Generalized Locally Toeplitz Matrix Sequences for Analysing Finite Element Block Matrices

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We consider general block matrices, arising from a finite element (FE) discretization of a system of partial differential equations and the task to precondition those matrices, when solving large scale linear systems. The classical preconditioning methods for block matrices usually require a high quality approximation of a Schur complement matrix, which is in general a rather difficult and very much problem dependent task. Recently, for FE matrices, a technique has been developed, that constructs a high quality sparse approximations of Schur complement matrices, based on element-wise techniques, manipulating small-sized, localy constructed Schur complement matrices. Various studies have shown that the element-wise FE approximation of the Schur complement is very efficient for some problems, such as scalar elliptic problems, linear elasticity problems in standard and mixed FE form, Stokes problem, convection-diffusion problems. The technique has been found less robust for other problems, such as Cahn-Hilliard and Navier-Stokes problems. Using Linear Algebra tools enables us to explain the experimentally observed high qualities of the element-wise Schur complement for the case when the system matrix is symmetric and positive definite as well as when it is symmetric indefinite and its pivot block is positive semi-definite. The available analysis tools, however, are not applicable for general matrices. Therefore, in this work, to get a better insight in the spectral properties of the matrices and the corresponding Schur complements, we apply the so-called Generalized Locally Toeplitz (GLT) framework, in which we construct the so-called *symbol* (or *generating function*) of the matrix, which is an analytical (block-)function with the following property. Asymptotically, a uniform sampling of the symbol gives a very precise idea of the spectrum of the corresponding matrix, up to a few outliers, and in practice the spectral approximation is good already for moderate sizes. The obtained results can be used for constructing efficient preconditioners and for analysing known preconditioning techniques. We illustrate the GLT technique for linear elasticity problems in mixed FEM form.

The Influence of Electrostatic Lenses on Wave Packet Dynamics

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The engineering and control of entangled quantum states within nanometer semiconductor structures is important in the emerging field of quantum computing and also for the experimental study of quantum mechanics.

The evolution of wave packets in a semiconductor can be manipulated using specially shaped potential profiles with convex or concave features, similar to refractive lenses used in optics. Such 'electrostatic lenses' offer the possibility, for instance, to concentrate a single wave packet which has been invoked by a laser pulse, or split it up into several wave packets. Moreover, the shape of the potential profile can be dynamically changed (by an externally applied potential), depending on the desired behavior of the entangled electron state.
We analyze the dynamics of a two-dimensional wave packet interacting with 'electrostatic lenses', by computing distributions of physical quantities using the Wigner function. The latter is obtained from Wigner Monte Carlo simulations employing the signed-particle method, which has made two-dimensional simulations numerically tractable. We explore the regions of interference, which distinguish an entangled state from a mixed state, by checking for the characteristic oscillations in the momentum and density distributions.
Furthermore, we investigate the role of absorbing boundaries, which can cause decoherence due to the loss of quantum information, by comparing the initial state with a time-reversed evolution of the final state – a discrepancy indicates that decoherence mechanisms are present.

A Non-Intrusive Parallel Time Integration Method Based on Multigrid Reduction

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Multigrid methods are important techniques for efficiently solving huge systems and they have already been shown to scale effectively on millions of cores. However, one of the major challenges facing computational science with future architectures is that faster compute speeds will be achieved through greater concurrency (more cores), since clock speeds are no longer increasing. Current petascale computers already have millions of cores, but future exascale machines are expected to have billions. This immense degree of parallelism requires a similar level of concurrency in the algorithms that run on them. One consequence of this is that time integration by traditional time marching will become a sequential bottleneck.
In this talk, we will discuss our efforts to develop multigrid methods for parallel time integration. In most multiphysics codes today, the space-time system is solved by marching from one time step to the next, much as you would in a forward solve for a lower-triangular matrix. This approach is computationally optimal, but sequential. The idea is to instead solve the same space-time system by computing multiple time steps at once in an iterative fashion. If the iterative method is also computationally optimal and exhibits enough concurrency, then additional parallel resources can be used to achieve a speedup. We will describe our new software library XBraid for doing parallel time integration based on multigrid reduction (MGR) techniques and present results for a variety of applications. The advantage of the XBraid approach is that it