

ANALYSIS OF THE HETEROGENEOUS MULTISCALE METHOD FOR ORDINARY DIFFERENTIAL EQUATIONS*

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1. Introduction

This paper is concerned with the analysis of a new class of efficient numerical methods for systems of ordinary differential equations (ODEs) with disparate time scales. We will be interested in stiff ODEs of the type that arise in chemical kinetics, for example:

$$\begin{cases} \dot{x} = -\frac{1}{\varepsilon}(x - f(y)) \\ \dot{y} = g(x, y) \end{cases} \quad (1.1)$$

as well as oscillatory systems of the type that arise in molecular dynamics and celestial mechanics, a simple example being the system

$$\begin{cases} \dot{\varphi} = \frac{1}{\varepsilon}\omega(I) + f(\varphi, I, \varepsilon) \\ \dot{I} = g(\varphi, I, \varepsilon) \end{cases} \quad (1.2)$$

studied in averaging methods [1]. Here f and g are assumed to be periodic in φ and bounded as $\varepsilon \rightarrow 0$. In the standard terminology of multiscale analysis, we would call x and φ the fast variables of these systems, y and I the slow variables. But we also have a particular interest on systems for which the fast and slow variables exist but cannot be explicitly identified beforehand.

At the present time, there does not exist a unified strategy for dealing with both problems of type (1.1) and (1.2). There is, however, a large literature on stiff systems of the type (1.1) and oscillatory systems of the type (1.2) separately. Starting from the pioneering work of Dahlquist and Gear [5], there has been extensive work on designing efficient numerical methods for stiff ODEs [7], such as the backward differentiation formula, implicit Runge-Kutta methods [5], extrapolation methods and Rosenbrock methods [7, 8, 6]. There is also extensive work on oscillatory systems, some of which are analytical [1], and some are numerical [9].

We will apply the framework of the heterogeneous multiscale method (HMM) [3], which is a general methodology for problems with multiscales. In the case of two scales, a macroscale and a microscale, HMM consists of two components: selection of a conventional macroscale solver, here a standard ODE solver, and estimating the effective forces used in the macroscale solver by performing numerical experiments using the microscale model and processing the data obtained. The procedure can be iterated if the system has more than two separated scales.

There are a number of related numerical methods for systems with multiple time scales, in particular for stiff ODEs. Even though the most popular numerical methods for stiff ODEs stem from implicit methods such as the backward differentiation formula, a number of explicit methods have also been proposed [8, 2, 7]. In the simplest version, these methods are Runge-Kutta in nature, each stage of which is a forward

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