Job Title	Computational Scientist
PVN ID	RC-2001-003469
Category	Research
Location	CUNY-ADVANCED SCIENCE RESEARCH CENTER
Department	Structural Biology Initiative
Status	Full Time
Salary	Depends on qualifications
Hour(s) a Week	35
Closing Date	Aug 04, 2020 (Or Until Filled)

General Description

The CUNY ASRC Structural Biology Initiative seeks applications from individuals with experience in software development and NMR (Nuclear Magnetic Resonance) spectroscopy, computational biology, computer science, biology or chemistry to serve as computational scientists. Several positions are available and the job description and level is dependent on the skills, experience and career goals of the candidates.

The Computational Scientists will be involved in several specific NMR related projects that are funded by three NIH grants. All projects will involve the production of state of the art software projects that will be used by an international audience of scientists.

The first project is part of the Center for Molecular Dynamics by NMR (an NIH P41 National Center) located at the New York Structural Biology Center (http://comdnmr.nysbc.org). The focus of CoMD/NMR is technical development and application of NMR spin relaxation and associated methods for characterizing protein and nucleic acid conformational dynamics in biological processes including ligand recognition, allostery, catalysis, and folding.

The second project is part of the Center of HIV RNA Studies (CRNA), an NIH P50 HIV Structural Biology Center (https://sites.google.com/a/umich.edu/the-center-for-hiv-rna-studies/). The CRNA consists of an integrated team of NMR spectroscopists, X-ray crystallographers, Cryo-EM microscopists, cell and computational biologists, chemists, and virologists located at multiple universities and dedicated to advancing understanding of the structures and molecular processes during HIV-1 replication that involve RNA.

The third project involves the development of an integrated software environment for NMR data analysis. This component is funded by an R01 grant (NMRFx: An Integrated software suite for macromolecular NMR analysis, https://nmrfx.org) and involves software development for NMR processing (NMRFx Processor), visualization and analysis (NMRViewJ – NMRFx Viewer), and structure calculation using torsion angle molecular dynamics (NMRFx Structure)

Other Duties

Other duties may include:

- Developing new algorithms for data analysis
- Maintaining hardware and software
- Writing documentation
- Developing software test suites
- Training users in use of the developed software
- Presenting at workshops and meetings.

Qualifications

Successful candidates must have significant experience in software development with either the Java or Python programming languages (preferably both) and should have an interest in computational science. Experience with other data science languages such as R, new machine learning technologies such as deep neural networks, and GPU programming would be an advantage. Other desirable skills (depending on the exact position) include applied mathematics, NMR (especially relaxation) theory, and software engineering skills (including source code management, integrated testing and documentation).

Minimum Qualifications (depending on position)

- A Master's Degree (or Bachelors with significant computational experience) from an accredited institution in Chemistry/Biochemistry/Computational Biology/Computer Science
- PhD preferred
- Software development experience in Python and/or Java
- Experience using standard software engineering tools including source code control (such as Git), integrated development environments (such as NetBeans), project management tools (such as Maven) and test suites (such as Junit).

Preferred Qualifications

- Coursework and/or experience in NMR spectroscopy (especially in NMR relaxation analysis).
- Course work or experience in numerical methods.
- Course work or experience in data mining and statistics
- Experience with GPU programming