Kim F. Wong

Center for Simulation and Modeling

1144 Benedum, University of Pittsburgh

May 18, 2015

Ken Jordan; Kay Brummond

University of Pittsburgh

Department of Chemistry

Chevron Science Center

219 Parkman AVE

Pittsburgh, PA 15260

Dear Professor Jordan and Professor Brummond:

My various professional activities for the 2014 academic year include:

1. Contributing to maintaining and administering the software environments within the Center for Simulation and Modeling (SaM) high-performance computing (HPC) facility
2. Providing software code development expertise to various collaborative projects and HPC consultation on effective workflow pipelines on the SaM cluster
3. Co-lecturer or guest lecturer: (1) Cluster Usage Training Workshops (2) Advanced Training Workshops (3) BioSc1540: Computational Biology

The above activities were undertaken in accordance with the mission of our Center for supporting and facilitating computational-based research across the University. These activities align with the education mission of our University as well as our Center’s goal of catalyzing multidisciplinary research.

During this prior academic year, I have been offered numerous opportunities to contribute to the education mission of our University. Through our cluster usage workshop at the start of each semester, we provide training to incoming students and new users on the basics of leveraging the University HPC facility for research. Through our intermediate/advance workshops (Special Howto Topics and MPI-X), we provide training to our seasoned users on the tools and skills required for effective scientific software development. Eric Polinko in the Department of Biological Sciences continues to utilize our Center’s HPC facility for his undergraduate BioSc1540 class and again extended an invitation for me to guest lecture. I also had the opportunity to mentor a Mathematics undergraduate and a Biology/Business Administrations undergraduate within the First Experiences in Research (FE-R) program. They were collaborating on a project to design, develop, and simulate the spread of diseases within a model of a UPMC hospital. Lastly, I had the pleasure of judging the Fall 2014 Chem. Dept. Undergraduate Laboratory Poster Session.

My prior contributions to the development of the WESTPA (Weighted Ensemble Simulation Toolkit with Parallelization and Analysis) project were recognized as a contributing author to the methodology paper. Since the Chong group are making extensive usage of the HPC facility, I continue to work with the group to ensure that our local instance of WESTPA and dependent software stack are optimized for their workflow. I also provide general support, maintenance, and benchmarking of molecular dynamics packages across our various types of CPUs and GPUs.

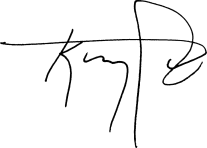
Although Bruce Lee has moved to Johns Hopkins University, I am still involved with the RHEA (Regional Healthcare Ecosystem Analyst) project for modeling disease dynamics within a healthcare setting. We are wrapping up the project from the CDC that funded my summer last year. The original scope of the project was to publish a Vital Signs during the fall of 2014; however, the emergent Ebola crisis diverted immediate CDC resources and the timeline got pushed back. The Vital Signs publication is now slated to come out during early Fall 2015, and it is supposed to be an important document that provides practical guidance on dealing with emerging public health issues. The CDC is happy with the modeling work we have accomplished and future opportunities may emerge.

On the proposal side, Lee Harrison (Pitt GSPH) and I submitted a Letter of Intent to the Simons Foundation to model the ecology of Clostridium difficile within the Western Pennsylvania area. The LOI was not selected for full proposal solicitation. While a bit disappointing, we have not totally given up. The undergraduate students I am mentoring under the FE-R program are designing and developing a smaller model that will become the seed for the larger model we envisioned. As we are convinced that the future will be in the modeling of ecology, we continue to seek out opportunities to place us in a good footing for when those solicitations become more prevalent.

With respect to administration of the HPC cluster, the following lists some of my key contributions:

* Installing and maintaining the license server and related software associated with Materials Studio, Lumerical FDTD, and CLC Genomics Server.
* Installing and maintaining the drivers and software stack for the GPUs on the cluster.
* Installing and maintaining software used by faculty in the Swanson School of Engineering. Examples include: Ansys, Diffpack, Abaqus, LAMMPS, Matlab, Comsol, FDTD, Materials Studio, Python.
* Installing and maintaining software used by faculty in Chemistry, Physics, Biology, Computational Biology, and Business. Examples include: Amber, Gromacs, LAMMPS, Tinker, WESTPA, VMD, Materials Studio, Matlab, FDTD, Python, R, SAS.
* Installing and maintaining software used by genomics researchers. Since Tony Ferreira has taken on the role of Executive Director, I have resumed my role as user support for genomics research until Health Sciences hires a replacement.

I believe the synergistic context of the broad professional activities enumerated above during the 2014 academic year specifically contributed to the education and research mission of our Center.

Sincerely,

Kim Wong