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**Center for Simulation and Modeling**

Dear Dr. Jordan,

This past academic year has most notably included my transition to Executive Director of the Center for Simulation and Modeling, which I formally began in October 2014. In that role, I have taken over the day-to-day management of the Consultants within the Center as well as other administrative duties. Since taking on that role, I have worked to establish an account to facilitate the collection and disbursement of funds for operational expenditures related to user payments for additional service units and storage space and I began an effort to solicit proposals from the faculty to support collaboration with the Center. I have also worked closely with faculty from the School of Medicine to develop a long-term plan for supporting their computational needs. In support of the Research Computing Committee (convened by the Provost), I worked closely with you in developing materials covering overall plans for hardware, software, staffing, and proposed budget levels.

As part of my outreach efforts for the Center, I attended SC14 in the Fall and the CASC meeting this Spring, for which I was an invited speaker and a member of the program committee. I have also served on the XSEDE technical program committee for the last two meetings. I have had several discussions with NETL personnel to pursue potential opportunities for research collaborations with the Center and played a significant role in the renewal of our CUDA Research Center designation. Additionally, I went to Lincoln Elementary School in Mt. Lebanon to do a chemistry demonstration for the 3rd grade classes with assistance from Dave Demilio for supplies and equipment.

On the purely academic side, I published a paper dealing with Bill Evans’ research group at St. Jude Children’s Research Hospital in *Nature Genetics*1 dealing with glucocorticoid inflammatory response in leukemia cells. My primary contribution to the paper was a set of quantum chemical calculations to estimate the interaction energies for Hoogsteen base pairings, which were then used to develop a modified version of the miRanda code (which we called Trident) to predict miRNA interactions crucial for the experimental design. I have served as a reviewer for the last two XSEDE meetings for both the poster and workshop committees and at the end of May 2015 I will be serving as an NSF panelist for the Advance Cyberinfrastructure division. I was listed as “Key Personnel” on two NIH proposals submitted by Peter Friedman (Pharmacology), although my effort was reduced to only 5% on each as he needed to retain salary support for a postdoc in his lab.

I was instrumental in the deployment of the SLASH2 filesystem in support of the Pittsburgh Genome Resource Repository (PGRR) and wrote custom software to automate and manage the data downloads from The Cancer Genome Atlas (TCGA) for use by the PGRR project. I also worked with Rebecca Jacobson to develop material for the PGRR training sessions (required for all users of the data). I also worked with our vendors to develop a plan to unify our fragmented InfiniBand fabric and oversaw the expansion and deployment of our Lustre array to 480 TB.

Sincerely,

Antonio M. Ferreira, PhD

(1) Paugh, S. W.; Bonten, E. J.; Savic, D.; Ramsey, L. B.; Thierfelder, W. E.; Gurung, P.; Malireddi, R. K. S.; Actis, M.; Mayasundari, A.; Min, J.; et al. NALP3 Inflammasome Upregulation and CASP1 Cleavage of the Glucocorticoid Receptor Cause Glucocorticoid Resistance in Leukemia Cells. *Nat. Genet.* **2015**.