PHYS 693 Core Skills for Computational Science

Content

This course provides students of computational sciences an introduction to the basic skills required to operate in the modern high performance computing (HPC) environment offered at the Arctic Region Supercomputing Center (ARSC). Topics include an introduction to HPC, basic Unix/batch/scripting skills, performance programming, shared and distributed memory parallelism, code profiling and debugging, data storage and management, and data visualization. Each of these topics will be presented in lecture format, however to provide additional applied knowledge, either a thorough case study by a guest speaker, and/or a hands-on lab session will be given in support of each. After completing this class you will be able to access high performance computers, write scripts to control jobs and data on those machines, write simple programs (in Fortran or C), profile and optimize programs on HPC machines, parallelize programs for massively parallel HPC machines and visualize the data outputted from these machine.

PHYS 693 as ARSC User Training

In the past, components of this class have been regularly offered as individual training sessions by the staff at ARSC. The impetus for creation of the 'core skills' class was to provide a more intensive training environment for new student users, while still providing distinct modules for more advanced researchers to refresh/update skills.

As such, the PHYS 693 lectures are open to any interested individuals. While the structure, lectures, labs and grading policies of this course are designed for UAF students enrolled in the course for credit, the course doubles as ARSC user training. ARSC users and prospective ARSC users are strongly encouraged to attend any lectures they would find beneficial. There will be no other formal ARSC user training on these topics offered this fall.

Instructors

This course will be taught by several instructors including Arctic Region Supercomputing Center staff, UAF Physics department faculty and guest speakers.

Contacting Us

The primary points of contact for the class are:

Tom Logan, Elvey 511-G, 474-5789, talogan@alaska.edu ARSC Help Desk, WRRB 105, 450-8602, consult@arsc.edu

Links to Course Syllabus, Homework, and References

Schedule & Lectures	<u>Homework</u>	References

In approaching this (and all) classes, please note the following ancient Chinese proverb: Teachers can open the door, but you must enter by yourself.

Prerequisites

Graduate standing in physical sciences; experience with FORTRAN or C programming language; or permission of instructor.

Lectures/Lab Meeting Time and Place

West Ridge Research Building 009, Tuesday/Thursday, 9:15 - 11:15am

Grading

The course grade will consist of the following components

Homeworks 40 % Semester project 30 % Mid-term 20 %

Attendance and Participation 10 9

Grading Components

Homework: There will be approximately one homework assignment per week. The assignment will be given out and posted on the web. These assignments help in assessing your understanding of the material, and will count as a major part of your final grade.

Project: There will be a semester project, which will require a final presentation and paper.

Mid-term Exam: A mid-term exam will be given.

Special Needs

The Office of Disability Services implements the Americans with Disabilities Act (ADA), and insures that UAF students have equal access to the campus and course materials. We will work with the Office

of Disabilities Services (208 WHIT, 474-5655) to provide reasonable accommodation to students with disabilities.

Plagiarism

Plagiarism and cheating are matters of serious concern for students and academic institutions. This is true in this class as well. The UAF Honor Code (or <u>Student Code of Conduct</u>) defines academic standards expected at the University of Alaska Fairbanks which will be followed in this class. (Taken from the <u>UAF plagiarism web site</u>, which has many links with good information about this topic)

Complaints and Concerns

You are always welcome to talk to the instructors about anything, however, if you have a non-subject matter question or concern that cannot be resolved by the instructors contact the department chair, Dr. Szuberla, Physics Department Office, room 110 Reichardt.

9 August 2013, Friday 17:02





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List of References

Unix for Dummies - Quick Reference (IDG Books)

Unix in a Nutshell (O'Reilly)

Linux in a Nutshell (O'Reilly)

Fortran 90/95 Explained, Metcalf & Reid, Oxford Univ Press, 1999

Fortran 90 for Engineers and Scientists, Larry Nyhoff and Sanford Leestma, Prentice-Hall, 1997

Parallel Programming in OpenMP (Chandra et al)

Using MPI (Gropp, Lusk, & Skjellum)

Parallel Programming with MPI (Pacheco)

List of Related Links

Introduction to Using PACMAN Cluster

Introduction to Using Cray Fish Cluster

ARSC HPC Newsletters

List of Fortran Tutorials

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This Site is Mobile Web Ready





PHYS 693

Core Skills for Computational Science

Date	Instructor Topic								
5-Sep	TL	Topic							
	ON	Introduction to ARSC & HPC							
10-Sep	TL	Introduction to Linux / Semester Project							
12-Sep	TL	Data Management / Unix Scripting							
17-Sep		Introduction to Fortran, Part 1							
19-Sep	TL	Introduction to Fortran, Part 2 (Lab session)							
24-Sep	TL -	Introduction to PACMAN and Fish Supercomputers							
26-Sep	TL	Makefiles (Lab session)							
1-Oct	TL	Viz 1: Basic Visualization Tools							
3-Oct	TL	Performance Programming Part I Part II							
8-Oct	TL	Performance Programming Part III / Debugging							
10-Oct	TL	Profiling and Introduction to CrayPat							
15-Oct	TL	Parallel Processing Concepts & Parallel Shared Memory Programming, Part 1							
17-Oct	TL	Parallel Shared Memory Programming, Part 2							
22-Oct	TL	Parallel Shared Memory Programming, Part 3 (Lab session)							
24-Oct	SM	Viz 2: Visualization Overview and Graphics Formats							
29-Oct	SM	Viz 3: Animation 101 (Lab session)							
31-Oct	DM	Parallel Programming Application (Example)							
5-Nov	TL	MIDTERM EXAM							
7-Nov	DN	Validation & Verification							
12-Nov		CANCELLED							
14-Nov		CANCELLED							
19-Nov	TL	Parallel Distributed Memory Programming, Part 1							
21-Nov	TL	Parallel Distributed Memory Programming, Part 2							
26-Nov	ΤL	Introduction to Co-Array Fortran							
28-Nov		Thanksgiving Holiday							
3-Dec	RT	GPGPU Programming							
5-Dec	KH	Version Control Systems							
10-Dec	DN	Giving Effective Presentations							
12-Dec		Open Session - Project Work							
17-Dec	TL	Final Presentations - Time TBD							
Key	Instructor		Position	E-mail	Office	Phone Ext			
DM	Don Morton		Research Professor	Don.Morton@alaska.edu	WRRB 105	8679			
DN	David Newman		Professor of Physics	denewman@alaska.edu	REIC 112	7858			
KH	Kate Hedstrom		Oceanographic Specialist	kshedstrom@alaska.edu	WRRB 105	8678			
ON	Oralee Nudson		User Consultant	onudson@alaska.edu	WRRB 105	8637			
RT	Bob Torgerson		HPC Systems Analyst	rltorgerson@alaska.edu	WRRB 105	8694			
SM	Sergei Maurits		HPC Specialist	samaurits@alaska.edu	WRRB 105	8697			
TL	Tom Logan		Associate Faculty	talogan@alaska.edu	Elvey 511-G	5789			