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On convergence of higher order schemes for the projective integration method for stiff ordinary differential equations

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ABSTRACT

We present a convergence proof for higher order implementations of the projective integration method (PI) for a class of deterministic multi-scale systems in which fast variables quickly settle on a slow manifold. The error is shown to contain contributions associated with the length of the microsolver, the numerical accuracy of the macrosolver and the distance from the slow manifold caused by the combined effect of micro- and macrosolvers, respectively. We also provide stability conditions for the PI methods under which the fast variables will not diverge from the slow manifold. We corroborate our results by numerical simulations.

1. Introduction

Many problems in the natural sciences are modelled by multidimensional ordinary differential equations with entangled processes running on widely separated time scales. One is often interested in resolving the behaviour of the slow processes over a long, macro time scale. However, the fast processes prevent direct solution of the system by traditional numerical methods. Recently two numerical methods designed to overcome the restriction to the small integration time step in these stiff dynamical systems have been much studied; the *projective integration method* within the equation-free framework and the *heterogeneous multiscale methods* (HMM). Each method exists in multiple formulations; in the PI method, we mention [1–8], and in the HMM, [9–15]. There is some debate on the similarities and differences between the methods; the interested reader is referred to [16,17] for a discussion.

Both methods assume that the fast variables in the full multiscale system quickly relax to a slow manifold, after which the dynamics of the slow variables is governed by a slow reduced system. Both methods estimate the effective influence of the fast variables on the dynamics of the slow variables by employing a *microsolver* to perform short fine-scale computations with small time steps (microsteps). This information is used to propagate the dynamics on the slow manifold for large time steps (macrosteps) in the *macrosolver*.

The philosophy behind each method is slightly different. The PI approach estimates the effective slow vector field via direct numerical evaluation, not assuming any knowledge on the form of the reduced vector field; this forms part of the equation-free approach. In contrast, the HMM philosophy utilises a priori analytical knowledge about the reduced vector field.

In this paper, we focus on numerical methods that are *seamless*; that is, the numerical methods do not explicitly separate the slow variables and the fast variables at any stage in the solver, but instead propagate all variables simultaneously. These

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methods are useful in systems where conceptually there exists a decomposition or transformation of the system into slow and fast variables, but where this transformation is unknown. The added complication of seamless numerical methods is that the fast variables are propagated simultaneously with the slow variables with the large time step of the macrosolver. This may lead to a more severe departure of the fast variables from the slow manifold over the macrosteps in comparison to nonseamless methods.

In first order PI methods the micro- and macrosolver are applied sequentially, so the error accrued by the micro- and macrosolver can be analysed separately, as for example in [11,18]. There are two different approaches to extend PI to higher order solvers. First, one can still apply the micro- and macrosolver sequentially, as in [19,12,5,20]. The analysis in [12,20] shows that such schemes can be accurate to second order in the size of the macrosolver. Alternatively, one can apply the microsolver multiple times during each time step of the macrosolver, as in [11,4,21]. The numerical schemes that we will consider take this approach. The analysis of such methods is complicated by the requirement that the errors accrued by the micro- and macrosolvers, which are intertwined due to the nonlinear nature of the dynamics, have to be estimated simultaneously. In [11], an error bound is proposed for a seamless HMM scheme of arbitrary order, albeit without proof. In [4,5,20], second order PI schemes are proposed and analysed. In [21], error bounds for the slow variables and stability conditions are derived for an arbitrary order Runge–Kutta macrosolver applied to a kinetic equation with linear relaxation.

In this paper we present a higher order seamless multiscale method as considered in [11,4], for a system of nonlinear stiff ordinary differential equations. We propose a slight modification of this method which, involving an additional application of the microsolver, constructs slow vector fields pointing towards the slow manifold. Both schemes reduce to Runge–Kutta methods if the microsolver is switched off. We establish rigorous convergence results for the slow variables of these methods. We find that both methods incur error terms proportional to the order of the macrosolver, the distance of the fast variables from the slow manifold, and an additional term due to the microsolver, independent of the order of the microsolver. This result confirms for the two methods we consider the error bound suggested in [11]. Furthermore, we find that the error due to the microsolver is smaller in our proposed method when both methods are employed at the same computational cost.

A known problem in seamless methods is that the macrosolver may lead to a departure of the fast variables from the slow manifold. To combat this divergence of the fast variables, several methods have been introduced [22–25]; analytical bounds on the departure of the fast variables from the slow manifold over a macrostep have received relatively little attention (with the notable exception of [12]). Estimates of the maximal deviation of the fast variables from the slow manifold are particularly important when bifurcations occur or when the dynamics transits to different solution branches (e.g. [19,1,7,26]); if the departure from the slow manifold is too large, the transitions may be premature.

We establish bounds on the departure of the fast variables from the slow manifold over the macrosolver. The bounds show that the numerically induced departure of the fast variables from the slow manifold scales one order better in the macrostep size in our modified version of PI. Furthermore, these bounds allow us to derive stability conditions for both methods under which the departure of the fast variables from the slow manifold remains finite over the macrosteps.

The paper is organised as follows. In Section 2 we discuss the class of dynamical systems studied, and briefly summarise in Section 3 classic Runge–Kutta methods for these systems. We then present two multiscale methods which enable the solution of these systems with macro length time steps in Section 4. In Section 5, the main part of this work, we derive rigorous error bounds for those numerical multiscale methods. In Section 6 we present results from numerical simulations corroborating our analytical findings. We conclude with a discussion in Section 7.

2. Model

We consider deterministic multiscale systems of the form

$$\dot{z}_\varepsilon = \mathcal{F}(z_\varepsilon, \varepsilon), \tag{2.1}$$

with $z_\varepsilon \in \mathbb{R}^{n+m}$ and time scale separation parameter $0 < \varepsilon \ll 1$. We assume there is a (possibly unknown) decomposition $z_\varepsilon = (x_\varepsilon, y_\varepsilon)$ into fast variables $x_\varepsilon \in \mathbb{R}^m$ and slow variables $y_\varepsilon \in \mathbb{R}^n$ which evolve according to

$$\dot{y}_\varepsilon = g(x_\varepsilon, y_\varepsilon), \tag{2.2}$$

$$\dot{x}_\varepsilon = \frac{1}{\varepsilon} f(x_\varepsilon, y_\varepsilon). \tag{2.3}$$

We consider here the particular fast vector fields of the form

$$f(x_\varepsilon, y_\varepsilon) = \frac{\Lambda}{\varepsilon}(-x_\varepsilon + h_0(y_\varepsilon)). \tag{2.4}$$

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 allow for a scaling of time such that $\min(\lambda_{ii}) = 1$ and define $\max(\lambda_{ii}) = \lambda$. We assume that there exists a slow manifold $x = h_\varepsilon(y) = h_0(y) + \mathcal{O}(\varepsilon)$, towards which initial conditions are attracted exponentially fast. On the slow manifold, the dynamics slows down and is approximately determined by

$$\dot{Y} = G(Y), \tag{2.5}$$