**Gordon Chalmers – Mentoring**

Mentoring as defined in the requested letter for the Computation Position is "to help train graduate students and post-doctoral fellows as they advance in their careers.” I believe that mentoring and spending time to help more junior scientists is equally important to research. I know the relevance of providing knowledgeable information in mentoring at the NIH and am willing to do this. I have spent much time in decades of work to educate and enable younger scientists (and older) to pursue excellent work. I appreciate the value of the time spent in helping junior scientists and also seeing the effect on their work and careers, and this is separate from my own work.

I have much experience in the formal and informal education of scientists and will describe this. First, I am also always available as a resource of the computing sciences, computational molecular work, programming, physics, and the use of mathematics to colleagues. I have made numerous contributions to other’s work at the graduate, postdoctoral, and professor level, over the years. This also includes small minor tasks, advice in problem solving, or coding.

My mentoring of junior scientists can be described as: 1) Discussions or collaborations involving algorithms, software development, and calculations with students and postdoctoral members, 2) Contributions to projects and papers in which I am not necessarily an author, 3) Teaching in a classroom. In the next paragraphs I give examples in which the work has enabled advance junior scientists’ careers and scientific knowledge.

During a multi-year long project, I worked in depth on a software package that enables automated assignment of sparsely labeled proteins. I was responsible for much of the machine learning genetic algorithm code, the C++ spin diffusion modeling from the MD trajectories, and importantly for informing other grad students of the principles of calculation and in using the software, notably Qi Gao and Rob Williams in the group of Jim Prestegard (UGA). The core software and use featured strongly in both of their PhD dissertations as well as in my own. I felt responsible for all my coworkers to know the basic principles of the genetic algorithm, and the computational aspects of the work including the subtle details having to do with the protein structures that were examined. Likewise, in another long project, in my collaborative work on the Skp1 protein, I wrote computational software to model NMR relaxation rates from MD simulations. In this context, I taught all those involved in the Skp1 project how to use the programs I had created, and one result was determination of ligand epitope and the resulting conformational change of the protein-ligand system necessary for function. David Thieker, one of Rob Wood’s graduate students and very adept at MD and protein structure, benefited in his PhD from the NMR software, training in C++, as well as statistical methods. In all projects I participated strongly in the molecular calculations, and having more experience in science, made sure that all involved knew the details of the calculations and the subtleties and limitations of any software use, not just my own. Furthermore, at RPI I managed the various software programs the group used and was always on hand for advice on how to use and implement. While there, I gave a graduate student about 20 microseconds of molecular dynamics (MD) trajectories of Arixtra and several charge modified forms, along with a range of different MD calculated NMR observables (Joel Janke’s thesis was about comparing Gromacs and Amber in particular conformational populations). Most recently, I used my newly developed software Ligand GA to initiate a portion of the PhD work of Xu Yang by generating an in silico designed glycoprotein enrichment tool; Xu learned basics of Matlab, genetic algorithms, and aspects of computationally generated small molecules and is now in the process of synthesis (poster listed in CV). I always am on hand to aid graduate students and postdocs (and faculty) with algorithms, computing, molecular chemistry, and physics and mathematical techniques. All of the graduate students I have worked with (except Xu Yang who is still in school) have graduated and gone on to successful careers in molecular work.

Due to my background and multiple PhDs, one in Computer Science, I amcan to solve problems or help in solving problems sometimes very quickly to aid the work of a junior scientist. I can program in many languages, and in Matlab, which is not as foreign as other scientific tools and more commonly used (I have used it for >20 years), I can offer strong and valuable advice when asked a question. My background in algorithms, the hard sciences, computing, and machine learning make me a relevant resource and I am quite happy to help in another’s work. I find it satisfying to do so, and I do this with the intent of encouraging confidence and enthusiasm.

On occasion I would give pedagogical seminars as introduction to some area that people would like to know about, such as a series of 4 1-hour presentations of the theory and measurement of residual dipolar couplings (RDCs) at RPI or an earlier multi-part series on chemical shifts and calculations for their prediction at UGA. One summer, I gave a weekly course in programming in C++. After the end of the course, I was told by several of the students that the practical introduction was greatly beneficial including in the postdoc positions that they held afterwards.

As an example of classroom education, I was a lecturer in the Physics Department at UCLA for one year. During this time, I taught 3 lower division classes and 3 upper division classes. I found the teaching rewarding, especially in the smaller upper division classes where there was more one-on-one discussion.

I also have served as an informal co-advisor to two graduate students in physics earlier in my career. One of these was Koenraad Schalm, and together, we published five papers. He is now a successful full professor at Leiden University in his home country of the Netherlands. I understand the importance of getting the computational tools in place for a junior scientist and in giving confidence in using the technical skills.

My training in mentoring junior scientists is rooted in my first postdoc, at the CN Yang Institute for Theoretical Physics, SUNY Stony Brook. The environment is known where there are ‘no stupid questions’ and has a very co-educational atmosphere. There are few as well regarded institutions with a reputation in which excellent mentoring is taught to junior postdocs.