This is a review text file submitted electronically to MR.

Reviewer: Werner M. Seiler

Reviewer number: 022262

Address:
Interdisziplinäres Zentrum für Wissenschaftliches Rechnen,
Universität Heidelberg,
69120 Heidelberg, Germany

Author: B. Leimkuhler, S. Reich

Short title: Simulating Hamiltonian Dynamics

Control number: 2132573

Primary classification: 37M15

Secondary classification(s): 65P10, 70-08

Review text:

The topic of geometric integrators, i.e., numerical methods for differential equations that preserve important qualitative features of the system, has attracted much interest in recent years. The first class of systems for which such methods were derived are Hamiltonian systems. Here symplectic integrators preserve the symplectic structure of the phase space and are known to possess superior stability properties, in particular for long time computations. This makes them very popular for applications in celestial mechanics and molecular dynamics.

The book is intended as an introduction to theory and application of symplectic integrators and written for a broad interdisciplinary audience. The only assumption is that the reader has a basic knowledge of linear algebra and ordinary differential equations. However, a reader without the necessary background in Hamiltonian mechanics or numerical analysis should also refer to some more specialised textbooks on the side (the authors give a number of recommendations).

The book consists of 12 chapters. After a short introduction, the second chapter reviews the basic numerical analysis of ordinary differential equations. The third chapter contains a survey of Hamiltonian mechanics mainly using classical coordinate language; differential forms are only briefly introduced and without any differential geometry. The main topic of the book, symplectic integrators, appears first in the fourth chapter. Already here, special emphasis is put on Hamiltonian splitting as a tool for the design to such methods.

Modified equations are used in Chapter 5 for a theoretical explanation of the stability properties of geometric integrators. The sixth chapter takes up again the idea of Hamiltonian splitting for the construction of higher order methods. It also briefly mentions the historically important approach via generating functions. In the seventh chapter the extension of symplectic integrators to constrained mechanical systems is studied. Here it is a bit surprising that the Dirac theory is hardly mentioned (the Dirac bracket not at all). As an important application the eighth chapter treats the rigid body as a constrained system. Instead of using a minimal set of coordinates like Euler angles with their well-known singularities, the rigid body is described with orthogonal matrices and the orthogonality condition leads to constraints. The rigid body is also a classical example of a system with a non-canonical symplectic structure.

It is well-known that symplectic integrators loose their favourable properties, when they are applied with variable step sizes. The ninth chapter studies how this problem can be partially circumvented using Sundman and Poincaré transformations. In the tenth chapter a number of approaches to deal with highly oscillatory problems are discussed; this includes in particular averaging and mollifying. A typical source for such problems is molecular dynamics to which the eleventh chapter is devoted with the main emphasis on modelling issues. The last chapter extends the method of symplectic integrators to Hamiltonian partial differential equations and culminates in the study of multi-symplectic discretisations.

Theoretical analysis and the discussion of concrete applications are well balanced throughout the text. Many references for further study are given. Each chapter closes with a set of exercises; some of the larger one may be considered as projects. The book should serve well as a text for an introductory course in computational Hamiltonian mechanics or as a reference for researchers intending to apply symplectic integrators.