Convergence of equation-free methods in the case of finite time scale separation with applications to deterministic and stochastic systems

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Summary. A common approach to studying high-dimensional systems with emergent low-dimensional behavior is based on lift-evolve-restrict maps (called equation-free methods): first, a lifting operator maps low-dimensional coordinates into the high-dimensional space, then the high-dimensional (microscopic) evolution is applied for some time, and finally a restriction operator maps down into a low-dimensional space again. We prove convergence of implicit equation-free methods for sufficiently large healing time. In contrast to previous results, our result does not require the time scale separation to be large. The results are demonstrated with Michaelis-Menten kinetics and a low-dimensional stochastic differential equation.

Dynamical systems with time scale separation have been studied for a long time with different methods with the aim to reduce the complexity of a high-dimensional (also called *microscopic*) system to a relatively simple low-dimensional (also called *macroscopic*) system. The justification for this reduction is simplest if the underlying dynamical system possesses a low-dimensional attracting slow manifold. After reduction, the long-term dynamics of the system can be analyzed on the slow manifold. There exists a range of well-established numerical methods (so-called equation-free methods) that avoid the explicit derivation of a macroscopic system by obtaining the required information from simulations [3, 4, 5]. The unknown macroscopic dynamics is evaluated by using a wrapper around existing microscopic simulators to achieve a closure on demand. The assumption behind equation-free computations is the existence of a time scale separation with a slow low-dimensional description (in $\mathbb{R}^d$) for some macroscopic quantities of the high-dimensional microscopic system (which is defined in $\mathbb{R}^D$). The framework also relies on the availability of a microscopic time stepper (a map $M(\delta;\cdot):\mathbb{R}^D\mapsto\mathbb{R}^D$) and two user-defined operators, the *lifting* $\mathcal{L}:\mathbb{R}^d\mapsto\mathbb{R}^D$ and the *restriction* $\mathcal{R}:\mathbb{R}^D\mapsto\mathbb{R}^d$, which are maps between the original high-dimensional ($\mathbb{R}^D$) microscopic level and the low-dimensional ($\mathbb{R}^d$) macroscopic level. The goal is to compose a macroscopic time stepper $\Phi_*(\delta;\cdot):\mathbb{R}^d\mapsto\mathbb{R}^d$, which is then amenable to higher-level tasks like a *macroscopic bifurcation analysis* of microscopic models. The central building block of equation-free methodology is the “lift-evolve-restrict” map $\mathcal{R}\circ M(\delta;\cdot)\circ\mathcal{L}$: for a given value $x\in\mathbb{R}^d$ of macroscopic quantities, one first applies the lifting $\mathcal{L}$ to x getting a microscopic state u, then one runs the simulation for time δ starting from u (applying the microscopic evolution $M(\delta;u)$), and finally one applies the restriction $\mathcal{R}$ to the result $M(\delta;u)$.

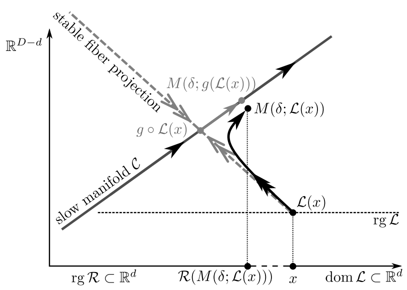


Figure 1: Geometry of lift-evolve-restrict map near slow manifold: macroscopic value x gets lifted to $\mathcal{L}(x)$, then evolved to $M(\delta;\mathcal{L}(x))$, then restricted back to $\mathcal{R}(M(\delta;\mathcal{L}(x))\in\mathbb{R}^d$. The aim is to approximate the slow flow $x\mapsto(g\circ\mathcal{L})^{-1}\circ M(\delta;g(\mathcal{L}(x)))$ using this map $\mathcal{R}\circ M(\delta;\cdot)\circ\mathcal{L}$, and assuming invertibility of $g\circ\mathcal{L}:\mathbb{R}^d\mapsto\mathcal{C}$.

Assuming that the D-dimensional microscopic problem has a d-dimensional attracting invariant slow manifold $\mathcal{C}$, one faces the geometric difficulty, illustrated in Fig. 1, that in general the lift-evolve-restrict map will not be compatible with the stable fibers of the slow manifold $\mathcal{C}$. More precisely, after lifting $x\in\mathbb{R}^d$ to $\mathcal{L}(x)\in\mathbb{R}^D$, the slow flow is effectively applied to a different point, $g\circ\mathcal{L}(x)$, which is the projection of $\mathcal{L}(x)$ onto the slow manifold $\mathcal{C}$ along the *stable fibers*. Thus, in the limit of infinite time-scale separation the dynamics of the lift-evolve-restrict map $P(t;\cdot)=\mathcal{R}\circ M(\delta;\cdot)\circ\mathcal{L}$ is a small perturbation of the map $\mathcal{R}\circ g\circ\mathcal{L}$. A faithful representation of the slow flow $\Phi_*(\delta;\cdot)$, using the coordinate x in the domain of the lifting $\mathcal{L}$ and the map $g\circ\mathcal{L}:\operatorname{dom}\mathcal{L}\mapsto\mathcal{C}$, mapping onto the manifold $\mathcal{C}$,

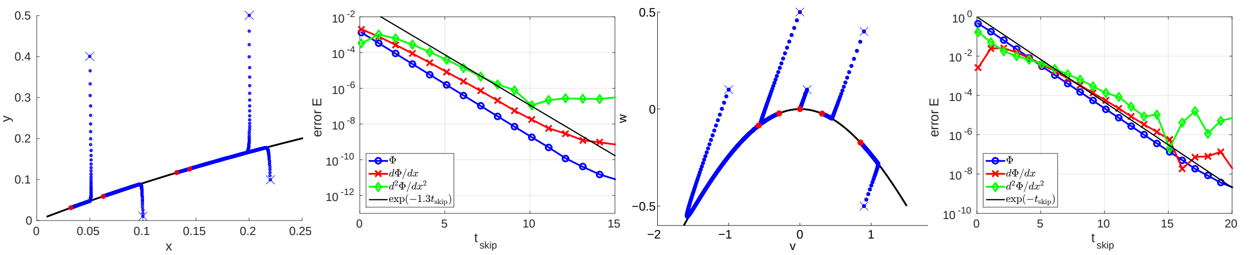
$$y_*=\Phi_*(\delta;x)=(g\circ\mathcal{L})^{-1}\circ M(\delta;\cdot)\circ g\circ\mathcal{L}(x), \tag{1}$$

(using the notation $(\cdot)^{-1}$ for the inverse map) is given by the implicit definition $\mathcal{R}\circ g\circ\mathcal{L}(y_*)=\mathcal{R}\circ M(\delta;\cdot)\circ g\circ\mathcal{L}(x)$. This definition is impractical since the nonlinear projection g and the slow manifold $\mathcal{C}$ are both unknown in general. One approach to overcome this problem is to introduce a *healing time* t_{skip}, exploiting that M attracts along the fibers [5, 1]. In our previous work [6] it is shown that the healing time t_{skip} can be justified by introducing an additional shift $M(t_{\mathrm{skip}};\cdot)$ and its inverse into (1) (note that $M(t_{\mathrm{skip}};\cdot)$ is invertible on the slow manifold $\mathcal{C}$):

$$y_*=\Phi_*(\delta;x)=(g\circ\mathcal{L})^{-1}\circ M(t_{\mathrm{skip}};\cdot)^{-1}\circ M(\delta+t_{\mathrm{skip}};\cdot)\circ g\circ\mathcal{L}(x). \tag{2}$$

Removing the inverses in (2) leads to an implicit equation for $y_*=\Phi_*(\delta;x)$ with the healing time t_{skip} as an parameter:

$$\mathcal{R}\circ M(t_{\mathrm{skip}};\cdot)\circ g\circ\mathcal{L}(y_*)=\mathcal{R}\circ M(\delta+t_{\mathrm{skip}};\cdot)\circ g\circ\mathcal{L}(x)$$



(a) (b) (c) (d)

Figure 2: Michaelis-Menten dynamics. (a) Phase space representation of dynamics for various initial conditions (crosses) which is very quickly approaching the slow manifold (black line) and evolves on much slower time scale. The final states for $t = 100$ are denoted by a red point. (b) Error as function of t_{skip}. (c,d) Same analysis for the rotated system where for our choice of lifting the degenerate situation that the stable fiber projection g is aligned with lifting and restriction is avoided. The initial large error in the flow of size 1 can be significantly reduced to an order of 10^{-8} for a larger healing time.

Replacing $M(t_{\mathrm{skip}};\cdot)\circ g$ with $M(t_{\mathrm{skip}};\cdot)$ results in a computable approximation $y_{t_{\mathrm{skip}}} = \Phi_{t_{\mathrm{skip}}}(\delta;x)$ of y_*, given implicitly by the equation

$$\mathcal{R}(M(t_{\mathrm{skip}};\mathcal{L}(y_{t_{\mathrm{skip}}}))) = \mathcal{R}(M(\delta + t_{\mathrm{skip}};\mathcal{L}(x))). \tag{3}$$

This approach was analyzed and illustrated in a traffic model in [6] and will also be studied here. We proved in [6] that the approximation $y_{t_{\mathrm{skip}}}$ is exponentially accurate if $d_{\tan}/d_{\mathrm{tr}} \to 0$: $\|y_{t_{\mathrm{skip}}} - y_*\| \sim \exp(-K d_{\mathrm{tr}}/d_{\tan})$ (for some constant K depending on t_{skip}). The error estimates in [6] requires that $t_{\mathrm{skip}} d_{\tan}/d_{\mathrm{tr}}$ and $(t_{\mathrm{skip}} + \delta)d_{\tan}/d_{\mathrm{tr}}$ stay bounded from above such that the convergence result is about the limit of infinite time scale separation $d_{\tan}/d_{\mathrm{tr}} \to 0$, similar to the results for constrained runs schemes [2, 8, 9]. The analysis left open if the error goes to zero for $t_{\mathrm{skip}} \to \infty$ but finite timescale separation: $d_{\tan}/d_{\mathrm{tr}} \in (0, 1)$.
We will present the general a-priori error estimate that $\|y_{t_{\mathrm{skip}}} - y_*\| \sim \exp((d_{\tan} - d_{\mathrm{tr}})t_{\mathrm{skip}})$ for $t_{\mathrm{skip}} \to \infty$ and fixed $d_{\tan} < d_{\mathrm{tr}}$ under some genericity conditions on $\mathcal{R}$ and $\mathcal{L}$. We will also give a convergence result for the derivatives of $y_{t_{\mathrm{skip}}}$ with respect to its argument x: $\|\partial^j y_{t_{\mathrm{skip}}} - \partial^j y_*\| \sim \exp(((2j+1)d_{\tan} - d_{\mathrm{tr}})t_{\mathrm{skip}})$ if $(2j+1)d_{\tan} < d_{\mathrm{tr}}$. An illustration is given in Fig. 2 for the Michaelis-Menten kinetics.
Equation-free analysis based on lift-evolve-restrict maps is more commonly applied to problems that are assumed to have a fast subsystem, where the fast time scale converges only in a statistical sense to a stationary measure conditioned on the slow variables, approximated by Monte Carlo simulations on ensembles of initial conditions. Barkley *et al* [1] investigated the behaviour of the lift-evolve-restrict map $P(\delta;\cdot) = \mathcal{R}\circ M(\delta;\cdot)\circ\mathcal{L}$ where the slow variables were leading moments (thus, P was called moment map in [1]) on prototype examples from the class of stochastic problems. The simplest example from [1] is a scalar stochastic differential equation (SDE), for which the evolution is governed by the (linear) Fokker-Planck equation (FPE) for the probability distribution and, hence, the measure of time-scale separation is the size of the spectral gap in the right-hand side of the FPE. The analysis in [1] found that the dynamics of the map P was qualitatively different from the dynamics of the underlying FPE. For example, P was nonlinear and metastable states were stabilized for certain choices of δ.
We will demonstrate for two different lifting operators $\mathcal{L}$ that the approximation $y_{t_{\mathrm{skip}}}$, defined by (3), behaves exactly as predicted by the presented convergence theorem. In particular, it preserves the metastability features and the linearity of the flow generated by the FPE. A detailed discussion will be given about the differences between observations of the behaviour in the SDE and the predictions from the theoretical result. These are caused by the numerical errors in the evaluations of lifting, evolution and restriction and their growth along trajectories.

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