ASU Research Computing
ARIZONA STATE UNIVERSITY

Research Computing Hands-On Seminars
MONDAYS, 10AM to NOON

This is a series of interactive seminars sponsored by the Research Computing Faculty Working Group. The seminars are intended to provide student and faculty researchers hands-on exposure to the research computing resources available at ASU and to provide an interactive opportunity for discussion, troubleshooting, and information sharing. These seminars will range from the introduction to high performance computing and basic programming, to discipline-specific workshops.

Where?
Life Sciences Center C, Room 180 (LSC 180)

When?
10 to 11 AM - Lecture
11 AM to Noon – Hands-on Practice

Who should attend?
Faculty, students or staff interested in using ASU Research Computing resources or current, discipline-specific users of these resources.

What are these seminars about?
This **interactive** workshop will begin with a lecture (10-11AM) and will be followed by hands-on practice (11AM to Noon). A member of the Research Computing training subgroup will be present at each seminar to facilitate discussion.

Monday August 29: Introduction to Supercomputing at ASU

Host: Brandon Mikkelsen, Director of Research Data Management
Audience: General (all faculty, staff and students)

This is the first in a series of training workshops being conducted to expose students and researchers to the high performance computing resources available at ASU. The presentation will provide a holistic overview of the cluster system hardware and software environment. A top level introduction to using an Unix/Linux based system with simple and useful commands and scripts, user environment including the Module system (used for software stack management), Compilers, SLURM, Moab and Gold for batch queuing, scheduling, and accounting will be provided. The talk will be very useful for first time users of the cluster to learn how to access and use the system effectively.

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Monday, September 12: Interacting with the Cluster: SSH/SFTP, SLURM Batch Scripts

Audience: General (all faculty, staff and students) / New Users
Host: Darren Thifault

This seminar is targeted to users who are comfortable running programs locally, but need a hands-on example of how to connect to the HPC, how to interact remotely with the cluster, how to move files, and how to execute jobs.

Monday, September 26: Useful Shell Scripting

Audience: General (all faculty, staff and students) / New Users
Host: Jeremy Mills

In everyday coding, shell scripting is extremely powerful and useful. This workshop will go over useful shell scripting for file manipulation and analysis.

Monday, October 24: Uncertainty Quantification and Sensitivity Analysis

Audience: Advanced Users
Host: Anuj Mubayi

Uncertainty and sensitivity quantification is a modern inter-disciplinary science that cuts across traditional research groups and combines statistics, numerical analysis and computational applied mathematics. *Uncertainty* captures how accurately does a mathematical model describe the true physics or biology and what is the impact of less precise known components in a model on its outputs? *Sensitivity* studies how the uncertainty in the output of a modeled system can be apportioned to different sources of uncertainty in its inputs.

Uncertainty is quantified using multiple approaches that uses statistical techniques directly to simulations via Monte Carlo simulation, Stratified sampling, Latin hypercube sampling, and Response surface method. Sensitivity analysis, which is used to reduce model uncertainty and suggest to empirical scientists what to collect in field, is categorized based on two different approaches: one-at-a-time and global measures.

In this workshop session, we will use simple mathematical models to simulate and show how uncertainty is quantified in both forward and inverse types as well as how to identify sensitive components of a system.

Monday, November 7: Designing and Implementing a Pipeline for Reference-based Genome Assembly

Audience: Advanced, discipline-specific users
Host: Tim Webster

Understanding genome-wide variation requires the 1) assembly of millions of short reads produced by high throughput sequencing technology into a single genomic sequence, and 2) accurate identification of genomic variants from this genomic sequence. The volume of data and many errors introduced during sequencing can make these tasks both bioinformatically challenging and computationally expensive. This session will present the design and implementation of a reproducible pipeline for reference-based and quality-controlled genome assembly and variant calling.

Monday, November 21: Protein Analysis

Audience: Advanced, discipline-specific users
Host: Darren Thifault

Characterizing and inferring protein dynamics is possible using bioinformatics software on the web, but large-scale analyses require installing and running this software on HPC. This session will present a series of software that are commonly used in protein analysis, I-TASSER (protein structure/function prediction), ClusPro (FFT based Docking), HADDOCK (Simulation based Docking), and give a brief overview of how these can be used on the HPC.

Monday December 5: Stochastic Modeling and Simulations

Audience: Advanced, discipline-specific users
Host: Lokam Dheeraj
Description: TBD

About Research Computing:

The Research Computing Working Group considers and recommends resources, policies, plans, and capabilities that affect faculty research computing and scholarly activities.

ASU Research Computing represents leading academic supercomputing capabilities — providing a high-performance computing environment, a high-end data intensive ecosystem (Big Data), a highly available 100 gigabit Internet2 connected network internal and external via Internet2 through an ESNET Science DMZ, large-scale data storage and elastic capacity to the public cloud. *Our mission is to eliminate boundaries to research computing by providing transformative advanced computing solutions in a cost-effective manner and to support the university's mission and goals as they apply to research, education and public service.*