

PROCEEDINGS

A High-Efficiency LBM Scheme for High-Throughput Predicting Effective Thermal Conductivity of 3D Complex Multi-Phase Media

Mingshan Yang¹, Xiangyu Li^{1,*}, and Weiqiu Chen²

¹Applied Mechanics and Structure Safety Key Laboratory of Sichuan Province, School of Mechanics and Aerospace Engineering, Southwest Jiaotong University, Chengdu, 610031, China

²School of Aeronautics and Astronautics, Zhejiang University, Hangzhou, 310000, China

*Corresponding Author: Xiangyu Li. Email: lixiangyu@swjtu.edu.cn

ABSTRACT

Lattice Boltzmann method is widely favored for simulating thermal transport in complex multi-phase media due to its straightforward implementation, simple boundary treatment, and inherent parallelism. However, as a kinetic-theory-based numerical approach, LBM often faces slow convergence and numerical instability when solving steady-state problems. These issues become particularly severe in multi-phase media with high thermal conductivity ratios, where millions of iterations may be required for convergence. High-throughput simulations of large-scale 3D representative volume elements (RVEs) are usually computationally prohibitive. This work proposes an efficient and implementation-friendly LB scheme to overcome these limitations. The primary innovation is the identification of an optimum convergence parameter, which enables the LB equation to converge to the steady heat conduction equation at the fastest possible speed without compromising accuracy. Compared to existing LB schemes, the proposed method achieves two to three orders of magnitude higher computational efficiency. In extreme cases, computation tasks that previously required hundreds of hours can now be completed within minutes. This scheme opens a new avenue for high-throughput simulations of 3D RVEs featuring large grid numbers and high thermal conductivity ratios. It may facilitate the application of data-driven techniques in study of thermal transport properties of emerging composite materials and structures [1,2].

KEYWORDS

Lattice Boltzmann method; high-throughput simulations; data-driven study; effective thermal conductivity

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