MATH 150-03 / COMP 150-07, High Performance Scientific Computing, Fall 2016

Department of Mathematics, Tufts University
Block F: (Tue, Thr, Fri, 12:00 - 12:50 PM), 26 Winthrop St Room 113
Instructor: Sergey Voronin (http://math.tufts.edu/faculty/svoronin/)
Email: sergey.voronin@tufts.edu
Office: 202 Bromfield-Pearson
Office Hours: Thr 3:30-5:30 PM, Fri after class and 3:00-4:00 PM
Prerequisites: Linear algebra (Math 70 or equivalent) and programming experience with Matlab.
Text: The following Tufts library electronically available textbooks will be used:
Numerical Linear Algebra with Applications by William Ford;
The C Programming Language, Second Edition by Brian W. Kernighan, Dennis M. Ritchie;
Linux Phrasebook, Second Edition by Scott Granneman;
An Introduction to Parallel Programming by Peter Pacheco;
Instructor supplied notes and source codes.

Description and learning objectives

This course will present the fundamentals of scientific computation using multi-core, multi-processor, and GPU computing architectures. We will look at some fundamental algorithms in numerical linear algebra and iterative methods with applications to some typical inverse problems and present the necessary steps to implement and run these algorithms on high performance shared and distributed memory systems, both from the ground up and using existing software libraries. The course will give the attendee the experience of prototyping, developing, and deploying efficient code for scientific applications on high performance computing platforms and research clusters.
Learning objectives for the course are $\{1b, 3a, 4c, 5a\}$, as specified in: http://ase.tufts.edu/faculty/committees/objectives/math.htm.

Homework and grading

There will be 5 homework assignments (individual) and one final project (for which you can work in small groups of at most 3 people). Grading is based on a maximum total of 100 points. Each homework is 15 points, for a total of 75 points. The final project is 25 points. Each student will apply for a Tufts research cluster account and the programming assignments will be tested and uploaded on the cluster for submission. All assignments (code and accompanying pdf file) are due on Sunday nights by 11:59 PM uploaded to a specific folder on the cluster (to be clarified). Late submissions are discouraged (20 % penalty is applied for .5 to 12 hours late; 40 % for 12 - 24; and so on).

Translation to letter grades will be based on your score relative to the class median out of 100 points and the IQR (the interquartile range). A score close to the median would correspond to the B letter (B-,B,B+) range. A total score below the median minus $1.5 \times$ IQR would be eligible for a failing grade.

- A range : $\approx$ median $+ 0.75 \times$ IQR, B range : $\approx$ median, C range : $\approx$ median $- 0.75 \times$ IQR
- D range : $\approx$ median $-$ IQR, F : $<$ median $- 1.5 \times$ IQR

The above are only rough guidelines! Exact grade cutoffs will be developed at the end of the course after all the scores have been compiled.

Note that you will be required to program in C and C++ for the assignments and to use a Linux command line interface when connected to the Tufts cluster. An introductory workshop on "*Basic Linux tools and C/C++*" will be given (in evening hours) as a supplement to the first unit.

Student accessibility services

If you need an accommodation due to a documented disability, you must register with the Student Accessibility Services Office at the beginning of the semester. To do so, call the Student Accessibility Services office at 617-627-4539 to arrange an appointment with Linda Sullivan, Program Director of Student Accessibility Services.

Schedule

The course is divided into five units, roughly as follows:

- Linux tools, Tufts cluster, Matlab, C/C++, mex files. Dense and sparse BLAS.
- Numerical linear algebra and iterative methods. Examples with the GNU GSL library.
- Multi-core computing with OpenMP and the Intel MKL library. Inverse problems 1.
- GPU computing using NVIDIA CUDA and associated tools. Inverse problems 2.
- Multi-processor computing with MPI and the PETSc and ScalaPACK packages. Additional topics.

We will follow the schedule below per local time. All homework will be posted on the instructor's website.

Unit 1	9/6, 9/8, 9/9	
	9/13, 9/15, 9/16	
	9/20, 9/22	
	Intro workshop on 9/9 and 9/12 (evenings, 7 - 8:30 PM). **HW 1 due 9/25 by 11:59 PM.**	
Unit 2	9/23	
	9/27, 9/29, 9/30	
	10/4, 10/6, 10/7	
	10/11	
	HW 2 due 10/16 by 11:59 PM.	
Unit 3	10/13, 10/14	
	10/18, 10/20, 10/21	
	10/25, 10/27, 10/28	
	11/1	
	HW 3 due 11/06 by 11:59 PM.	
Unit 4	11/3, 11/4	
	11/8, 11/10	
	11/15, 11/17, 11/18	
	11/22	
	HW 4 due 11/27 by 11:59 PM.	
Unit 5	11/29	
	12/1, 12/2	
	12/6, 12/8, 12/9	
	HW 5 due 12/11 by 11:59 PM.	
Final project due 12/18 by 11:59 PM.		