Summer 2017

High performance computing tools

**Course Coordinator:**

Najeh Jisrawi, [njisrawi@sharjah.ac.ae](mailto:njisrawi@sharjah.ac.ae)

Office: +971-6-5050350. @JisrawiTeach.

**Learning Outcomes :**

After completely this course, students will be able to:

1. Setup and install linux on a personal computer and carry out basic system administration tasks including networking issues.
2. Use the linux/unix commandline to install and compile scientific software, and write simple shell scripts to automate tasks.
3. Use python for numerical solutions of scientific problems and visualization of scientific data.
4. Use git for project version control.
5. Use jupyter and ipython notebooks as IDEs for coding, visualization, and other desktop tasks.
6. Install and run atomistic modeling software including lammps, abinit, and quantum espresso.
7. Efficiently use University of Sharjah HPC resources for building and executing scientific computing projects.

**Course Schedule and Format:**

The course will be taught online and with a flexible schedule allowing students to run at their own pace. There will be some mild management and tasks will be different for different users.

The course home will be <https://elearning.sharjah.ac.ae/> and will use blackboard collaborate for synchronous sessions and office hours.

The course will run for the duration of the summer and continue into the fall of 2017/2018.

Syllabus

# Course Overview

To get started right away, just tap any placeholder text (such as this) and start typing.

## What you need: Hardware

### To easily apply any text formatting you see in this outline with just a tap, on the Home tab of the ribbon, check out Styles.

### For example, this paragraph uses Heading 3 style.

## What you need: software

## Setting up your desktop

## UoS resources

## Working in the cloud

## Open source resources

# linux and open source

## Install and optimize

## Linux GUI for routine tasks

## Commandline basics

## Shell scripting

## Sysadmin: networking

# Python for high performance computing

## Installation and optimization of python:

### Python under linux

### Anaconda

## Using Python:

### Python as a calculator

### Numpy

### Matplotlib

### Pandas

# numerical methods for Hpc

## Analytical versus computational: the third leg of science!

## Algebraic methods: Newton’s, secant, search techniques for solving nonlinear equations.

## Integration and differentiation: discrete calculus

## Ordinary differential equations

## Partial differential equations

## Random methods and Monte Carlo

## Fourier transforms

# Notebooks: jupyter and ipython

## <http://jupyter.org/>

### mix text, code, and media.

### Use ipython notebooks

## Installation

## Getting started with notebooks

# git and version control

## Why should we use git

## Installation

## Commandline usage

## HPC with git

# data analytics and visualization

## Data analytics with Python (pandas) and R

## Visualization of scientific data:

### Matplotlib

### Bokeh

### Plotly

### Non-python open source tools

# modeling and simulations for advancaed materials

## Scientific computing tools

## Classical modeling with lammps

## Quantum modeling: abinitio; abinit, quantum espresso

## Simulation data visualization and analysis: VMD, VESTA

# advnaced tools:

## MedeA

## AIIDA

# HPC @Sharjah

## Local HPC guide

## Hardware resources

## Software resources

## A brief history and future plans