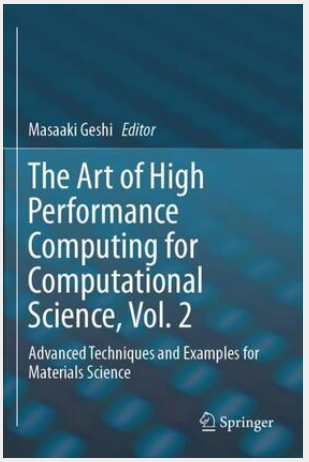
Geshi

The Art of High Performance Computing for Computational Science, Vol. 2

Advanced Techniques and Examples for Materials Science



This book presents advanced and practical techniques for performance optimization for highly parallel processing. Featuring various parallelization techniques in material science, it is a valuable resource for anyone developing software codes for computational sciences such as physics, chemistry, biology, earth sciences, space science, weather, disaster prevention and manufacturing, as well as for anyone using those software codes. Chapter 1 outlines supercomputers and includes a brief explanation of the history of hardware. Chapter 2 presents procedures for performance evaluation, while Chapter 3 describes the set of tuned applications in materials science, nanoscience and nanotechnology, earth science and engineering on the K computer. Introducing the order-N method, based on density functional theory (DFT) calculation, Chapter 4 explains how to extend the applicability of DFT to large-scale systems by reducing the computational complexity. Chapter 5 discusses acceleration and parallelization in classical molecular dynamics simulations, and lastly, Chapter 6 explains techniques for large-scale quantum chemical calculations, including the order-N method. This is the second of the two volumes that grew out of a series of lectures in the K computer project in Japan. The first volume addresses more basic techniques, and this second volume focuses on advanced and concrete techniques.

106,99 €
99,99 € (zzgl. MwSt.)

Lieferfrist: bis zu 10 Tage

Artikelnummer: 9789811398049
Medium: Buch
ISBN: 978-981-13-9804-9
Verlag: Springer Nature Singapore
Erscheinungstermin: 15.10.2020
Sprache(n): Englisch
Auflage: 1. Auflage 2019
Produktform: Kartoniert
Gewicht: 335 g
Seiten: 206
Format (B x H): 155 x 235 mm