Postdoctoral Research Associate
Supercomputing for Crystallography and Drug Development

The SSRL (Stanford Synchrotron Radiation Lightsource) Directorate at SLAC National Accelerator Laboratory is accepting applications for a Postdoctoral Research Associate to join the **SuperBio project** aimed at promoting supercomputer access for light-source users.

The chosen applicant will be expected to lead the development of three supercomputing workflows that directly support the **Macromolecular Crystallography (MC) Group** at SSRL and crystallographic fragment screening pipelines currently in development at the facility.

Additionally, the work will involve facilitating the adoption of supercomputer capabilities by the MC group user community, ultimately to enrich the process of scientific discovery at the SSRL. In essence, the SuperBio project is being developed to mask the complexities of supercomputer operations from the light-source user.

This project will be done in partnership with the Joint Genome Institute and will utilize their JGI Analysis Workflow Service (JAWS). A main thrust of the project will be the development of an SSRL-JAWS client portal that users can interact with to launch and track jobs.

This role offers the chance to gain expertise in industry standards for running computational workflows, as well as learning about structural biology, macromolecular crystallography, and high-performance computing.

Key responsibilities

- **Workflow system leadership:** Implement, test, and deploy the SSRL-JAWS client and ensure user accessibility. This may include development of a dedicated SSRL-JAWS user portal.
- **Workflow development:** Build, test, and maintain three supercomputing workflows for:
    - **Advanced modeling:** Using forward models in data reduction for increased structural accuracy.
    - **Virtual Ligand Screening (VLS):** Running molecular docking and molecular dynamics simulations to support drug development pipelines.
    - **Fast processing**: Real time processing of lossy diffraction data.
- **Container maintenance:** Create and maintain Docker containers for each of the above-listed workflows and for each supercomputer facility (e.g., NERSC Perlmutter/Doudna).
- **Feature integration:** For the **"Fast processing"** workflow, integrate the results for the user-facing Blu-ICE GUI, so that results are observed in real-time.
- **Promotion of future developments:** Establish a general framework and set of instructions outlining the steps needed for future SSRL-JAWS workflow developments and custom user workflows, including those outside of macromolecular crystallography.

- **Feedback management:** Work with key users and MC staff to test the workflows and setup a user portal for feedback.
- **Results dissemination:** Lead the publication of a peer-reviewed scientific article demonstrating the new capability. Present results at relevant conference.

Required qualifications

- Ph.D. in a relevant computational or experimental field (e.g., Physics, Computational Chemistry, Computer Science, Statistics, Bioinformatics, Structural Biology, or a related discipline) completed within the last three years.
- Extensive experience with Python, and professional software development practices (including test-driven code development and version control).
- Proficiency working in a Unix shell environment and shell (e.g. BASH) scripting.
- Excellent data processing and statistical analysis skills, as well as strong interpersonal acumen, with the ability to work effectively in a large, multi-disciplinary team.
- A strong desire to build user-friendly computational tools that promote scientific discovery.

Preferred qualifications

- Knowledge of common parallelization strategies and frameworks (e.g. MPI, CUDA).
- Prior experience with diffraction data analysis software (e.g., DIALS, XDS) and/or molecular dynamics simulations / molecular docking software.
- Prior experience with High-Performance Computing systems.
- Experience using Docker for packaging and deploying software environments
- Modern machine learning approaches.

This is a **fixed-term staff position**, expected to be a **2-year appointment**.

Application materials should include a **cover letter**, a **statement of research area** including a summary of accomplishments, a **curriculum vitae** (CV), a **list of publications**, and names of **three references for future letters of recommendation**.

Please email all application materials to Dr. Derek Mendez; dermen@slac.stanford.edu

SLAC is a U.S. Department of Energy (DOE) laboratory operated by Stanford University and based in Menlo Park, CA. The **Macromolecular Crystallography Group** is part of the Structural and Molecular Biology division of the SSRL directorate.