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# Class Intro

CSE 380: Tools and Techniques of Computational Science

# Welcome

- Class outline
  - Syllabus
  - Canvas
  - Computer Accounts
  - Field Trip

# Class Outline

- Office Hours
  - After class in POB (ACES) 6.340
- Grading
  - 5 Homeworks (50%)
  - 1 Project (40% each)
  - Final is a presentation (10%)
- Lecture notes posted on Canvas the day after class

# Other Related Classes

- Fall
  - CSE 380: Tools and Techniques o Computational Science
    - Prerequisites include:
      - numerical analysis
      - some *nix familiarity
      - C/C++/F90 programing background
  - SSC 335/394 Scientific and Technical Computing
    - Less stringent prerequisites
- Spring: SSC Parallel Computing for Science and Engineering
- Summer: SSC introduction to programming classes

# Class Goals — at the end, students should be able to …

- Understanding floating point arithmetic and how cache hierarchy works
- Understand “speeds and feeds”; disk access times vs. interconnect vs. memory vs. cache
- Understand the fundamentals of instruction sets and vectorization
- Grok the Unix Operating System and get a good intro to the tools available
- Use version control as well as good software engineering practices
- Perform both code and solution verification across a wide range of problem types
- Debug, profile, optimize code
- Produce reproducible “well-documented” research and be the envy of their peers

# More goals …

- Exposure to:
  - on-node, off-node and Hybrid parallelization
  - offloading including GPGPUs and Xeon Phis (MICs)
- **Improve your (research group's) software**
- **Learn what tools are available for a range of applications**
- **Learn to be productive on HPC systems**
- **Learn the foundations of reproducible science/computing**
- possibly enabling you to get closer to graduation?

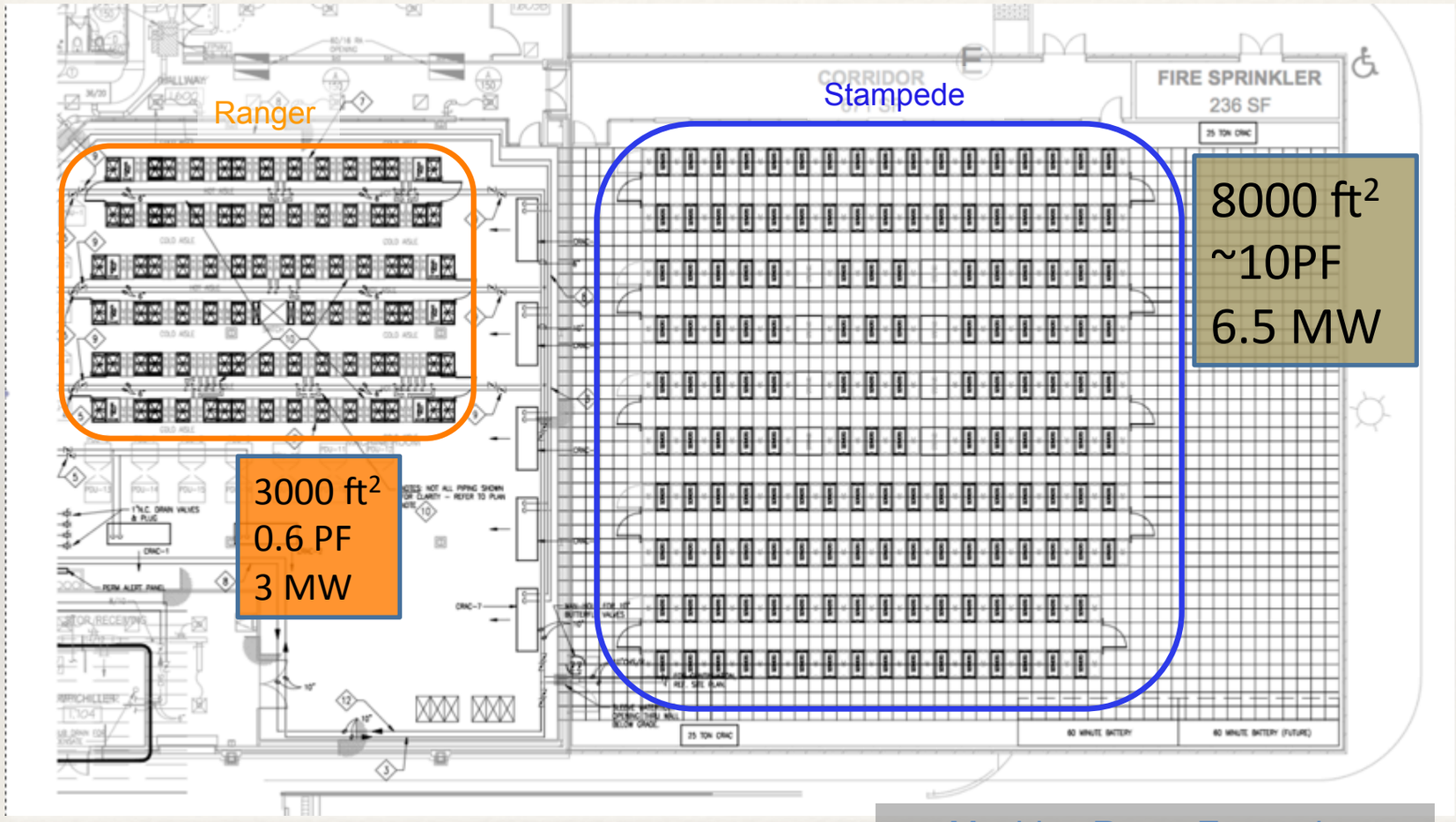
# Computer Accounts

- We will use 3 primary resources for this class
- UT's newest supercomputer, Stampede
- Canvas
- Bitbucket or Github (haven't decided yet)

# Stampede – High Level Overview

- Dell/Intel/Mellanox
  - Intel Sandy Bridge processors
  - 6,400 compute nodes
  - 56 Gb/s Mellanox FDR Infiniband Interconnect
  - More than 100k cores, 2.2 petaflops peak performance
- Co-processors
  - Intel Xeon Phi “MIC” Many Integrated Core processors
  - 61 cores per card
  - 7.3 petaflops additional performance

# Supercomputer Sizes




Machine Room Expansion

Added 6.5MW of additional power

# Production Environment

- Jobs run in a managed environment
  - login to the login node
  - submit jobs to the scheduler
  - wait
  - collect results
  - …
  - profit?

# Final Comments

- You will need to have access to a laptop or desktop to do this class
- This should be a "fun" class that provides practical computing exposure, introduction to some best practices and to fill the gap in computational science education
- I do have a day job, but feel free to email me with any questions or suggestions
  - csim@ices.utexas.edu
  - **make sure to include CSE380 in the subject line!**

# First Assignment

- Checkout the Canvas site for this class
  - http://canvas.utexas.edu/
- Sign up for a TACC account
  - http://portal.tacc.utexas.edu
- Email me your TACC account infos
- Start thinking about your projects and discussing this with your advisor; come to office hours to discuss possibilities

# Field Trip?

- TACC Visit — Tour of Stampede and TACC Facilities
- Directions — http://www.tacc.utexas.edu/about/contact-us/directions
- Doodle pool will be created to come up with times once everyone sends me their TACC usernames