

Computing Singularly Perturbed Differential Equations

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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

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Roman Wölfel



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Table of Contents Singularly Perturbed Differential Equations

1. Understanding the eBook Singularly Perturbed Differential Equations
 - The Rise of Digital Reading Singularly Perturbed Differential Equations
 - Advantages of eBooks Over Traditional Books
2. Identifying Singularly Perturbed Differential Equations
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Singularly Perturbed Differential Equations
 - User-Friendly Interface
4. Exploring eBook Recommendations from Singularly Perturbed Differential Equations
 - Personalized Recommendations
 - Singularly Perturbed Differential Equations User Reviews and Ratings
 - Singularly Perturbed Differential Equations and Bestseller Lists
5. Accessing Singularly Perturbed Differential Equations Free and Paid eBooks
 - Singularly Perturbed Differential Equations Public Domain eBooks
 - Singularly Perturbed Differential Equations eBook Subscription Services
 - Singularly Perturbed Differential Equations Budget-Friendly Options
6. Navigating Singularly Perturbed Differential Equations eBook Formats

- ePub, PDF, MOBI, and More
- Singularly Perturbed Differential Equati Compatibility with Devices
- Singularly Perturbed Differential Equati Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Singularly Perturbed Differential Equati
 - Highlighting and Note-Taking Singularly Perturbed Differential Equati
 - Interactive Elements Singularly Perturbed Differential Equati
- 8. Staying Engaged with Singularly Perturbed Differential Equati
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Singularly Perturbed Differential Equati
- 9. Balancing eBooks and Physical Books Singularly Perturbed Differential Equati
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Singularly Perturbed Differential Equati
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Singularly Perturbed Differential Equati
 - Setting Reading Goals Singularly Perturbed Differential Equati
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Singularly Perturbed Differential Equati
 - Fact-Checking eBook Content of Singularly Perturbed Differential Equati
 - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
- 14. Embracing eBook Trends
 - Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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