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STOCHASTIC MODELS FOR SELECTED SLOW VARIABLES IN LARGE DETERMINISTIC SYSTEMS

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Abstract

A new stochastic mode-elimination procedure is introduced for a class of deterministic systems. Under assumptions of mixing and ergodicity, the procedure gives closed-form stochastic models for the slow variables in the limit of infinite separation of timescales. The procedure is applied to the truncated Burgers-Hopf (TBH) system as a test case where the separation of timescale is only approximate. It is shown that the stochastic models reproduce exactly the statistical behavior of the slow modes in TBH when the fast modes are artificially accelerated to enforce the separation of timescales. It is shown that this operation of acceleration only has a moderate impact on the bulk statistical properties of the slow modes in TBH. As a result, the stochastic models are sound for the original TBH system.

Key words

Stochastic Mode-Reduction, Deterministic Conservative Systems

1 Stochastic models for deterministic systems

The stochastic mode-reduction strategy introduced in this paper is particularly relevant in the context of high-dimensional systems of ODEs arising as projections of conservative partial differential differential equations. Consider a set of real variables $\{u_k(t)\}_{k\in S}$ with index k varying in some set S. The variables $\{u_k(t)\}_{k\in S}$ can be thought of as coefficients in the some appropriate representation (Fourier, etc.), and the set S is the set of indexes retained in the Galerkin projection. We also assume that the dependent variables $\{u_k(t)\}_{k\in S}$ can be decomposed in two sets, $\{a_i\}_{i\in S_a}$ and $\{b_j\}_{j\in S_b}$, where $\{a_i\}_{i\in S_a}$ represent the slow essential degrees of freedom and $\{b_j\}_{j\in S_b}$ represent the fast unresolved modes. The indices i and j vary over some index sets $S_a = \{1,..,M\}$ and $S_b = \{1,..,N\}$. M and N are the numbers of slow and fast variables, respectively.

We consider a general quadratic system of equations for the variables $a = \{a_i\}$ and $b = \{b_i\}$

$$
\begin{aligned}
\dot{a}_i &= \sum m^{aaa}_{ijk} a_j a_k + \\
&\quad 2\varepsilon^{-1} \sum m^{aab}_{ijk} a_j b_k + \varepsilon^{-1} \sum m^{abb}_{ijk} b_j b_k, \\
\dot{b}_i &= \varepsilon^{-1} \sum m^{baa}_{ijk} a_j a_k + \\
&\quad 2\varepsilon^{-1} \sum m^{bab}_{ijk} a_j b_k + \varepsilon^{-2} \sum m^{bbb}_{ijk} b_j b_k,
\end{aligned}
\tag{1}
$$

where $\varepsilon < 1$ is a parameter measuring the difference in timescales between the slow and fast modes, and we will be interested in the asymptotic behavior of (1) in the limit as $\varepsilon \to 0$. Summations in (1) are taken over the repeated indexes which vary in the set S_a or S_b, depending on the indexed variable. The right-hand sides in (1) have been explicitly decomposed into the self-interactions of slow modes (a with a), interactions between the slow and fast dynamics (a and b), and fast self-interactions (b with b). The interaction coefficients are denoted as m^{xzy}_{ijk} where each x, y, z stands for a or b. Without the loss of generality we can make the symmetry assumption $m^{xyz}_{ijk} = m^{xzy}_{ikj}$.

We also assume that (i) $m^{xyz}_{ijk} + m^{yzx}_{jki} + m^{zxy}_{kij} = 0$; this assumption guarantees that the dynamics in (1) conserves energy

$$
E = \sum a_i^2 + \sum b_i^2 =: |a|^2 + |b|^2, \tag{2}
$$

and (ii) divergence of the right-hand side of the system in (1) is zero; the second assumption ensures that the dynamics in (1) is volume-preserving (Liouville property). If we also assume that (1) is ergodic on the hypersphere defined in (2) then it follows that the unique invariant measure for (1) is the uniform distribution on the sphere $E = \mathrm{Const}$. Finally, we will assume that the dynamics in (1) is exponentially mixing.

1.1 Stochastic models for small ε

It has been demonstrated in (Majda *et al.*, 2006) that under the conditions described in the previous section, the limiting behavior of $a(t)$ in (1) as $\varepsilon \to 0$ can be captured by a stochastic model

$$da_i = \sum m_{ijk}^{aaa} a_j a_k dt + B_i(a)dt \\ + \sum \frac{\partial}{\partial a_j} D_{ij}(a)dt + \sqrt{2} \sum \sigma_{ij}(a)dW_j, \tag{3}$$

where W_j is a M-dimensional Wiener process and $\sigma_{ij}(a)$ satisfies $\sum \sigma_{ik}(a)\sigma_{jk}(a) = D_{ij}(a)$.

The proposition can be formally established by singular perturbation analysis of the backward equation associated with (1), see e.g. (Majda *et al.*, 2001). A rigorous proof can be found e.g. in (Freidlin and Wentzell, 1998).

The drift and diffusion in (3) are given by

$$B_i(a) = -(1 - 2N^{-1})\mathcal{E}^{-1} \sum D_{ij}(a)a_j, \tag{4}$$

where $\mathcal{E} := \mathcal{E}(a) := N^{-1}(E - |a|^2)$ and

$$D_{ij}(a) = \sqrt{\mathcal{E}} \int_0^\infty \int P_i(c) P_j\left(C(t)\right) d\mu dt, \tag{5}$$

with

$$P_i(c) = 2 \sum m_{ijk}^{aab} a_j c_k + \sqrt{\mathcal{E}} \sum m_{ijk}^{abb} c_j c_k. \tag{6}$$

Here $C(t)$ is the solution of the fast auxiliary subsystem

$$\dot{c}_i = \sum m_{ijk}^{bbb} c_j c_k, \tag{7}$$

with initial condition $C(0) = c$ consistent with the energy requirement $|c|^2 = N$, and $d\mu$ is the uniform measure on the sphere of constant energy $|c|^2 = N$, where N is the number of fast variables.

The proof of this Proposition uses a rescaling on the sphere of radius N of the fast subsystem. After this rescaling the system (7) must be solved with an initial condition consistent with $|C(0)|^2 = |c|^2 = N$, which is therefore independent of a. In other words, the diffusion tensor $D_{ij}(a)$ can be estimated for all a from a single calculation with (7).

The integrals with respect to the invariant measure $d\mu$ correspond to microcanonical averages of the fast subsystem on the energy shell $|C|^2 = N$. Therefore, averages in (5) can be expressed as the area under the graph of the two-point autocorrelation function. These terms are evaluated numerically from a single realization of the fast subsystem.

2 Truncated Burgers-Hopf system

We apply a recently developed stochastic mode-reduction strategy for deterministic conservative systems (see (Majda *et al.*, 2006) for complete details) to the spectral truncation of the inviscid Burgers-Hopf model. These equations can be recast as a finite-dimensional system of equations for the Fourier amplitudes, $\hat{u}_k$ with $0 < |k| \le \Lambda$

$$\dot{\hat{u}}_k = -\frac{ik}{2} \sum_{\substack{k+p+q=0 \\ |p|,|q| \le \Lambda}} \hat{u}_p^* \hat{u}_q^*, \tag{8}$$

with the reality condition $\hat{u}_{-k} = \hat{u}_k^*$. The spectral truncation of the inviscid Burgers-Hopf model (TBH) was introduced in (Majda and Timofeyev, 2000; Majda and Timofeyev, 2002); this system exhibits many of the desirable properties found in more complex systems, but has the virtue of allowing a relatively complete analysis of statistical properties and extensive numerical studies. The key property is the conservation of energy

$$E = \frac{1}{4\pi} \int_0^{2\pi} u_\Lambda^2 dx = \sum_{k=1}^{\Lambda} |\hat{u}_k|^2. \tag{9}$$

The vector field in (8) is volume-preserving and in (Majda and Timofeyev, 2000; Majda and Timofeyev, 2002) an equilibrium statistical theory for the TBH was developed. The marginal on each Fourier mode $k \neq 0$ of the microcanonical distribution approaches Gaussian probability distribution $\mu(d\hat{u}_k) = C_\beta e^{-\beta|\hat{u}_k|^2} d\hat{u}_k$ in the limit $\Lambda \to \infty$ with $E = \Lambda/\beta$ for some β playing the role of an inverse temperature. This implies equipartition of energy in this limit $\forall k \neq 0$: $\text{var}\{\text{Re}\ \hat{u}_k\} = \text{var}\{\text{Im}\ \hat{u}_k\} = \frac{1}{2\beta}$. These predictions were verified for a wide variety of regimes and random and deterministic initial data. In addition, it was demonstrated that for low wavenumbers an empirical scaling law for correlation times, defined as the area under the normalized auto-correlation functions for mode $\hat{u}_k$, holds: $\text{corr\_time}\{\hat{u}_k\} \sim |k|^{-1}$.

3 Selectively accelerated TBH systems

The results in Section 1 hold provided that the timescale separation between fast and slow variables is infinite. In practical applications the timescale separation between these two groups of variables is moderate, at best. Therefore, for any such system it is in principle necessary to verify the applicability of asymptotic expansions a priori. A systematic way to address this issue is to artificially accelerate the dynamics of the fast variables and observe the effect this induces on the statistical behavior of the slow variables. This procedure can be implemented as follows on TBH: (i) fix a wave number $\Lambda_1 < \Lambda$ such that any mode with $|k| \le \Lambda_1$ is considered as slow, and any mode with $\Lambda_1 < |k| \le \Lambda$

is considered as fast; (ii) modify (8) by introducing ε into the equation consistent with the general form of (1). The original TBH system is recovered by setting $\varepsilon = 1$.

Since the timescale separation is only approximate in the original TBH, the grouping into fast and slow modes is somewhat arbitrary. Here we illustrate the approach outlined in the previous section for $\Lambda_1 = 1$, i.e. u_1 is the only slow mode.

3.1 One slow mode, $\hat{u}_1$

Taking the first Fourier coefficient as the only slow mode amounts to choosing $\Lambda_1 = 1$, in which case the Selectively-Accelerated TBH (SA-TBH) system is given by

$$\begin{aligned}\dot{\hat{u}}_1 &= -\frac{i}{2\varepsilon} \sum_{\substack{p+q+1=0\\2\le|p|,|q|\le\Lambda}} \hat{u}_p^* \hat{u}_q^*,\\ \dot{\hat{u}}_k &= -\frac{ik}{2\varepsilon}\left(\hat{u}_{k+1}\hat{u}_1^* + \hat{u}_{k-1}\hat{u}_1\right)\\ &\quad - \frac{ik}{2\varepsilon^2} \sum_{\substack{k+p+q=0\\2\le|p|,|q|\le\Lambda}} \hat{u}_p^*\hat{u}_q^*, \qquad (k \ge 2)\end{aligned} \tag{10}$$

where we used the reality condition $\hat{u}_{-k} = \hat{u}_k^*$ to simplify the right-hand side of the second equation.

The SA-TBH systems in (10) preserve the energy in (9) for all ε. If the dynamics is ergodic and mixing on the surface of constant energy, then equilibrium statistical mechanics predicts that the equilibrium distribution is the microcanonical distribution on the surface of constant energy. Then (10) (written in terms of Re $\hat{u}_k$ and Im $\hat{u}_k$) is a special case of (1), and its behavior as $\varepsilon \to 0$ is given by the stochastic system in (3).

Notice that the slowest of the fast modes, $\hat{u}_2$, is only twice as fast as the designated slow mode, i.e. *corr_time*$\{\hat{u}_1\}$/*corr_time*$\{\hat{u}_2\} \approx 2$ when $\varepsilon = 1$. Of course, the situation changes when $\varepsilon \to 0$, and the main goal for considering the SA-TBH system in (10) is investigate the effect of this operation on the statistical behavior of $\hat{u}_1$.

We perform direct numerical simulations of the equations in (10) with three values of $\varepsilon = 0.5,\ 0.25,\ 0.1$, and compare them with the original system with $\varepsilon = 1$. The other parameters were chosen to be $\Lambda = 20,\ E = 0.4\ (\beta = 50)$.

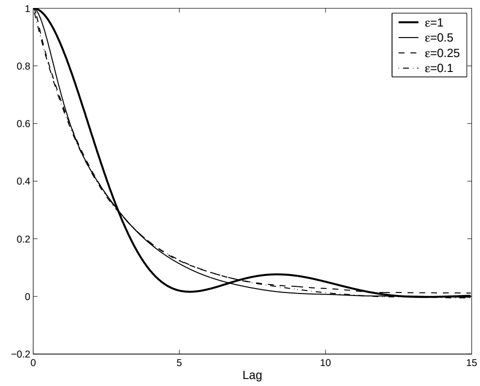

Figure 1: Normalized correlation function of Re u_1 from the simulations of the SA-TBH system in (10).

All statistics are computed as time-averages from a single microcanonical realization of length $T \approx 10^5$.

The behavior of correlation functions for various values of ε is presented in Figure 1. There is a significant difference between the simulations with $\varepsilon = 1$ and $\varepsilon = 0.5$; a small difference between $\varepsilon = 0.5$ and $\varepsilon = 0.25$; and almost no difference between $\varepsilon = 0.25$ and $\varepsilon = 0.1$. This demonstrates convergence of the correlation functions in the limit as $\varepsilon \to 0$. However, the shape of the correlation functions in this limit also shows that the artificial acceleration in TBH does have an effect on the dynamics. The correlation functions at $\varepsilon = 0.5 \ldots 0.1$ are close to exponential, while the correlation function in the original TBH systems has a complicated shape with the "bump" in the middle and smoother behavior at zero. Nevertheless, the mean decay rate is reproduced correctly by the simulations of the accelerated model. The correlation times (area under the graph of the corresponding normalized correlation function) of Re $\hat{u}_1$ in the simulation with $\varepsilon = 1$ and $\varepsilon = 0.1$ are

$$\text{corr\_time}\{\hat{u}_1\}^{\varepsilon=1} \approx 2.63,$$
$$\text{corr\_time}\{\hat{u}_1\}^{\varepsilon=0.1} \approx 2.4.$$

4 Stochastic model for $\hat{u}_1$

In this section we use the effective SDE in (3) to study the statistical behavior of $\hat{u}_1$. In principle, the solution of this SDE should behave similarly as the solutions of (10) at small ε. In practice, however, additional discrepancies can be introduced because the coefficients in the SDE are obtained numerically with finite precision only.

In order to write the SDEs in a more compact form we denote the slow variables as

$$a = (a_1, a_2) \equiv (\text{Re}\ \hat{u}_1, \text{Im}\ \hat{u}_1). \tag{11}$$

Then the SDE in (3) obtained from (10) in the limit as $\varepsilon \to 0$ can be written explicitly as:

$$da_k = [B(a) + H(a)]a_k dt + \sqrt{2}\sigma(a)dW_k(t), \tag{12}$$

for $k = 1, 2$, where

$$B(a) = -(1 - N^{-1}) \left(\mathcal{E}^{1/2} I_2 |a|^2 + \mathcal{E}^{3/2} I_f \right) / \mathcal{E},$$
$$H(a) = 2\mathcal{E}^{1/2} I_2 - (\mathcal{E}^{-1/2} |a|^2 I_2 + 3\mathcal{E}^{1/2} I_f)/N,$$
$$\sigma^2(a) = \mathcal{E}^{1/2} |a|^2 I_2 + \mathcal{E}^{3/2} I_f,$$

where $B(a)$ and $H(a)$ are the drift and Itô terms in (3), respectively. $\mathcal{E}(a)$ denotes the energy per mode of the fast subsystem, i.e.

$$\mathcal{E}(a) = N^{-1}(E - |a|^2), \tag{13}$$

where $N = 2\Lambda - 2$ is the number of fast degrees of freedom and E is the total energy of the full TBH model.

The integral of $P_i(c) P_j(C(t))$ in (5) can be recast as the cross-correlation between right-hand sides of the slow variables projected onto the fast dynamics alone. Therefore, we have also defined

$$I_2 = I[\text{Re}\,\hat{u}_2, \text{Re}\,\hat{u}_2] = I[\text{Im}\,\hat{u}_2, \text{Im}\,\hat{u}_2], I_f = I[f^r, f^r] = I\left[f^i\right. \tag{14}$$

where $I[\cdot,\cdot]$ is a short-hand notation for the area under the graph of a correlation function

$$I[g,h] = \int_0^\infty \langle g(t) h(t+\tau) \rangle_t d\tau, \tag{15}$$

where $\langle \cdot \rangle_t$ denotes the temporal average, and

$$f^r(t) = \text{Re}\left(-\frac{i}{2} \sum_{\substack{p+q+1=0 \\ 2 \le |p|,|q| \le \Lambda}} \hat{u}_p^* \hat{u}_q^* \right),$$
$$f^i(t) = \text{Im}\left(-\frac{i}{2} \sum_{\substack{p+q+1=0 \\ 2 \le |p|,|q| \le \Lambda}} \hat{u}_p^* \hat{u}_q^* \right) \tag{16}$$

denote the real and the imaginary parts of the right hand-side of the equation for $\hat{u}_1$ in (10). The various correlation functions in the expressions above must be computed on the fast subsystem (7), which in the present situation corresponds to a TBH system with wavenumbers $2 \le |k| \le \Lambda$

$$\dot{\hat{u}}_k = -\frac{ik}{2} \sum_{\substack{k+p+q=0 \\ 2 \le |p|,|q| \le \Lambda}} \hat{u}_p^* \hat{u}_q^*, \qquad (2 \le |k| \le \Lambda). \tag{17}$$

The derivation of (12) is somewhat tedious but straightforward. In addition to the general assumptions stated in Section 1 the derivation utilizes specific properties of the TBH system to simplify the expressions for the stochastic model further. First, it uses the fact that the correlations of the real and imaginary parts of the same mode are identical by symmetry. Second, it utilizes the property (verified to very good precision for large Λ in (Majda and Timofeyev, 2000; Majda and Timofeyev, 2002)) that the joint distributions of any two modes is Gaussian with a diagonal correlation matrix. Therefore, all third moments can be neglected. Finally, it uses the fact that the cross-correlation between f^r and f^i, and Re $\hat{u}_2$ and Im $\hat{u}_2$ are negligible

$$\langle f^r(0) f^i(t) \rangle_t = \langle \text{Re}\,\hat{u}_2(0)\,\text{Im}\,\hat{u}_2(t) \rangle_t \approx 0,$$

which is also verified to very good precision in the simulations.

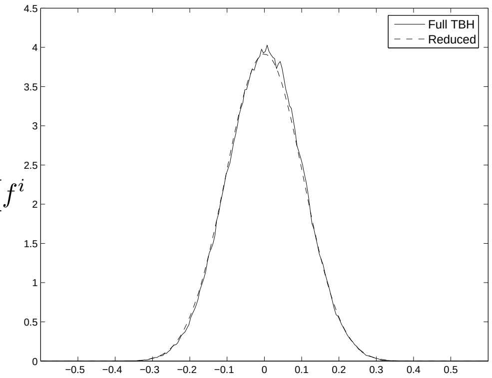

Figure 2: Marginal probability density function of Re $\hat{u}_1$ in the simulations of the original TBH system (8) with $\Lambda = 20$ (solid line) and the corresponding SDE in (12) (dashed line).

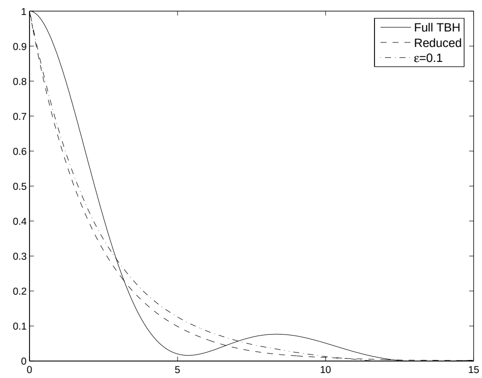

Figure 3: Normalized correlation function of Re $\hat{u}_1$ in the simulation of the original TBH system in (8) with $\Lambda = 20$ (solid line), the SA-TBH system in (10) with $\varepsilon = 0.1$ (dash-dotted line) and the SDE in (12) (dashed line).

We consider two cases $\Lambda = 20$ and $\Lambda = 40$. The values of coefficients are $(I_2, I_f)_{\Lambda=20} = (0.14, 4.3)$, and $(I_2, I_f)_{\Lambda=40} = (0.092, 6.1)$ were computed from the simulations of the auxiliary fast subsystem for $\Lambda = 20$ and $\Lambda = 40$ on energy levels consistent with $\beta = 1/2$ for several sets of initial conditions. Fluctuations of these parameters do not exceed 1.5%.

Statistical behavior of the stochastic model The comparison between the direct numerical simulations of the original TBH system in (8) and the SDEs in (12) is depicted in Figures 2 and 3. The one-time statistics is Gaussian in both simulations with perfect agreement between the simulations of the full TBH system and the stochastic model. To illustrate this, marginal distribution of Re $\hat{u}_1$ is presented in Figure 2.

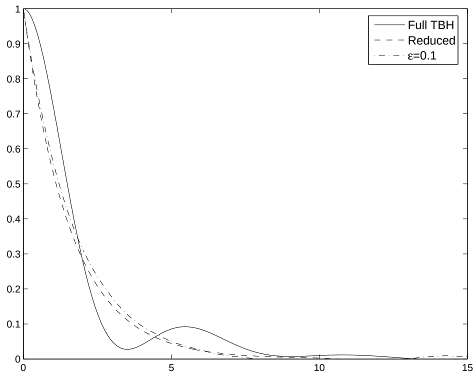

Figure 4: Normalized correlation function of Re $\hat{u}_1$ in the simulation of the original TBH system in (8) with $\Lambda = 40$ (solid line), the SA-TBH system in (10) with $\varepsilon = 0.1$ (dash-dotted line) and the SDE in (12) (dashed line).

Unlike the one-time statistics, the correlation functions of Re $\hat{u}_1$ and Im $\hat{u}_1$ differ more considerably between the original TBH system and the stochastic model. The detailed structure of the correlations is no longer represented in the stochastic model. Instead, correlation functions of Re $\hat{u}_1$ and Im $\hat{u}_1$ are exponentials with the averaged rate of decay reflecting the decorrelation times of the full model. But, as expected, the correlation functions of the stochastic model agree with the simulations of the SA-TBH system in (10) within a few percent. The correlation functions of Re $\hat{u}_1$ for truncation sizes $\Lambda = 20$ and $\Lambda = 40$ in the simulation of the original TBH system, the SA-TBH system with $\varepsilon = 0.1$, and corresponding stochastic models is depicted in Figures 3 and 4, respectively. Decorrelation times of the mode $\hat{u}_1$ are presented in Table 1.

	$\Lambda = 20$	$\Lambda = 40$
Original TBH	2.63	1.81
SDE in (12)	2.17	1.61
SA-TBH ($\varepsilon = 0.1$)	2.38	1.84

Table 1: Estimates for decorrelation times (1/area of the normalized correlation function) of Re $\hat{u}_1$ in simulations with $\Lambda = 20$ and $\Lambda = 40$.

5 Conclusions

A modified stochastic mode-reduction strategy for conservative systems was presented. One of the main advantages of the current approach is that no ad-hoc modifications of the underlying equations are necessary. Under assumptions of mixing and ergodicity, the procedure gives closed-form stochastic differential equations for the slow dynamics which are exact in the limit of infinite timescale separation between fast and slow modes. Only bulk statistical quantities of the fast dynamics enter the stochastic equations as coefficients and these can be computed for all energy levels from a single microcanonical realization on an auxiliary subsystem.

In any realistic system, the separation of timescale is only approximate. In this case, the stochastic model captures the behavior of the slow modes in a system where the fast modes have been artificially accelerated. This viewpoint allows, at least in principle, to test the validity and relevance of the stochastic model by assessing the impact of the artificial acceleration on the original dynamics. This approach was tested here on the TBH system. It was shown that the statistical properties of the slow modes in the SA-TBH system are, in the bulk if not in the detail, similar to the properties of these modes in the original TBH system. As a result, the stochastic models with only one or two modes retained out of 102 perform surprisingly well. The transportability of these conclusions to other systems is difficult to test, but they offer hope that the stochastic mode-elimination approach is applicable to problems without substantial timescale separation, as is the case in most applications of interest.

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