Computational material design: Efficient solvers & optimal approximation

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Abstract

The design of new materials to improve existing technologies or enable new applications is a key aspect of research in multiple disciplines, including materials science and engineering, condensed matter physics, and materials chemistry. To this end, multiscale modeling as well as data analysis of experimental and simulation data are employed successfully in different applications. In this presentation, we focus on applications in which experimental data is scarce yet simulation data can in principle be generated with arbitrary resolution. However, the computational costs associated with the simulation data is substantial and very often dominated by the solution of the resulting algebraic equations so that the key enabler to carrying out large scale data analysis on very large simulation data is in fact the linear solver. We consider the design of rubber materials for advanced tires and present an algebraic multigrid method for this challenging application. Moreover, we consider laminated composite plates and discuss how small scale structural details that are typically ignored in design and margin of safety applications due to excessive computational costs when using classical approximation methods such as finite elements. Here, we present the construction of optimal basis functions that implicitly resolve these details so that it becomes feasible to consider these details also in design.

Speaker Biography

2002	Dr. rer. nat., University of Bonn
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The development of efficient meshfree methods for partial differential equations is at the center of my research work. Since these modern methods do not require the availability of an appropriate computational mesh they alleviate the treatment of applications in complex domains, especially in time-dependent settings.

The particle-partition of unity method, a meshfree generalization of the finite element method I have developed together with Prof. Dr. M. Griebel, furthermore allows for the easy incorporation of a priori information about special local behavior of the solution (e.g. discontinuities and singularities) by so-called enrichment. If such information is available (analytically or numerically) this enrichment technique reduces the computational complexity substantially since it eliminates the need for classical adaptive refinement. This enrichment technique can also be interpreted as a multiscale coupling.

In fracture mechanics for instance good enrichment information is often available from asymptotic expansions of the solution. Hence, the use of enriched approximation techniques is becoming well-established in this field. In general however the numerical construction of appropriate enrichment information is necessary. Here, the use of adaptive refinement or microscale simulations must be employed. The automatic computation of fine

scale enrichment information and its incorporation in a coarse scale simulation is a very important research topic with wide application and thus shall be further explored also in the future.