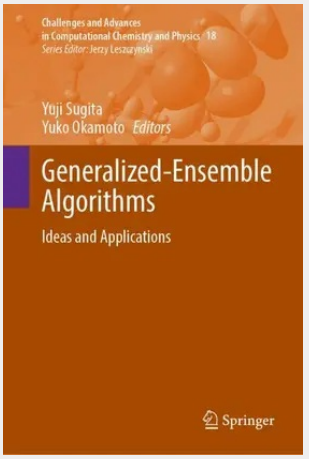
Sugita / Okamoto

Generalized-Ensemble Algorithms

Ideas and Applications



This book presents the generalized-ensemble algorithms, which are powerful algorithms to simulate complex systems and greatly speed up the convergence to thermal equilibrium. By using the algorithms, one can perform random walks of certain physical quantities or their conjugate parameters, which alleviates the difficulty of conventional methods in which simulations tend to get trapped in states of local-minimum free energy states. In this book, one of the most commonly used generalized-ensemble algorithms, namely, replica-exchange method (REM) is explained first. The original version performs a random walk in temperature space. The authors then present various extensions of REM by introducing multidimensional replica-exchange method in which multivariable random walks are realized by further enhancing the configurational sampling. Other generalized-ensemble algorithms are also presented for wide applications to many complex systems. The book explains the basic ideas in detail, and it is not only useful for researchers in academia and industry in the field of computational physics, chemistry, biology, pharmacology, medicine, materials science but also can be used as a textbook for undergraduate and graduate students.

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