University of Puerto Rico at Mayagüez
Monzón Building
XSEDE Workshop Agenda

Monday, January 26, 2015

8am	Sign-In & Consulting & Coffee Room 201	
9:00am	Opening Session Room M-201 – Welcome – *Coastal & Ocean Modeling Research Presentation* - Aurelio Mercado, UPRM – *Graduate Student Research Lightning Talks* – *XSEDE @UPR Mayaguez* - Ana Carmen Gonzalez – *XSEDE Overview* – Linda Akli	
Noon	Lunch & Consulting Room, M-213	
1:00pm – 5:00pm	*Getting Started: XSEDE New User Training* Instructor: Marcela Madrid Room: M-119	*Linux/Unix Basics for High Performance Computing* Instructor: Daniel Lucio Room: M-107
5:00pm	Consulting	

Tuesday, January 27, 2015

8:00am – Noon	*CUDA™: GPU Programming* Instructor: Vince Betro Room: M-119	*Intro to Parallel Computing with MPI and Open MP* Instructor: Daniel Lucio Room: M-110
Noon	Lunch & Consulting, Room 213	
1:00pm – 4:30pm	*Getting Started: XSEDE New User Training* Instructor: Marcela Madrid Room: M-119	*Introduction to Scientific Visualization* Instructor: Vince Betro Room: M-107

Session Descriptions

XSEDE New User Training

This tutorial will help new users become comfortable with the steps needed to access XSEDE resources, and to successfully use those resources to accomplish their research or educational goals. Topics will include how to request an allocation, find documentation, ask for help, login and run on an XSEDE supercomputer, submit a job and troubleshoot a job that has not run. The practice section of the tutorial will consist of hands-on activities including submitting a job, figuring out why it has not run and transferring files between supercomputers. Participants who know no Unix at all will benefit from attending the Linux/Unix Basics tutorial beforehand, but if unable to do so, we will provide personalized help during this session.

Linux/Unix Basics for High Performance Computing

An introduction to the Linux and Unix basics will be provided in this session. An overview of interacting with clusters and HPC resources will also be provided through interactive teaching. While there are no labs associated with this session, participants will be able to follow along with the instructor to gain experience and familiarity with the Linux/Unix environment.

Introduction to Parallel Computing with MPI and OpenMP

An overview of a typical XSEDE high performance computing (HPC) resource and the user-environment will be provided in this session. There are no labs associated with this session. The topics that will be discussed are:

- HPC System Overview
- Theoretical Background
- Parallel computing systems
- Parallel programming models
- MPI/OpenMP examples
- HPC User-Environment

CUDA™: GPU Programming

This training module is a beginners/intermediate course on programming NVIDIA GPUs with CUDA. After a short segment on why we are using accelerators in High Performance Computing and on accelerator hardware I will describe all pieces necessary to write a program in C and FORTRAN. The example will be a stencil update, which is simple enough to be written in a few lines of code. The specific code design will be guided by the hardware and I will put emphasis on motivating common design principles by the desire to write fast code for GPU accelerators. In the second part of the presentation I will focus on two common optimization strategies, namely the use of shared memory and data streams. Some experience with writing serial code in C or FORTRAN will be helpful to follow the examples.

Introduction to Scientific Visualization

This session will discuss the visualization systems available to XSEDE users. This will include an overview of the hardware on-site, the services available for remote-access visualization, and the software available for scientific visualization, including Visit and ParaView. A hands-on training session for ParaView will be offered. Discussion of information visualization will also be included as interest indicates.

Consulting

Have questions, need help? Bring your project ideas, code problems, questions about tools and resources and XSEDE staff will be there to answer. We can help you get started or solve a problem with an existing project using High Performance Computing.

Speaker Bios

Linda Akli is the Assistant Director of Training Education and Outreach at the Southeastern Universities Research Associate, a non-profit university membership organization that manages the Department of Energy Jefferson Lab, Coastal and Environmental Research, and Information Technology programs. As the lead for XSEDE Underrepresented Community Engagement, she delivers programs and events to promote, education, and involve faculty and students from traditionally underrepresented groups as users and contributors to XSEDE and the national cyberinfrastructure ecosystem.

Dr. Vincent Charles Betro received his Ph.D. in Computational Engineering from the University of Tennessee SimCenter at Chattanooga in 2010, where he became research faculty and the STEM Outreach coordinator. Since 2012, he is a Computational Scientist at the University of Tennessee National Institute for Computational Sciences at Oak Ridge National Laboratory, where he focuses his research on porting and optimizing applications for several accelerator architectures and developing Computational Fluid Dynamics codes for the Application Acceleration Center of Excellence. Additionally, due to his background as a middle and high school mathematics teacher and college mathematics and engineering instructor, Vince enjoys working with students in his community to broaden their understanding of and interest in STEM careers and is actively involved in leadership in the XSEDE User Engagement and Campus Champions programs.

Daniel Lucio is a HPC consultant at the National Institute for Computational Sciences at Oak Ridge National Laboratory. He has more than fourteen years of experience working with Supercomputers and HPC resources. He has spent the last seven years working at NICS and being involved at several TeraGRID/XSEDE events. He loves training and helping other people to succeed. He is constantly looking for new ways to bring knowledge for the masses and get minorities to get engaged in science and engineering.

Marcela Madrid is a Senior Computational Scientist at the Pittsburgh Supercomputing Center. She specializes in computational biology and structural bioinformatics. She collaborates with other scientists with the aim of applying high performance computing to the advancement of scientific problems and teaching. Using quantum mechanics and molecular dynamics simulations, she has studied hemoglobin, HIV-1 Reverse Transcriptase, Peptide Nucleic Acids and heat transfer in Silicon thin films. She develops and delivers training and outreach activities on XSEDE leading-edge high performance computers. Dr. Madrid holds a Ph.D. in Physics from Instituto Balseiro, Argentina.