Esteban Meneses

Research Assistant Professor Center for Simulation and Modeling University of Pittsburgh emeneses@pitt.edu

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Professor Kenneth Jordan and Professor Kay Brummond Department of Chemistry University of Pittsburgh

Dear Kenneth and Kay,

I started my position in the Center for Simulation and Modeling (SaM) at the University of Pittsburgh in the Fall semester of 2013. During those 20 months I have had the opportunity to develop my career as a young scientist thanks to my participation in a combination of education and research projects on high performance computing (HPC). At the same time, I was involved in multiple activities that are aligned with the goals of SaM and my individual responsibilities at the center. I will proceed to list the main professional activities I participated in during the last 8 months, grouped into broad categories.

Education	• Python for Scientific Computing Workshop. Organized by the whole SaM team in April, 2015. My main role was to help with the organization and design lecture slides for one of the sessions. I was in charge of teaching the lecture on high performance computing Python.
	• Intel Xeon Phi Workshop. Helped in the organization of a workshop on the accelerator technology of Intel (Xeon Phi coprocessor). The workshop itself was imparted by instructors from Colfax International.
	• CS1645: Introduction to High Performance Computing Systems. I was the instructor of an undergraduate-level course in the Department of Computer Science at Pitt during the Spring semester, 2015. The name of the class is "Introduction to High Performance Computing Systems" (CS1645/CS2045). This class was registered by 43 people, and was attended by three graduate students from the departments of Physics, Electrical and Computer Engineering, and Computer Science. The class received an educational allocation on Stampede, the seventh most powerful supercomputer in the world as of early 2015. Therefore, the students had the opportunity to interact with a state-of-the-art supercomputer and learn the languages and tools to run simulations on it.
Invited Talks/ Presentations	• Exploring the Interplay of Reliability and Energy Efficiency in HPC Systems. Hosted by the Institute for Scientific Computing at Lawrence Livermore National Laboratory. In this research seminar, I presented a collection of results from different projects related to reliability and energy consumption of HPC applications. The feedback received during the presentation was useful in the development of new ideas and projects.
	• Load Balancing and Data Migration in a Hybrid Computational Fluid Dynamics Application. Organized by the Parallel Programming Laboratory at the University of Illinois at Urbana-Champaign, the 13th Annual Workshop on Charm++ and its Applications gathered speakers from multiple institutions. I presented the ongoing work on one research project I participate along with other Pitt researchers. In particular, this talk was focused on comparing two tools in HPC to provide dynamic load balancing capabilities to applications. My colleague Dr. Patrick Pisciuneri and I have been working on this project and felt it was a good time to get some feedback.
Published Papers	• Using Migratable Objects to Enhance Fault Tolerance in Supercomputers. Published online-first on IEEE Transactions on Parallel and Distributed Systems (TPDS). This paper surveys the work on migratable objects to improve the reliability of different techniques for fault tolerance in HPC.
	• Scalable Replay with Partial-Order Dependencies for Message-Logging Fault Tolerance. Published in the proceedings of IEEE International Conference on Cluster Computing (CLUSTER). This paper explores a novel theoretical framework to describe different properties of applications and the matching minimal message-logging protocol.
	• Dynamic Load Balancing Strategies for Parallel Reacting Flow Simulations. Published as an abstract in the 67th Annual Meeting of the APS Division of Fluid Dynamics. This work describes the efforts of a research project at Pitt as part of a collaboration between the School of Engineering, the Department of Computer Science and the Center for Simulation and Modeling.
	• CAMEL: Collective-Aware Message Logging. Published in Springer's The Journal of Supercomputing. This paper describes a new technique to reduce the memory overhead of message-logging protocols in reliable HPC systems.
	• Analyzing the Interplay of Failures and Workload on Titan Supercomputer. Published in the proceedings of the Cray User Group Conference. This meeting gathers participantes from multiple institutions that traditionally use Cray machines, including NCSA, CSCS, and NERSC.

 $\bullet \ Load \ Balancing, Dynamic \ Repartitioning, and \ Data \ Migration \ in \ Turbulent \ Reactors. \ Published \ as \ an$

abstract in 15th International Conference on Numerical Combustion.

Research Projects	 Computational Fluid Dynamics (CFD). Along with my colleague Dr. Patrick Pisciuneri, I have been exploring the use of Charm++ (the language of NAMD) to solve a prominent problem in CFD codes, namely load imbalance. I am in charge of migrating the IPLMCFD code to Charm++. This code was developed at Prof. Peyman Givi's group. We currently have a design of the code and we have a working benchmark in Charm++. Fault Tolerance in High Performance Computing. This is my major research area and spans multiple topics. I am broadly interested in making HPC applications reliable on faulty hardware. Future supercomputers will inevitably have a smaller mean-time-between-failures (MTBF) than current machines. Therefore, it is imperative to provide a solid solution for this problem. There are multiple opportunities in the HPC community for this type of work.
Outreach	 Advancing Research through HPC. I played a minor role in contacting speakers and coordinating other activities for the annual seminar on HPC that the SaM organizes. Brown-bag seminar series. I was the leader in organizing a brown-bag seminar for the Fall semester in 2014. The SaM team officially sponsored this seminar that included three one-hour presentations on languages for HPC: Julia, Charm++, and Global Arrays.
Grants	I participated with Computer Science professors Rami Melhem and Taieb Znati to submit a proposal for the Department of Energy call "Resilience for Extreme Scale Supercomputing Systems". The proposal defines a new computation framework that targets systems with unreliable hardware and allows applications to run through node crashes. In addition, the energy dimension is considered by decreasing the power required by the resilient framework. We have not received the official approval of the proposal yet.
Consulting	Helping researchers, students, and professors with their technical problems is one of the mayor responsibilities of my position at SaM. I have fulfilled this role by attending tickets in our ticketing system (SaM Core). My focus has been tickets on accelerators (GPUs). In addition, I have interacted with professors, postdoctoral associates, and students in the use of Matlab, multithreading libraries, graph partitioning tools, and others.
Computer Science Liaison	Other of my roles at SaM is to work as a liaison with the Computer Science Department. I have had a strong interaction with multiple professors, including Prof. Daniel Mossé, Prof. Taieb Znati, Prof. Rami Melhem, Prof. Panos Chrysanthis, Prof. Alex Labrinidis, and others. I have participated in several discussions with Prof. Melhem and Prof. Znati on research projects regarding fault tolerance for HPC. In addition, Prof. Chrysanthis and Prof. Labrinidis are part of a large collaboration with other Pitt faculty and members of SaM.
Accelerator Technologies	I was assigned the responsibility to foster the use of accelerator technologies at Pitt. Here is a summary of my activities in that role: • I submitted a proposal to renew our CUDA center. The proposal was approved and the University of Pittsburgh is currently an official CUDA Research Center for the year 2015-2016. I am acting as the Pitt contact, along with Prof. Ken Jordan. As part of the grant we received two GPU Tesla K40c cards from NVIDIA. These cards are meant for research on CUDA technology. • I worked on having an Intel Xeon Phi installed in one of the servers of SaM. The accelerator was installed in its own machine and accesses were granted to users for testing the accelerator. • I worked on a proposal for a new GPU-enabled cluster to Silicon Mechanics. The proposal was not accepted, but it generated some momentum in the Pitt community. Currently, we have people in the departments of Chemistry, Chemical and Petroleum Engineering, and Computer Science with a specific project description for this type of hardware.

Sincerely	yours,	
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Esteban Meneses