

Computational Methods

CMSC/AMSC 460

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Course Goals

- Introduction to the use of scientific computing techniques to solve problems in various domains
- Understand principles behind algorithms
- Intelligent choice and use of available software
- Understand how to
 - Convert a model into a discrete system on the computer
 - How to deal with data
 - Perform simulations for applications
 - Display and evaluate simulation results
 - Appreciate which computations are feasible
 - Understand how erroneous the computations could be

“New Paradigm”

- Scientific Discovery through Computing
- Paradigm?
 - A set of assumptions, concepts, values, and practices that constitutes a way of viewing reality for the community that shares them, especially in an intellectual discipline.
- Engineering (aeronautics, fluid dynamics, circuit design, radar, antennas, signal processing, ...)
- Physics (stellar dynamics, materials, ...)
- Economics/Sociology (modeling and analyzing data, computational statistics, stock picking, ...)
- Biology (biostatistics, computational biology, genomics and proteomics, ...)
- Chemistry (molecular dynamics, drug design, activity recognition ...)
- Computer Science (modeling systems/network performance, information retrieval, ...)
- Your field ...

Another “paradigm”: Data driven science

- Grab data and process it
- Audio, video, text, MRI, X-Ray, weather, strain-gage, flow, gene-chip, seismograph, ...
- Moore’s law drives both processing power, memory, sensor cost and capability
 - Moore’s law: Processor speed doubles every 18 months
 - More generally: Technology X capability will double in Y months
- Need algorithms to process larger and larger data sets, and extract information from them
 - Fit data, Extract model parameters, Learn relationships
 - In general compute with the data

The Course

- Three lectures a week
- Homework every week or other week
- 30% homework, 20% exam 1, 20% exam 2, 30 % final
 - Attendance/participation will be a factor
 - No make up exam ... will scale your other exam grade
- Class web site:
<http://www.umiacs.umd.edu/~ramani/cmssc460/index.html>
- Required Book

Numerical Computing with MATLAB by Cleve Moler

- The good news: complete book is online!
- Book is also not as expensive as some others (~\$40)

Software: Matlab

- Matlab is essential
- Two choices
 - Choice 1: Use university computers that already have Matlab on them
 - Choice 2: Buy the student edition of Matlab for your personal use
- Can give pointers, but cannot support the installation or access to the software
- Book comes with Matlab software that is downloadable from the book web site
 - Some homework will use that software

Homework

- Homework will involve programming in MATLAB
- mainly problems from the text
- Style/Clarity/Cleanliness of output will count
- Work/Results must be easily understood to be interpreted
 - Visualization (graphs)
 - Commented code
- Remember the grader is a busy student doing his own courses/research

Syllabus

- **Introduction, Computer Arithmetic and Errors** (Chapter 1) (approx. 4 lectures)
 - course survey
 - introduction to Matlab
 - machine arithmetic and error analysis
 - stability and conditioning
- **Solving Linear Systems of Equations** (Chapter 2) (approx. 6 lectures)
 - Gaussian elimination
 - well-conditioning vs. ill-conditioning, matrix and vector norms
 - Notions of algorithm complexity
 - sparse systems: direct and iterative methods