TITLE: Improving the performance of ab initio molecular dynamics simulations and band structure calculations for actinide and geochemical systems with new algorithms and new machines

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Abstract: Methods for directly simulating the behavior of complex strongly interacting atomic systems (molecular dynamics, Monte Carlo) have provided important insight into the behavior of nanoparticles, biochemical systems, actinide systems and geofluids. The limitation of these methods to even wider applications is the difficulty of developing accurate atomic level potential interactions that can capture their complex chemistry. Plane wave DFT methods have provided a means to simulate the both the electronic structure and dynamics from molecules and simple crystals to large nanoscale systems. However, these methods, because of their computational expense, have been limited to smaller systems sizes and short time-scales compared to classical molecular dynamics. Thus the performance of software is always an important consideration and the changing computing technologies based on Intel MICs are requiring major reformulations of our ab initio molecular dynamics and band structure codes.

This talk will focus on our developments in two areas: implementation of plane-wave electronic structure methods into NWChem on hybrid HPC architectures, including exact exchange, fast localization based on the real space density matrix, integration with FEFF, and the development of parallel in time algorithms. The talk will focus on the fundamentals of these methods and the realities in terms of system size, computational requirements and simulation times that are required for their application. Recent applications of these methods will be shown for solvated mineral surfaces and their interaction with metal cations.