

Computing Singularly Perturbed Differential Equations

Sabyasachi Chatterjee*

Amit Acharya*

Zvi Artstein†

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Abstract

A computational tool for coarse-graining nonlinear systems of ordinary differential equations in time is discussed. Three illustrative model examples are worked out that demonstrate the range of capability of the method. This includes the averaging of Hamiltonian as well as dissipative microscopic dynamics whose ‘slow’ variables, defined in a precise sense, can often display mixed slow-fast response as in relaxation oscillations, and dependence on initial conditions of the fast variables. Also covered is the case where the quasi-static assumption in solid mechanics is violated. The computational tool is demonstrated to capture all of these behaviors in an accurate and robust manner, with significant savings in time. A practically useful strategy for initializing short bursts of microscopic runs for the accurate computation of the evolution of slow variables is also developed.

1 Introduction

This paper is concerned with a computational tool for understanding the behavior of systems of evolution, governed by (nonlinear) ordinary differential equations, on a time scale that is much slower than the time scales of the intrinsic dynamics. A paradigmatic example is a molecular dynamic assembly under loads, where the characteristic time of the applied loading is very much larger than the period of atomic vibrations. We examine appropriate theory for such applications and devise a computational algorithm. The singular perturbation problems we address contain a small parameter ϵ that reflects the ratio between the slow and the fast time scales. In many cases, the solutions of the problem obtained by setting the small parameter to zero matches solutions to the full problem with small ϵ , except in a small region - a boundary/initial layer. But, there are situations, where the limit of solutions of the original problem as ϵ tends to zero does not match the solution of the problem obtained by setting the small parameter to zero. Our paper covers this aspect as well. In the next section we present the framework of the present study, and its sources. Before displaying our algorithm

*Dept. of Civil & Environmental Engineering, Carnegie Mellon University, Pittsburgh, PA 15215. sabyasac@andrew.cmu.edu (S. Chatterjee), acharyasamit@cmu.edu (A. Acharya).

†Dept. of Mathematics, The Weizmann Institute of Science, Rehovot, Israel, 7610001. zvi.artstein@weizmann.ac.il.

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Evgeniĭ Frolovich Mishchenko



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