CCT Colloquium Series

High Performance Multiple Scattering Methods for Materials Simulation

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Johnston Hall 338
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Abstract:
Multiple scattering theory (MST) techniques have a history in electronic structure calculations dating back to the pioneering work of Korringa and of Kohn and Rostoker that resulted in initial implementations of the KKR band structure method in the mid 60s. More recently, MST methods underpin a number of first principles – density functional theory based – methods for calculating the electronic structure and properties of a variety of complex systems. Here, I will outline the theoretical and algorithmic aspects of MST – Greens function methods, optimal use of the complex energy plane, efficient parallelization and matrix methods – that, when combined with modern high performance computers, lead to powerful approaches for dealing with materials ranging from disordered alloys to nanoparticles. Specifically, I will illustrate how MST Green's functions methods for solving the Schrodinger and Dirac equations can effectively exploit parallelism and, at the cost of some accuracy, to approaches that scale linearly (O[N]) with the number of atoms (N) being treated. In particular, in the Locally Self-consistent Multiple Scattering (LSMS) method, the basic equations are recast in a manner that yields an approach that is parallel by construction. As a result, the LSMS method naturally maps on massively parallel computers and produces scaling that is close to O[N]; rather than O[N3] as in conventional electronic structure methods and a prerequisite for dealing with large numbers of atoms. I will demonstrate the performance of LSMS code on state of the art supercomputers with data gathered on the Cray XT3/4 systems at the ORNL Center for Computational Sciences. This data shows near ideal strong scaling for systems containing tens of thousands of atoms and for parallelization across thousands of cores. Finally, I will discuss some applications of MST methods to magnetic properties of nanostructures that are of current experimental interest including Fe and Co nanowires at Pt-surface step-edges and FePt-nanoparticles. Work supported by the DOE-OS through the Office of Basic Energy Sciences (BES), Division of Materials Sciences and Engineering.

Speaker's Bio:
Dr. G. Malcolm Stocks is a Corporate Fellow and Group Leader of the Materials Theory Group of the Materials Science and Technology Division at Oak Ridge National Laboratory. His major research activities are in the development and application of first principles multiple scattering theory electronic structure methods, the theory of magnetism, alloy theory, theoretical methods for strongly correlated electron systems, and the application of parallel algorithms and computers to extend the size and complexity of systems amenable to treatment by first principles methods. Dr. Stocks was instrumental in developing the widely used first principles KKR-CPA method for calculating the electronic structure of substitutionally disordered systems as well as the order-N Locally Self-consistent Multiple Scattering (LSMS) method which is capable of performing electronic structure calculations for systems containing many thousands of atoms. He has twice been awarded the Gordon Bell Prize for the application of these methods on parallel computers. His current research is focused on the continued development of LSMS and related approaches and their application to the theory of equilibrium and non-equilibrium properties of inhomogeneous itinerant magnets and magnetic nano-structures. Other interests include the development of new first principles electronic structure approaches for strongly correlated electron materials, such as 3d-transition metal oxides and 5f-actinide containing materials. Continuing interests include the first principles theory of the electronic structure and energetics of substitutionally disordered systems, ordering mechanisms in alloys, and alloy phase stability.

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