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ON CONVERGENCE OF THE PROJECTIVE INTEGRATION METHOD FOR STIFF ORDINARY DIFFERENTIAL EQUATIONS*

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Abstract. We present a convergence proof of the projective integration method for a class of deterministic multi-dimensional multi-scale systems which are amenable to center manifold theory. The error is shown to contain contributions associated with the numerical accuracy of the microsolver, the numerical accuracy of the macrosolver and the distance from the center manifold caused by the combined effect of micro- and macrosolvers, respectively. We corroborate our results by numerical simulations.

Key words. Multi-scale integrators, projective integration, heterogeneous multiscale methods.

AMS subject classifications. 37Mxx, 65Pxx, 37Mxx, 34.

1. Introduction

Devising efficient computational methods to simulate high-dimensional complex systems is of paramount importance to a wide range of scientific fields, ranging from nanotechnology, biomolecular dynamics, and material science to climate science. The dynamics of large complex systems is made complicated by their high dimensionality and by the possible existence of active entangled processes running on temporal scales varying by several orders of magnitude. To resolve all variables in a high-dimensional system and capture the whole range of temporal scales is impossible given current computing power. In many applications, however, the modeler is only interested in the dynamics of a few relevant slow macroscopic coarse-grained variables. How to extract from a dynamical system the relevant dynamics of the slow degrees of freedom while ensuring that the collective effect of the unresolved variables is implicitly represented is one of the most challenging problems in computational modeling. There are two separate scenarios when such a dimension reduction is possible: scale separation and weak coupling [9]. We restrict ourselves here to the big class of time scale separated systems, in particular to deterministic stiff dissipative systems.

Recently two numerical methods to deal with multi-scale systems have received much attention: the *projective integration method* (PI) within the equation-free framework [8, 13] and the *heterogeneous multiscale method* (HMM) [3, 7]. These powerful methods have successfully been applied to a wide range of problems, including modeling of water in nanotubes, micelle formation, chemical kinetics, and climate modeling [18, 5, 12]. The general strategy of both methods is the following: Provided there exist closed (but possibly unknown) equations for the slow variables, the simulation is split between a macrosolver employing a large integration time-step and a microsolver, in which the full high dimensional system is integrated for a short burst employing a small integration time step. The two methods differ in the way the information of the microsolver is utilized in the macrosolver to evolve the slow variables. In the equation-free approach this is done without any assumptions on the actual form of the

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reduced equations, using the microsolver to estimate the temporal derivative of the slow variable, which is then subsequently propagated over a large time step. The underlying assumption is that the fast variables quickly relax to their equilibrium value (conditioned on the slow variables), and that subsequently the dynamics evolves on a reduced slow manifold. In heterogeneous multiscale methods, on the other hand, information available (i.e. through perturbation theory such as for example center manifold theory, averaging theorems, or homogenization [1, 14, 15, 19]) is used to determine the functional form of the reduced slow vector field; the microsolver is then used to estimate the coefficients of this slow vector field conditioned on the slow variables. For further details we refer the reader to [12, 13, 6, 22].

The question we address here is the convergence of the numerical PI approximation to the true solution of a full multi-scale system of stiff deterministic ordinary differential equations. There exists a body of analytical work on the convergence of HMM [3, 2, 7], including formulations for stochastic differential equations [4, 17]. Convergence results for PI were obtained for specific deterministic systems and for on-the-fly local error estimates in numerical algorithms [8, 16]. Stochastic differential equations were treated in [10]. Here we provide global error estimates for PI for a subclass of systems amenable to center-manifold theory.

The paper is organized as follows. In Section 2 we discuss the class of dynamical systems studied, and briefly summarize in Section 3 HMM and PI for these systems. In Section 4, the main part of this work, we derive rigorous error bounds for those numerical multiscale methods. In Section 5 these are numerically verified. We conclude with a summary in Section 6.

2. Model

We consider deterministic multiscale systems for slow variables $y_\varepsilon \in \mathbb{R}^n$ and fast variables $x_\varepsilon \in \mathbb{R}^m$ of the form

$$\dot{y}_\varepsilon = g(x_\varepsilon, y_\varepsilon)\,, \tag{2.1}$$

$$\dot{x}_\varepsilon = \frac{1}{\varepsilon}(-\Lambda x_\varepsilon + f(y_\varepsilon))\,, \tag{2.2}$$

with time scale separation parameter $0 < \varepsilon \ll 1$. Without loss of generality we assume that $(x_\varepsilon, y_\varepsilon) = (0,0)$ is a fixed point. We assume there is a coordinate system such that the matrix $\Lambda \in \mathbb{R}^{m\times m}$ is diagonal with diagonal entries $\lambda_{ii} > 0$. We further assume that we allowed for a scaling of time such that $\min(\lambda_{ii}) = 1$ and define $\max(\lambda_{ii}) = \lambda$. We assume that the vector field of the slow variable $g(x,y)$ is purely nonlinear with $\det \mathrm{D}g(0,0) \neq 0$, where $\mathrm{D}g$ denotes the Jacobian of $g(x,y)$, so that there exists a center manifold $x = h_\varepsilon(y)$ on which the slow dynamics evolve according to

$$\dot{Y} = G(Y)\,, \tag{2.3}$$

with $Y = y + \mathcal{O}(\varepsilon)$. The reduced slow vector field is given by (see for example [1])

$$G(y) = g(h_\varepsilon(y), y)\,. \tag{2.4}$$

Initial conditions close to the fixed point are exponentially quickly attracted towards the center manifold along the stable manifold of the fast variables x_ε. Near the center manifold the dynamics slow down and are approximately determined by the dynamics of the slow variables (2.3) only. Center manifold theory assures that on times $T \sim \mathcal{O}(1)$ the dynamics of (2.1) are well approximated by the reduced slow system (2.3) (see for example [1]).

It is worthwhile to formulate center manifold theory in the framework of averaging [9], and view the effect of the fast variables on the slow variables through their induced empirical measure which is approximated by $\mu_y(dx)=\delta(x-h_\varepsilon(y))dx$, conditioned on the slow variables. The dynamical system (2.1)-(2.2) can equivalently be described by its associated Liouville equation for the probability density function $\rho(x_\varepsilon,y_\varepsilon)$. After an initial transient, the solution of the Liouville equation is approximated by

$$\rho(x,y)=\delta(x-h_\varepsilon(y))\hat{\rho}(y)+\mathcal{O}(\varepsilon)\,. \tag{2.5}$$

We can now reformulate (2.4) as

$$\begin{aligned} G(y) &= \int g(x,y)\mu_y(dx) \\ &= g(h_\varepsilon(y),y)\,. \end{aligned} \tag{2.6}$$

The underlying assumption is that the measure $\mu_y(dx)=\delta(x-h_\varepsilon(y))dx$ is the physically observable measure on the y-fibre; that is, Lebesgue almost all initial conditions of the fast variables will evolve to generate $\mu_y(dx)$, if sufficiently close to the center manifold. Center manifold theory [1] makes this approach rigorous and $\hat{\rho}(y)$ is the invariant density of the reduced system (2.3). This is exploited explicitly in HMM and implicitly in PI. In the following we will approximate the center manifold $h_\varepsilon(y)$ by $h_\varepsilon(y)\approx\Lambda^{-1}f(y)+\mathcal{O}(\varepsilon)$.

3. Numerical multiscale methods

We consider here two numerical methods to deal with the deterministic multiscale system (2.1)-(2.2), namely heterogeneous multiscale methods and projective integration. We use the formulation of PI as in [8, 13] and of heterogeneous multiscale methods as in [3, 7]. We will see that both methods can be formulated in the same framework.

We denote by x^n and y^n the numerical approximations to the solutions of (2.1)-(2.2) evaluated at the discrete time t^n, $x_\varepsilon(t^n)$ and $y_\varepsilon(t^n)$ respectively. Further we denote by $Y(t^n)$ the time-continuous solution of the reduced ordinary differential equation (2.3) evaluated at time t^n. Throughout the paper superscripts denote discrete variables whereas brackets are reserved for continuous variables. We will employ a forward Euler method for both the micro- as well as the macrosolver.

3.1. Heterogeneous multiscale methods. The microsolver consists of M microsteps with micro-time step δt [3]. The slow variables are held fixed during the microsteps, assuming infinite time scale separation. Let us denote by $x^{n,m}$ the mth microstep of the fast variables which was initialized at the nth macrostep at $t^n=n\Delta t$ with $x^{n,0}=x^{n-1,M}=x^n$ and $y^{n,0}=y^n$. The microstep for a forward Euler scheme then is

$$x^{n,m+1}=x^{n,m}-\frac{\delta t}{\varepsilon}\left(\Lambda x^{n,m}-f(y^n)\right),$$

for $m=0,\ldots,M$. Invoking the Birkhoff ergodic theorem, the time series of the fast variables $x^{n,m}$ is used to estimate the average in the reduced slow vector field (2.6), and the macrosolver is initialized at the previous macrostep y^n and is written for a forward Euler step as

$$y^{n+1}=y^n+\Delta t\,\hat{g}(x^n,y^n), \tag{3.1}$$

with the time-discrete approximation of the reduced slow vector field (2.4)

$$G(y_\varepsilon(t^n)) \approx \hat{g}(x^n, y^n) = \sum_{m=0}^{M} W_m g(x^{n,m}, y^n),$$

for some weights W_m. This is justified as long as the slow variable remains constant while integrating over the fast fibres. Being associated with the empirical approximation of the invariant density induced by the fast dynamics (cf. (2.6)), the weights W_m satisfy the normalization constraint

$$\sum_{m=0}^{M} W_m = 1\,. \tag{3.2}$$

The weights should be chosen to best approximate the invariant density of the fast variable. A natural choice for our system (2.1)-(2.2), where the fast dynamics rapidly settle on the center manifold, and do not advance significantly on the center manifold in M microsteps, is to set

$$W_m = \begin{cases} 0, & \text{for } m < M, \\ 1, & \text{for } m = M. \end{cases} \tag{3.3}$$

The convergence of this scheme has been analyzed in [2]. More general weights were discussed in [7].

It is pertinent to mention that for this formulation of HMM the fast variables must be initialized before each application of the microsolver; see for example [6] for a discussion on initializations. In PI, as described in the next subsection, the fast variables are initialized on the fly.

The *seamless* heterogeneous multiscale method [2, 7] can be applied to the case when the slow and fast variables are not explicitly known. The seamless HMM formulation for our system (2.1)-(2.2) advances both fast and slow variables simultaneously first through M microsteps, and then subsequently through one macrostep. We adopt here the formulation described in [2] for deterministic dissipative systems. Introducing $y^{n,m}$ analogously to $x^{n,m}$ the M microsteps are executed as

$$x^{n,m+1} = x^{n,m} - \frac{\delta t}{\varepsilon}(\Lambda x^{n,m} - f(y^{n,m})), \tag{3.4}$$

$$y^{n,m+1} = y^{n,m} + \delta t\, g(x^{n,m}, y^{n,m})\,. \tag{3.5}$$

The macrostep is initialized at $(x^n, y^n) = (x^{n,0}, y^{n,0})$ and takes the form

$$x^{n+1} = x^n - \frac{\Delta t}{\varepsilon}\sum_{m=0}^{M} W_m \left(\Lambda x^{n,m} - f(y^{n,m})\right), \tag{3.6}$$

$$y^{n+1} = y^n + \Delta t\, \tilde{g}(x^n, y^n)\,, \tag{3.7}$$

with the time-discrete approximation of the slow vector field

$$\tilde{g}(x^n, y^n) := \sum_{m=0}^{M} W_m g(x^{n,m}, y^{n,m})\,. \tag{3.8}$$

Again, the weights W_m need to satisfy (3.2) (see [7] for choices of weights W_m).

3.2. Projective integration. We present a formulation of projective integration which is close to the seamless formulation of HMM. PI advances both slow and fast variables at the same time, as done in seamless HMM. However, the PI scheme proposed in [8] does not start the macrostep at $(x^{n,0}, y^{n,0})$ as done in our adopted formulation of seamless HMM, but at $(x^{n,M}, y^{n,M})$, allowing for nontrivial dynamics of the slow variables during the M microsteps. This takes into account finite time scale separation ε, ignored in HMM. The microsteps of PI are exactly as in seamless HMM, (3.4)–(3.5). The macrostep of PI is given by estimating the temporal time derivative of the slow (and fast) variables using the microsolver according to

$$x^{n+1} = x^{n,M} + \Delta t \frac{x^{n,M} - x^{n,M-1}}{\delta t},$$
$$y^{n+1} = y^{n,M} + \Delta t \frac{y^{n,M} - y^{n,M-1}}{\delta t},$$

which becomes, upon using the Euler step of the microsolver (3.4)–(3.5),

$$x^{n+1} = x^{n,M} - \frac{\Delta t}{\varepsilon}(\Lambda x^{n,M} - f(y^{n,M})), \tag{3.9}$$
$$y^{n+1} = y^{n,M} + \Delta t\, g(x^{n,M}, y^{n,M}). \tag{3.10}$$

Here the time between two macrosteps is $t_\Delta = \Delta t + M\delta t$ and we have $t^n = nt_\Delta$. Upon substituting the microsteps (3.4)–(3.5) into the macrosolver (3.9)–(3.10) we reformulate PI, such that it formally resembles seamless HMM, as

$$x^{n+1} = x^n - \frac{t_\Delta}{\varepsilon} \sum_{m=0}^{M} W_m (\Lambda x^{n,m} - f(y^{n,m})), \tag{3.11}$$
$$y^{n+1} = y^n + t_\Delta \tilde{g}(x^n, y^n), \tag{3.12}$$

with the weights W_m now defined as

$$W_m = \begin{cases} \dfrac{\delta t}{t_\Delta}, & \text{for } m < M, \\ \dfrac{\Delta t}{t_\Delta}, & \text{for } m = M. \end{cases} \tag{3.13}$$

Hence PI with a microstep of δt and macrostep of Δt is equivalent to seamless HMM with a microstep of δt, a macrostep of t_Δ, and a particular choice of weights W_m.

4. Error analysis for projective integration

We will now provide rigorous error bounds for PI in the formulation (3.11)–(3.13). We follow the general line of proof used in [2] for error bounds of HMM with the choice of weights (3.3).

Throughout this work we assume the following conditions on the global growth and smoothness of solutions of our system and on the numerical discretization parameters of PI.

ASSUMPTIONS

A1: The vector field $f(y)$ is Lipschitz continuous; that is there exists a constant L_f such that

$$|f(y_1) - f(y_2)| \le L_f |y_1 - y_2|.$$

A2: The vector field $g(x,y)$ is Lipschitz continuous; that is there exists a constant L_g such that

$$|g(x_1,y_1)-g(x_2,y_2)|\leq L_g(|x_1-x_2|+|y_1-y_2|)\,.$$

A3: The vector field $f(y)$ is bounded for all y; that is there exists a constant C_f such that

$$C_f=\sup|f(y)|\,.$$

A4: The vector field $g(x,y)$ is bounded for all x,y; that is there exists a constant C_g such that

$$C_g=\sup|g(x,y)|\,.$$

A5: The reduced vector field $G(Y)$ of the slow dynamics is of class C^1; that is there exists a constant C^* such that

$$C^*=\sup|\ddot{Y}(t)|\,.$$

A6: The microstep size δt resolves the fastest of the fast variables, while the macrostep size Δt resolves the dynamics of the slow system, so that

$$0<\delta t\leq\frac{2\varepsilon}{\lambda}<\Delta t\,.$$

A7: The total time $M\delta t$ of the microsteps is sufficiently short so that

$$L_G M\delta t\leq L_g(1+L_f)M\delta t\leq 1\,,$$

where $L_G\leq L_g(1+L_f)$ is the Lipschitz constant of the reduced dynamics (2.3).

A8: The macrostep size Δt, number of microsteps M, and microstep size δt are chosen such that

$$\Delta t\exp\left(-\frac{M\delta t}{\varepsilon}\right)<\frac{\varepsilon}{\lambda}\qquad\text{if}\quad 0<\delta t\leq\frac{2\varepsilon}{\lambda+1}\,,$$
$$\textit{or}$$
$$\Delta t\exp\left(-\frac{M\delta t^\star}{\varepsilon}\right)<\frac{\varepsilon}{\lambda}\qquad\text{if}\quad \frac{2\varepsilon}{\lambda+1}<\delta t<\frac{2\varepsilon}{\lambda}\,.$$

with $\delta t^\star=2\varepsilon-\lambda\delta t$. The range $2\varepsilon/(\lambda+1)<\delta t<2\varepsilon/\lambda$ corresponds to $0<\delta t^\star<2\varepsilon/(\lambda+1)$. This assumption is necessary to bound the distance of the fast variables from the center manifold over the macrosteps.

The global Lipschitz conditions can be relaxed to local Lipschitz conditions by the usual means.

We will establish bounds for the error $\mathcal{E}^n$ between the PI estimate y^n and the solution of the full system $y_\varepsilon(t^n)$:

$$\mathcal{E}^n=|y_\varepsilon(t^n)-y^n|\,.$$

Our main result is provided by the following theorem.

THEOREM 4.1. *Given the assumptions (A1)–(A8), there exists a constant C such that on a fixed time interval T, for each n such that $nt_\Delta \leq T$, the error between the PI estimate and the exact solution of the full multiscale system (2.1)-(2.2) is given by*

$$\mathcal{E}^n \leq \begin{cases} C\left(t_\Delta + \varepsilon + \left(\dfrac{\varepsilon}{t_\Delta} + \varepsilon + e^{-\frac{M\delta t}{\varepsilon}}\right)|d^n|\right), & \text{if } \ 0 < \delta t \leq \dfrac{2\varepsilon}{\lambda+1}, \\ C\dfrac{\delta t}{\delta t^*}\left(t_\Delta + \varepsilon + \left(\dfrac{\varepsilon}{t_\Delta} + \varepsilon + e^{-\frac{M\delta t^*}{\varepsilon}}\right)|d^n|\right), & \text{if } \ \dfrac{2\varepsilon}{\lambda+1} < \delta t < \dfrac{2\varepsilon}{\lambda}, \end{cases}$$

where d^n measures the maximal distance of the fast variables x from the approximate center manifold $x = \bar{f}(y) := \Lambda^{-1} f(y)$ over all macrosteps and is estimated by

$$|d^n| \leq \begin{cases} \left|x^0 - \bar{f}(y^0)\right| + \dfrac{\varepsilon L_f C_g (1+\lambda)\Delta t}{\varepsilon - \Delta t \lambda e^{-\frac{M\delta t}{\varepsilon}}}, & \text{if } \ 0 < \delta t \leq \dfrac{2\varepsilon}{\lambda+1}, \\ \left|x^0 - \bar{f}(y^0)\right| + \dfrac{\varepsilon L_f C_g (1+\frac{\delta t}{\delta t^*}\lambda)\Delta t}{\varepsilon - \Delta t \lambda e^{-\frac{M\delta t^*}{\varepsilon}}}, & \text{if } \ \dfrac{2\varepsilon}{\lambda+1} < \delta t < \dfrac{2\varepsilon}{\lambda}, \end{cases}$$

with $\delta t^* = 2\varepsilon - \lambda \delta t$.

Before proceeding to the proof of the theorem, it is worthwhile to interpret the bounds on $\mathcal{E}^n$. The term proportional to $t_\Delta = \Delta t + M\delta t$ reflects the first order convergence of the forward Euler numerical scheme used to propagate the micro- and macro-solver respectively. The terms proportional to the time scale parameter ε represent the error made by the reduction as well as an additional error incurred during the drift of the slow variable over the microsteps. The term proportional to $\exp(-M\delta t/\varepsilon)|d^n|$ measures the exponential decay of the fast variables towards the slow manifold.

4.1. Error analysis. We split the error into two parts according to

$$\begin{aligned} \mathcal{E}^n &= |y_\varepsilon(t^n) - y^n| \\ &\leq |y_\varepsilon(t^n) - Y(t^n)| + |y^n - Y(t^n)|, \end{aligned}$$

where the first term describes the error between the exact solution of the full system (2.1)-(2.2) and the reduced slow system (2.3), which we label *reduction error*, and the second term the error between PI and the exact solution of the reduced slow system (2.3), which we denote by *discretization error*. We will bound the two terms separately in the following.

4.2. Reduction error. Defining the error between the exact solution of the full system (2.1)-(2.2) and the reduced slow system (2.3) by

$$|E_c^n| = |y_\varepsilon(t^n) - Y(t^n)|, \tag{4.1}$$

and setting the initial conditions close to the slow manifold with $y_\varepsilon(0) = Y(0) + c_{0,y}\varepsilon$ and $x_\varepsilon(0) = f(y_\varepsilon(0)) + c_{0,x}$, we can formulate the following theorem.

THEOREM 4.2. *Given the assumptions (A1)–(A3), there exists a constant C_1 such that on a fixed time interval T, for each $t^n \leq T$, the error between the exact solutions of the reduced and the full system is bounded by*

$$|E_c^n| \leq C_1 \varepsilon,$$

with

$$C_1 = \max\left(|y_\varepsilon(0) - Y(0)|, L_f L_g C_g t^n, L_g |d_\varepsilon(0)|\right) e^{L_g(1+L_f)t^n}\,,$$

where $d_\varepsilon = x_\varepsilon - f(y_\varepsilon)$ measures the distance of the fast variables from the approximate slow manifold.

Proof. The proof is standard in center manifold theory and is included for completeness. Using assumptions (*A1*)–(*A2*) on the Lipschitz continuity of f and g we estimate

$$\begin{aligned}
\frac{d}{dt}|y_\varepsilon(t) - Y(t)| &= |g(x_\varepsilon, y_\varepsilon) - g(\bar{f}(Y), Y)| \\
&\le |g(x_\varepsilon, y_\varepsilon) - g(x_\varepsilon, Y)| + |g(x_\varepsilon, Y) - g(\bar{f}(Y), Y)| \\
&\le L_g |y_\varepsilon - Y| + L_g |x_\varepsilon - \bar{f}(Y)| \\
&\le L_g |y_\varepsilon - Y| + L_g |x_\varepsilon - \bar{f}(y_\varepsilon)| + L_g |\bar{f}(y_\varepsilon) - \bar{f}(Y)| \\
&\le L_g (1 + L_f) |y_\varepsilon - Y| + L_g |x_\varepsilon - \bar{f}(y_\varepsilon)|\,, \qquad (4.2)
\end{aligned}$$

To estimate the second term, we differentiate the distance of the fast variable to the slow manifold $d_\varepsilon = x_\varepsilon - \bar{f}(y_\varepsilon)$ with respect to time, using (2.2), as

$$\dot{d}_\varepsilon = -\frac{\Lambda}{\varepsilon} d_\varepsilon - D\bar{f}(y_\varepsilon)\, g(x_\varepsilon, y_\varepsilon)\,,$$

where $\mathrm{D}\bar{f}$ denotes the Jacobian matrix of $\bar{f}$. Integrating and using the boundedness Assumption (*A4*) on g and the Lipschitz continuity Assumption (*A1*) on f, we readily estimate

$$\begin{aligned}
|d_\varepsilon(t)| &\le \exp\Big(-\frac{\Lambda}{\varepsilon} t\Big) |d_\varepsilon(0)| + \left| \int_0^t \exp\Big(-\frac{\Lambda}{\varepsilon}(t-s)\Big) D\bar{f}(y_\varepsilon(s))\, g(x_\varepsilon(s), y_\varepsilon(s))\, ds \right| \\
&\le e^{-\frac{t}{\varepsilon}} |d_\varepsilon(0)| + \sup_{|g| \le C_g} |Dfg| \int_0^t e^{-\frac{t-s}{\varepsilon}}\, ds \\
&\le e^{-\frac{t}{\varepsilon}} |d_\varepsilon(0)| + \varepsilon L_f C_g\,, \qquad (4.3)
\end{aligned}$$

which signifies the exponential attraction of the fast dynamics towards the slow center manifold. Substituting (4.3) into (4.2) yields, upon application of the Gronwall lemma,

$$|y_\varepsilon(t) - Y(t)| \le e^{L_g(1+L_f)t} \left(|y_\varepsilon(0) - Y(0)| + \varepsilon L_f L_g C_g t + \varepsilon L_g |d_\varepsilon(0)| \right)\,,$$

which immediately yields the desired result using the initial condition $d_\varepsilon(0) = c_{0,x}$ and $y_\varepsilon(0) = Y(0) + c_{0,y}\varepsilon$. ∎

4.3. Discretization error. In order to bound the discretization error $|y^n - Y(t^n)|$ we first estimate how close the fast variables remain to the center manifold during the application of the microsolver. Defining the deviation of the PI approximation of the fast variables from the approximate center manifold at time $t^n + m\delta t$ as

$$d^{n,m} = x^{n,m} - \bar{f}(y^{n,m})\,, \qquad (4.4)$$

we formulate the following lemma which constitutes the discrete time version of (4.3).

LEMMA 4.3. *Given assumptions (A1), (A4), and (A6), the error between the fast variables and the approximate center manifold during the application of the PI microsolver is bounded for all* $0 \le m \le M$ *by*

$$|d^{n,m}| \le \begin{cases} \left(1-\dfrac{\delta t}{\varepsilon}\right)^m |d^{n,0}| + \varepsilon L_f C_g, & \text{if } 0<\delta t \le \dfrac{2\varepsilon}{\lambda+1}, \\ \left(1-\dfrac{\delta t^*}{\varepsilon}\right)^m |d^{n,0}| + \dfrac{\delta t}{\delta t^*}\varepsilon L_f C_g, & \text{if } \dfrac{2\varepsilon}{\lambda+1} < \delta t < \dfrac{2\varepsilon}{\lambda}. \end{cases}$$

The first term is a manifestation of the exponential decay of the fast variables towards the slow center manifold along their stable eigendirection. The second term proportional to ε describes, as we will see below, the cumulative effect of changes of the slow variables y during the microsteps causing a departure from the center manifold for nonconstant $\bar{f}(y)$.

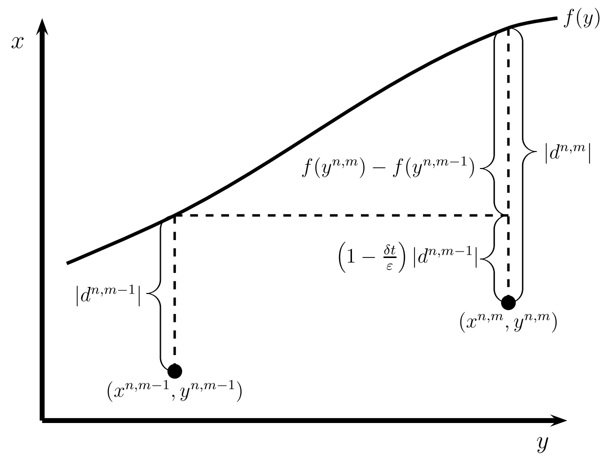

Fig. 4.1: *Illustration of equation* (4.5) *for* $x_\varepsilon \in \mathbb{R}$*, so that* $\Lambda = 1$*. The two dots show one microstep in PI.*

Proof. Using the definition of the PI microsolver (3.4), a recursive relationship for $d^{n,m}$ is readily established as

$$\begin{aligned} d^{n,m} &= x^{n,m} - \bar{f}(y^{n,m}) \\ &= \left(\mathbb{I} - \frac{\delta t}{\varepsilon}\Lambda\right) d^{n,m-1} - \left(\bar{f}(y^{n,m}) - \bar{f}(y^{n,m-1})\right). \end{aligned} \tag{4.5}$$

Let us pause here for a moment to discuss the terms appearing in this equation. The first term illustrates that at each microstep the distance between the ith fast variable and the approximate slow manifold decreases by a factor of $1-\delta t \lambda_{ii}/\varepsilon$. The second term represents the change in the approximate slow manifold during the drift of the slow variable y in one microstep. This is illustrated in figure 4.1.

The cumulative effect of M microsteps on $d^{n,m}$ is easily obtained from (4.5) as

$$d^{n,m} = \left(\mathbb{I} - \frac{\delta t}{\varepsilon}\Lambda\right)^m d^{n,0} - \sum_{k=0}^{m-1}\left(\mathbb{I} - \frac{\delta t}{\varepsilon}\Lambda\right)^k \left(\bar{f}(y^{n,m-k}) - \bar{f}(y^{n,m-1-k})\right). \tag{4.6}$$

Taking absolute values and using the Lipschitz condition on f *(A1)*, the bound on the slow vector field g *(A4)*, and (3.5), the cumulative effect of M microsteps on the distance $|d^{n,m}|$ of the fast variables to the approximate center manifold is

$$\begin{aligned}|d^{n,m}| &\le \left|\mathbb{I}-\frac{\delta t}{\varepsilon}\Lambda\right|^m |d^{n,0}| + L_f C_g \delta t \sum_{k=0}^{m-1}\left|\mathbb{I}-\frac{\delta t}{\varepsilon}\Lambda\right|^k \\ &= \left|\mathbb{I}-\frac{\delta t}{\varepsilon}\Lambda\right|^m |d^{n,0}| + L_f C_g \delta t \frac{1-|\mathbb{I}-\frac{\delta t}{\varepsilon}\Lambda|^m}{1-|\mathbb{I}-\frac{\delta t}{\varepsilon}\Lambda|}\,.\end{aligned}$$

To avoid divergence from the center manifold we require

$$\left|\mathbb{I}-\frac{\delta t}{\varepsilon}\Lambda\right| = \max\left\{1-\frac{\delta t}{\varepsilon}, \lambda\frac{\delta t}{\varepsilon}-1\right\} < 1\,,$$

implying the standard condition $0<\delta t<2\varepsilon/\lambda$. For $0<\delta t\le\frac{2\varepsilon}{\lambda+1}$, $\left|\mathbb{I}-\frac{\delta t}{\varepsilon}\Lambda\right| = 1-\frac{\delta t}{\varepsilon}$ and we obtain the bound

$$|d^{n,m}| \le \left(1-\frac{\delta t}{\varepsilon}\right)^m |d^{n,0}| + \varepsilon L_f C_g\left[1-\left(1-\frac{\delta t}{\varepsilon}\right)^m\right]. \tag{4.7}$$

Furthermore for $\frac{2\varepsilon}{\lambda+1}<\delta t<\frac{2\varepsilon}{\lambda}$, introducing $\delta t^\star = 2\varepsilon-\lambda\delta t$, $\left|\mathbb{I}-\frac{\delta t}{\varepsilon}\Lambda\right| = \lambda\frac{\delta t}{\varepsilon}-1 = 1-\frac{\delta t^*}{\varepsilon}$, yielding

$$|d^{n,m}| \le \left(1-\frac{\delta t^*}{\varepsilon}\right)^m |d^{n,0}| + \frac{\delta t}{\delta t^*}\varepsilon L_f C_g\left[1-\left(1-\frac{\delta t^*}{\varepsilon}\right)^m\right]. \tag{4.8}$$

Lemma 4.3 follows from (4.7)–(4.8). Note that the term proportional to ε was generated by a sum of error terms in δt related to the change in the manifold during the drift of the slow variable $y^{n,m}$ over each microstep. ∎

Remark 4.1. In the limit $\delta t^\star \to 0$ (i.e. $\delta t \to 2\varepsilon/\lambda$) the term $\left[1-\left(1-\frac{\delta t^*}{\varepsilon}\right)^m\right]$ in (4.8), which is neglected in Lemma 4.3, is crucial to obtain a finite estimate $|d^{n,m}| \le |d^{n,0}| + m\delta t L_f C_g$.

Remark 4.2. In the case $x_\varepsilon \in \mathbb{R}$ with $\Lambda = 1$, a direct estimation of (4.5) implies that for the particular choice $\delta t = \varepsilon$ we have $|d^{n,m}| \le L_f C_g \delta t$, i.e. there is no dependence on initial conditions for the fast variable; this is a peculiarity of the underlying forward Euler scheme used (cf. (3.4)) where for $\delta t = \varepsilon$ we have $x^{n,m+1} = f(y^{n,m})$.

We have bounded the distance of the PI approximation of the fast variables $x^{n,m}$ from the slow center manifold $\bar{f}(y^{n,m})$ over the microsteps. We now establish bounds on the distance of the PI approximation of the slow variables $y^{n,m}$ from the solution of the reduced dynamics on the center manifold over the microsteps. We therefore introduce the auxiliary time-continuous system

$$\dot{Y}^{(n)}(s) = G(Y^{(n)}(s)), \tag{4.9}$$

$$Y^{(n)}(0) = y^n\,, \tag{4.10}$$

which resolves the reduced slow dynamics (2.3) initialized after each macrostep at time $t^n = nt_\Delta$ with the PI approximation of the slow variables y^n. Further we introduce the discrete Euler approximation of the reduced slow dynamics (2.3)

$$\varphi_\eta^m = \varphi_\eta^{m-1} + \delta t G(\varphi_\eta^{m-1}), \tag{4.11}$$

$$\varphi_\eta^0 = \eta\,, \tag{4.12}$$

for arbitrary initial conditions η. Note that for the particular choice $\eta = y^n$, (4.11)-(4.12) corresponds to an Euler discretization of the system (4.9)-(4.10).

LEMMA 4.4. *Assuming (A1), (A2), (A5), and (A7), the numerical estimate $y^{n,m}$ of the slow variable is close to $\varphi_{y^n}^m$ with*

$$|y^{n,m} - \varphi_{y^n}^m| \le \begin{cases} 3L_g\varepsilon|d^{n,0}| + 2\dfrac{L_f C_g \varepsilon}{L_f+1} + \mathcal{O}(m\delta t^2), & \text{if } \ 0 < \delta t \le \dfrac{2\varepsilon}{\lambda+1}, \\ \left(3L_g\varepsilon|d^{n,0}| + 2\dfrac{L_f C_g \varepsilon}{L_f+1}\right)\dfrac{\delta t}{\delta t^*} + \mathcal{O}(m\delta t^2), & \text{if } \ \dfrac{2\varepsilon}{\lambda+1} < \delta t < \dfrac{2\varepsilon}{\lambda}. \end{cases}$$

Proof. Employing the auxiliary system (4.9)-(4.10), we split the error into

$$|y^{n,m} - \varphi_{y^n}^m| \le |y^{n,m} - Y^{(n)}(m\delta t)| + |Y^{(n)}(m\delta t) - \varphi_{y^n}^m|\,. \tag{4.13}$$

The second term above can be readily bounded by the standard proof for Euler convergence (see for example [11]). The first term is bounded by a slight variation of the same proof. For completeness we provide the proof of the bounds for both terms, beginning with the bound on the second term. By Taylor expanding we write, upon using the auxiliary dynamics (4.9),

$$Y^{(n)}(m\delta t) = Y^{(n)}\big((m-1)\delta t\big) + \delta t\, G\big(Y^{(n)}\big((m-1)\delta t\big)\big) + \mathcal{O}(\delta t^2)\,. \tag{4.14}$$

Note that assumptions (*A1*) and (*A2*) imply a Lipschitz constant $L_G \le L_g(1+L_f)$ for the reduced vector field G. Using the Euler discretization (4.11) of the reduced auxiliary system (4.9)-(4.10) with initial condition y^n, and employing Assumption (*A5*) with $C^* = \sup|\ddot{Y}(t)|$ to bound the $\mathcal{O}(\delta t^2)$-term in (4.14), we obtain

$$\begin{aligned} |Y^{(n)}(m\delta t) - \varphi_{y^n}^m| \le & \left|Y^{(n)}\big((m-1)\,\delta t\big) - \varphi_{y^n}^{m-1}\right| \\ & + \delta t \left|G\big(Y^{(n)}\big((m-1)\delta t\big)\big) - G(\varphi_{y^n}^{m-1})\right| + C^*\delta t^2 \\ \le & (1+L_G\delta t)\left|Y^{(n)}\big((m-1)\,\delta t\big) - \varphi_{y^n}^{m-1}\right| + C^*\delta t^2 \\ \le & C^*\delta t^2 \sum_{k=0}^{m-1}(1+L_G\delta t)^k\,, \end{aligned}$$

since we initialize with $Y^{(n)}(0) = \varphi_{y^n}^0$. Evaluating the sum we find

$$\begin{aligned} |Y^{(n)}(m\delta t) - \varphi_{y^n}^m| & \le C^*\delta t^2\,\frac{(1+L_G\delta t)^m - 1}{L_G\delta t} \\ & \le 2C^* m\delta t^2\,, \end{aligned} \tag{4.15}$$

where Assumption (*A7*), that $L_G M\delta t \le 1$, was used to bound $e^{L_G m\delta t} - 1 \le 2L_G m\delta t$. To bound the first term in (4.13), $|y^{n,m} - Y^{(n)}(m\delta t)|$, we analogously obtain

$$\begin{aligned} \left|y^{n,m} - Y^{(n)}(m\delta t)\right| \le & \left|y^{n,m-1} - Y^{(n)}\big((m-1)\delta t\big)\right| \\ & + \delta t\left|g(x^{n,m-1}, y^{n,m-1}) - G(y^{n,m-1})\right| \end{aligned}$$

$$
\begin{aligned}
&+\delta t\Big|G(y^{n,m-1})-G\big(Y^{(n)}\big((m-1)\delta t\big)\big)\Big|+C^*\delta t^2\\
\le&(1+L_G\delta t)\Big|y^{n,m-1}-Y^{(n)}\big((m-1)\delta t\big)\Big|\\
&+L_g\delta t\left|d^{n,m-1}\right|+C^*\delta t^2\,.
\end{aligned}
\tag{4.16}
$$

Employing Lemma 4.3 with $0<\delta t<\frac{2\varepsilon}{\lambda+1}$, we obtain

$$
\begin{aligned}
\Big|y^{n,m}-Y^{(n)}(m\delta t)\Big|\le&\delta t\,L_g|d^{n,0}|\sum_{k=0}^{m-1}(1+L_G\delta t)^k\left(1-\frac{\delta t}{\varepsilon}\right)^{m-1-k}\\
&+\left[L_gL_fC_g\varepsilon\delta t+C^*\delta t^2\right]\sum_{k=0}^{m-1}(1+L_G\delta t)^k\,,
\end{aligned}
$$

since $y^{n,0}=y^n=Y^{(n)}(0)$. Evaluating the sums and using Assumption $(A7)$ yields

$$
\begin{aligned}
\Big|y^{n,m}-Y^{(n)}(m\delta t)\Big|\le&L_g\delta t|d^{n,0}|\frac{(1+L_G\delta t)^m-\left(1-\frac{\delta t}{\varepsilon}\right)^m}{L_G\delta t+\frac{\delta t}{\varepsilon}}+2C^*m\delta t^2\\
&+2L_gL_fC_g\varepsilon m\delta t\\
\le&L_g\varepsilon|d^{n,0}|(1+2L_Gm\delta t)+2C^*m\delta t^2+2\frac{L_fC_g\varepsilon}{L_f+1}\\
\le&3L_g\varepsilon|d^{n,0}|+2C^*m\delta t^2+2\frac{L_fC_g\varepsilon}{L_f+1}\,,
\end{aligned}
$$

which concludes the proof of the lemma for $0<\delta t<\frac{2\varepsilon}{\lambda+1}$. Analogously for $\frac{2\varepsilon}{\lambda+1}<\delta t<\frac{2\varepsilon}{\lambda}$, Lemma 4.3 is used to estimate (4.16) as

$$
\begin{aligned}
\Big|y^{n,m}-Y^{(n)}(m\delta t)\Big|\le&\delta t\,L_g|d^{n,0}|\sum_{k=0}^{m-1}(1+L_G\delta t)^k\left(1-\frac{\delta t^*}{\varepsilon}\right)^{m-1-k}\\
&+\left[L_gL_fC_g\varepsilon\frac{\delta t^2}{\delta t^*}+C^*\delta t^2\right]\sum_{k=0}^{m-1}(1+L_G\delta t)^k\\
\le&L_g\delta t|d^{n,0}|\frac{(1+L_G\delta t)^m-\left(1-\frac{\delta t^*}{\varepsilon}\right)^m}{L_G\delta t+\frac{\delta t^*}{\varepsilon}}+2C^*m\delta t^2\\
&+2L_gL_fC_g\varepsilon m\frac{\delta t^2}{\delta t^*}\\
\le&3L_g\varepsilon\frac{\delta t}{\delta t^*}|d^{n,0}|+2C^*m\delta t^2+2\frac{L_fC_g\varepsilon}{L_f+1}\frac{\delta t}{\delta t^*}.
\end{aligned}
$$

□

Lemma 4.4 established bounds on the PI approximation of the slow variables and an Euler approximation of the reduced system during the microsteps. We will now establish bounds on the PI approximation of the slow variables and an Euler approximation of the reduced system during one macrostep. In order to do so we introduce the vector field

$$
\tilde{G}(\eta):=\sum_{m=0}^{M}W_mG(\varphi_\eta^m)\,,
\tag{4.17}
$$

with weights W_m given by (3.13) as in PI. We now proceed to bound $|\tilde{g}(x^n,y^n)-\tilde{G}(y^n)|$.

Lemma 4.5. *Assuming (A1)-(A6), the auxiliary vector field $\tilde{G}$ is close to the vector field $\tilde{g}$ of PI, with*

$$|\tilde{g}(x^n,y^n)-\tilde{G}(y^n)|\le\begin{cases} L_g\left(\dfrac{\varepsilon}{t_\Delta}+3L_g(1+L_f)\varepsilon\right)|d^{n,0}| \\ \quad +L_g e^{-\frac{M\delta t}{\varepsilon}}|d^{n,0}|+3L_gL_fC_g\varepsilon, & \text{if } 0<\delta t\le\dfrac{2\varepsilon}{\lambda+1}, \\ \\ L_g\left(\dfrac{\delta t}{\delta t^*}\dfrac{\varepsilon}{t_\Delta}+3\dfrac{\delta t}{\delta t^*}L_g(1+L_f)\varepsilon\right)|d^{n,0}| \\ \quad +L_g e^{-\frac{M\delta t^*}{\varepsilon}}|d^{n,0}|+3\dfrac{\delta t}{\delta t^*}L_gL_fC_g\varepsilon, & \text{if } \dfrac{2\varepsilon}{\lambda+1}<\delta t<\dfrac{2\varepsilon}{\lambda}. \end{cases}$$

Proof. Employing the Lipschitz condition (*A1*) on f and (*A2*) on g, we write

$$\begin{aligned} &|\tilde{g}(x^n,y^n)-\tilde{G}(y^n)| \\ &=\left|\sum_{m=0}^{M}W_m\Big[g(x^{n,m},y^{n,m})-G(\varphi_{y^n}^m)\Big]\right| \\ &\le\sum_{m=0}^{M}W_mL_g\Big[|x^{n,m}-\bar{f}(\varphi_{y^n}^m)|+|y^{n,m}-\varphi_{y^n}^m|\Big] \\ &\le\sum_{m=0}^{M}W_mL_g\Big[|x^{n,m}-\bar{f}(y^{n,m})|+|\bar{f}(y^{n,m})-\bar{f}(\varphi_{y^n}^m)|+|y^{n,m}-\varphi_{y^n}^m|\Big] \\ &\le\sum_{m=0}^{M}W_mL_g\Big[|d^{n,m}|+(1+L_f)|y^{n,m}-\varphi_{y^n}^m|\Big]. \end{aligned} \tag{4.18}$$

Using lemmas 4.3 and 4.4 for the case when $0<\delta t<\frac{2\varepsilon}{\lambda+1}$, we expand

$$\begin{aligned} |\tilde{g}(x^n,y^n)-\tilde{G}(y^n)|\le\sum_{m=0}^{M}W_m\left[L_g\left(1-\frac{\delta t}{\varepsilon}\right)^m|d^{n,0}|\right]+3L_gL_fC_g\varepsilon \\ +3L_g^2(1+L_f)\varepsilon|d^{n,0}|. \end{aligned} \tag{4.19}$$

Inserting the weights W_m (3.13) which characterize PI, and evaluating the geometric series, we obtain

$$\begin{aligned} |\tilde{g}(x^n,y^n)-\tilde{G}(y^n)|\le&\sum_{m=0}^{M-1}\frac{\delta t}{t_\Delta}L_g\left(1-\frac{\delta t}{\varepsilon}\right)^m|d^{n,0}|+\frac{\Delta t}{t_\Delta}L_g\left(1-\frac{\delta t}{\varepsilon}\right)^M|d^{n,0}| \\ &+3L_gL_fC_g\varepsilon+3L_g^2(1+L_f)\varepsilon|d^{n,0}| \\ \le&L_g\left(\frac{\varepsilon}{t_\Delta}+3L_g(1+L_f)\varepsilon+e^{-\frac{M\delta t}{\varepsilon}}\right)|d^{n,0}|+3L_gL_fC_g\varepsilon, \end{aligned}$$

which concludes the proof for that case. Using lemmas 4.3 and 4.4 for $\frac{2\varepsilon}{\lambda+1}<\delta t<\frac{2\varepsilon}{\lambda}$ in (4.18), we obtain analogously

$$|\tilde{g}(x^n,y^n)-\tilde{G}(y^n)|$$

$$\le \sum_{m=0}^{M} W_m \left[L_g \left(1 - \frac{\delta t^*}{\varepsilon}\right)^m |d^{n,0}| \right] + 3\frac{\delta t}{\delta t^*} L_g L_f C_g \varepsilon + 3\frac{\delta t}{\delta t^*} L_g^2 (1+L_f)\varepsilon |d^{n,0}| \tag{4.20}$$

$$\le L_g \left(\frac{\delta t}{\delta t^*}\frac{\varepsilon}{t_\Delta} + 3\frac{\delta t}{\delta t^*} L_g (1+L_f)\varepsilon + e^{-\frac{M\delta t^*}{\varepsilon}} \right) |d^{n,0}| + 3\frac{\delta t}{\delta t^*} L_g L_f C_g \varepsilon.$$

∎

REMARK 4.3. The above estimates (4.19) and (4.20) not only hold for PI, but also for the seamless formulation of HMM, since they are independent of the particular choice for the weights W_m and of the method of reinitialization of the fast variables x^n.

We have established in Lemma 4.5 that the vector field $\tilde{G}$ given by (4.17) is close to the PI approximation $\tilde{g}$ of the slow dynamics over a time step of t_Δ. In the following lemma we demonstrate that $\tilde{G}$ can be used to step forward the reduced slow variables in a macrostep.

LEMMA 4.6. *$\tilde{G}(Y(t^n))$ provides a numerical estimate of the reduced slow vector field with*

$$Y(t^{n+1}) - Y(t^n) = t_\Delta \tilde{G}(Y(t^n)) + \mathcal{O}(t_\Delta^2),$$

where the error term $\mathcal{O}(t_\Delta^2)$ is bounded by $2C^* t_\Delta^2$.

Proof. By Taylor expanding we write

$$Y(t^{n+1}) - Y(t^n) = t_\Delta \tilde{G}(Y(t^n)) + t_\Delta \Big(G(Y(t^n)) - \tilde{G}(Y(t^n)) \Big) + \mathcal{O}(t_\Delta^2),$$

where according to Assumption (*A5*) the $\mathcal{O}(t_\Delta^2)$-term is bounded by $C^\star t_\Delta^2$. We now bound

$$\begin{aligned} \Big| G(Y(t^n)) - \tilde{G}(Y(t^n)) \Big| &= \left| G(Y(t^n)) - \sum_{m=0}^{M} W_m G(\varphi^m_{Y(t^n)}) \right| \\ &\le \sum_{m=0}^{M} W_m L_G \left| Y(t^n) - \varphi^m_{Y(t^n)} \right| \\ &\le L_G C_G t_\Delta, \end{aligned}$$

where $C_G \le C_g$ is the maximum of $|G|$. Noting that $C^* = \sup|\ddot{Y}| = \sup|DG(Y)G(Y)| = L_G C_G$ completes the proof. ∎

Using lemmas 4.3, 4.4, 4.5, and 4.6 we now proceed to bound the discretization error

$$|E_d^n| = |y^n - Y(t^n)|, \tag{4.21}$$

and formulate the following theorem.

THEOREM 4.7. *Given the assumptions (A1)–(A8), there exists a constant C_2 such that on a fixed time interval T, for each $n\Delta t \le T$, the error between the solution of the projective integration scheme and the exact solutions of the reduced system is bounded by*

$$E_d^n \le \begin{cases} C\left(t_\Delta + \varepsilon + \left(\frac{\varepsilon}{t_\Delta} + \varepsilon + e^{-\frac{M\delta t}{\varepsilon}} \right) |d^n| \right), & \text{if } \ 0 < \delta t \le \frac{2\varepsilon}{\lambda+1}, \\ C\frac{\delta t}{\delta t^*}\left(t_\Delta + \varepsilon + \left(\frac{\varepsilon}{t_\Delta} + \varepsilon + e^{-\frac{M\delta t^*}{\varepsilon}} \right) |d^n| \right), & \text{if } \ \frac{2\varepsilon}{\lambda+1} < \delta t < \frac{2\varepsilon}{\lambda}, \end{cases}$$

where $|d^n| := \max_{0\le i\le n-1}|d^{i,0}|$.

REMARK 4.4. The error estimate involves the well known exponential decay of the fast variable towards the approximate center manifold, leading to a loss of memory of the fast initial condition; PI, however, involves an additional error term proportional to the maximal distance of the fast variable to the approximate center manifold which involves no memory loss with $M \to \infty$.

Proof. We estimate the difference $E_d^n = y^n - Y(t^n)$, applying Lemma 4.6, as

$$\begin{aligned} E_d^n - E_d^{n-1} &= y^n - y^{n-1} - \big(Y(t^n) - Y(t^{n-1})\big) \\ &= \tilde{g}(x^{n-1}, y^{n-1})t_\Delta - \tilde{G}\big(Y(t^{n-1})\big)\, t_\Delta + \mathcal{O}(t_\Delta^2) \\ &= \Big(\tilde{G}(y^{n-1}) - \tilde{G}(Y(t^{n-1}))\Big)\, t_\Delta + \Big(\tilde{g}(x^{n-1}, y^{n-1}) - \tilde{G}(y^{n-1})\Big)\, t_\Delta + \mathcal{O}(t_\Delta^2) \\ &= \mathcal{L}_G^{n-1} E_d^{n-1} t_\Delta + \alpha_{n-1} t_\Delta\,. \end{aligned} \tag{4.22}$$

We used the mean value theorem for vector-valued functions to introduce

$$\mathcal{L}_G^n := \int_0^1 \mathrm{D}\tilde{G}\big(Y(t^n) + \theta(y^n - Y(t^n))\big)\, d\theta\,,$$

where $\mathrm{D}\tilde{G}$ is the Jacobian matrix of $\tilde{G}$, and we set

$$\alpha_n := \tilde{g}(x^n, y^n) - \tilde{G}(y^n) + \mathcal{O}(t_\Delta)\,,$$

where according to Lemma 4.6 we have

$$|\alpha_n| \le |\tilde{g}(x^n, y^n) - \tilde{G}(y^n)| + 2C^* t_\Delta\,. \tag{4.23}$$

Taking absolute values we obtain

$$|E_d^n| \le \big(1 + t_\Delta ||\mathcal{L}_G^{n-1}||\big)\left|E_d^{n-1}\right| + |\alpha_{n-1}| t_\Delta\,.$$

Employing Assumption (*A4*) on the boundedness of g, we define

$$\hat{\alpha} = \max_{0\le i\le n-1} |\alpha_i|\,,$$

and using (*A5*) on the boundedness of G it is easy to show that

$$L_G = \max_{0\le i\le n-1} ||\mathcal{L}_G^i||.$$

We obtain, evaluating the geometric series,

$$\begin{aligned} |E_d^n| &\le (1 + t_\Delta L_G)^n \left|E_d^0\right| + \hat{\alpha} t_\Delta \sum_{m=0}^{n-1} (1 + t_\Delta L_G)^m \\ &\le \frac{\hat{\alpha}}{L_G} e^{n t_\Delta L_G}, \end{aligned} \tag{4.24}$$

where we used that at $n=0$ we initialize with $E_d^0 = 0$. Recalling the bound (4.23) for $|\alpha_n|$ and employing Lemma 4.5 for $0 < \delta t < \frac{2\varepsilon}{\lambda+1}$ we obtain for the bound of the discretization error

$$|E_d^n| \le \frac{e^{n t_\Delta L_G}}{L_G} \left\{ 2C^* t_\Delta + L_g \left(\frac{\varepsilon}{t_\Delta} + 3L_g(1 + L_f)\varepsilon + e^{-\frac{M\delta t}{\varepsilon}} \right) |d^n| + 3L_g L_f C_g \varepsilon \right\}. \tag{4.25}$$

Employing Lemma 4.5 for $\frac{2\varepsilon}{\lambda+1}<\delta t<\frac{2\varepsilon}{\lambda}$ we analogously obtain

$$|E_d^n|\leq\frac{e^{nt_\Delta L_G}}{L_G}\left\{2C^*t_\Delta+L_g\left(\frac{\delta t}{\delta t^*}\frac{\varepsilon}{t_\Delta}+3\frac{\delta t}{\delta t^*}L_g(1+L_f)\varepsilon+e^{-\frac{M\delta t^*}{\varepsilon}}\right)|d^n|\right.$$
$$\left.+3\frac{\delta t}{\delta t^*}L_gL_fC_g\varepsilon\right\}. \tag{4.26}$$

Theorem 4.7 follows realizing $\delta t^\star<\delta t$ for $\delta t>2\varepsilon/(\lambda+1)$. ∎

Besides the parameters used in the numerical scheme, i.e. the macrostep size Δt, the number of microsteps M with microstep size δt, and the time scale parameter ε, the error bound also involves the maximal deviation $|d^n|$ of the fast variables to the approximate center manifold.
The bound on $|d^n|$ is established in the following Lemma.

LEMMA 4.8. *Assuming (A1), (A4), (A6), and (A8), the maximal deviation of the fast variables from the approximate center manifold over n macrosteps* $|d^n|=\max_{0\leq i\leq n-1}|d^{n,0}|$ *satisfies*

$$|d^n|\leq\begin{cases}\left|d^{0,0}\right|+\dfrac{\varepsilon L_fC_g(1+\lambda)\Delta t}{\varepsilon-\Delta t\lambda e^{-\frac{M\delta t}{\varepsilon}}}, & \text{if } \ 0<\delta t\leq\dfrac{2\varepsilon}{\lambda+1},\\ \left|d^{0,0}\right|+\dfrac{\varepsilon L_fC_g\left(1+\lambda\frac{\delta t}{\delta t^*}\right)\Delta t}{\varepsilon-\Delta t\lambda e^{-\frac{M\delta t^*}{\varepsilon}}}, & \text{if } \ \dfrac{2\varepsilon}{\lambda+1}<\delta t<\dfrac{2\varepsilon}{\lambda}.\end{cases}$$

Proof. We bound for $0\leq i\leq n$

$$\begin{aligned}|d^{i,0}|&=|x^i-\bar f(y^i)|\\&=\left|x^{i-1,M}-\frac{\Delta t}{\varepsilon}\left(\Lambda x^{i-1,M}-f(y^{i-1,M})\right)-\bar f(y^i)\right|\\&\leq\Delta t\frac{\lambda}{\varepsilon}\left|d^{i-1,M}\right|+\left|\bar f(y^{i-1,M})-\bar f(y^i)\right|,\end{aligned}$$

where we have used Assumption (*A6*) to simplify

$$\left|\Delta t\frac{\Lambda}{\varepsilon}-\mathbb{I}\right|=\Delta t\frac{\lambda}{\varepsilon}-1<\Delta t\frac{\lambda}{\varepsilon}.$$

Employing Lemma 4.3 for $0<\delta t<\frac{2\varepsilon}{\lambda+1}$, and assumptions (*A1*) and (*A4*), we obtain

$$\begin{aligned}|d^{i,0}|&\leq\Delta t\frac{\lambda}{\varepsilon}\left|d^{i-1,M}\right|+L_f\left|y^{i-1,M}-y^i\right|\\&\leq\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t}{\varepsilon}}\left|d^{i-1,0}\right|+L_fC_g(1+\lambda)\Delta t.\end{aligned} \tag{4.27}$$

Evaluating this recursive relationship yields

$$\begin{aligned}|d^{i,0}|&\leq\left[\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t}{\varepsilon}}\right]^i\left|d^{0,0}\right|+L_fC_g(1+\lambda)\Delta t\frac{1-\left[\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t}{\varepsilon}}\right]^i}{1-\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t}{\varepsilon}}}\\&\leq\left|d^{0,0}\right|+\frac{L_fC_g(1+\lambda)\Delta t}{1-\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t}{\varepsilon}}},\end{aligned} \tag{4.28}$$

where we used Assumption $(A8)$ with $0<\delta t<\frac{2\varepsilon}{\lambda+1}$. Using Lemma 4.3 for $\frac{2\varepsilon}{\lambda+1}<\delta t<\frac{2\varepsilon}{\lambda}$ in (4.27), we obtain

$$
\begin{aligned}
|d^{i,0}| &\leq \Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t^*}{\varepsilon}}\left|d^{i-1,0}\right|+L_fC_g\left(1+\lambda\frac{\delta t}{\delta t^*}\right)\Delta t\\
&\leq \left[\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t^\star}{\varepsilon}}\right]^i\left|d^{0,0}\right|+L_fC_g(1+\lambda\frac{\delta t}{\delta t^\star})\Delta t\frac{1-\left[\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t^\star}{\varepsilon}}\right]^i}{1-\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t^\star}{\varepsilon}}}\\
&\leq \left|d^{0,0}\right|+\frac{\varepsilon L_fC_g\left(1+\lambda\frac{\delta t}{\delta t^*}\right)\Delta t}{\varepsilon-\Delta t\lambda e^{-\frac{M\delta t^*}{\varepsilon}}},
\end{aligned}
\tag{4.29}
$$

where we used Assumption $(A8)$ with $\frac{2\varepsilon}{\lambda+1}<\delta t<\frac{2\varepsilon}{\lambda}$. ∎

REMARK 4.5. In the limits of Assumption $(A8)$, $\Delta t\exp\left(-\frac{M\delta t}{\varepsilon}\right)\to\frac{\varepsilon}{\lambda}$ and $\Delta t\exp\left(-\frac{M\delta t^\star}{\varepsilon}\right)\to\frac{\varepsilon}{\lambda}$, the terms $1-\left[\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t}{\varepsilon}}\right]^i$ in (4.28) and $1-\left[\Delta t\frac{\lambda}{\varepsilon}e^{-\frac{M\delta t^\star}{\varepsilon}}\right]^i$ in (4.29), which are neglected in Lemma 4.8, are crucial to obtain finite estimates $|d^n|\leq\left|d^{0,0}\right|+n\Delta tL_fC_g(1+\lambda)$ and $|d^n|\leq\left|d^{0,0}\right|+n\Delta tL_fC_g\left(1+\frac{\delta t}{\delta t^*}\lambda\right)$, respectively.

Theorem 4.1 follows by combining theorems 4.2 and 4.7 with Lemma 4.8, realizing $\delta t^\star<\delta t$ for $\delta t>2\varepsilon/(\lambda+1)$.

5. Numerical confirmation of the error bound $|E_d^n|$

We now illustrate the error bound $|E_d^n|$ of Theorem 4.7, equation (4.25), which we recall here including the constants as obtained in the proof:

$$
|E_d^n|\leq 3\frac{e^{nt_\Delta L_G}}{L_G}\left\{C^*t_\Delta+L_g\left(\frac{\varepsilon}{t_\Delta}+L_g(1+L_f)\varepsilon+e^{-\frac{M\delta t}{\varepsilon}}\right)|d^n|+L_gL_fC_g\varepsilon\right\},\tag{5.1}
$$

for $0<\delta t<\frac{2\varepsilon}{\lambda+1}$, and

$$
|E_d^n|\leq 3\frac{e^{nt_\Delta L_G}}{L_G}\frac{\delta t}{\delta t^*}\left\{C^*t_\Delta+L_g\left(\frac{\varepsilon}{t_\Delta}+L_g(1+L_f)\varepsilon+e^{-\frac{M\delta t^*}{\varepsilon}}\right)|d^n|+L_gL_fC_g\varepsilon\right\},\tag{5.2}
$$

for $\frac{2\varepsilon}{\lambda+1}<\delta t<\frac{2\varepsilon}{\lambda}$.

We demonstrate the scaling of $|E_d^n|$ with respect to the macrostep size Δt, the timescale parameter ε, and the reinitialization error of the fast variable $|d^n|$ for fixed final time $T=nt_\Delta$. Note that the dependencies of ε and Δt are complicated through the dependency of $|d^n|$ on those parameters. We show results for simulations using the following multiscale system:

$$
\dot{y_\varepsilon}=-x_\varepsilon y_\varepsilon-ay_\varepsilon^2,\tag{5.3}
$$

$$
\dot{x_\varepsilon}=\frac{-x_\varepsilon+\sin^2(by_\varepsilon)}{\varepsilon},\tag{5.4}
$$

which has, at lowest order in ε, the slow limit system

$$
\dot{Y}=-Y\sin^2(bY)-aY^2.\tag{5.5}
$$

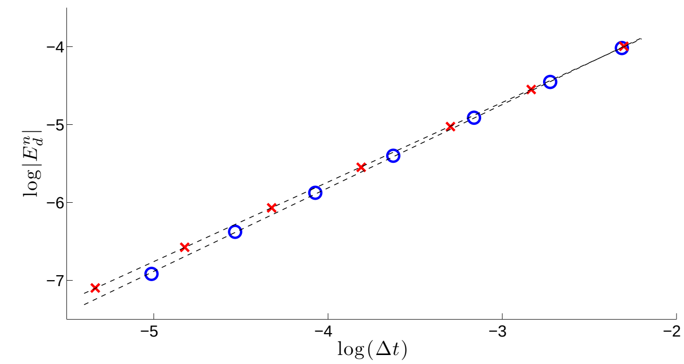

Fig. 5.1: *Plot of* $\log|E_d^n|$ *versus* $\log\Delta t$ *for fixed time of integration* $T=1$*. The dots represent results from numerical PI simulations of the system* (5.3)-(5.4)*, with the crosses representing results from a system with* $\delta t=0.1\varepsilon$ *and the circles representing a system with* $\delta t=1.6\varepsilon$*. The dashed lines are linear regression lines with a slopes of* 1.02 *and* 1.07*, respectively.*

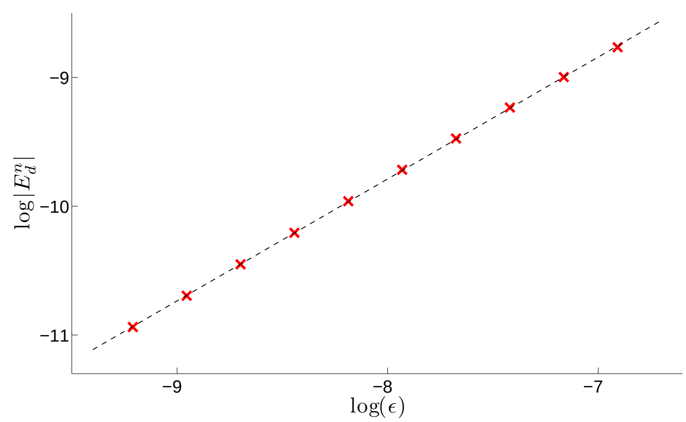

Fig. 5.2: *Plot of* $\log|E_d^n|$ *versus* $\log\varepsilon$*. The dots represent results from numerical PI simulations of the system* (5.3)-(5.4)*. The line is a linear regression with a slope of* 0.947*.*

For higher order approximations of the center manifold and the associated coordinate transformations relating y and Y the reader is referred to the very useful webpage [21] (see also [20]).

The system (5.3)-(5.4) with initial condition $y_\varepsilon(0)>0$ is locally Lipschitz with Lipschitz constant $L_f\le b$ and $L_g=\max(|x_\varepsilon|+2a|y_\varepsilon|)$, where the maximum is taken over the local region around the fixed point at $(x_\varepsilon,y_\varepsilon)=(0,0)$ under consideration. The vector field of the slow dynamics (5.3) is locally bounded by $C_g=\max(|x_\varepsilon y_\varepsilon|+a|y_\varepsilon|^2)$, with the maximum taken over the same region. The free parameters a and b are used to control the Lipschitz constants L_f and L_g. Here $\lambda=1$, implying $\frac{2\varepsilon}{\lambda+1}=\varepsilon$. Therefore (5.1) holds for $0<\delta t<\varepsilon$ and (5.2) holds for $\varepsilon<\delta t<2\varepsilon$.

We first investigate how $|E_d^n|$ scales with the macrostep Δt. We ensure that the term proportional to C^*t_Δ is the dominant term in (5.1) by initializing the fast

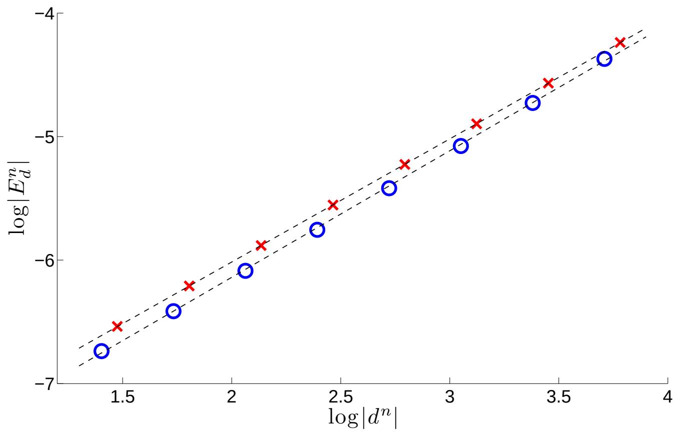

Fig. 5.3: *Plot of* $\log|E_d^n|$ *versus* $\log|d^n|$. *The dots represent results from numerical PI simulations of the system* (5.3)-(5.4). *The crosses are results from simulations with* $\delta t = 0.01\varepsilon$ *and the circles are results from simulations with* $\delta t = 1.99\varepsilon$. *The dashed lines are linear regression lines with a slope of* 1.00 *and* 1.03*, respectively.*

variables on the approximate slow manifold with $|d^{0,0}| = 0$. Figure 5.1 illustrates the linear scaling of $|E_d^n|$ with Δt. System parameters are $a = 1$, $b = 0.1$. The scale separation parameter is $\varepsilon = 10^{-5}$. We used $M = 90$ microsteps with microstep size $\delta t = 0.1\varepsilon$ and $\delta t = 1.6\varepsilon$. The number of iterations n varied from 48 to 918 to keep $T = nt_\Delta = 1$ fixed for all values of Δt. Initial conditions are chosen to lie on the approximate slow center manifold with $y^0 = 1$, $x^0 = \sin^2(0.1)$. The Lipschitz constants are $L_g = 2$ and $L_f = 0.2$, the bound on the vector field of the slow dynamics is $C_g = 1$, and the maximal second derivative of the reduced slow dynamics is $C^* = 2$.

We now present results for the scaling of $|E_d^n|$ with the time scale parameter ε. To focus on the linear scaling suggested by the term $L_g L_f C_g \varepsilon$ in (5.1), we will have to control the term proportional to $|d^n|$ and the $C^* t_\Delta$ term. The $|d^n|$-term is controlled by setting initial conditions on the center manifold and employing $M \gg 1$, allowing for relaxation to the center manifold. The $C^* t_\Delta$ term we control by choosing $t_\Delta < \varepsilon$, violating Assumption (A6) (note that this implies $\delta t < \varepsilon$). System parameters are $a = 0.1$, $b = 1$. Initial conditions are $y^0 = 5$, $x^0 = \sin^2(5)$, i.e. $|d^{0,0}| = 0$. We used $M = 100$ microsteps with microstep size $\delta t = 10^{-6}$, macrostep size $\Delta t = 10^{-4}$, for $n = 50$ iterations of PI with $T = 0.01$. The Lipschitz constant for the slow dynamics is $L_g = 2$ and for the center manifold is $L_f = 1$, the bound on the vector field of the slow dynamics is $C_g = 7$, and the maximal second derivative of the reduced slow dynamics is $C^* = 6$. Figure 5.2 illustrates the linear dependence of $|E_d^n|$ on ε in this situation.

We now illustrate the linear scaling of $|E_d^n|$ with the maximal distance $|d^n|$ of the fast variable from the approximate center manifold after a macrostep. To ensure that the error is not dominated by the initial initialization error $|d^{0,0}|$, we choose parameters which render the scheme unstable and violate Assumption (*A8*), allowing for divergence of the fast variables from the center manifold over the macrosteps, i.e. $|d^{n,0}| > |d^{0,0}|$. Figure 5.3 shows clearly the linear dependence of $|E_d^n|$ on $|d^n|$. System parameters are $a = 1$, $b = 1$. Initial conditions are $y^0 = 1$, $x^0 \in [\sin^2(1) + 0.01, \sin^2(1) + 0.5]$. The scale separation is $\varepsilon = 10^{-4}$. We used $M = 100$ microsteps with microstep size $\delta t=0.01\varepsilon$ and $\delta t=1.99\varepsilon$, and $n=5$ macrosteps with macrostep size $\Delta t=10^{-3}$, implying $T=0.0055$ or $T=0.1$. The Lipschitz constants are $L_g=1$ and $L_f=1$, the bound on the vector field of the slow dynamics is $C_g=290$, and the maximal second derivative of the reduced slow dynamics is $C^*=6$.

6. Discussion

We have established bounds on the error of a numerical approximation of the solution of a multiscale system by Projective Integration. The error contains terms stemming from the inherent error made by reducing the full dynamics on the center manifold as well as errors specific to the numerical discretization. In particular, the order of the numerical scheme features, as well as errors due to inaccurately approximating the dynamics on the center manifold. Although the constants involved in our error estimates are not optimal, the numerical simulations suggest that the scaling obtained is correct.

In future work it is planned to use the analytical results obtained here as well as a trivial extension of our results to seamless HMM and the results obtained for the non-seamless version of HMM (see [2]) to shed light on the important question in what circumstances one method or the other may lead to better performance. These methods exhibit different error bounds due to their different weights as well as due to differing reinitialization procedures for the fast variables.

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