

Eigenvalue Problems in Nanoscale Material Modeling

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Together with a group of material scientist, we intend to calculate the atomic and electronic structure of nanoparticles on a quantum-mechanical level. The mathematical core of this modeling is a sequence of large and sparse eigenvalue problems. In this talk, I will present the special requirements of the solutions, the challenges on the computational method, and our algorithmic approach and software development. Numerical implementation on the advanced distributed computers will be demonstrated.
