Research

Colloquium

High-Performance Computing for 3D Maxwell Equations with fourteen Bravais Lattices

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摘　要：

The numerical simulation of the band structure of three-dimensional photonic crystals leads to large-scale generalized eigenvalue problems (GEPs). Due to a high dimensional subspace associated with the eigenvalue zeros, it is very challenging to solve the GEP. In this paper, we focus on developing a high-performance computing method to solve GEP for all fourteen Bravais lattices. For each lattice, we derive the explicit matrix form of the discrete double-curl operator by using Yee's scheme and classify all the matrices into four general types. The eigen-decompositions of these four general matrices are then derived. Based on these eigen-decompositions, the nullspace-free method is applied to exclude the zero eigenvalues from the associated generalized eigenvalue problem. Applying these theoretical results, a high-performance computing package FAME (Fast Algorithm for Maxwell's Equations) with GPU acceleration is proposed to find the target eigenpairs for any lattices. Numerical results illustrate that FAME successfully solves each of a set of 5.184 million dimension eigenvalue problems within 18 to 50 seconds on a workstation with NVIDIA Tesla P100 GPUs.