t) = \sum_{n=-\frac{N}{2}}^{\frac{N}{2}-1} |\psi_n(t)|^2 \tag{6}$$

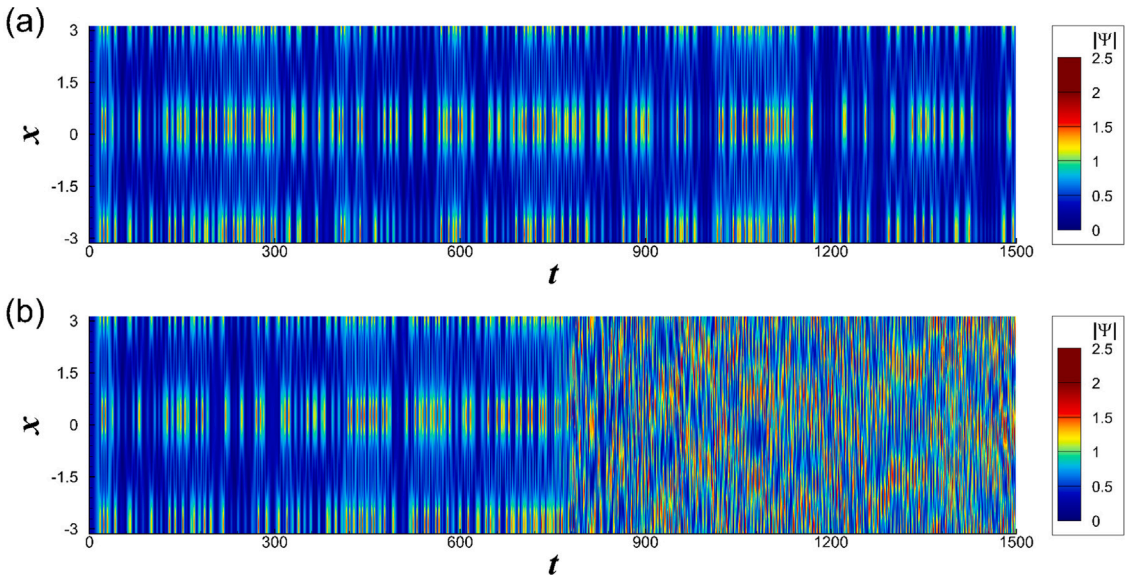

Fig. 1. Spatio-temporal plots of $|\Psi(x,t)|$ obtained from Eqs. (2)–(5) solved by (a) CNS and (b) RKwD.

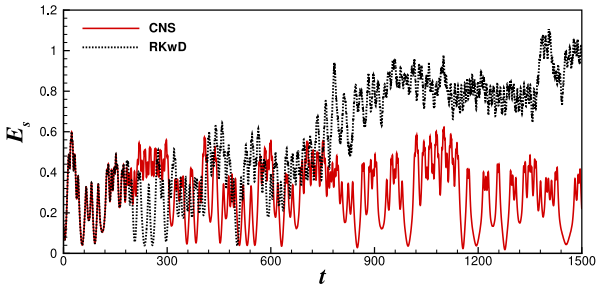

Fig. 2. Time histories of total spectrum energy (6) obtained from Eqs. (2)–(5) solved by CNS (red) and RKwD (black).

predicted by the CNS and RKwD schemes, where $\psi_n(t)$ is defined by the following Fourier spectral expression

$$\Psi(x,t) \approx \sum_{n=-\frac{N}{2}}^{\frac{N}{2}-1} \psi_n(t) e^{in(\frac{2\pi}{L}x+\pi)}, \tag{7}$$

which can be easily obtained via the CNS algorithm for 1D NLSE (see Supplementary Material). $E_s(t)$ denotes the total energy of the chaotic dynamical system. Note that $E_s(t)$ given by CNS and RKwD are almost the same when $t \le 150$, because the corresponding numerical noise of RKwD is still at a micro-level and thus negligible. Later, the deviation between the CNS and RKwD results becomes increasingly distinct, as the numerical noise increases to a macroscopic level. Even so, the two sets of results remain at the same order of magnitude until $t \approx 800$ when the spatio-temporal chaos emerges in the RKwD result. For $t > 800$, $E_s(t)$ given by RKwD is several times larger than that of the CNS benchmark solution, indicating the appearance of spatio-temporal chaos.

Furthermore, following Shlizerman & Rom-Kedar [25], the normalized correlation function

$$C_T(\Psi, y; t) = \frac{\int_{t-\frac{T}{2}}^{t+\frac{T}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \Psi(x,s)\overline{\Psi}(x+y,s)dxds}{\int_{t-\frac{T}{2}}^{t+\frac{T}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} |\Psi(x,s)|^2 dxds} \tag{8}$$

is calculated over a time window T. The normalized correlation function $C_{70}(\Psi, L/2; t)$ given by CNS and RKwD are as shown in Fig. 3(a),

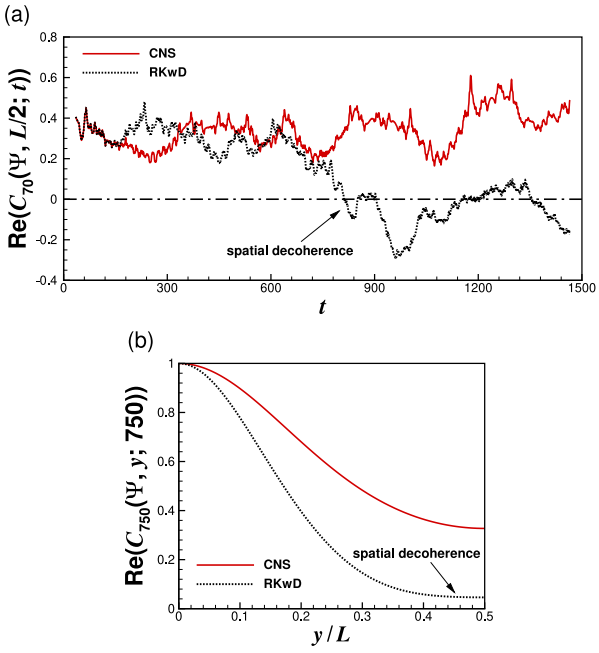

Fig. 3. Normalized spatial correlation function (8) obtained from Eqs. (2)–(5) solved by CNS (red) and RKwD (black). (a) $C_{70}(\Psi, L/2; t)$ and (b) $C_{750}(\Psi, y; 750)$.

where $T = 70$. For $t > 800$, $C_{70}(\Psi, L/2; t)$ predicted using RKwD fluctuates around zero, clearly indicating the spatial decoherence that corresponds to spatio-temporal chaos. The same conclusion can be obtained by considering the normalized spatial correlation function $C_{750}(\Psi, y; 750)$ given by the RKwD result, as shown in Fig. 3(b). In other words, when $150 < t < 800$, the numerical noise transfers to a macroscopic level only in the temporal dimension, and thereafter in both spatial and temporal dimensions leading to spatio-temporal chaos. On the contrary, the CNS solution maintains the spatial coherence pretty well throughout the whole time interval $t \in [0, 1500]$, as shown in Fig. 3. This indicates that numerical noise can greatly affect spatial/temporal correlation and might lead to spatial decoherence of the chaotic system of the NLSE (2)–(5).

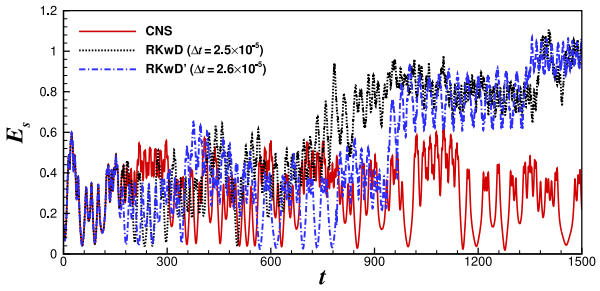

Fig. 4. Temporal evolutions of total spectrum energy (6) given by the CNS benchmark solution, the RKwD simulation (with $\Delta t = 2.5 \times 10^{-5}$), and the RKwD′ simulation (with $\Delta t = 2.6 \times 10^{-5}$).

Here we give an explanation for the above-mentioned phenomenon. The NLSE (2)–(5) might have two final states: temporal chaos and spatio-temporal chaos, which can be regarded as two minima of a double-well potential. Once the CNS benchmark solution falls in one of the two minima, say, temporal chaos, it remains there for a long time because the corresponding numerical noise is much less than the 'true' physical solution and thus cannot trigger the transition to another minimum. By contrast, the RKwD simulation can perform the transition from a state of temporal chaos to one of spatio-temporal chaos because its 'false' numerical noise (in the form of artificial stochastic disturbances) can be of the same order of magnitude as the 'true' physical solution. Hence the RKwD simulation might depart far away from its 'true' solution and thus be attracted to the other minimum, i.e. spatio-temporal chaos. If so, transition of the RKwD simulation from the temporal chaos to the spatio-temporal chaos of the NLSE (2)–(5) should occur at random times for different numerical noise as a kind of artificial stochastic disturbances. To verify the above-mentioned guess, we perform a new RKwD simulation of the NLSE (2)–(5) with the same initial/boundary conditions and the same physical parameters as the previous case, but using a different time-step $\Delta t = 2.6 \times 10^{-5}$, marked by RKwD′. Fig. 4 shows the temporal evolution of the total spectrum energy $E_s(t)$, where the transition from temporal chaos to spatio-temporal chaos (i.e. parabolic resonance) of the RKwD′ simulation (with $\Delta t = 2.6 \times 10^{-5}$) occurs at a different time $t \approx 950$, compared with the transition time $t \approx 800$ predicted by the previous RKwD simulation (with $\Delta t = 2.5 \times 10^{-5}$). This confirms our explanation mentioned above.

4. Concluding remarks and discussions

In summary, using the NLSE (2)–(5) as an example, we illustrate that numerical noise of a chaotic system as tiny artificial stochastic disturbances increases exponentially to a macro-level so that numerical simulations given by traditional algorithms in double precision are readily polluted. This leads to huge deviations at large scale from the 'true' solution not only in trajectory but also, sometimes, even in statistics and qualitative properties. Therefore, it should be better to pay more attention to the large-scale influence of numerical noise on chaotic systems, not only quantitatively but also qualitatively. The present work also illustrates that CNS provides us with a new way by which to investigate chaotic systems more accurately because it can reveal physical truths by effectively clearing away numerical noise.

It is a general belief [1,3,4] that randomness and uncertainty might come from chaos governed by a deterministic equation. This is a paradox in logic for the authors. In this paper, we give rigorous evidence that the so-called 'randomness' and 'uncertainty' of chaos arise from the butterfly-effect, and that numerical noise as it increases exponentially might finally reach the order of magnitude as the 'true' solution. From a mathematical viewpoint, the so-called 'uncertainty' of chaos does not exist so long as numerical noise remains sufficiently small over a prescribed, long interval of time and all initial/boundary conditions are 'exact'. However, even if all initial/boundary conditions could be exactly given, small physical disturbances in time and space are unavoidable, which are often much larger than artificial numerical noise. So, from a physical viewpoint, it would be wrong to neglect small physical disturbances in time and space of a chaotic system, because such disturbances might have huge influence not only on chaotic trajectory but also on its statistics and/or certain qualitative properties, as illustrated in this paper. Thus, it is advisable to consider random, small spatio-temporal disturbances in chaotic systems: in short, chaos should not be described by deterministic equations.

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CRediT authorship contribution statement

Shijie Qin: Writing – original draft, Validation, Software, Formal analysis, Data curation. **Shijun Liao:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors report no conflict of interest.

Data availability

Data will be made available on request.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.physd.2024.134355.

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