Postdoctoral Appointee - Computational Multiscale Research

Location: Albuquerque, NM
Full-time, Temporary Position

What Your Job Will Be Like

Are you looking to be a member of a highly motivated team? We are seeking a Postdoctoral Appointee in the areas of multiscale materials modeling, machine learning, and high-performance scientific computing. You will address challenges in the development of novel interatomic potentials for molecular dynamics, the creation of multiscale simulation capabilities (e.g., electronic structure, atomistic scale, continuum scale), and the application of machine learning to problems in materials modeling. This position provides the opportunity to collaborate with a diverse set of colleagues including researchers from your own field, applications specialists, and others, and to engage with the broader research community through publications and participation in leading scientific conferences. Join our team of scientists and researchers and make a difference! You may work with export controlled information which requires US Person status.

The Computer Science Research Institute is committed to nurturing a culture compatible with a broad group of people and perspectives in accordance with the changing makeup of the workforce. In support of this vision, the center actively recruits applicants from diverse backgrounds and fosters an inclusive community.

Qualifications We Require

- You have, or are pursuing, a PhD in Physics, Chemistry, Mathematics, Chemical Engineering, Materials Science, Computer Science, or related science or engineering field, and possess a bachelor's degree in science, technology, engineering, mathematics (STEM) or related science or engineering field
- Experience in research, development, and programming of atomistic simulation methods, primarily molecular dynamics
- Experience in high-performance scientific computer programming
- Record of research as demonstrated by publications in peer-reviewed journals or competitive conference proceedings
- Due to U.S. export-control laws, only U.S. Persons (U.S. citizens, lawful permanent residents, asylees, or refugees) are eligible for consideration

Qualifications We Desire

- Experience with the LAMMPS software package (http://lammps.sandia.gov), both in code development and application
- Experience using and developing machine learned models (neural networks, kernel methods, etc.) and mathematical/computational theory of AI/ML
- Experience with electronic structure codes such as Gaussian, NWChem, or VASP
- Proficiency in C++ and Python software development, code verification, and modern software quality practices
- Experience with developing and running complex science and engineering codes on massively parallel computing clusters, including GPU+CPU hybrid platforms
- A commitment to fostering an inclusive culture, as demonstrated in your application materials
- Interest in impacting applications and customers in support of DOE missions
- Ability to acquire and maintain a DOE security clearance

About Our Team

The Computational Multiscale Department performs outstanding research and development in physics-based materials modeling and high-performance computing. We combine expertise across multiple fields to solve science and engineering problems in support of the DOE mission. Our team brings together authorities in density functional theory, molecular dynamics, direct simulation Monte Carlo, microstructure modeling, continuum mechanics, equations of state, and peridynamics. We lead a number of software development efforts, including the LAMMPS molecular dynamics code and the FitSNAP machine learning interatomic potential software, and strive to advance the state of the art in materials modeling through a wide range of collaborations across the laboratories.

Apply online at:
sandia.gov/careers
Job #: 672016

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