Cambridge University Press
0521019168 - Many-Body Tree Methods in Physics
Susanne Pfalzner and Paul Gibbon
Frontmatter
More information

Studying the dynamics of a large number of particles interacting through long-range forces, commonly referred to as the N-body problem, is a central aspect of many different branches of physics. In recent years, significant advances have been made in the development of fast N-body algorithms to deal efficiently with such complex problems. This book is the first to give a thorough introduction to these so-called tree methods, setting out the basic principles and giving practical examples of their use.

After a description of the key features of the hierarchical tree method, a variety of general N-body techniques are presented. Open boundary problems are then discussed, as well as the optimization of tree codes, periodic boundary problems, and the fast multipole method.

No prior specialist knowledge is assumed, and the techniques are illustrated throughout with reference to a broad range of applications. The book will be of great interest to graduate students and researchers working on the modeling of systems in astrophysics, plasma physics, nuclear and particle physics, condensed-matter physics, and materials science.

MANY-BODY TREE METHODS IN PHYSICS

MANY-BODY TREE METHODS IN PHYSICS

SUSANNE PFALZNER
Max-Planck-Research Unit
"Dust in Starforming Regions,"
University of Jena

PAUL GIBBON
Max-Planck-Research Unit
"X-Ray Optics,"
University of Jena

CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, São Paulo

Cambridge University Press
The Edinburgh Building, Cambridge CB2 2RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9780521495646

First published 1996
This digitally printed first paperback version 2005

A catalogue record for this publication is available from the British Library

Library of Congress Cataloguing in Publication data
Pfalzner, Susanne.
Many-body tree methods in physics / Susanne Pfalzner, Paul Gibbon.
p. cm.
Includes bibliographical references and index.
ISBN 0-521-49564-4 (hardcover)
1. Many-body problem. 2. Algorithms. 3. Mathematical physics.
I. Gibbon, Paul. II. Title
QC174.17.P7P44 1996 95-36237
530.1′44 – dc20 CIP

ISBN-13 978-0-521-49564-6 hardback
ISBN-10 0-521-49564-4 hardback

ISBN-13 978-0-521-01916-3 paperback
ISBN-10 0-521-01916-8 paperback

Cambridge University Press
0521019168 - Many-Body Tree Methods in Physics
Susanne Pfalzner and Paul Gibbon
Frontmatter
More information

To our daughter, Theresa,
and our parents, Helga and Hans and Elin and David

Contents

Preface

The difficulty in writing a 'how-to' book on numerical methods is to find a form which is accessible to people from various scientific backgrounds. When we started this project, hierarchical N-body techniques were deemed to be 'too new' for a book. On the other hand, a few minutes browsing in the References will reveal that the scientific output arising from the original papers of Barnes and Hut (1986) and Greengard and Rohklin (1987) is impressive but largely confined to two or three specialist fields. To us, this suggests that it is about time these techniques became better known in other fields where N-body problems thrive, not least in our own field of computational plasma physics. This book is therefore an attempt to gather everything hierarchical under one roof, and then to indicate how and where tree methods might be used in the reader's own research field. Inevitably, this has resulted in something of a pot-pourri of techniques and applications, but we hope there is enough here to satisfy the beginners and connoisseurs alike.

Errata

1. In the derivation of the tree algorithm scaling starting on p. 20, the inner shell radius r_1 is defined as the radius beyond which particles can be grouped together in clusters. This can begin as soon as the inter-cluster distance θr_1 exceeds the mean particle separation a, i.e.:

$$\theta r_1 > a = n^{-1/3}$$

2. On p. 27, the initial expression for the potential in Cartesian coordinates should read:

$$\Phi_i(\mathbf{R} - \mathbf{r}_i) = -\frac{m_i}{\sqrt{(x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2}}.$$

3. Equation (2.11) for the quadrupole moment of the parent cell on p. 30 should read:

$$\begin{aligned} Q_{xy}^{parent} &= \sum_d \left(\sum_i m_i x_i y_i - x_{sd} \sum_i m_i y_i \right. \\ &\qquad \left. - y_{sd} \sum_i m_i x_i + x_{sd} y_{sd} \sum_i m_i \right) \\ &= \sum_d \left(Q_{xy}^d - x_{sd} D_y^d - y_{sd} D_x^d + x_{sd} y_{sd} M^d \right). \end{aligned}$$

4. The Ewald summation for the potential (5.2) on p. 93 is missing the 'self-energy' correction $\Phi_s = -2\alpha q_i/\pi^{1/2}$. This is needed to cancel an identical, unphysical term contained in the k-space sum Φ_{II}. The latter is also missing a normalisation factor $|\mathbf{h}|^{-\mathbf{2}}$, so that the net potential should actually read:

$$\begin{aligned} \Phi_p &= \Phi_I + \Phi_{II} + \Phi_s \\ &= \sum_{\mathbf{n}} \sum_i q_i \frac{\operatorname{erfc}(\alpha r_{\mathbf{n}i})}{r_{\mathbf{n}i}} \\ &\quad + \frac{1}{\pi L} \sum_i \sum_{\mathbf{h} \neq 0} \frac{q_i}{|\mathbf{h}|^{\mathbf{2}}} \exp\left(\frac{-\pi^2 |\mathbf{h}|^2}{\alpha^2 L^2} \right) \cos(\mathbf{k} \cdot \mathbf{r}_{oi}) - \frac{2\alpha}{\pi^{1/2}} q_i, \end{aligned}$$

where $\mathbf{k} = 2\pi \mathbf{h}/L$.

5. As for the potential above, a factor $|\mathbf{h}|^{-2}$ is missing from the k-space force term F_x^{II} on p. 94, which should read:

$$F_x^{II} = \frac{2}{L^2}\sum_i \sum_{\mathbf{h}\neq 0} \frac{q_i h_x}{|\mathbf{h}|^2} \exp\left(\frac{-\pi^2|\mathbf{h}|^2}{\alpha^2 L^2}\right) \sin\left(\mathbf{k}\cdot\mathbf{r}_{os}\right).$$

6. In the multipole expansion of the Ewald sum (5.5) the term $A(h)$ on p. 98 is also missing this factor, and should read:

$$A(h) = \frac{1}{|\mathbf{h}|^2} \exp\left(\frac{-\pi^2|\mathbf{h}|^2}{\alpha^2 L^2}\right).$$

7. The shifting formulae on p. 99 should correspond to those on p. 30 and p. 31, namely:

$$\sum_i q_i x_i \rightarrow \sum_i q_i x_i - x_{sd}\sum_i q_i$$

$$\sum_i q_i x_i^2 \rightarrow \sum_i q_i x_i^2 - 2x_{sd}\sum_i q_i x_i + x_{sd}^2 \sum_i q_i$$

$$\sum_i q_i x_i y_i \rightarrow \sum_i q_i x_i y_i - x_{sd}\sum_i q_i y_i - y_{sd}\sum_i q_i x_i + x_{sd} y_{sd} \sum_i q_i$$

8. The plasma frequency in (6.2) is normally referred to by the angular frequency ω_p, rather than the inverse period $\nu_p \equiv \tau_p^{-1}$, and is defined (in c.g.s. units) by:

$$\omega_p = \left(\frac{4\pi n_e e^2}{m_e}\right)^{1/2}.$$