

CS/MATH-4414 (CRN 17864/18511)
Issues in Scientific Computing
Spring 2012

Essential information.

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Teaching assistant	Ji Wang (wji@cs.vt.edu)
Office hours	Thu 12:45–1:45, 122 McBryde Hall

Lecture	Tue–Thu, 11:00–12:15, 307 McBryde Hall
Web Page	http://www.cs.vt.edu/~asandu/Courses/CS4414/CS4414.html
Prerequisites	MATH 2214, MATH 3214
Final Exam	Section 11T, May 4, 2012, 10:05–12:05

Textbook.

Our main textbook is Michael T. Heath: “Scientific Computing: An Introductory Survey”, 2nd ed., McGraw-Hill, 2002. Web materials from this text are available at <http://www.cse.illinois.edu/heath/scicomp>.

Another good reference textbook is Cleve Moler’s “Numerical Computing with MATLAB” available online at <http://www.mathworks.com/moler>.

Additional materials will be indicated in class and posted on the web.

Topics.

- **Floating point arithmetic. Roundoff errors.** From PC’s to supercomputers, all systems have special floating point hardware; compilers are called upon to optimize floating point implementations; and operating systems are designed to properly respond to floating point exceptions such as overflow. We will discuss the IEEE standard, floating point formats, rounding errors and rounding modes, floating point exceptions, and error propagation. IEEE standard, floating point formats.
- **Accuracy of algorithms. Truncation errors.** We will discuss the basic aspects of approximation; how a continuous mathematical model is turned into a discrete model, which is suitable for computer implementation. Truncation errors, due to approximations in the mathematical formulation. Examples from interpolation and function approximation, and from discretization of differential equations.
- **Conditioning of problems.** Some problems are more sensitive to approximation errors than others, being less amenable to computer formulations. We will talk about well and ill conditioning, error propagation, and forward and backward error analysis.
- **Stability of algorithms.** Propagation of errors through numerical algorithms and its effect on the solution. Examples from linear algebra and differential equations.

- **Efficiency of algorithms. Sparse matrices.** Specialized data structures and algorithms that exploit the special particularities of a problem can greatly enhance performance. Different representations of sparse matrices and several associated algorithms will be discussed.
- **Efficiency of computer implementations. Cache friendly programming.** Many times scientific and engineering (floating point) models take hours, days or even weeks to complete. Can we speed up the computations while preserving the quality of the results? Sometimes a simple loop rearrangement can make a considerable impact on the code performance. Other times we need to rethink the whole computational algorithm, for example, we may look for and exploit the inherent parallelism in the problem. Examples using matrix multiplication techniques; blocking; BLAS level 1 through level 3.
- **Examples and numerical software.** Algorithms from linear algebra, approximation, optimization, finite difference and finite element methods, numerical ODE's and PDE's, etc. will be discussed. Mathematical software packages like BLAS and LAPACK will be used to exemplify the concepts exposed in this course.

Grading.

Homework will consist of programming assignments (in Matlab and {Fortran or C}) and of written exercises. Homework will be submitted via Scholar. No late homework will be accepted. Homework will account for 30% of your grade. There will be one midterm exam/project and one final exam/project, each accounting for 35% of the total grade.

Disclaimer.

Some information given to you in class may supersede the information in this syllabus.

Student Complaints and Academic Misconduct.

The Virginia Tech Honor Code applies. If you have any problems, the first step is to discuss with me directly. Should you need to speak with the Chair of the C.S. Department, you can make an appointment by speaking with the Departmental Secretary in Knowledgeworks II.

Disabilities.

Please let me know if you have a disability which requires special arrangements.