<<分子模拟入门>>

图书基本信息

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前言

Why did we write a second edition ?
A minor revision of the first editionwould have been adequate to correct the （admittedly many）typographicalmistakes. However, many of the nice comments that we received from stu-dents and colleagues alike, ended with a remark of the type: "unfortunately,you don't discuss topic x". And indeed, we feel that, after only five years,the simulation world has changed so much that the title of the book was nolonger covered by the contents.The first edition was written in 1995 and since then several new tech-niques have appeared or matured. Most （but not all） of the major changesin the second edition deal with these new developments. In particular, wehave included a section on.

内容概要

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章节摘录

插图：It is difficult to talk about Monte Carlo or Molecular Dynamics programs inabstract terms. The best way to explain how such programs work is to writethem down. This will be done in the present section.Most Monte Carlo or Molecular Dynamics programs are only a few hun- dred to several thousand lines long. This is very short compared to, forinstance, a typical quantum-chemistry code. For this reason, it is not un- common that a simulator will write many different programs that are tailor-made for specific applications. The result is that there is no such thing as a standard Monte Carlo or Molecular Dynamics program. However, the cores of most MD/MC programs are, if not identical, at least very similar. Next,we shall construct such a core. It will be very rudimentary, and efficiency has been traded for clarity. But it should demonstrate how the Monte Carlomethod works.

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