Interdisciplinary Computational Graduate Education

CHEM 243, COGS 243, EECS 243, MATH 243, ME 243, PHYS 243, PSY 243, QSB 243

Spring 2018 Syllabus

This one-credit course is designed as the primary educational vehicle for the Interdisciplinary Computational Graduate Education (ICGE) Program, a National Research Training program funded by the National Science Foundation. The goal of this program is to create a systematic, integrated approach to decreasing attrition among first-year graduate students in computational science-related fields, including underrepresented minority and first-generation graduate students. The program ties this explicitly to career preparation for research positions in industry and national laboratories, as well as academia. This course consists of team-taught modules on topics including scientific programming, planning and managing team-based projects, creating effective technical presentations, as well as providing advice on success in graduate school and in future careers. See below for module descriptions.

The ICGE program and this course have five **Course Learning Outcomes**:
1. ***Professionalization*** within the context of an interdisciplinary computational science research project
2. ***Team science*** and project management skills pertaining to managing knowledge-intensive projects
3. Fundamental ***research skills*** including writing scientific papers, literature reviews, scientific presentation, and research ethics
4. ***Computational skills*** including techniques for managing data, coding, data structures, visualization, and analytic techniques
5. ***Career preparation*** to work in and with industry and the national labs as well as the academy

These **Course Learning Outcomes** for this cross-listed course support student development in the following **Program Learning Outcomes** for seven different graduate programs:

Applied Mathematics

PLO #4, Model real-world problems mathematically and analyze those models using their mastery of the core concepts.

Chemistry & Chemical Biology

PLO #4, Be proficient in laboratory, theoretical, and/or computational techniques necessary to contribute to knowledge in their chosen subfield of chemistry.

Cognitive & Information Sciences

PLO #4, Ability to integrate knowledge across the disciplines that compose cognitive and information sciences.

Electrical Engineering & Computer Science

PLO #3, Are able to design and conduct experiments and computational simulations for the purpose of evaluating and comparing proposed solutions on the basis of empirical evidence.

Mechanical Engineering

PLO #3, Are able to design and conduct experiments and/or simulations of mechanical systems, and to analyze and evaluate.

Physics

PLO #2, Have the experimental, theoretical, and/or computational skills necessary to conduct and lead independent responsible research and contribute to knowledge in their chosen subfield.

Psychology

PLO #2, Statistics and Methods: Graduate students will demonstrate skills in the use of the basic data gathering methods and statistical techniques used for typical analyses in conducting research in the Psychological Sciences.

Quantitative & Systems Biology

PLO #1, Knowledge and understanding of quantitative (statistical, computational, and model dependent) and high-throughput experimental systems approaches to biological problems, and demonstrated ability to conceive, plan, execute and/or interpret the applications of these approaches to research questions.

The faculty for this course are:
Marjorie Zatz (PI), Paul Maglio (Co-PI), Michael Spivey (Co-PI), and Michael Colvin, Sayantani Ghosh, Arnold Kim, Ashlie Martini, Suzanne Sindi, and Mukesh Singhal. We can best be reached by email.

Grading Policy: Students will be expected to participate fully in all training modules, including (a) programming exercises, (b) performance on team projects, (c) oral presentation of project results, and (d) contribution to discussion. Students will receive grades that are based on their performance in all four categories (with equal weighting). As per Graduate Division policy, a minimum letter grade of B is required to pass this course.

Class Policy: Students are expected to attend all class times, and participate courteously and respectfully in group discussion and team projects. Students are encouraged to bring their own laptops to class (with appropriate software installed) for programming exercises. Instructions for software installation will be provided via email. If a student must miss a class for personal reasons, he/she should inform one of the instructors in advance of this upcoming absence. Missed programming exercises cannot be made up.

Integrity Policy: This course is committed to promoting an ethically responsible approach to science and education. Any reports of academic misconduct, such as cheating, fabrication, plagiarism, or facilitating academic dishonesty, should be referred to the Office of Student Conduct: `studentconduct@ucmerced.edu`

Disability Services Information: This course is committed to promoting equal educational access and full participation by and for students with disabilities. Reasonable accommodations will be made for any student requesting them, with the assistance of the Disability Services Office of UCM: `disabilitiservices@ucmerced.edu`

Schedule of Activities:
The Interdisciplinary Computational Graduate Education Program will meet every Friday during the spring semester from 2-5 pm for instruction and team-based work.

<u>Jan 19 – Instructional Module 1:</u>
Practices and Habits of Successful Graduate Students in the Interdisciplinary Computational Sciences. *Lead faculty*: Zatz, Ghosh, Maglio, and Spivey

<u>Jan 26 - Instructional Module 5:</u>
Team Science and Project Management. *Lead faculty*: Maglio, Zatz and Spivey
Finalize project teams, topics, and expert advisers

<u>Feb 2 – Instructional Module 2:</u>
Interactive Programming with Matlab**.** *Lead faculty*: Spivey

<u>Feb 9 – Instructional Module 2:</u>
Interactive Programming with Matlab**.** *Lead faculty*: Spivey

<u>Feb 16 Instructional Module 3:</u>
The Linux Operating System and Shell Scripting. *Lead faculty*: Sindi

<u>Feb 23 – Instructional Module 2:</u>
Interactive Programming with Python**.** *Lead faculty*: Colvin
with pointer to C++ workshop outside of class

<u>March 2 – Instructional Module 2:</u>
Interactive Programming with Python**.** *Lead faculty*: Colvin
Progress update on team projects

<u>March 9 – Instructional Module 2:</u>
Interactive Programming with R**.** *Lead faculty*: Colvin

<u>March 16 – Instructional Module 4:</u>
High Performance Clusters and Remote Supercomputers. *Lead faculty*: Martini and Singhal, assisted by Jeffrey Weekley (Director of Cyber Infrastructure and Research Computing)

March 23 – Project Team Work Day: *Lead faculty: All team faculty mentors*

April 6 – Instructional Module 5:
Team Science and Project Management. *Lead faculty*: Ghosh, Maglio, Zatz
with a focus on interfacing computation and experimental data collection

April 13 – Instructional Module 1:
Practices and Habits of Successful Graduate Students in the Interdisciplinary Computational Sciences. *Lead faculty*: Zatz, Ghosh, Maglio, and Spivey
with a focus on team projects

April 20 – Presentation Training. *Lead faculty*: Zatz, Maglio, and Ghosh

April 27 – Project Presentations by 2 student teams

May 4 – Project Presentations by 2 student teams

May 11 – Celebration and recognitions

A description of the six instructional modules, including their format, objectives, and anticipated outcomes, follows below:

Module 1: **Practices and Habits of Successful Graduate Students in the Interdisciplinary Computational Sciences.** *Lead faculty*: Zatz
Format: In addition to the orientation, four 30-minute instructional sessions plus continuous hands-on experience in project teams and at final group presentation.
Objectives: Provide students expectations and goals for graduate school and beyond. *Student Learning Objectives*: 1 (Professionalization) and 5 (Career Preparation).
Description: This module will provide students the fundamental, non-technical skills needed in graduate school such as clarifying the nature of the Ph.D. and how it differs from undergraduate studies, ethical practices in research, and preparing publications, presentations, webpages, curriculum vitae, etc. through participation in discussions and activities with an inclusive community of scholars. In addition, students will be introduced to the value of interdisciplinary and transdisciplinary research and to the broad spectrum of career opportunities in the computational and data sciences. To hone their oral communication skills, project participants will participate in GradSlam, a UC system-wide competition in which students must present their research in three minutes. Writing skills will be addressed through Dissertation Boot Camp and through the publishing and grant writing workshops offered by the Graduate Division. Students may also participate in our Preparing Future Faculty and Preparing Future Professionals series, which include forums on choosing between academic and nonacademic careers, the

postdoctoral research experience, interviewing for academic positions and negotiating the job offer, surviving and thriving as faculty of color, employment opportunities for Ph.D.s in industry, business, government, and nongovernmental organizations, preparing for jobs in industry, and National Labs Day (see http://graduatedivision.ucmerced.edu/GEARS). In addition, UC Merced has a subscription to the National Center for Faculty Development and Diversity and the Versatile Ph.D. and we will draw on webinars and other resources from these clearinghouses.
Outcomes: Upon completing this module, students will have adjusted to graduate school, and will have developed a curriculum vitae, personal webpage, and Independent Development Plan.

Module 2: **Interactive Programming.** *Lead faculty*: Colvin and Spivey, assisted by Jeffrey Weekley, Director of Cyber Infrastructure and Research Computing
Format: Four 45-minute instructional sessions plus continuous hands-on experience in project teams.
Objectives: Provide experience successfully writing, testing, and validating programs in several interactive and scripting programming environments such as Matlab, R, Python, and CalVR. *Student Learning Objectives:* 2 (Team Science), 3 (Research Skills) and 4 (Computational Skills).
Description: This module will teach students fundamentals of programming such as data structures, logical operations, loops, and data management and visualization using interactive programming environments. Data visualization will include virtual immersion demonstrations in our Virtual Reality CAVE (Computer Assisted Virtual Environment), an intracampus facility housed in the Digital Humanities Lab.
Outcomes: Upon completing this module, teams of students will have developed, tested and cross-validated codes in Matlab, R, Python, and CalVR to solve problems relevant to their own research and, in so doing, gained team science skills.

Module 3: **The Linux Operating System and Shell Scripting.** *Lead faculty*: Sindi
Format: Four 45-minute instructional sessions plus continuous hands-on experience in project teams.
Objectives: Provide experience working with the Linux operating system and developing shell scripts. *Student Learning Objectives*: 3 (Research Skills) and 4 (Computational Skills).
Description: This module will teach students how to manage files, transfer data, and execute programs in the Linux operating system.
Outcomes: Upon completing this module, the students will be able to use commands in the Linux operating system to organize and parse data files, to transfer data between computer systems, and write scripts to automate program execution and data analysis.

Module 4: **High Performance Clusters and Remote Supercomputers.** *Lead faculty*: Martini and Singhal, assisted by Jeffrey Weekley (Director of Cyber

Infrastructure and Research Computing) *Format*: Two 60-minute instructional sessions plus continuous hands-on experience in project teams.
Objectives: Provide experience accessing and using high performance clusters and remote supercomputer systems, such as those on the NSF-funded XSEDE network. *Student Learning Objective*: 4 (Computational Skills).
Description: Each student will be provided an account on an XSEDE supercomputer as part of an educational allocation, learn about accessing and using this computer, write scripts to run programs in the supercomputer's queuing system, and run a series of benchmark simulations.
Outcomes Achieved: Upon completing this module, students will be able to effectively use local and remote supercomputing resources for their graduate research.

Module 5. **Team Science and Project Management.** *Lead faculty*: Maglio
Format: In addition to the orientation, four 30-minute instructional sessions plus continuous hands-on experience in project teams and at final group presentation.
Objectives: Provide experience with managing projects using a team science approach, and provide deep understanding of the technological and social challenges and opportunities associated with team science. *Student Learning Objectives*: 1 (Professionalization) 2 (Team Science), 3 (Research Skills), and 5 (Career Preparation).
Description: In this module, students will learn project management and teamwork skills. The weekly project team activities will teach participants about the technology-based tools that enable collaboration and project management and how to identify and structure a project, organize the team, break the work into subprojects, and assess team performance. They will learn to identify and address different types of problems and the scientific skills necessary to complete those projects. We will place additional emphasis on training them to connect their interpretation to experimental data and outcomes. In particular, they will learn to describe a set of data using appropriate statistical methods,
evaluate the accuracy of their analysis in the context of physical problems and communicate the results of computations in meaningful and effective ways. The goal of this exercise will be to close the bridge between computation and experimental assessments.We will also familiarize students with basic team science tools, skills and principles as well as different frameworks for developing solutions to real-world problems, thus enabling our students to transition from incremental research to transformational breakthroughs. Students will utilize various cloud-based tools and platforms for cooperation and coordination.
Outcomes Achieved: Upon completing this module, students will be able to efficiently and effectively participate in team science projects, and be able to assess and diagnose issues related to team effectiveness and efficiency.

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Example Interdisciplinary Projects from previous year:

Project Name: "Network Analysis of Power Grid Integrity"
Team Name: "Power Rangers"
Team: Jon Anzules (QSB), Ayme Tomson (CIS), Taran Rallings (QSB) Advisory Board
Mentor: Mihai Anitescu (Argonne)
Faculty Mentors: Ashlie Martini, Paul Maglio, Michael Spivey

Project Name: "Sense Air: Custom Air Quality Reports"
Team Name: "Sense Air"
Team: Amin Boroomand (QSB), Adolfo Ramirez-Aristizabal (CIS), Imtiaz Ali (Physics), Jackie Shay (QSB)
Advisory Board Mentor: Spike Narayan (IBM) and Janice Zdankus (HPE)
Faculty Mentors: Michael Colvin

Project Name: "Cosmological Data Analysis"
Team Name: "Pale Blue Dot"
Team: Jose Zamora (BEST), Alyssa Funk (QSB), Farnaz Golnaraghi (Physics), Thomas Thayer (EECS)
Advisory Board Mentor: David Brown (LBNL)
Faculty Mentors: Arnold Kim, Juan Meza

Project Name: "SADI: Smart Archeology Investigator"
Team Name: "Indiana Drones"
Team: Derek Hollenbeck (ME), Jeramias Gonzalez (Physics), Katherine Shurik (IH)
Advisory Board Mentor: David Berger (NASA)
Faculty Mentors: Mukesh Singhal