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Numerical solution of nonlinear matrix equations arising from Green's function calculations in nano research

The Green's function approach for treating quantum transport in nano devices requires the solution of nonlinear matrix equations of the form $X + (C^* + i\eta D^*)X^{-1}(C + i\eta D) = R + i\eta P$, where R and P are Hermitian, $P + \lambda D^* + \lambda^{-1} D$ is positive definite for all λ on the unit circle, and $\eta \to 0^+$. For each fixed $\eta > 0$, we show that the required solution is the unique stabilizing solution X_η. Then $X_* = \lim_{\eta \to 0^+} X_\eta$ is a particular weakly stabilizing solution of the matrix equation $X + C^* X^{-1} C = R$. In nano applications, the matrices R and C are dependent on a parameter, which is the system energy $\mathcal{E}$. In practice one is mainly interested in those values of $\mathcal{E}$ for which the equation $X + C^* X^{-1} C = R$ has no stabilizing solutions or, equivalently, the quadratic matrix polynomial $P(\lambda) = \lambda^2 C^* - \lambda R + C$ has eigenvalues on the unit circle. We point out that a doubling algorithm can be used to compute X_η efficiently even for very small values of η, thus providing good approximations to X_*. We also explain how the solution X_* can be computed directly using subspace methods such as the QZ algorithm by determining which unimodular eigenvalues of $P(\lambda)$ should be included in the computation.
(Based on joint work with Yueh-Cheng Kuo and Wen-Wei Lin.)