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The Development of High Performance Scientific Applications

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Abstract:

The development of high performance applications on large-scale parallel architectures requires the close collaboration with the domain scientist, computer scientist and applied mathematicians. In this presentation I will describe the theoretical development and the numerical implementation of three first principles density functional theory methods based on multiple scattering theory that all achieved high performance (80-90% efficiency) via a multi-disciplinary approach. This work resulted in a number of high performance computing awards including several Gordon Bell Awards, Computerworld Smithsonian Laureate Award, and a Cray Gigaflop award. These methods represented new approaches and the ability to address scientific problems that were not treatable due their inherent complexity that required considerable computational resources rendering them untenable at that time on modern high performance systems.

Speaker's Bio:

Dr. Shelton began his career in 1990 as National Academy of Sciences/National Research Council Postdoctoral fellow in the Complex Systems Theory Group at the Naval Research Laboratory. He then joined Oak Ridge National Laboratory as a staff scientist in 1992. Dr. Shelton was a group leader of the Computational Condensed Matter Physics group until 2001 and a Distinguished Senior Research Staff member of the Computational Chemical Sciences group prior to coming to EMSL in September 2010. He also spent a year during his Ph.D. studies at the University of Bristol in Bristol, England working with Professor Balaz Gyorffy. The main body of his work is in the general area of disorder systems, alloy theory and surface science where he has worked on incorporating magnetic and chemical disorder including point defects, such as vacancies and antisites in both materials and chemistry. Early in his career he worked superconductivity, magnetic multilayers, intermetallics and later he worked on surface science problems including recent investigations in Li-Air battery systems.
Dr. Shelton is currently associate director of WR Wiley Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory.

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