Lothar-Collatz-Seminar

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Scalable Domain Decomposition Eigensolvers for Schrödinger Operators in Anisotropic Structures

Abstract:

This talk presents the construction and analysis of scalable preconditioning strategies for the linear Schroödinger eigenvalue problem with periodic potentials in anisotropic structures. As only some dimensions of the computational domain expand to infinity, the resulting eigenvalue gap between the first and second eigenvalue vanishes, posing a significant challenge for iterative solvers. For these iterative eigenvalue solvers, we provide a quasi-optimal shift-and-invert preconditioning strategy such that the iterative eigenvalue algorithms converge in constant iterations for different domain sizes. In its analysis, we derive an analytic factorization of the eigenpairs and use directional homogenization to analyze the asymptotic behavior. The resulting easy-to-calculated unit cell problem can be used within a shift-and-invert preconditioning strategy. This approach leads to a uniformly bounded number of eigensolver iterations. Numerical examples illustrate the effectiveness of this quasi-optimal preconditioning strategy if direct solvers are used since the shifting strategy, by definition, leads to a smaller eigenvalue for the resulting shifted operator, which, in turn, results in a high condition number.

We also provide a two-level domain decomposition preconditioner for iterative linear solvers to overcome this issue. As the calculation of the quasi-optimal shift already offered the solution to a spectral cell problem as limiting eigenfunction, it is logical to use it as a generator to construct a coarse space. Indeed, it is the case that the resulting two-level additive Schwarz preconditioner is independent of the domain's anisotropy since we obtain a condition number bound using the theory of spectral coarse spaces despite the need for only one basis function per subdomain for the coarse solver. We provide several numerical examples illustrating the effectiveness of both methods separately and combine them in the end to show their combined scalability.

For further information please contact

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www.c3s.uni-hamburg.de/news-events/seminar-c3s.html