New Stochastic Mode Reduction Strategy for Dissipative Systems

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We present a new methodology for studying non-Hamiltonian nonlinear systems based on an information theoretical extension of a renormalization group technique using a modified maximum entropy principle. We obtain a rigorous dimensionally reduced description for such systems. The neglected degrees of freedom by this reduction are replaced by a systematically defined stochastic process under a constraint on the second moment. This then forms the basis of a computationally efficient method. Numerical computations for the generalized Kuramoto-Sivashinsky equation support our method and reveal that the long-time underlying stochastic process of the fast (unresolved) modes obeys a universal distribution that does not depend on the initial conditions and which we rigorously derive by the maximum entropy principle.

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Many nonlinear time-dependent problems in science and engineering are too complex to be fully resolved, and hence some degrees of freedom need to be neglected. Popular examples of high-dimensional problems, which can only be solved or studied by model reduction and approximation, are models for weather and climate prediction, cell biology processes, nonlinear networks, or economics. These problems involve many different time scales; e.g., oceans show a characteristic behavior over years whereas atmosphere does over days. More generally, any process governed by nonlinear partial differential equations (PDEs) is infinite dimensional and hence requires a reliable finite dimensional representation for numerical purposes. This gives rise to the central question of how can one systematically and reliably reduce the complexity of such high-dimensional systems without neglecting essential information contained in the unresolved or neglected degrees of freedom.

As in the case of weather and climate modeling, time-scale separation is a central feature of many dissipative processes in physical and industrial applications. Such a scale separation can be conveniently expressed in Fourier space by differentiating the so-called fast modes, which are characterized with large wave numbers and converge towards equilibrium much faster than the slow (low wave number) modes. As a consequence, the long-time behavior of the system is primarily contained in the latter. There are several mode reduction techniques in the literature that take advantage of such scale decomposition, including deterministic methodologies such as adiabatic elimination [1] and the classical center-manifold theory [2], which usually requires the system to be close to criticality and to equilibrium, i.e., close to an invariant solution that is expected to be part of a finite-dimensional center manifold [3]. A different line of thought follows the so-called stochastic mode reduction strategies, where the aim is to convert an infinite-dimensional deterministic dynamical system (PDE) into a low-dimensional stochastic one. In the case of Hamiltonian-like systems, there exist well-known powerful techniques such as optimal prediction and the Mori-Zwanzig formalism [4] for the derivation of mode-reduced (low-dimensional) stochastic equations. Both approaches make use of the existence of an invariant or canonical probability distribution given by the Hamiltonian structure. Other examples of these include Ref. [5] where a Galerkin truncated Burgers-Hopf equation is considered to obtain a Hamiltonian structure and a canonical Gibbs measure.

However, a stochastic methodology available for problems that do not have a Hamiltonian structure does not seem to exist. It is precisely our purpose to study this open problem. To this end, we properly extend the evolutionary renormalization group (ERG) method [6], which asymptotically defines equations for slow and fast modes, towards a stochastic mode reduction by adapting the principle of maximum information entropy (PMIE) [7] appropriately extended to PDEs, which allows us to extract the relevant information from the fast modes to obtain a closed equation for the slow modes only. Separation of scales (slow or fast) can be physically justified by the presence of dissipation. We observe that the ERG method provides a systematic and rigorous (in terms of error estimates) tool to separate a dissipative nonlinear problem into fast (w^ϵ) and slow (v^ϵ) modes

$$\partial_t v^\epsilon = f(v^\epsilon, w^\epsilon), \qquad \partial_t w^\epsilon = \frac{1}{\epsilon} g(v^\epsilon, w^\epsilon), \tag{1}$$

where the parameter $0 < \epsilon \ll 1$ measures the time scale separation. It is important to note that in the aforementioned deterministic mode reduction strategies such as invariant manifolds, one generally assumes that the model of interest decomposes as Eq. (1) from the beginning

without further specification $\epsilon \ll 1$. However, such a decomposition and the associated definition of ϵ needs to be checked carefully from a practical and theoretical point of view, and in particular for systems exhibiting spatiotemporal chaos, it is expected that many characteristic spatiotemporal scales can be present. A well-known example of such systems is the generalized Kuramoto-Sivashinsky (gKS) equation [8] which retains the fundamental ingredients of any nonlinear process involving spatiotemporal transitions and pattern formation: nonlinearity, instability or energy production, stability or energy dissipation, and dispersion. In our methodology, we systematically define the parameter ϵ, which mediates the time scales and depends on the number of the resolved degrees of freedom represented by v^ϵ. We can further place our low-dimensional approximation on a solid theoretical basis by rigorous error estimates [9] controlled by ϵ. Moreover, our stochastic mode reduction based on the PMIE rigorously supports theoretically Stinis's computational approach [10]. Using the dissipation property defined by the renormalized fast modes, which implies that the fast Fourier modes are independently distributed, we show via PMIE that they are Gaussian distributed with zero mean and variance $\sigma^2 > 0$. This leads to a rigorous methodology to rationally and systematically derive stochastic low-dimensional representations of deterministic, nonlinear, and non-Hamiltonian PDEs and further explain the arising randomness as the extracted information from the neglected fast modes, which is important from the point of view of noise-induced phenomena [11,12]. Finally, our new stochastic mode reduction strategy rigorously supports the formal RG approach applied to the gKS equation by Chow and Hwa [13].

General methodology: ERG and PMIE.—Consider dissipative nonlinear PDEs of the form

$$\partial_t u = \mathcal{A}u + \mathcal{F}(u), \tag{2}$$

where $u(x, t)$ is a one-dimensional variable with space and time dependence; $\mathcal{A}$ denotes a linear spatial differential operator and $\mathcal{F}$ denotes a nonlinear term. For ease of presentation, we consider deterministic initial conditions (ICs) with high enough spatial regularity (i.e., differentiability), and for simplicity, we restrict ourselves to periodic boundary conditions. The ERG method consists in approximating $u := v + w$ by $u^\epsilon := v^\epsilon + w^\epsilon$, where v^ϵ are the slow and w^ϵ the fast modes, i.e.,

$$\begin{aligned} \partial_t v^\epsilon &= \mathcal{A}_v v^\epsilon + P_N \mathcal{F}(v^\epsilon, w^\epsilon), \\ \partial_t w^\epsilon &= \mathcal{A}_w w^\epsilon + Q_N \mathcal{F}(v^\epsilon, w^\epsilon), \end{aligned} \tag{3}$$

where P_N and $Q_N := I - P_N$ are the orthogonal projections to the first N Fourier modes and its complement. We have also applied formally the notation $\mathcal{A}_v := P_N \mathcal{A}$ and $\mathcal{A}_w := \epsilon Q_N \mathcal{A}$ where $\epsilon := 1/N^\beta$ and $\beta > 0$ denotes the highest order of spatial derivatives defined by the operator $\mathcal{A}$. The separation (3) can be made rigorous by error estimates [9], which indicate how large one should choose $N > 0$. Next, we insert the asymptotic expansion $u^\epsilon = u^0 + \epsilon u^1 + \epsilon^2 u^2 + \cdots$ into Eq. (3) reformulated for a vectorial $u^\epsilon := [v^\epsilon, w^\epsilon]'$, leading to the ERG equation

$$\partial_t U = \mathcal{F}_R(U), \tag{4}$$

with $U(0) = u_0$, which removes secular terms growing in time (see e.g., Ref. [14] for classical homogenization with respect to space). U is the RG solution, which turns out to be the Galerkin approximation with N Fourier basis functions, and also decomposes into slow V and fast W modes. The resonant part $\mathcal{F}_R$ of $\mathcal{F}$ is defined via

$$e^{L\tau}\mathcal{F}(e^{-L\tau}u_0) - \mathcal{A}v_0 =: \mathcal{F}_R(u_0) + \tilde{\mathcal{F}}_{\mathrm{NR}}(\tau, u_0), \tag{5}$$

where L is the system size, $\tilde{\mathcal{F}}_{\mathrm{NR}}$ represents the nonresonant part, and τ is the rescaled time. The slow variable V of the RG Eq. (4) solves the standard Galerkin approximation of Eq. (2) for $2N + 1$ modes, i.e.,

$$\partial_t V = \mathcal{A}_v V + P_N \mathcal{F}(V). \tag{6}$$

Putting things together finally leads to the renormalized solutions

$$\mathrm{v}^\epsilon = P_N u^\epsilon = V(t) + \epsilon P F_{\mathrm{NR}}(t/\epsilon, U), \tag{7a}$$

$$\mathrm{w}^\epsilon = Q_N u^\epsilon = e^{-Q_N \mathcal{A} t/\epsilon}[W(t) + \epsilon Q F_{\mathrm{NR}}(t/\epsilon, U)], \tag{7b}$$

where $F_{\mathrm{NR}}(s, U) := \int_0^s \tilde{\mathcal{F}}_{\mathrm{NR}}(\tau, U)d\tau$. Note that the fast modes W [required in Eq. (4)] are still infinite dimensional. To obtain a finite-dimensional representation, we replace w^ϵ with a random process that is defined by the original (i.e., not renormalized) fast variable w^ϵ, which contains more information about the dynamics. We obtain the probability distribution for w^ϵ via PMIE by maximizing the information entropy

$$\mathcal{S}_I(f(w_j^\epsilon)) := -\int_\Omega f(w_j^\epsilon) \log\left(\frac{f(w_j^\epsilon)}{\nu(\omega)}\right) d\omega \tag{8}$$

under the constraint

$$\int_\Omega f(w_j^\epsilon) \frac{d}{dt} \mathcal{C}_N(w_j^\epsilon) d\omega = \delta_j(t), \tag{9}$$

where Ω is the space of events and $f(w_j^\epsilon)$ is the probability density of the jth fast mode $w_j^\epsilon(t, \omega)$; $\delta_j(t)$ is a characteristic dissipation rate, which for simplicity we approximate by the jth Fourier mode $\tilde{W}_j(t) := e^{-\rho_j^w t/\epsilon} w_j(0)$ of the leading order term in Eq. (7b) by setting $\delta_j(t) := d/dt\mathcal{C}_N(\tilde{W}_j) := -(1/2)d/dt\tilde{W}_j^2$. The measure ν is defined by prior or background knowledge on the system, such as uncertainties associated with the model (which turns out to be a uniform distribution after applying the PMIE), and the stochastic process W defined via Eqs. (8) and (9) finally leads to a random process for the solution v^ϵ in Eq. (7a).

The gKS equation.—We exemplify the above procedure with the gKS equation, i.e.,

$$\mathcal{A} := -(\partial_x^2 + \kappa\partial_x^3 + \partial_x^4), \qquad \mathcal{F}(u) := -u\partial_x u,$$

defined on the periodic domain $\mathcal{D}_L :=]-L/2, L/2[$. The ERG provides the deterministic approximation [(7a) and (7b)] via Eq. (6) and

$$PF_{\mathrm{NR}}(s,U) = 2i\lambda \sum_{|j|\le N} e^{i(j/\alpha)x} \sum_{\substack{k+l=j \\ |k|\le N<|l|}} \frac{e^{-\rho_l^w s}}{\rho_l^w} V_k \frac{j}{\alpha} W_l + i\lambda \sum_{|j|\le N} e^{i(j/\alpha)x} \sum_{\substack{k+l=j \\ |k|,|l|>N}} \frac{e^{-(\rho_k^w+\rho_l^w)s}}{\rho_k^w+\rho_l^w} W_k \frac{j}{\alpha} W_l,$$

where $\rho_l^w := -(1/N^\beta)((l/\alpha)^2 + i\kappa(l/\alpha)^3 + (l/\alpha)^4)$ are the eigenvalues of $\mathcal{A}_w$ with eigenvectors $e^{i(k/\alpha)x}$, and $\alpha := L/2\pi$.

We choose $\mathcal{C}_N[w_j^\epsilon(t,\omega)] := -(1/2)(w_j^\epsilon)^2(t,\omega)$, and hence from the solutions of the equation for w_j^ϵ we obtain

$$\frac{d}{dt}\mathcal{C}_N(w_j^\epsilon) = \rho_j^w (w_j^\epsilon)^2 + i w_j^\epsilon \sum_{\substack{|k|\le N \\ |j-k|>N}} v_k \frac{j-k}{\alpha} w_{j-k}^\epsilon.$$

Maximizing now the information entropy (8) under the constraint of Eq. (9) [see Ref. [7], Chap. 9] leads to the following probability density

$$f(w_j^\epsilon) := \frac{1}{Z_j} m_j \frac{1}{\sigma_j\sqrt{2\pi}} \exp - \frac{(w_j^\epsilon - \mu_j)^2}{2\sigma_j^2},$$

where $m_j := c_j^{-1}\sigma_j\sqrt{2\pi}\exp -\mu_j^2/(2\sigma_j^2)$, and

$$\mu_j := \frac{i}{2\rho_j^w} \sum_{\substack{|k|\le N \\ |j-k|>N}} v_k^\epsilon \frac{j-k}{\alpha} \mu_{j-k}, \qquad \sigma_j^2 := \frac{1}{2\lambda_j \rho_j^w}. \quad (10)$$

Note that if one replaces Eq. (9) by $\int_{-\infty}^{\infty} f(w_j^\epsilon)(w_j^\epsilon)^2 d\omega = \sigma^2$, we get the classical result $w_j \sim \mathcal{N}(0,\sigma^2)$. We apply the PMIE with respect to the original dynamics w^ϵ in Eq. (8) and hence added complete dynamical information to the Fourier modes W_j of W in Eq. (10) leading to $W_j \sim \mathcal{N}(\mu_j, \sigma_j^2)$. It follows from Eq. (10) and $\overline{\mu_j} = \mu_{-j}$, where $\overline{\mu}_j$ denotes the complex conjugate of μ_j, that $\mu_j = 0$ for $|j| > N$, and the constraint (9) finally defines $\lambda_j = 1/(2\delta_j(t))$ where $\delta_j(t) = d/dt\mathcal{C}_N(\tilde{W}_j) = \rho_j^w e^{-2\rho_j^w t} w_j^2(0)$ for the dissipation rate in Eq. (9). For random ICs, the above methodology carries over but $w_k^2(0)$ is replaced with $\langle w_k^2(0)\rangle$, where brackets denote average over different ICs.

From the formula for $f(w_j^\epsilon)$, we deduce that the normalization constant, i.e. the partition function, is $Z_j := m_j$. On the basis of f, the distribution of the fast renormalized variable $W(x,t) := \sum_{|j|>N} W_j e^{ij/\alpha(x+2V_0 t)}$ can be determined as $W \sim \mathcal{N}(\mu_W, \sigma_W^2)$ where $\mu_W := \sum_{|j|>N} e^{ij/\alpha(x+2V_0 t)}\mu_j$, and $\sigma_W^2 := \sum_{|j|>N} e^{i2j/\alpha(x+2V_0 t)}\sigma_j^2$. Using $W \sim \mathcal{N}(\mu_W, \sigma_W^2)$ in Eq. (7a) gives the final result of our stochastic mode reduction method. This result not only offers a systematic way of accurately representing deterministic equations with low-dimensional stochastic ones but also allows for efficient computations, as we only need to solve the reduced model and add the noise *a posteriori*.

Numerical results and physical interpretations.—We start by looking at the statistics of the fast modes by numerically solving the gKS equation for $2\Lambda + 1$ Fourier modes with $\Lambda = 2048$, $\kappa = 0.1$, and using different types of random ICs of the form $u_0(x) = a\xi(x)$, where $\xi(x)$ corresponds to either spatial white noise [i.e., $\langle\xi(x)\xi(x')\rangle = 2\delta(x-x')$] with zero mean and unit variance or a uniform distribution $\xi(x) \in [-1, 1]$. We also choose different values for the noise amplitude, namely, $a = 0.1$, 1, 3, 6, and perform 2000 noise realizations each. The spatiotemporal solution of $u(x,t)$ rapidly evolves into a complex dynamics characterized by a chaotic behavior (see e.g., Ref. [8]). Figures 1(a) and 1(c) show that after some time, the distribution of the fast modes relaxes to a universal probability density function (PDF) that is independent of the ICs and corresponds to a Gaussian distribution $\mathcal{N}(0,\sigma_k^2)$. This relaxation can also be seen by computing the evolution of the entropy S_I, observing that the final state is independent of the ICs [cf. Fig. 1(b)]. Our results also suggest that the variance of the fast modes has a k dependency, which is an exponential decay as a consequence of dissipation.

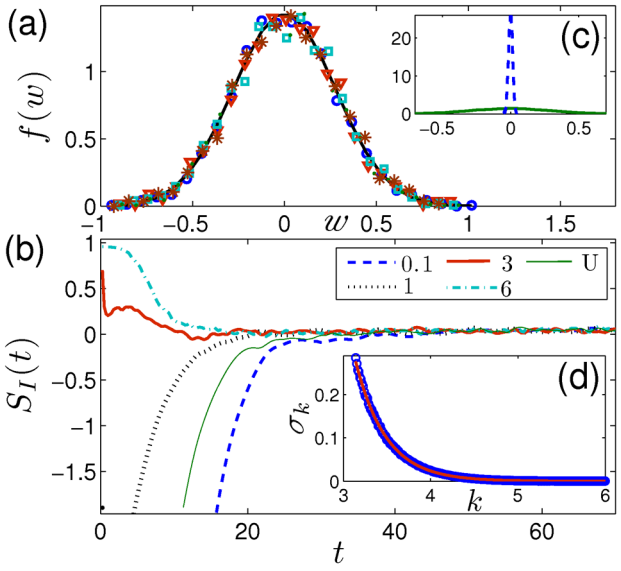

FIG. 1 (color online). (a) Long-time behavior of $f(w_k)$ for the first fast mode ($k = N + 1$) and five different ICs (represented by different symbols). The solid line is a Gaussian PDF with $\mu = 0$ and $\sigma = \sigma_{N+1} = 0.27$. The inset (c) shows snapshots of $f(w)$ at $t = 0$ (dashed line) and long times (solid line). (b) Time evolution of the entropy S_I for $k = N + 1$ and random initial conditions of the form $u_0(x) = a\xi(x)$ with $a = 1$ for a uniform distribution (U), and $a = 0.1$, 1, 3, and 6 for a Gaussian distribution. For simplicity, we have considered $\nu(w) = 1$ to compute S_I in Eq. (8). (d) Exponential k dependency of σ at long times where the solid line is a data fit with $\sigma_k = \exp(-2.86k + 7.73)$. k is rescaled here by $\alpha = L/2\pi$.

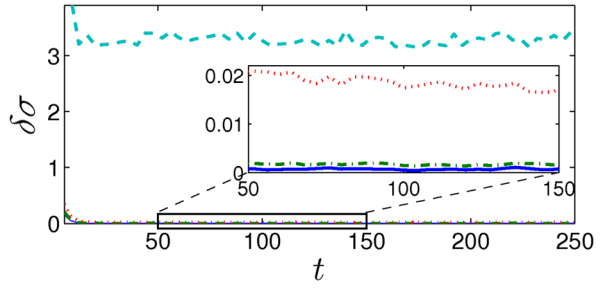

FIG. 2 (color online). Difference between the second moment of the full and ERG solutions as function of time and for $N = 768$ (cyan dashed line), 896 (red dotted line), 960 (green dot-dashed line), and 1024 (blue solid line). The inset shows a zoom into the marked area.

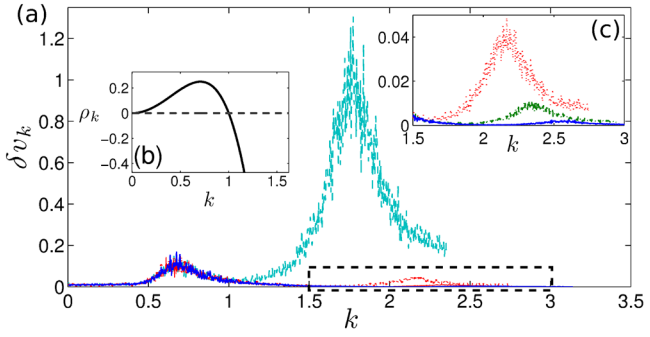

FIG. 3 (color online). Difference between the modes obtained from the full and ERG solution by taking $N = 768$ (cyan dashed line), 896 (red dotted line), 960 (green dot-dashed line), and 1024 (blue solid line). k is rescaled here by $\alpha = L/2\pi$, and the maximum values correspond to $k_{\max} = 2.35$, 2.74, 2.94, and 3.13, respectively. (b) Eigenvalues ρ_k of the linear operator $\mathcal{A}$. (c) Zoom into the area marked with dashed lines.

Next, we demonstrate the performance of our new mode reduction strategy by comparing numerical results obtained from the full system, i.e., the solution $u(x, t)$ that takes into account all the modes up to Λ, and the reduced system, i.e., the solution $v^{\epsilon}(x, t)$ obtained with a lower number $N < \Lambda$ of modes. We note that the efficiency of the method relies on the fact that we only need to solve the system with $N < \Lambda$ modes and add the ERG corrections *a posteriori* [see Eqs. (7a) and (7b)] where the fast modes W_k are given as random variables of zero mean and variance σ_k, the k dependency of which is the one observed numerically in Fig. 1. We compute first the second moment of both the full spatiotemporal solution, i.e., $\sigma_F = (\overline{u^2} - \overline{u}^2)^{1/2}$, where the overline denotes spatial average, and the ERG solution $v^{\epsilon}(x, t)$, which we denote as σ_R. Figure 2 depicts the error distance between both magnitudes $\delta\sigma := \langle(\sigma_F - \sigma_R)^2\rangle$, for different values of N. We observe that the ERG solution converges to the full solution (with $\delta\sigma < 10^{-3}$) as $N \to \Lambda/2$.

We also compute the error distance between each Fourier mode by defining $\delta v_k = \langle[(v_k - v_k^{\epsilon})/\max(v_k)]^2\rangle$, where v_k and v_k^{ϵ} correspond to the absolute value (amplitude) of the slow modes from the full and ERG solution. Figure 3 shows the results for sufficiently long times (i.e., the entropy function has already equilibrated) and for different values of N. It is interesting to note that the error distance for the linearly unstable (slow) modes, which are defined as those with positive eigenvalues $\rho_k > 0$ [see Fig. 3(b)], is practically unaffected as we change N. On the other hand, the stable modes in $1 < k < 3$ largely depend on the truncation number N observing as before a rapid convergence to zero as $N \to \Lambda/2$. This indicates that (a) the dynamics of the unstable modes is robust and seems not to depend on the number of stable modes used for the reduced model and (b) less than half of the stable modes, i.e., $N < \Lambda/2$, already provides a reliable representation of the full system solution.

Finally, we also look at how time correlations of a single mode can be well represented by the reduced model. To this end, we compute the frequency power spectrum of the absolute value of a given mode for $0 < t < T$, i.e., $s_f(k, w) = (1/T)\sum_t v_k(t)\exp(iwt)$ [see the Supplemental Material [15]]. As before, all solutions with different N values give similar results for the unstable modes, whereas the difference between both solutions for the stable slow modes grows as N is decreased [see Fig. 1 in the Supplemental Material [15]].

To conclude, we have outlined a new stochastic mode reduction methodology for dissipative dynamical systems of the general form (2). It was exemplified with a paradigm for nonlinear evolution and pattern formation, the gKS equation. The cornerstone of our methodology is the information entropy, which combined with an ERG formalism, gives a rigorous and systematic justification of fast-slow scale separation as well as of randomness in dissipative systems. We demonstrated numerically the validity of the method and its efficiency, i.e., that one only needs to solve the reduced model (which can contain as few as half of the whole number of modes), and then add the particular type of the underlying stochastic process resulting from the maximum entropy principle. We further showed that the methodology enables us to uncover new physical insights. These include a universal PDF for the fast modes that emerges independently of the ICs and a clear distinction between the modes that are relevant to describe the dynamics of the full system based on a reduced model, from those that have a faster decay. Moreover, our method uncovers an appropriate definition of entropy for dissipative nonequilibrium processes that show a universal characteristic such as a Gaussian PDF, thus providing a systematic means for quantifying the evolution of dissipative systems.

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[15] See the Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.110.244101 for time-correlations of a single mode, full system and the reduced model.