Research

Colloquium

Computing the full spectrum of large sparse palindromic quadratic eigenvalue problems arising from nano research

主講人：田恒 博士
國立交通大學應用數學系

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摘　要：

Full spectrum of a large sparse T-palindromic quadratic eigenvalue problem (T-PQEP) is needed in the calculation of surface Green's functions (SGFs) of nano-transistors with a tremendous non-periodic cross-section. For this problem, general purpose eigensolvers are not efficient, nor is advisable to resort to the decimation method etc.to obtain the Wiener–Hopf factorization. After reviewing some rigorous understanding of SGF calculation from the perspective of nonlinear matrix equation, we present our new approach to this problem. In a nutshell, the unit disk where the spectrum of interest lies is broken down adaptively into pieces small enough that they each can be locally tackled by the generalized T-skew-Hamiltonian implicitly restarted shift-and-invert Arnoldi (GTSHIRA) algorithm with suitable shifts and other parameters, and the eigenvalues missed by this divide-and-conquer strategy can be recovered thanks to the accurate estimation provided by our newly developed scheme. Notably the novel non-equivalence deflation is proposed to avoid as much as possible duplication of nearby known eigenvalues when a new shift of GTSHIRA is determined. We demonstrate our new approach by calculating the SGF of a realistic nanowire whose unit cell is described by a matrix of size 4000 by 4000 at the density functional tight binding level, corresponding to an 8 by 8 nm^2 cross-section.