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Parameterization of stochastic multiscale triads

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Abstract. We discuss applications of a recently developed method for model reduction based on linear response theory of weakly coupled dynamical systems. We apply the weak coupling method to simple stochastic differential equations with slow and fast degrees of freedom. The weak coupling model reduction method results in general in a non-Markovian system; we therefore discuss the Markovianization of the system to allow for straightforward numerical integration. We compare the applied method to the equations obtained through homogenization in the limit of large timescale separation between slow and fast degrees of freedom. We numerically compare the ensemble spread from a fixed initial condition, correlation functions and exit times from a domain. The weak coupling method gives more accurate results in all test cases, albeit with a higher numerical cost.

1 Introduction

Many models of physical systems are too complex to be solved analytically, or even numerically if a large range of temporal and spatial scales is involved. For some high-dimensional dynamical systems it is, however, possible to derive lower-dimensional reduced models (Givon et al., 2004; Huisinga et al., 2003). The reduced model is easier to solve analytically and faster to integrate numerically, while still preserving some of the essential characteristics of the full system. This line of research lies at the heart of many applications, for example, in molecular dynamics (Hijón et al., 2009; Lu and Vanden-Eijnden, 2014) and climate modeling

(Lucarini et al., 2014; Imkeller and Von Storch, 2001; Palmer and Williams, 2009).

The derivation of a reduced model is possible, for example, in the presence of a timescale separation between slow resolved and fast unresolved variables, as is assumed in the homogenization method (Pavliotis and Stuart, 2008). This method applies to slow–fast systems of the form

$$\dot{x} = f_0(x, y) + \frac{1}{\varepsilon} f_1(x, y)$$
$$\dot{y} = \frac{1}{\varepsilon^2} g_1(x, y) + \frac{1}{\varepsilon} \beta(y)\xi(t), \qquad (1)$$

in the limit of infinite timescale separation $\varepsilon \to 0$, where ξ denotes a standard Brownian motion (i.e., the equations should be considered equivalent to a stochastic integral in the Itô interpretation) (Khas'minskii, 1963; Papanicolaou, 1976). It is evident from the dynamical equation that the y variables evolve on a faster timescale than the x variables. For finite values of ε, there is an intricate feedback between the evolution of the x and y variables. The situation simplifies in the limit of $\varepsilon \to 0$ where the slow variables do not evolve on the timescales on which y strongly fluctuates. As a result, the slow dynamics converge to a stochastic evolution, where the effect of y is completely replaced by statistical quantities related to the motion of y for a fixed value of x. On a more technical note, the precise expression for the quantities entering in the reduced dynamics can be easily obtained through an expansion in ε of the backward Kolmogorov equation (the adjoint of the Fokker–Planck equation) $\partial_t v(x, t) = (\mathcal{L}_0 + \mathcal{L}_1 / \varepsilon + \mathcal{L}_2 / \varepsilon^2) v(x, t)$ corresponding to the slow–fast dynamics (where $\mathcal{L}_0 = f_0 \partial_x$, $\mathcal{L}_1 = f_1 \partial_x$ and $\mathcal{L}_2 = g_1 \partial_y + (\beta/2)\partial_y^2$) (Pavliotis and Stuart, 2008).

The method of homogenization has found a great number of applications in different fields of physics and mathematics (Pavliotis and Stuart, 2008). Many physical systems, however, do not feature a timescale separation. As an example, the climate system has variability on many different temporal (and spatial) scales, but no clear spectral gaps can be identified (Mitchell, 1976). This creates fundamental difficulties in the theoretical investigation of climate dynamics and in the construction of climate models. As a result, approximate equations are used for dealing with scales of motions belonging to a range of scales of interest, and numerical models are able to explicitly resolve only a fraction of the full range of scales. The dynamics taking place on scales that are too small and/or fast to be resolved need to be parameterized. Consider the case of convective motion in the Earth's atmosphere. Convective clouds are significant for the climate, yet can only be resolved at a spatial resolution of 10–100 m (Sakradzija et al., 2015), whereas climate models only resolve scales of the order of 100 km (Intergovernmental Panel on Climate Change, 2013). Unresolved convective motion however features a so-called gray zone, a range of timescales overlapping with the dynamical timescales of the resolved large-scale flow (Sakradzija et al., 2015); therefore, homogenization can not be applied. It is a formidable challenge to derive dimension reduction methods that do not require a timescale separation. One should underline that when facing a lack of timescale separation, we would like to be able to construct self-adaptive parameterizations as opposed to empirical ones, so that when the resolution of a numerical model is changed we do not need to redo the exercise of fitting a reduced model.

Going beyond the familiar setting of infinite timescale separation requires a novel approach to the derivation of closed equations for the reduced system. Recently, we have developed a model reduction technique that does not rely on the presence of such a separation (Lucarini et al., 2014; Wouters and Lucarini, 2012, 2013). The alternative method for model reduction makes use of a weak coupling approach, in which response theory (Ruelle, 2009, 1997) is used to derive a closure. The systems of interest follow dynamics determined by

$$\dot{x} = \varepsilon \psi_x(x, y) + f_x(x)$$
$$\dot{y} = \varepsilon \psi_y(x, y) + g_y(y), \tag{2}$$

where x is the variable of interest. Exploiting the weak coupling form of this equation, response theory can be employed to expand expectation values of x-dependent observables under the invariant measure in orders of ε. This expansion yields a series in terms of ε, reminiscent of the Dyson series in scattering theory, each representing a sequence of interactions between the x and y subsystems, corresponding to a certain Feynman diagram (Maggiore, 2005).

The truncation of this series up to a given order yields an approximation of the response of the x subsystem to the coupling to the y subsystem. More importantly, it allows to

determine the statistical quantities of the y system that dictate this response. The first-order correction to the dynamics of the x system can be written as the expectation value $\varepsilon \int dy \psi_x(x, y)\rho_y(y)$, where ρ_y is the invariant density of the uncoupled $\dot{y} = g_y(y)$ dynamics. At second order, two correction terms appear: one due to double ψ_x interactions from y to x, determined by a correlation function of the uncoupled y dynamics, and a feedback term, determined by a response function of the uncoupled y dynamics. This knowledge can then be exploited to derive a surrogate dynamic for x that reproduces the effect of the coupling of x to y up to second order in ε. This theory has been originally developed assuming that the uncoupled systems are Axiom A dynamical systems. This assures, thanks to properties such as structural stability, the existence of linear and higher-order response (Ruelle, 1998, 1997). The theory can, however, be equally applied in the case where the uncoupled dynamics are stochastic, with only the requirement to have a physical measure (an ergodic measure is called physical if, for a set of initial conditions of nonzero Lebesgue measure, the temporal average of a typical observable converges to the spatial average over this measure). Interestingly, the results obtained using response theory match what one can derive by constructing a perturbative expansion of the dynamics of the system using the Mori–Zwanzig projection method (Wouters and Lucarini, 2013).

Previously, we have proposed a surrogate dynamical equation for the x variable that introduces an ε-dependent perturbing term to the dynamics f_x to match the response of the statistics of the full system. The perturbing term contains a non-Markovian memory term and a correlated noise, with the memory kernel and correlation functions depending on the statistics of the uncoupled dynamics $\dot{y} = g_y$. In a recent study of the applicability of the weak coupling approach to a simple ocean–atmosphere system, the method has been shown to give a good result for sufficiently weak coupling between the ocean and the atmosphere (Demaeyer and Vannitsem, 2016), even if it is clear that a systematic investigation of the performance of the weak coupling approach is indeed still needed.

We remark that Chekroun et al. (2015a, b) have recently proved that, indeed, constructing reduced-order models entails introducing deterministic, stochastic and memory correction to the dynamics of the variables of interest.

Here, we will apply and extend the weak coupling approach of Wouters and Lucarini (2012, 2013) for the development of parameterizations for various stochastic triad models. Triad interactions arise from quadratic nonlinearities with energy-conserving properties (see, e.g., Gluhovsky and Tong, 1999). The triad models considered here appear in applications of the homogenization technique to construction of parameterizations in climate modeling (see, e.g., Majda et al., 2001, 2002; Franzke et al., 2005; Franzke and Majda, 2006; Dolaptchiev et al., 2013b, a). The non-Markovian memory kernel in the weak coupling approach will be calculated for these simple stochastic multiscale models and approximated by a Markovian stochastic process, in order to

allow for easier numerical implementation. The systems we investigate can be written in both the weak coupling form of Eq. (2) and the slow–fast form of Eq. (1); therefore, direct comparison is possible and will be performed on a number of metrics, namely initial ensemble spread, correlation functions and exit times from an interval. We intend our results to be of relevance for providing sound foundations for stochastic parameterizations in weather and climate models (Palmer and Williams, 2009; Franzke et al., 2015; Berner et al., 2016).

2   The additive triad

The first model we look at is the stochastically forced additive triad. This system is a low-dimensional model that has nonlinear interactions reminiscent of those occurring between the Fourier modes of a fluid flow. It is stochastically forced to mimic the interaction with further unresolved modes. The system has three variables: one slow variable x and two fast variables y_1 and y_2. The fast dynamics are dominated by two independent Ornstein–Uhlenbeck processes. The dynamical equations for this triad are

$$\frac{dx}{dt} = B^{(0)} y_1 y_2$$

$$\frac{dy_1}{dt} = B^{(1)} x y_2 - \frac{\gamma_1}{\varepsilon} y_1 + \frac{\sigma_1}{\sqrt{\varepsilon}} \xi_1(t)$$

$$\frac{dy_2}{dt} = B^{(2)} x y_1 - \frac{\gamma_2}{\varepsilon} y_2 + \frac{\sigma_2}{\sqrt{\varepsilon}} \xi_2(t). \tag{3}$$

By scaling the time by powers of ε, this process is of the form of Eq. (1), with $f_0 = 0$, and also of the form of Eq. (2), with $f_x = 0$. The processes ξ_i are independent Brownian motions in the Itô sense. Here and below, a differential equation featuring a Brownian motion will be interpreted as the equivalent stochastic integral. In addition, we require $\sum_i B^{(i)} = 0$, which guarantees energy conservation in the case $\gamma_i = \sigma_i = 0$.

2.1   Homogenization

On the timescale t, when increasing the timescale separation $1/\varepsilon$ to infinity, we have trivial dynamics of the averaged equations $\dot{\bar{x}} = B^{(0)} \langle y_1 y_2 \rangle_{\rho_{OU}} = 0$ where ρ_{OU} is the Gaussian invariant measure of the fast Ornstein–Uhlenbeck process generated by taking $B^{(i)} = 0$ for $i = 1, 2, 3$. In the setting of homogenization, one looks at the convergence of the distribution of paths on a longer timescale. The time is scaled to the diffusive timescale $\theta = \varepsilon t$ and on this longer diffusive timescale, deviations from the averaged dynamics develop.

By expanding the backward Kolmogorov equation for the slow–fast system in orders of ε, a Kolmogorov equation for only the slow variables can be derived (see Pavliotis and Stuart, 2008). The dynamical equation corresponding to this Kolmogorov equation is, in this case, a one-dimensional
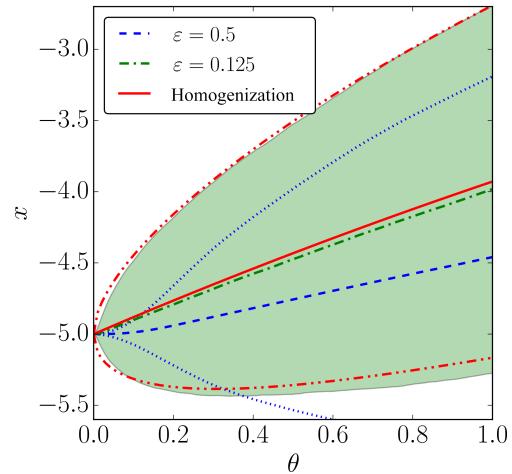

Figure 1. Convergence to the homogenized equations for the additive triad (Eq. 3) in $\theta = \varepsilon t$ timescale. The red solid and double-dotted dash lines show the analytically calculated mean and 2σ intervals, respectively, for an ensemble evolving according to the homogenized equation (Eq. 4) from an initial condition $x = -5$. The blue dashed and dotted lines show the mean and 2σ intervals for a 10 000 member ensemble of the additive triad (Eq. 3) for $\varepsilon = 0.5$ from an initial condition $(x, y_1, y_2) = (-5, 0, 0)$ with $B^{(0)} = -0.75$, $B^{(1)} = -0.25$, $B^{(2)} = 1$, $\gamma_1 = 1/\delta$, $\sigma_1 = \sqrt{2/\delta}$, $\gamma_2 = 1$ and $\sigma_2 = \sqrt{2}$ with $\delta = 0.75$. The green dash-dotted line and the green shaded area show the same for $\varepsilon = 0.125$.

Ornstein–Uhlenbeck process (Majda et al., 2002):

$$\frac{\partial x}{\partial \theta} = C_0 x + \sqrt{2 A_0} \xi(\theta), \tag{4}$$

where

$$C_0 = \frac{B^{(0)}}{\gamma_1 + \gamma_2} \left(B^{(1)} \frac{\sigma_2^2}{2\gamma_2} + B^{(2)} \frac{\sigma_1^2}{2\gamma_1} \right)$$

$$A_0 = \frac{B^{(0)2}}{\gamma_1 + \gamma_2} \frac{\sigma_1^2}{2\gamma_1} \frac{\sigma_2^2}{2\gamma_2}.$$

See Fig. 1 for an illustration of the homogenization principle for the additive triad (Eq. 3). The mean and variance of the triad converge to those of the Ornstein–Uhlenbeck process (Eq. 4) for small ε.

2.2   Weak coupling limit

We will now discuss the weak coupling method as described in Wouters and Lucarini (2012, 2013). By rescaling the time as $\tau = \varepsilon^{-1} t$, we can write the stochastically forced additive triad equation (Eq. 3) as a two-dimensional Ornstein–Uhlenbeck system, weakly and nonlinearly coupled to a triv-

ial zero-gradient x system:

$$\frac{dx}{d\tau} = \varepsilon \psi_x(y_1, y_2)$$

$$\frac{dy_1}{d\tau} = \varepsilon \psi_{y,1}(x, y) - \gamma_1 y_1 + \sigma_1 \xi_1(\tau)$$

$$\frac{dy_2}{d\tau} = \varepsilon \psi_{y,2}(x, y) - \gamma_2 y_2 + \sigma_2 \xi_2(\tau), \tag{5}$$

with $\psi_x(y_1, y_2) = B^{(0)} y_1 y_2$ and $\psi_y(x, y) = (B^{(1)} x y_2, B^{(2)} x y_1)^T$. The stochastic parameterization derived in Wouters and Lucarini (2012, 2013) is given by a non-Markovian equation:

$$\frac{d\widetilde{x}}{d\tau} = \varepsilon \eta(\tau)$$

$$+ \varepsilon^2 \int\limits_0^\infty ds \, R(s, \widetilde{x}(\tau - s)), \tag{6}$$

where the memory kernel $R(s, \widetilde{x})$ and first two moments of the stochastic process $\eta(\tau)$ are derived using the weak coupling method to the following statistics of the uncoupled y Ornstein–Uhlenbeck dynamics:

$$\langle \eta(\tau) \rangle = 0$$

$$C(\tau) := \langle \eta(0) \eta(\tau) \rangle$$

$$= \langle \psi_x(y_1, y_2) \psi_x(y_1(\tau), y_2(\tau)) \rangle_{\rho_{OU}} \tag{7}$$

$$R(\tau, x) = \langle \psi_y(x, y_1, y_2) . \nabla_y \psi_x(y_1(\tau), y_2(\tau)) \rangle_{\rho_{OU}}, \tag{8}$$

where the evolution of y_1 and y_2 into $y_1(\tau)$ and $y_2(\tau)$ are taken to be the uncoupled Ornstein–Uhlenbeck dynamics $dy_i / d\tau = -\gamma_i y_i + \sigma_i \xi_i$. For the case of the additive triad (Eq. 3), we have

$$C(\tau) = (B^{(0)})^2 \langle y_1(0) y_1(\tau) \rangle \langle y_2(0) y_2(\tau) \rangle_{\rho_{OU}}$$

$$= (B^{(0)})^2 \exp(-(\gamma_1 + \gamma_2)\tau) \frac{\sigma_1^2}{2\gamma_1} \frac{\sigma_2^2}{2\gamma_2} \tag{9}$$

and

$$R(\tau, x) = B^{(0)} B^{(1)} x \langle y_2(0)(\partial_{y_1} y_1(\tau)) y_2(\tau) \rangle_{\rho_{OU}} \tag{10}$$

$$+ B^{(0)} B^{(2)} x \langle y_1(0) y_1(\tau)(\partial_{y_2} y_2(\tau)) \rangle_{\rho_{OU}}$$

$$= x B^{(0)} \exp(-(\gamma_1 + \gamma_2)\tau) \left(\frac{\sigma_2^2}{2\gamma_2} B^{(1)} + \frac{\sigma_1^2}{2\gamma_1} B^{(2)} \right).$$

2.2.1 Markovian parameterization

Due to the identical timescale $\gamma_1 + \gamma_2$ in both memory and noise correlation, the memory equation (Eq. 6) can be transformed to a Markovian parameterization. We want to find a parameterizing two-level Markovian dynamical system of

the form

$$\frac{dz_1}{d\tau} = \varepsilon C_1 z_2$$

$$\frac{dz_2}{d\tau} = -\gamma z_2 + \sigma_z \xi(\tau) + \varepsilon C_2 z_1, \tag{11}$$

such that the second-order response of this system to changes in ε is the same as the response of Eq. (6). In other words, we want to determine the parameters C_1, C_2, γ and σ_z in Eq. (11) such that the correlation and memory functions of the fast equation in Eq. (11) are equal to Eqs. (9) and (10), respectively. The correlation function $C(\tau)$ and memory function $R(\tau, z_1)$ of the fast equation of Eq. (11) are

$$C(\tau) = \langle (C_1 z_2(0))(C_1 z_2(\tau)) \rangle = C_1^2 e^{-\gamma \tau} \frac{\sigma_z^2}{2\gamma} \tag{12}$$

$$R(\tau, z_1) = \langle (C_2 z_1) \partial_{z_2}(C_1 z_2(\tau)) \rangle = C_1 C_2 z_1 e^{-\gamma \tau}, \tag{13}$$

where the evolution of z_2 to $z_2(\tau)$ is now given by $dz_2/d\tau = -\gamma z_2 + \sigma_z \xi(\tau)$. By equating these functions to their counterparts in Eqs. (9) and (10), we see that by choosing

$$C_1 = B^{(0)}$$

$$C_2 = \frac{\sigma_2^2}{2\gamma_2} B^{(1)} + \frac{\sigma_1^2}{2\gamma_1} B^{(2)} = \beta_2 B^{(1)} + \beta_1 B^{(2)}$$

$$\gamma = \gamma_1 + \gamma_2$$

$$\sigma_z^2 = 2 \frac{\sigma_1^2}{2\gamma_1} \frac{\sigma_2^2}{2\gamma_2}(\gamma_1 + \gamma_2) = 2\beta_1 \beta_2 \gamma,$$

the reduced z_1 dynamics of the parameterized dynamical system (Eq. 11) in the weak coupling method are of the same form as those of the stochastic triad (Eq. 3).

This Markovian reduced equation (Eq. 11) is in fact a reformulation of the non-Markovian equation (Eq. 6). To see this, we write an explicit solution for z_2 as a function of the history of z_1 and ξ as

$$z_2(\tau) = e^{-\gamma \tau} z_2(0)$$

$$+ \int\limits_0^\tau dt' \left(\sigma_z \xi(t') + \varepsilon C_2 z_1(t') \right) e^{-\gamma(\tau - t')}.$$

This solution can then be inserted into Eq. (11) to obtain

$$\frac{dz_1}{d\tau} = \varepsilon C_1 e^{-\gamma \tau} z_2(0)$$

$$+ \varepsilon C_1 \int\limits_0^\tau dt'(\sigma_z \xi(t') + \varepsilon C_2 z_1(t')) e^{-\gamma(\tau - t')}, \tag{14}$$

which agrees with Eq. (6), with the first two terms being an Ornstein–Uhlenbeck process with the required correlation plus a memory term with the required memory kernel.
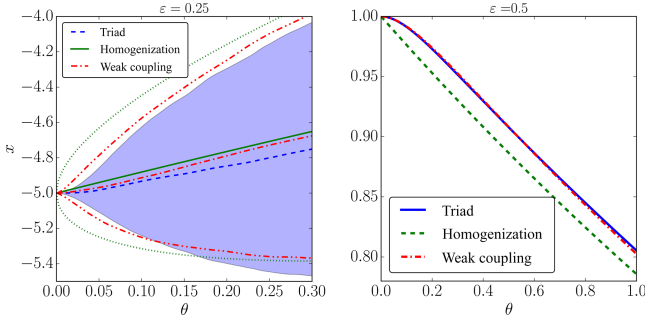
Figure 2. Left: comparison of the ensemble spread for the original additive triad system for $\varepsilon = 0.25$ from an initial condition $(-5, 0, 0)$ (the ensemble mean is the blue dashed line, 2σ interval is the blue shaded area), the two-level Ornstein–Uhlenbeck process from the weak coupling method (Eq. 11) from an initial condition $(-5, 0)$ (ensemble mean: red dash-dotted line, 2σ interval: red dash–dot-dotted lines) and the one-level Ornstein–Uhlenbeck process from homogenization (Eq. 4) from $x = -5$ (ensemble mean: green solid line, 2σ interval: dotted lines). Right: comparison of the autocorrelation functions of the slow variable $\langle x(t)x(0) \rangle$ in the full triad for $\varepsilon = 0.5$ (blue dash-dotted line), $\langle z_1(t)z_1(0) \rangle$ in the weak coupling model (green solid line) and $\langle x(t)x(0) \rangle$ for the homogenized equation (red dashed line). Both plots use parameter values $B^{(0)} = -0.75$, $B^{(1)} = -0.25$, $B^{(2)} = 1$, $\gamma_1 = 1/\delta$, $\sigma_1 = \sqrt{2/\delta}$, $\gamma_2 = 1$ and $\sigma_2 = \sqrt{2}$ with $\delta = 0.75$; the ensemble size is 1000.

This Markovian formulation allows for a straightforward numerical implementation of the parameterization, compared to the non-Markovian equation (Eq. 6) which requires one to store the history of the process in memory.

A comparison of the performance of the two model reductions is shown in Fig. 2. Shown are the spread of an ensemble initiated at a fixed value for the slow variables $x = z_1 = -5$ and the autocorrelation function of the slow variables. The weak coupling method clearly gives better results.

By correctly rescaling time and taking the limit of $\varepsilon \to 0$ in the Markovian parameterization (Eq. 11), one can furthermore verify that in this limit it converges to the homogenization of the original triad equation (Eq. 4).

3 The slowly oscillating additive triad

The additive triad, as specified in Eq. (3), can be generalized to allow for an additional interaction between the y variables on the slow timescale that is independent of x. The dynamical equations for this slowly oscillating triad are

$$\frac{dx}{dt} = B^{(0)} y_1 y_2$$
$$\frac{dy_1}{dt} = B^{(1)} y_2 x - \frac{\gamma_1}{\varepsilon} y_1 + \omega y_2 + \frac{\sigma_1}{\sqrt{\varepsilon}} \xi_1(t)$$
$$\frac{dy_2}{dt} = B^{(2)} x y_1 - \frac{\gamma_2}{\varepsilon} y_2 - \omega y_1 + \frac{\sigma_2}{\sqrt{\varepsilon}} \xi_2(t). \tag{15}$$

3.1 Homogenization

The homogenized equation is similar to the one for the additive triad (Eq. 3) (see Eq. 4), with an added constant forcing C_r in the reduced stochastic differential equation (SDE):

$$\frac{\partial x}{\partial \theta} = C_0 x + C_r + \sqrt{2A_0} \xi(t)$$
$$C_r = \frac{B^{(0)}}{\gamma_1 + \gamma_2} \omega \left(\frac{\sigma_2^2}{2\gamma_2} - \frac{\sigma_1^2}{2\gamma_1} \right). \tag{16}$$

3.2 Weak coupling limit

The coupling functions ψ_x and ψ_y are now

$$\psi_x(y) = B^{(0)} y_1 y_2$$
$$\psi_y(x, y) = x \begin{pmatrix} B^{(1)} y_2 \\ B^{(2)} y_1 \end{pmatrix} + \omega \begin{pmatrix} y_2 \\ -y_1 \end{pmatrix}.$$

The correlation function (Eq. 7) of the coupling to x, determining the correlations of the parameterization noise σ is

$$\langle \psi_x(y)\psi_x(y(\tau)) \rangle = B^{(0)^2} \langle y_1(0)y_1(\tau) \rangle \langle y_2(0)y_2(\tau) \rangle$$
$$= B^{(0)^2} \exp(-(\gamma_1 + \gamma_2)\tau) \frac{\sigma_1^2}{2\gamma_1} \frac{\sigma_2^2}{2\gamma_2}.$$

The response function (Eq. 8) of ψ_x to ψ_y, determining the memory kernel of the parameterization, is similar to the one for the additive triad (see Eq. 10), with an added exponential function, the integral of which gives the same constant C_r of the homogenized equations:

$$R(\tau, x) = \langle \psi_y(x, y) \partial_y \psi_x(y(\tau)) \rangle$$
$$= \exp(-\gamma\tau)(D_1 x + D_0)$$
$$D_1 = B^{(0)} \left(B^{(1)} \frac{\sigma_2^2}{2\gamma_2} + B^{(2)} \frac{\sigma_1^2}{2\gamma_1} \right) = \gamma C_0$$
$$D_0 = \omega B^{(0)} \left(\frac{\sigma_2^2}{2\gamma_2} - \frac{\sigma_1^2}{2\gamma_1} \right) = \gamma C_r.$$

Combined, this then results in the following non-Markovian parameterized equations:

$$\frac{d\widetilde{x}}{d\tau} = \varepsilon\eta(\tau) + \varepsilon^2 \int_0^\infty ds\, R(s, \widetilde{x}(\tau - s))$$
$$= \varepsilon\eta(\tau) + \varepsilon^2 \int_0^\infty ds\, \exp(-\gamma s)(D_1 \widetilde{x}(\tau - s) + D_0)$$
$$= \varepsilon\eta(\tau) + \varepsilon^2 \int_0^\infty ds\, \exp(-\gamma s)\widetilde{x}(\tau - s) + \varepsilon^2 C_r. \tag{17}$$

Table 1. The relative error on the mean exit time $|\mathbb{E}_1(\tau) - \mathbb{E}_0(\tau)|/\mathbb{E}_0(\tau)$ where $\mathbb{E}_0(\tau)$ is the mean exit time from $[-1, 1]$ of the full triad system (Eq. 15) and $\mathbb{E}_1(\tau)$ is the mean exit time of the parameterized systems of Eqs. (18) and (16), with $B^{(0)} = -0.75$, $B^{(1)} = -0.25$, $B^{(2)} = 1$, $\omega = 0.25$, $\gamma_1 = 1/\delta$, $\sigma_1 = \sqrt{2/\delta}$, $\gamma_2 = 1$ and $\sigma_2 = \sqrt{2}$ with $\delta = 0.75$. These values are calculated from 1000 independent trials.

ε	0.5	0.25	0.125
Homogenization	0.403	0.184	0.0982
Weak coupling	0.205	0.0839	0.0589

Table 2. The relative error on the standard deviation of the exit times $|\sigma_1(\tau) - \sigma_0(\tau)|/\sigma_0(\tau)$ where $\sigma_0(\tau)$ is the standard deviation of exit times from $[-1, 1]$ of the full triad system (Eq. 15) and $\sigma_1(\tau)$ is the standard deviation of exit times of the parameterized systems of Eqs. (18) and (16). Parameters are chosen as in Table 1. These values are calculated from 1000 independent trials.

ε	0.5	0.25	0.125
Homogenization	0.420	0.217	0.115
Weak coupling	0.232	0.0814	0.0395

3.2.1 Markovian parameterization

The non-Markovian equation (Eq. 17) can again be Markovianized by a two-level Ornstein–Uhlenbeck process of the form

$$\frac{dz_1}{d\tau} = \varepsilon C_1 z_2$$
$$\frac{dz_2}{d\tau} = -\gamma z_2 + \sigma_z \xi(t) + \varepsilon(C_2 z_1 + C_3). \tag{18}$$

The corresponding correlation and memory terms are

$$C(\tau) = C_1^2 e^{-\gamma\tau} \frac{\sigma_z^2}{2\gamma} \tag{19}$$

$$R(\tau, z_1) = C_1 e^{-\gamma\tau} (C_2 z_1 + C_3). \tag{20}$$

We can therefore take

$$C_3 = D_0/C_1$$
$$= \omega \left(\frac{\sigma_2^2}{2\gamma_2} - \frac{\sigma_1^2}{2\gamma_1} \right).$$

In the limit $\varepsilon \to 0$ in the Markovian parameterization (Eq. 18), we again recover the homogenized equations (Eq. 16).

3.3 Exit times

When comparing initial ensemble spread and autocorrelation functions for the slow variable of this system with the weak coupling parameterization (Eq. 18) and the homogenized system (Eq. 16), the results are similar to those presented for the additive triad above. Additionally, here we perform a comparison of a rare event statistic: the first exit time of the slow variable from an interval $[-1, 1]$ when the slow variable is initialized at 0.

The results in Tables 1 and 2 show that the statistics of exit times are approximated significantly better in the weak coupling parameterization.

4 The rapidly oscillating additive triad

A further generalization of the additive triad (Eq. 3) is to introduce an interaction between the y variables on the fast timescale (Dolaptchiev et al., 2013a). The dynamical equations for the rapidly oscillating triad are

$$\frac{dx}{dt} = B^{(0)} y_1 y_2$$
$$\frac{dy_1}{dt} = B^{(1)} y_2 x - \frac{\gamma_1}{\varepsilon} y_1 + \frac{\omega}{\varepsilon} y_2 + \frac{\sigma_1}{\sqrt{\varepsilon}} \xi_1(t)$$
$$\frac{dy_2}{dt} = B^{(2)} x y_1 - \frac{\gamma_2}{\varepsilon} y_2 - \frac{\omega}{\varepsilon} y_1 + \frac{\sigma_2}{\sqrt{\varepsilon}} \xi_2(t). \tag{21}$$

Note the difference in scaling on the oscillatory terms ωy_i compared to Eq. (15). The invariant measure of the fast system is a correlated Gaussian measure,

$$\rho(y) = \exp(-y^T (2S)^{-1} y)/\mathcal{Z},$$

determined by

$$\Gamma S + (\Gamma S)^T = \Sigma^T \Sigma,$$

with

$$\Gamma = \begin{pmatrix} \gamma_1 & -\omega \\ \omega & \gamma_2 \end{pmatrix}$$

and

$$\Sigma = \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix}.$$

Homogenization leads to a solvability condition on the system of Eq. (21), whereby the mean of $B^{(0)} y_1 y_2$ under the fast process has to equal zero. This condition is fulfilled if either $\omega = 0$ or $\sigma_1^2/\gamma_1 = \sigma_2^2/\gamma_2$. The homogenized equation is now given by

$$\dot{x} = \gamma_\omega x + \sqrt{2A_\omega} \xi(t), \tag{22}$$

with

$$\gamma_\omega = b B^{(1)} S_{22} + 2(a B^{(1)} + c B^{(2)}) S_{12} + b B^{(2)} S_{11} \quad (23)$$

$$A_\omega = B^{(0)} (3 a S_{11} S_{12} + b(S_{11} S_{22} + S_{12}^2) + 3 c S_{22} S_{12}) \quad (24)$$

$$b = \frac{B^{(0)}}{\left(\frac{\omega^2}{\gamma_1} + \frac{\omega^2}{\gamma_2} + \gamma_1 + \gamma_2 \right)}$$

$$a = (-\omega / 2\gamma_1) b$$

$$c = (\omega / 2\gamma_2) b.$$

4.1 Weak coupling

The coupling functions of Eq. (21) have the following form:

$$\psi_x(y_1, y_2) = B^{(0)} y_1 y_2 \quad (25)$$

$$\psi_y(x, y_1, y_2) = x (B^{(1)} y_2, B^{(2)} y_1)^T. \quad (26)$$

The correlation function $\langle \psi_x(y_1, y_2) \psi_x(y_1(t), y_2(t)) \rangle$ appearing in the weak coupling expansion can again be calculated explicitly. Solutions of the fast Ornstein–Uhlenbeck system $\dot{y} = -\Gamma y + \Sigma \xi$ can be written as

$$y_i(t) = [e^{-\Gamma t} y(0)]_i + \int_0^t d\tau [e^{-\Gamma(t-\tau)} \Sigma \xi(\tau)]_i.$$

Inserting this expression into the autocorrelation function gives

$$\begin{aligned} C_\omega(t) :=& \langle \psi_x(y_1, y_2) \psi_x(y_1(t), y_2(t)) \rangle \\ =& \left(B^{(0)} \right)^2 \langle y_1(0) y_2(0) y_1(t) y_2(t) \rangle \\ =& \left(B^{(0)} \right)^2 \left([e^{-\Gamma t}]_{11} [e^{-\Gamma t}]_{21} (3 S_{11} S_{12}) \right) \\ &+ \left([e^{-\Gamma t}]_{11} [e^{-\Gamma t}]_{22} + [e^{-\Gamma t}]_{12} [e^{-\Gamma t}]_{21} \right) \\ &\cdot \left(S_{11} S_{22} + 2 S_{12}^2 \right) \\ &+ \left([e^{-\Gamma t}]_{12} [e^{-\Gamma t}]_{22} (3 S_{22} S_{12}) \right) \\ &+ \left(B^{(0)} \right)^2 R_{12} \int_0^t d\tau_1 d\tau_2 \left\langle \left[e^{-\Gamma(t-\tau_1)} \Sigma \xi(\tau_1) \right]_1 \right. \\ &\left. \cdot \left[e^{-\Gamma(t-\tau_2)} \Sigma \xi(\tau_2) \right]_2 \right\rangle, \end{aligned}$$

since the noise ξ is white and has zero mean.

The memory term $R_\omega(\tau, x)$ can be calculated by performing integration by parts on the response function, resulting in a fluctuation–dissipation-type expression:

$$\begin{aligned} R_\omega(\tau, x) =& \left\langle \left(-\frac{\nabla \cdot (\rho \psi_y)}{\rho} \right) \psi_x(\tau) \right\rangle \\ =& B^{(0)} x \left\langle \right. \\ &+ B^{(2)} \left[S^{-1} \right]_{22} \right) y_1(0) y_2(0) \\ &+ B^{(2)} \left[S^{-1} \right]_{12} y_1^2(0) \right) y_1(\tau) y_2(\tau) \right\rangle. \end{aligned}$$

4.1.1 Markovian parameterization

Guided by the Markovian form of the previous triad systems, we again want to derive a Markovian parameterization with a reduced one-level Ornstein–Uhlenbeck system as the fast component:

$$\begin{aligned} \dot{z}_1 &= \varepsilon C_1 z_2 \\ \dot{z}_2 &= \varepsilon C_2 z_1 - \gamma z_2 + \sigma_z \xi_z(t). \end{aligned} \quad (27)$$

In this case, there is no exact match between the autocorrelation and response functions of this Markovian system and the non-Markovian weak coupling parameterization. The choice of the parameterization parameters is therefore not exactly determined and one needs to choose a parameterization such that the autocorrelation and response functions of the coupling function in the fast component of the full system are approximated in some sense. A further restriction comes from the fact that in the limit $\varepsilon \to 0$ the limiting path distribution of the full system is determined by the homogenized equation (Eq. 22) and we therefore want to retain this limiting behavior in the parameterized system. To have this limiting property, we have the following constraints on the parameters in Eq. (27):

$$\frac{C_1^2 \sigma_z^2}{2\gamma^2} = A_\omega$$

$$\frac{C_1 C_2}{\gamma} = \gamma_\omega,$$

where A_ω and γ_ω are the forcing and friction parameters obtained through homogenization (see Eqs. 23–24). With the remaining free parameters we can match the response and correlation functions in a more precise manner; for example, by matching the values of these functions at time $t = 0$. In this way, we get

$$C_2 = \frac{R_y(0)}{C_1}$$

$$\gamma = C_\omega(0)$$

and

$$\sigma_z^2 = \frac{2\gamma C_\omega(0)}{C_1^2},$$

where $R_y = R_\omega / x$. This leaves the parameter C_1 undetermined. With the above choice of C_2, γ and σ_z, the memory and correlation functions of the system of Eq. (27) no longer depend on C_1. The weak coupling method therefore can not give further guidance in determining its value. The numerical results appear to be insensitive to the choice of C_1. The results presented here are for the case where we take $C_1 = B^{(0)}$.

A simulation of the ensemble spread from a fixed initial condition is shown in Fig. 3. It demonstrates that the weak
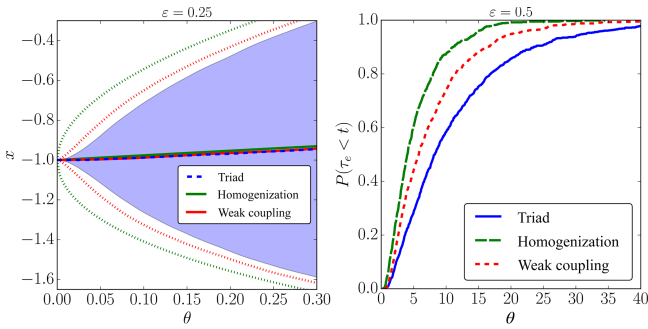
Figure 3. Left: comparison of the ensemble spread for the original oscillating triad system of Eq. (21) for $\varepsilon = 0.25$ from an initial condition $(-1, 0, 0)$ (the ensemble mean is the blue dashed line, 2σ interval the blue shaded area), the two-level Ornstein–Uhlenbeck process from the weak coupling method of Eq. (27) from an initial condition $(-1, 0)$ (ensemble mean: red dashed line, 2σ interval: red dotted lines) and the one-level Ornstein–Uhlenbeck process from homogenization (Eq. 22) from $x = -5$ (ensemble mean: green solid line, 2σ interval: dotted lines) $B^{(0)} = -0.75$, $B^{(1)} = -0.25$, $B^{(2)} = 1$, $\omega = 1/12$, $\gamma_1 = 1/\delta$, $\sigma_1 = \sqrt{2/\delta}$, $\gamma_2 = 1$ and $\sigma_2 = \sqrt{2}$ with $\delta = 0.75$. The ensemble size is 4000. Right: cumulative histograms of exit times from $[-1, 1]$ for the rapidly oscillating triad (Eq. 21) with $\varepsilon = 0.5$, the homogenized equation (Eq. 22) and the two-level Ornstein–Uhlenbeck process from the weak coupling method (Eq. 27), calculated from 1000 independent trials.

Table 3. The relative error on the mean exit time $|\mathbb{E}_1(\tau) - \mathbb{E}_0(\tau)| / \mathbb{E}_0(\tau)$ where $\mathbb{E}_0(\tau)$ is the mean exit time from $[-1, 1]$ of the full triad system of Eq. (21) and $\mathbb{E}_1(\tau)$ is the mean exit time of the parameterized systems of Eqs. (22) and (27). The parameters are the same as those used for Fig. 3. These values are calculated from 1000 independent trials.

ε	0.5	0.25	0.125
Homogenization	0.534	0.262	0.118
Weak coupling	0.322	0.127	0.0619

coupling parameterization (Eq. 27) outperforms the homogenized reduced system of Eq. (22). A longer simulation (not plotted here) shows that over time the difference between the methods decreases and all three systems relax to nearly the same invariant measure.

4.2 Exit times

The same experiment on exits from an interval has been performed as described in Sect. 3.3. The results are displayed in Table 3. As before, the weak coupling reduced system gives a much better result when compared to the homogenized system.

Table 4. The relative error on the standard deviation of the exit times $|\sigma_1(\tau) - \sigma_0(\tau)| / \sigma_0(\tau)$ where $\sigma_0(\tau)$ is the standard deviation of exit times from $[-1, 1]$ of the full triad system of Eq. (21) and $\sigma_1(\tau)$ is the standard deviation of exit times of the parameterized systems of Eqs. (22) and (27). The parameters are the same as those used for Fig. 3. These values are calculated from 1000 independent trials.

ε	0.5	0.25	0.125
Homogenization	0.583	0.286	0.118
Weak coupling	0.362	0.109	0.0503

5 The multiplicative triad

A final type of interactions is given by the multiplicative triad equations (Majda et al., 2002):

$$\frac{dx_1}{dt} = B^{(1)} x_2 y$$
$$\frac{dx_2}{dt} = B^{(2)} x_1 y$$
$$\frac{dy}{dt} = B^{(3)} x_1 x_2 - \frac{\gamma_m}{\varepsilon} y + \frac{\sigma_m}{\sqrt{\varepsilon}} \xi(t), \tag{28}$$

which describe the interplay between two x modes and a stochastically forced single y mode. In the absence of forcing and dissipation, energy conservation is satisfied if $\sum_i B^{(i)} = 0$. In the system of Eq. (28), the y mode can be eliminated directly by integrating the last equation of Eq. (28):

$$y(t) = e^{-\frac{\gamma_m}{\varepsilon} t} y(0)$$
$$+ \int_0^t dt' \left(\frac{\sigma_m}{\sqrt{\varepsilon}} \xi(t') + B^{(3)} x_1(t') x_2(t') \right) e^{-\frac{\gamma_m}{\varepsilon}(t-t')}.$$

By inserting this result in the equations for the x variables, one obtains

$$\frac{d}{dt} \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} = \begin{pmatrix} B^{(1)} x_2(t) \\ B^{(2)} x_1(t) \end{pmatrix} \left\{ e^{-\frac{\gamma_m}{\varepsilon} t} y(0) + \int_0^t dt' \right.$$
$$\left. \left(\frac{\sigma_m}{\sqrt{\varepsilon}} \xi(t-t') + B^{(3)} x_1(t-t') x_2(t-t') \right) e^{-\frac{\gamma_m}{\varepsilon} t'} \right\}. \tag{29}$$

Note that the first two terms on the right-hand side result from a Ornstein–Uhlenbeck process with zero mean and stationary time autocorrelation function given by

$$\frac{\sigma_m^2}{2\gamma_m} e^{-\frac{\gamma_m}{\varepsilon} t}.$$

5.1 Weak coupling

The coupling functions for the multiplicative triad are

$$\psi_x(x, y) = (B^{(1)}x_2 y, B^{(2)}x_1 y)^T,$$
$$\psi_y(x) = B^{(3)}x_1 x_2.$$

The coupling terms in the x equations are separable:

$$\psi_{x,i}(x, y) = a_i \psi'_{x,1,i}(x)\psi'_{x,2,i}(y) \tag{30}$$

with $\langle \psi'_{x,2,i}(y) \rangle_{\rho_{OU}} = 0$, where

$$a_1 = B^{(1)}, \psi'_{x,1,1}(x) = x_2, \psi'_{x,2,1}(y) = y,$$
$$a_2 = B^{(2)}, \psi'_{x,1,2}(x) = x_1, \psi'_{x,2,2}(y) = y.$$

The resulting parameterization in the weak coupling approach (Wouters and Lucarini, 2012, 2013) is

$$\frac{\mathrm{d}x_i}{\mathrm{d}\tau} = \varepsilon a_i \psi'_{x,1,i}\eta_i(\tau) + \varepsilon^2 \int_0^\infty \mathrm{d}s\, R_i(s, x(\tau - s)), \tag{31}$$

with a noise term η_i with zero mean and correlation given by

$$\langle \eta_i(0)\eta_j(\tau) \rangle = \langle \psi'_{x,2,i}(y)\psi'_{x,2,j}(y(\tau)) \rangle_{\rho_{OU}} = \frac{\sigma_m^2}{2\gamma_m}e^{-\gamma_m \tau}.$$

The memory kernel has the form

$$R_i(s, x) = \langle \psi_y(x, y) \cdot \nabla_y \psi_{x,i}(x(s), y(s)) \rangle_{\rho_{OU}},$$
$$R(s, x) = B^{(3)}x_1 x_2 e^{-\gamma s}\begin{pmatrix} B^{(1)}x_2(s) \\ B^{(2)}x_1(s) \end{pmatrix}.$$

Thus, Eq. (31) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\begin{pmatrix} x_1(\tau) \\ x_2(\tau) \end{pmatrix} = \begin{pmatrix} B^{(1)}x_2(\tau) \\ B^{(2)}x_1(\tau) \end{pmatrix}\Big\{ \sigma(\tau) \tag{32}$$
$$+ \int_0^\infty \mathrm{d}s\, B^{(3)}x_1(\tau - s)x_2(\tau - s)e^{-\gamma_m s}\Big\},$$

which is exactly the same result as in Eq. (29), if we rescale time and assume $x_1(t) = x_2(t) = 0$ as the initial condition for $t < 0$. In this case, the weak coupling approach recovers exactly the full model. The original three-component system was reduced to a two-component non-Markovian system but there is no efficiency gain using the parameterization since the corresponding Markovian system is again a three-component one.

5.2 Homogenization

Introducing a longer timescale $\theta = \varepsilon^2 \tau$ in Eq. (32) and taking the limit $\varepsilon \to 0$, one recovers the homogenization result in

Stratonovich formulation:

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{B^{(3)}}{\gamma}x_1 x_2\begin{pmatrix} B^{(1)}x_2 \\ B^{(2)}x_1 \end{pmatrix}$$
$$+ \frac{\sigma_m}{\gamma_m}\begin{pmatrix} B^{(1)}x_2 \\ B^{(2)}x_1 \end{pmatrix}\xi(\theta). \tag{33}$$

The latter corresponds to an Itô stochastic differential equation of the form

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{B^{(3)}}{\gamma}x_1 x_2\begin{pmatrix} B^{(1)}x_2 \\ B^{(2)}x_1 \end{pmatrix}$$
$$+ \frac{\sigma_m^2}{2\gamma_m^2}B^{(1)}B^{(2)}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$
$$+ \frac{\sigma_m}{\gamma_m}\begin{pmatrix} B^{(1)}x_2 \\ B^{(2)}x_1 \end{pmatrix}\xi(\theta). \tag{34}$$

An extensive numerical comparison of the statistics of the multiplicative triad and the homogenized model has been performed in Majda et al. (2002). It demonstrates a good agreement on various quantities, such as autocorrelation functions up to values of $\varepsilon = 0.4$. For details, we refer to Majda et al. (2002).

6 Conclusions

In this work, we have worked out a first application of the weak coupling response method of Wouters and Lucarini (2012, 2013) to a multiscale stochastic system. Through the choice of system, we were able to perform both homogenization and the weak coupling reduction on this system, thereby allowing for a direct comparison between the two reduction methods.

The response method yields a non-Markovian equation, making it cumbersome to integrate numerically. We have demonstrated here that, for the systems studied, the non-Markovian equation can be further reduced to a Markovian equation. Even with this further reduction the system gives a better match to the original system than the homogenized equations.

In the case of the additive triad (Eq. 3), the system of Eq. (11) that is obtained through the Markovianization procedure is of intermediate complexity, between the full system of Eq. (3) and the homogenized limit of Eq. (4). In the systems studied here, the retention of a fast timescale in the reduced system means that the reduction in simulation complexity is modest (one variable instead of two and a linear coupling instead of a nonlinear one). In the case of the multiplicative triad (Eq. 28), the weak coupling parameterization recovers exactly the full model and there is no efficiency gain. In many applications of practical relevance, however, the number of degrees of freedom of the unresolved variables is considerably larger than those of the slow variables of interest. A reduction to a system of one or a few variables will

constitute a significant reduction in complexity in this case. This approach can be compared to the superparameterization approach to convection, where convection is parameterized by a model that is still dynamical in nature, yet significantly simpler than the full convective motion (Randall et al., 2003; Grooms and Majda, 2013, 2014).

The methodology discussed here provides a framework for deriving rather then heuristically constructing (stochastic) parameterizations for multiscale systems, even if further investigations are indeed needed (see the promising results by Demaeyer and Vannitsem (2016)).

7   Data availability

The plots and data for this article were generated using Jupyter 4.0.6, Python 3.4.3, NumPy 1.8.2 and Matplotlib 1.4.2. The source code is available under doi:10.5281/zenodo.167533.

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