Dear LANL Hiring Team,

I am very excited to be applying for this position because it represents a great opportunity to expand and hone my current skillset as a computational scientist. My greatest intellectual interest is in computational physics and I have been lucky enough to leverage this interest into a career path. I believe my scientific skillset, work experience, and interests are particularly well suited to the demands of this position. My experience with computational physics lies in two primary domains: molecular simulations of complex fluids, and simulations of charged particle optical systems.

As a graduate student at the University of Oregon, my research focused on using computational methods to build models of individual macromolecules or ensembles of macromolecules using a Langevin equation or the Ornstein–Zernike equation, respectively. In general, this required developing a theoretical model and using data from molecular dynamics (MD) simulations to calculate or validate statistics predicted by the model. To generate simulation data, I used either GROMACS or LAMMPS simulation software to run parallelized MD simulations on a high performance computing platform. Processing simulation data required developing reusable and scalable code for data analysis in Python and Fortran. This work demanded a strong understanding of computational methods for modeling many-particle systems, applying these methods in a parallel computing environment, and contributing to a repository of software tools for data analysis and visualization.

At Thermo Fisher Scientific, I am currently working with the Focused Ion Beam (FIB) research group using computational methods to study novel FIB technologies.

I am interested in this position because the job description aligns very well with my professional goals. I am currently looking for a career doing work that leverages computational power to solve complex problems in science. I have been lucky enough to do this kind of work in an academic setting and in industry, and to have been exposed to multiple fields in which this work is done.

The primary experience I have that is relevant to this position is in developing software and data analysis techniques for scientific research. This work has taken three forms: writing code to produce data from simulations or hardware, writing code to process data, and writing code to create and optimize workflows for performing the latter two tasks.

In my work at University of Oregon, I developed theoretical models of macromolecules, and validated these models using molecular dynamics simulation data. Typically, this involved writing shell scripts to run simulations in GROMACS on a High Performance Computing System, and processing the output using a combination of Python and Fortran. To do this properly, I had to develop a deep understanding of the physics of both the theoretical model and the simulated physical models. This work also required writing code for data analysis that scaled to $\sim$1-10TB of data, and communicating the results of my analysis to a research group through data visualizations.

At Thermo Fisher Scientific, I have been working in the Advanced Technology division doing research on Focused Ion Beam (FIB) technology. Initially, this involved running experiments on a Thermo Fisher dual-beam system, which required careful programming to control delicate hardware for experiment automation. More recently, I have been working on a project to optimize novel column designs using FIB simulations in the General Particle Tracer simulation engine. My work at Thermo Fisher has been an exciting opportunity to see theoretical results validated experimentally, and vice versa, with excellent agreement between the two.

I am very excited to be applying for jobs doing scientific research at UCLA and I hope to hear from you soon. Thank you.

Sincerely,
Jeremy Welsh-Kavan

In my work as a graduate student at the University of Oregon, my research goal was to develop coarse-grained models for macromolecules and validate them using computational methods. This research focused on constructing models of individual macromolecules or ensembles of macromolecules using a Langevin equation or the Ornstein–Zernike equation, respectively. The primary computational method used to build these models