A Variational Approach to Small-Scale Parameterization for Nonlinear and Stochastic Dynamical Systems

Honghu Liu[1], Mickael Chekroun[2], and James McWilliams[3]

[1]Virginia Tech
[2]University of California Los Angeles
[3]University of California in Los Angeles

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Abstract

The modeling of physical phenomena oftentimes leads to partial differential equations (PDEs) that are usually nonlinear and can also be subject to various uncertainties. Solutions of such equations typically involve multiple spatial and temporal scales, which can be numerically expensive to fully resolve. On the other hand, for many applications, it is large-scale features of the solutions that are of primary interest. The closure problem of a given PDE system seeks essentially for a smaller system that governs to a certain degree the evolution of such large-scale features, in which the small-scale effects are modeled through various parameterization schemes. We will present an approach to parameterize the unresolved small-scale dynamics using the resolved large scales for forced dissipative systems. We will show that efficient parameterizations can be explicitly determined as parametric deformations of geometric objects constructed from dynamically based analytical formulas. The minimizers are intimately tied to the conditional expectation of the original system. We will highlight, within a variational framework, a simple semi-analytic approach to determine such parameterizations based on backward-forward auxiliary systems and short solution data. Concrete examples arising from geophysical considerations will also be presented to illustrate the effectiveness of the approach.

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Mickaël Chekroun[1,2], Honghu Liu*[,3], James C McWilliams[1]

[1]Department of Atmospheric & Oceanic Sciences, University of California, Los Angeles, CA 90095-1565;

[2]Department of Earth and Planetary Sciences, Weizmann Institute of Science, Rehovot 76100, Israel;

[3]Department of Mathematics, Virginia Tech, Blacksburg, VA 24061, hhliu@vt.edu.

Contribution

An efficient way to construct low-dimensional closures for (stochastic) nonlinear dissipative systems is proposed. The unobserved small-scale variables are parameterized through nonlinear functions of large-scale variables. Such nonlinear functions are constructed from the constitutive terms of the governing equations, with a few scalar parameters optimized via a variational framework based on solution data. For stochastic systems, the proposed parameterization brings extrinsic memory into the closure, which can play an essential role for the closure to capture rare tail events. At the same time, memory terms become secondary provided that a Markovian parameterization already provides a good approximation of the underlying conditional expectation and that the associated residual dynamics is mainly orthogonal to it, as illustrated on the paradigmatic Lorenz 80 model.

A motivating example of E. Lorenz [1, 3]

While the Mori-Zwanzig formalism [6, 9, 10, 11] of statistical mechanics suggests that the optimal closure models consist of a Markovian part, a part carrying memory effects, and a noise term that is uncorrelated with the resolved variables, it does not offer an explicit way of constructing such terms. We illustrate through the following reduced primitive model of E. Lorenz (L80) that when high-quality parameterization of the unresolved variables are available, it not only simplifies the construction of the memory and the noise terms, but also can render the memory terms unnecessary when the parameterization residual is mainly orthogonal to the observed variables.

The L80 model is the nine-variable system of ODEs derived in [8] as a truncation of the shallow-water equations onto three Fourier spatial basis functions (see [1] for the formulation adopted here):

$$\begin{aligned}
\epsilon^2 a_i \frac{\mathrm{d}X_i}{\mathrm{d}t} &= \epsilon^3 a_i b_i X_j X_k - \epsilon^2 c(a_i - a_k) X_j Y_k + \epsilon^2 c(a_i - a_j) Y_j X_k - 2\epsilon c^2 Y_j Y_k - \epsilon^2 N_0 a_i^2 X_i + a_i(Y_i - Z_i),\\
a_i \frac{\mathrm{d}Y_i}{\mathrm{d}t} &= -\epsilon a_k b_k X_j Y_k - \epsilon a_j b_j Y_j X_k + c(a_k - a_j) Y_j Y_k - a_i X_i - N_0 a_i^2 Y_i,\\
\frac{\mathrm{d}Z_i}{\mathrm{d}t} &= -\epsilon b_k X_j (Z_k - H_k) - \epsilon b_j (Z_j - H_j) X_k + c Y_j (Z_k - H_k) - c(Z_j - H_j) Y_k + g_0 a_i X_i - K_0 a_i Z_i + \mathcal{F}_i,
\end{aligned} \tag{1}$$

which are written for each cyclic permutation of the set of indices $(1,2,3)$: $(i,j,k) \in \{(1,2,3),(2,3,1),(3,1,2)\}$.

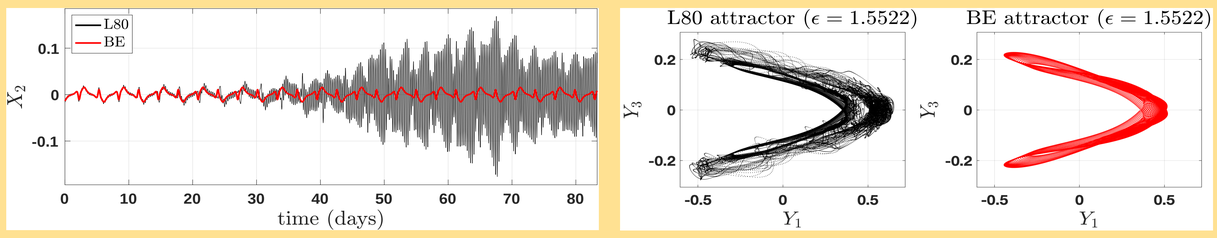
The scaling parameter ϵ is related to the Rossby number, which helps reveal the relative importance of the terms appearing in the "fast" variables $\boldsymbol{X}$ when ϵ is small. Such a consideration led the authors of [7] to consider a Balance Equation (BE) parameterization of the fast variables $\boldsymbol{X}$ and $\boldsymbol{Z}$ in terms of the slow variables $\boldsymbol{Y}$, which takes the following functional form (see [1, Sec. 3.1]):

$$Z_i = G_i(\boldsymbol{Y}) \stackrel{\text{def}}{=} Y_i - \frac{2\epsilon c^2}{a_i} Y_i Y_k, \quad \text{and} \quad \boldsymbol{X} = \Phi(\boldsymbol{Y}) \stackrel{\text{def}}{=} [M(\boldsymbol{Y}, G(\boldsymbol{Y}))]^{-1} \begin{pmatrix} d_{1,2,3}(\boldsymbol{Y}, G(\boldsymbol{Y})) \\ d_{2,3,1}(\boldsymbol{Y}, G(\boldsymbol{Y})) \\ d_{3,1,2}(\boldsymbol{Y}, G(\boldsymbol{Y})) \end{pmatrix}, \tag{2}$$

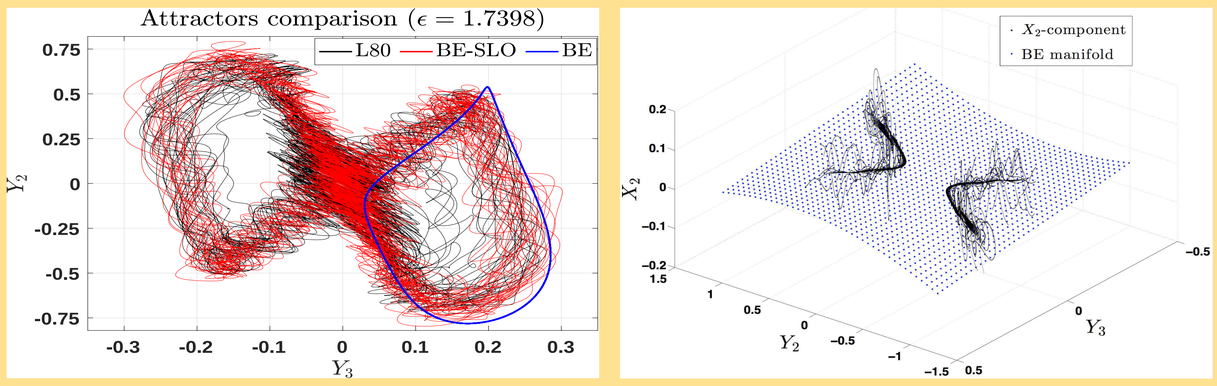
where M is a nonlinear matrix function of $\boldsymbol{Y}$ (and $\boldsymbol{Z}$ through the parameterization $G(\boldsymbol{Y})$), and $d_{i,j,k}$ are scalar functions of $\boldsymbol{Y}$. All constituent terms of M and $d_{i,j,k}$ are analytically constructed from the vector field of (1). The BE closure for $\boldsymbol{Y}$ is then obtained by simply replacing $\boldsymbol{X}$ by $\Phi(\boldsymbol{Y})$ in the $\boldsymbol{Y}$-equations of the system (1):

$$a_i \frac{\mathrm{d}Y_i}{\mathrm{d}t} = -\epsilon a_k b_k \Phi_j(\boldsymbol{Y}) Y_k - \epsilon a_j b_j Y_j \Phi_k(\boldsymbol{Y}) + c(a_k - a_j) Y_j Y_k - a_i \Phi_i(\boldsymbol{Y}) - N_0 a_i^2 Y_i. \tag{3}$$

When ϵ is small, fast oscillations are either not visible or arise with small amplitudes; the BE parameterization $(\Phi(\boldsymbol{Y}), G(\boldsymbol{Y}))$ approximates almost exactly the true dynamics of $(\boldsymbol{X}, \boldsymbol{Z})$. But when ϵ exceeds a critical threshold ϵ^*, explosive fast oscillations can appear in $\boldsymbol{X}$ and $\boldsymbol{Z}$ as shown here for the time series of X_2 in the right column. The BE parameterization still captures the corresponding slow averaged motion extremely well. When ϵ is not too far above ϵ^*, the BE closure is able to reproduce the coarse-grained topological features (corresponding to the slow Rossby wave dynamics) of the projected attractors as shown below for ϵ at the critical value $\epsilon^* \approx 1.5522$.



However, when ϵ is further increased, the BE closure is no longer sufficient as shown below for the projected attractor with $\epsilon \approx 1.7398$ (left panel, back vs blue). Careful analysis of the dynamical properties of the BE residual reveals that such residuals can be effectively emulated by a network of Stuart-Landau oscillators (SLOs) [3]. This SLO rectification of the BE is clearly successful as shown by comparing the projected attractors below (black vs red). In the formulation of the SLOs, no conditioning of any sort on the slow variables $\boldsymbol{Y}$ is enforced.



The success here relies heavily on the remarkable ability of BE to separate the averaged dynamics (conditional expectation) from the fast dynamics. The latter turns out to be mostly orthogonal to the former as shown on the right panel above, where the blue dots correspond to the BE manifold in a reduced phase space representation, and the black curves are from the L80 dynamics. Thus, the SLOs provide essentially the noise terms in the Mori-Zwanzig formalism while no memory terms were needed in this efficient BE-SLO closure.

A variational framework for small-scale parameterization [2, 5]

How can we extend the idea of the BE parameterization to general nonlinear models? Through the works [2, 4, 5], we established a variational framework, called **optimal parameterizing manifold (OPM)**, for such a parameterization problem for both deterministic and stochastic dissipative systems without assuming a slow-fast structure. We present below the key ideas in a deterministic, autonomous setting.

Motivated from fluid dynamics applications, we consider forced dissipative systems of the form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = Lu + B(u,u) + F, \tag{4}$$

where the state space E is either high- or infinite-dimensional, L is a linear differential operator, B a quadratic nonlinearity and F an autonomous forcing. Assume u is decomposed into a large-scale resolved part $u_{\mathfrak{c}}$ and a small-scale unresolved part $u_{\mathfrak{s}}$. Using insights from approximations of invariant manifolds in dynamical systems theory, we seek optimal approximation of $u_{\mathfrak{s}}$ in terms of a nonlinear function of $u_{\mathfrak{c}}$ within broad classes of dynamically-based analytical formulas. The optimality is in the sense of minimizing certain cost function by calibrating a few scalar parameters in the analytical formula based on short solution data.

One such class of parameterizations arises from a flow-interpretation of the leading-order approximation of invariant manifolds ([2, Section 4.3]), which is based on the following auxiliary backward-forward system

$$\frac{\mathrm{d}u_{\mathfrak{c}}^{(1)}}{\mathrm{d}s} = \Pi_{\mathfrak{c}} L u_{\mathfrak{c}}^{(1)}(s) + \Pi_{\mathfrak{c}} F, \qquad s \in [-\tau_n, 0], \quad u_{\mathfrak{c}}^{(1)}(0) = X \in E_{\mathfrak{c}}, \tag{5a}$$

$$\frac{\mathrm{d}u_n^{(1)}}{\mathrm{d}s} = \beta_n u_n^{(1)}(s) + \Pi_n B\big(u_{\mathfrak{c}}^{(1)}(s), u_{\mathfrak{c}}^{(1)}(s)\big) + \Pi_n F, \qquad s \in [-\tau_n, 0], \quad u_n^{(1)}(-\tau_n) = 0, \tag{5b}$$

where the decomposition of E is based on eigenfunctions of L, $\Pi_{\mathfrak{c}}$ (resp. Π_n) denotes the orthogonal projector onto the resolved subspace $E_{\mathfrak{c}}$ associated with $u_{\mathfrak{c}}$ (resp. the unresolved eigenmode $\boldsymbol{e}_n$), and $\tau_n > 0$ is a free scalar parameter. Eq. (5a) is first solved backward from $s = 0$ with $u_{\mathfrak{c}}^{(1)}(0) = X$; its solution $u_{\mathfrak{c}}^{(1)}$ is then used in (5b) to solve for $u_n^{(1)}$ forward from $s = -\tau$. The solution of $u_n^{(1)}$ at $s = 0$ is taken as the parameterization of the unobserved component u_n given the observed variable $u_{\mathfrak{c}} = X$. Since Eq. (5a) and Eq. (5b) are only "one-way" coupled and both are linear forced equations in the respective variables, the parameterization of u_n admits an explicit formula given below assuming L is diagonal under the eigenbasis:

$$\Psi_n(\tau_n, X) = u_n^{(1)}(s; X, \tau_n)|_{s=0} = \sum_{i,j=1}^{m} \Big(U_{ij}^n(\tau_n, \boldsymbol{\beta}) F_i F_j + V_{ij}^n(\tau_n, \boldsymbol{\beta}) F_i X_j + D_{ij}^n(\tau_n, \boldsymbol{\beta}) X_i X_j \Big), \tag{6}$$

where $m = \dim(E_{\mathfrak{c}})$, U_{ij}^n, V_{ij}^n, and D_{ij}^n are coefficients involving the eigenvalues of L (collected into $\boldsymbol{\beta}$) and nonlinear interactions among the eigenfunctions of L through the nonlinearity B.

Collecting the above parameterization for each unresolved mode u_n and denoting $\boldsymbol{\tau} = (\tau_{m+1}, \tau_{m+2}, \ldots)$, we obtain the following class of parameterizations of the unresolved dynamics $u_{\mathfrak{s}}$ called the *leading-interaction approximation* (LIA($\boldsymbol{\tau}$)) parameterization:

$$\Psi_{\boldsymbol{\tau}}(X) = \sum_{n \geq m+1} \Psi_n(\tau_n, X) \boldsymbol{e}_n, \; X \in E_{\mathfrak{c}}. \tag{7}$$

Training for the optimal $\boldsymbol{\tau}$: Given numerical solution of (4), $u(t) = u_{\mathfrak{c}}(t) + u_{\mathfrak{s}}(t)$, over a training interval $[0, T]$, we optimize τ_n for each $n \geq m+1$ by minimizing the parameterization residual $\mathcal{Q}_n(\tau_n)$:

$$\min_{\tau_n} \mathcal{Q}_n(\tau_n), \quad \text{where } \mathcal{Q}_n(\tau_n) \stackrel{\text{def}}{=} \int_0^T \big| u_n(t) - \Psi_n(\tau_n, u_{\mathfrak{c}}(t)) \big|^2 \, \mathrm{d}t \text{ with } \Psi_n(\tau_n, X) \text{ given by (6)}. \tag{8}$$

The resulting minimizers τ_n^* whose collection is denoted by $\boldsymbol{\tau}^*$, allows us to define the following optimal parameterization within the LIA($\boldsymbol{\tau}$)-class

$$\Psi_{\boldsymbol{\tau}^*}(X) = \sum_{n \geq m+1} \Psi_n(\tau_n^*, X) \boldsymbol{e}_n. \tag{9}$$

Then, the corresponding optimal LIA($\boldsymbol{\tau}^*$)-closure for the large-scale variable $u_{\mathfrak{c}}$ of (4) is given by:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \Pi_{\mathfrak{c}} L X + \Pi_c B(X + \Psi_{\boldsymbol{\tau}^*}(X), X + \Psi_{\boldsymbol{\tau}^*}(X)) + \Pi_{\mathfrak{c}} F. \tag{10}$$

Generalization: The above procedure for deriving the optimal LIA($\boldsymbol{\tau}^*$)-closure can be generalized in a few ways. Different classes of dynamically-based parameterizations can be used in place of the LIA-class, as long as they admit backward-forward flow interpretations in the spirit of (5); other cost function instead of $\mathcal{Q}_n(\tau_n)$ can be used in the minimization problem (8) as well to determine the optimal $\boldsymbol{\tau}^*$ ([2, Section 4.4 and Section 6]; see also the KS application on the right column). The framework also covers broader classes of equations than (4) in which the forcing can be time dependent [2, Section 7] or stochastic [5, Chapter 5-7]. If needed, further modeling of the OPM residual can be added to the OPM closure (10), while the actual form of the additional model will depend obviously on the dynamical properties of the residual; see again the L80 model above for an example.

Closures of KS equation resolving only unstable modes [2]

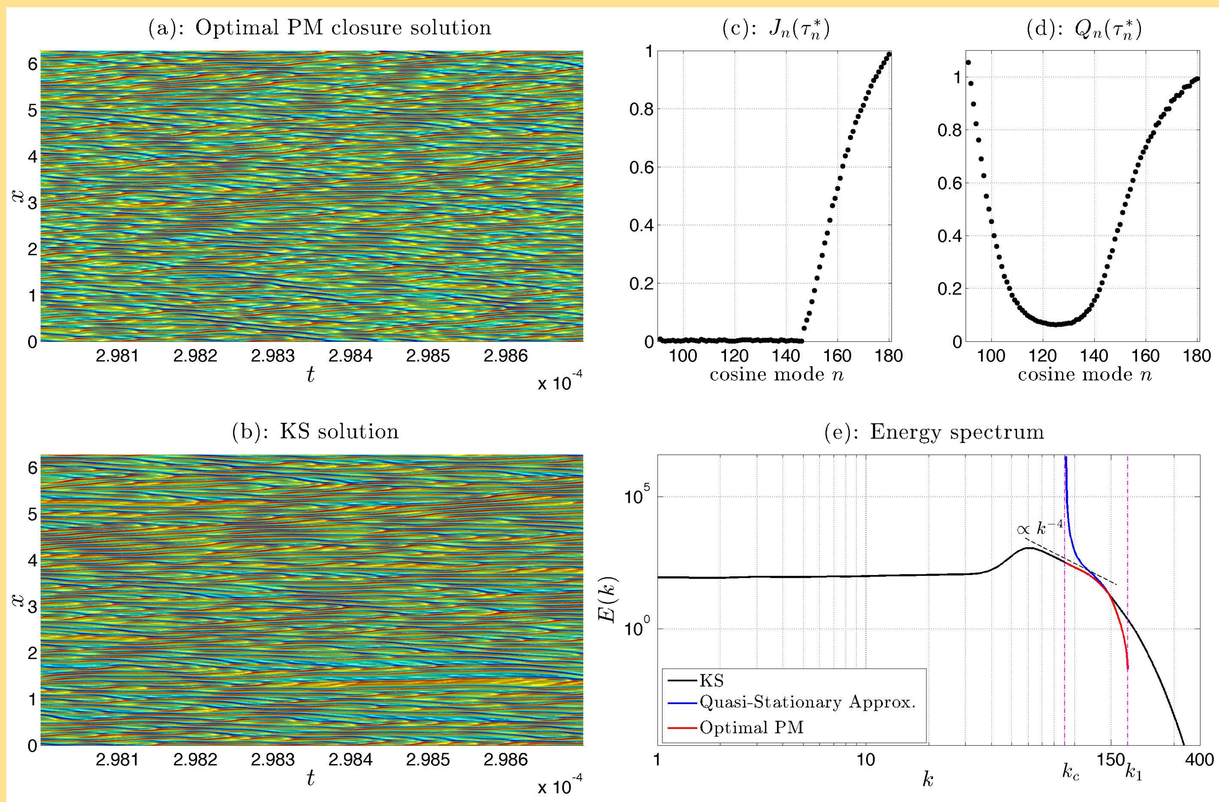
As an application of the variational reduction framework, we consider the Kuramoto-Sivashinsky (KS) equation posed on the interval $(0, 2\pi)$ under periodic boundary conditions:

$$\partial_t u = -4\partial_{xxxx} u - \alpha\big(\partial_{xx} u + u \partial_x u\big). \tag{11}$$

The KS equation is commonly considered as a basic case study for spatiotemporal chaos. Previous studies concerning the closure/reduction problem of the KS equation usually focused on regimes with only a few pairs of unstable modes. Here, we place the equation in a strongly chaotic regime with $\alpha = 33000$, leading to 90 pairs of unstable Fourier modes. We show below that the proposed approach is able to provide an efficient closure when the resolved variables consist only of the unstable modes.

For the chosen regime, traditional parameterizations such as the quasi-stationary approximation (QSA) scheme provide an *over-parameterization* of the neglected scales (blue curve in panel (e) below), leading to an incorrect reproduction of the backscatter transfer of energy due to nonlinear interactions between the modes, especially near the cutoff scale k_c marked in panel (e). Such an *inverse error cascade* originated from the parameterized small scales gradually contaminates the larger scale dynamics and spoils the corresponding closure skills.

This over-parameterization problem near the cutoff scales is fixed almost perfectly by using a parametric form of the QSA within the proposed variational framework as shown by the red curve in panel (e) below. Indeed, the flow interpretation of QSA leads to auxiliary systems analogous to (5b), which resulting in the corresponding QSA($\boldsymbol{\tau}$)-class parameterizations. To optimize $\boldsymbol{\tau}$, instead of using the parameterization defect $\mathcal{Q}_n$ defined in (8), a new cost function J_n is adopted that ensures closeness of the energy spectrum; see panel (c) for the actual cost values at the optimal parameter τ_n^*'s. The corresponding optimal QSA($\boldsymbol{\tau}^*$)-closure is able to reproduce faithfully the spatiotemporal dynamics of the KS equation (panel (a) vs. panel (b)). As a comparison, when the cost function $\mathcal{Q}_n$ is used for determining the τ_n^*'s, the corresponding optimal cost value (after normalized by the energy of each mode u_n) is shown in panel (d). The energy spectrum near the cutoff scale is slightly less well captured when $\boldsymbol{\tau}^*$ is determined by minimizing $\mathcal{Q}_n$, while the skill of the corresponding closure is slightly less good than that shown in panel (a); see [2, Section 6.3]. Comparable performance is also achieved when the LIA($\boldsymbol{\tau}$)-class (7) is used instead of the QSA($\boldsymbol{\tau}$)-class as shown in [2, Section 6.3].



Acknowledgments

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