



## Parallel-replica dynamics study of tip-surface and tip-tip interactions in atomic force microscopy and the formation and mechanical properties of metallic nanowires

PI: Arthur F. Voter (T-12) [afv@lanl.gov](mailto:afv@lanl.gov)

### Abstract

Metallic nanowires, with diameters of a few atoms down to even a single atom, will play an important role in future-generation nanodevices, such as electrical conductors, and electrical and perhaps even mechanical switches. Enabling this technological paradigm shift will require a deep understanding of the unique formation mechanisms and mechanical properties of nanoscale structures. Up to now, atomistic simulations aimed at understanding these processes have been necessarily limited to time scales that are short of the experimental reality by a factor  $10^3$  to  $10^7$ . By porting the parallel-replica dynamics (Par-Rep) code to Roadrunner, we will be able to perform the first-ever atomistic simulations of the formation (through AFM tip to surface contact and withdrawal), and tensile test behavior of metallic nanowires of silver and copper on experimentally accessible time scales of milliseconds. The Par-Rep method, an accelerated molecular dynamics method developed at LANL, gives exact long-time evolution of an infrequent-event system. Based on initial benchmark calculations, we expect to achieve a speed of  $\sim 0.5$  ms of simulation time per wall-clock hour on Roadrunner.