Professional Statement
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I dedicated myself to interdisciplinary research when I was a sophomore at University of Science and Technology of China (USTC). At that time, I was an engineering major and worked in a computational lab that using mathematical and physical models to help experimentalists to explain experimental phenomena and reveal mechanisms. Unsatisfied about only developing explanatory models, I switched my interest to computational biochemistry when I was a senior student, hoping to develop predictive models to better assist researchers to design experiments.

At UMD, I'm advised by Prof. David Fushman, a structural biologist and Prof. Max Leiserson, a computational scientist and computational biologist. In Prof. Fushman's lab, my research focus on studying conformations of proteins via the integration of different NMR data. In Prof. Leiserson's lab, I develop algorithms to study peptides presented on cell surfaces (antigen presentation), and work on missing link prediction methods for biological networks. I study different proteins in both labs, but the major goal is unified: help experimentalists to integrate experiment data from different sources to gain insights into biological interactions.

Gradually, I realized that many scientific programs are not easy to use for general researchers since they don't have graphical user interfaces and require some knowledges in Java/MATLAB. Moreover, they are separate programs and if someone wants to do a bunch of analysis, they have to install multiple programs and deal with different runtime environments of different languages. When I work with biochemists, I find them are often unwilling to install and run those heterogenous programs. More importantly, it's not easy for biochemists to find those programs. Some algorithms published on prestigious journals, for example, Prof. David Fushman's group published PATI (Prediction of Alignment Tensor through Integration) on Journal of American Society of Chemistry (JACS), but the huge potential applications in biochemistry may be overshadowed by complicated theoretical details in that paper. As a result, even biochemists who need the software can't find the software if only at a glimpse of the paper.

Therefore, as a first-year PhD, my short-term goal is to transform our off-line software into web-based applications and make them more accessible to biochemists. The first time I heard about GenApp, I realized that's exactly the framework I'm looking for. I hope by utilizing GenApp, any biochemist in this world can easily find our programs if they want to do similar analysis, and they can run programs on web server smoothly without any prior knowledge in MATLAB/Java. Hopefully, we can even collect feedback from them to make further improvement.

Sponsored by Science Gateways Community Institute, I realized my goal this summer. With the assistance of Dr. Emre Brookes, Dr. Alexey Savelyev and Dr. David Fushman, I modified an existing program ROTDIF, a versatile software package that enables researchers to perform accurate and comprehensive analysis of NMR relaxation data in order to determine the rotational diffusion tensors and characterize the amplitudes and time scales of internal motions in biological macromolecules (proteins and nucleic acids). Using the GenApp technology for scientific gateways (https://genapp.rocks), I successfully developed a science gateway for ROTDIF that

provides advanced computational functionalities, streamlines data input, storage, and output, and enables interactive 2D and 3D plotting and visualization. These features will dramatically improve the user experience and broaden the number of potential users of this gateway. I will present specific examples illustrating data input, functionality, and output visualization in my poster. I also firmly believe that others in science gateways related to biological structural community will be able to use these new tools to advance their research capabilities and to enhance their research experience.

In the future, I intend to transform and make available through GenApp other software packages and modules for NMR data analysis that we developed. Moreover, I will also take GenApp into account at the beginning of designing any original program.

I will continue devoting myself to developing useful algorithms combined with the first-hand information gained by experimentalists and cutting-edge algorithms for biochemists who always look for rationale in performing experiments. Meanwhile, I determine to join more projects like science gateways since it successfully bridges researchers in experimental and computational areas.