

CSC 7700: Scientific Computing

Course Introduction

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Our Goals

- Building the experience and confidence that will encourage **you** to seek out and use national cyberinfrastructure and scientific computing techniques
Make you not shy away from large computers
- Demonstrating best practices of using and extending research software
Make you not shy away from programming in teams
- Showing how to efficiently collaborate with colleagues both locally and remote
Make you not shy away from working in distributed teams



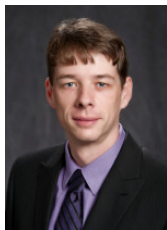
- Class time: Fridays 8:20am-11:20am
- Class location
 - Today: Tureaud Hall, Room 0101
 - Later: LDMC (announced on class email list)
- Email list for class: sci-comp-2013-class@mail.cct.lsu.edu
- Email list instructors: sci-comp-2013-instructors@mail.cct.lsu.edu
- Class web page: https://wiki.cct.lsu.edu/sci-comp/Main_Page
- Materials Subversion repository:
<https://svn.cct.lsu.edu/repos/courses/sci-comp-2013/public>



Course Organization

- 5 overall topics
- 5 instructors
- 2-3 classes (Fridays) each instructor
- topics:
 - A: Basic Skills
 - B: Advanced Programming Tools
 - C: Parallel Computing
 - D: Simulations and Application Frameworks
 - E: Distributed Scientific Computing





- Module A: Basic Skills
- Staff position at Center for Computation and Technology (CCT)
- Relativistic Astrophysics
- High-Performance Computing



Challenge with “incoming” graduate students into research groups:

- Wide variability in basic computer and computational skills and experience
- Unless students had already been partially trained in other research groups:
 - Rarely have previous experience with HPC
 - Would not know about the existence of, or the use of local, state-wide or national computing resources
 - Rarely worked in large, distributed teams
 - Often didn't work on large software projects yet



- ① Survival skills for Unix environments
- ② Revision control systems; Collaboration / project management
- ③ Simple data visualization
- ④ Three-dimensional data visualization





- Module B: Advanced Programming Tools
- Faculty at CCT, Computer Science
- Software development specialist
- HPC expert

- Compiling
- Debugging
- Profiling
- Programming (best) practices
- Accelerator computing

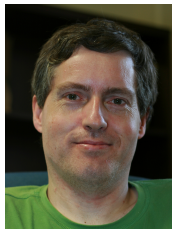




- Module C: Parallel Computing
- Assistant Professor at CCT, Computer Science
- Parallel programming and HPC expert
- C++ “guru”

- The future of computing: going parallel
 - MPI
 - OpenMP
 - other choices
- Challenges in parallel computing
 - typical bottlenecks
 - possible (future) solutions





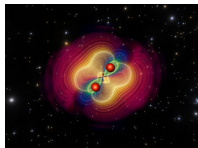
- Module D: Simulations and Application Frameworks
- Assistant Professor at CCT
- Relativistic Astrophysics
- High-Performance Computing

Simulations and Application Frameworks

Aim: explain the essential elements of modern simulation codes that are run on parallel supercomputers, especially Xsede systems.

Examples at LSU:

- modeling black holes
- predicting the effects of hurricanes
- optimizing oil and gas production from underground reservoirs



Often not understood by students:

- typical code structure
- scientific goals and needs
- hardware and technology limitations





- Module E: Distributed Scientific Computing
- Assistant Professor, ECE, Rutgers University
- Former director of Cyberinfrastructure Development at CCT
- Distributed computing expert



Distributed Scientific Computing

- Introduction to the Practice of Distributed Computing
 - Definition and application examples
 - Comparison to HPC
- Introduction to SAGA
- Examples of “production” grid infrastructure
- Building own distributed applications
- Introduction to Cloud computing
 - Commercial/Enterprise Clouds
 - FutureGrid
- When to compute distributed and when rather not



- Emphasis on practical work and experience
- No aim at tricky exam questions: convince with your experience
- Don't leave coursework until the last moment: it does **not** work here
- Course work of each module counts.
- No midterm, but review session
- Final Exam will be oral and will cover all modules.

Module A course work	15%
Module B course work	15%
Module C course work	15%
Module D course work	15%
Module E course work	15%
Final Exam	25%



Famous Last (First) Words

- This class is for **YOU**
- Ask questions
- Give suggestions
- Do course work **early**
- Let us know of problems right away



Course Work: some general remarks

- Do it early!
- Course work will form 75% of your grade!
- If you have problems: contact us. This will not lower your grade. The only change it might have on your grade is positive.
- To be submitted electronically (see below)
- Deadlines are strict (end of the deadline day)



Course Work: some general remarks

- If not asked otherwise, submit reports in pdf, as single file. Other formats will not be accepted.
- If you are asked to write a program, submit the source code (text file, no pdf here) and, if applicable, a makefile - not the executable
- Make the reports look nice. This is (also) an exercise in report/paper writing.
- Include your name, the class number (CSC 7700) and a date.
- If you have graphs or pictures, include them in the pdf file. Don't submit separate files unless asked for.



Course Work A1

No pdf reports yet, but:

<https://portal.xsede.org/>

- Create Account
- Submit all necessary information and verify account
- **ASAP!**
- Send us email with your Xsede user name to sci-comp-2013-instructors@mail.cct.lsu.edu

https://accounts.hpc.lsu.edu/login_request.php

- Request login
- Submit all necessary information and verify account
- LSU contact: Frank Löffler (Center for Computation and Technology)
- **ASAP!**
- Send us email with HPC user name to sci-comp-2013-instructors@mail.cct.lsu.edu

