# Scientific Computing, Spring 2012

## Logistics

*Course webpage*
`http://cims.nyu.edu/~donev/Teaching/SciComp-Spring2012/`
including links to textbook and software, assignments, and lecture slides

*Registration* 3pts per semester, MATH-GA.2043 (math) or CSCI-GA.2112 (computer science)

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*Graders* Juan Calvo (*calvo@cims.nyu.edu*), office hours Mondays, 4-6pm, 705 Warren Weaver Hall
Aaron Eastburn (*ae593@cims.nyu.edu*), office hours Fridays, 4-6pm, 705 Warren Weaver Hall

*Lectures:* 5:10 - 7 pm Thursdays, 109 Warren Weaver Hall (Courant Institute)

*Office Hours:* 4 - 6 pm Tuesdays, or by appointment

*Communication* Blackboard (accessible via NYU Home) will be used for messages, assignments, and grading.

## Content

This course is a graduate-level introduction to practical introduction to computational problem solving, including both mathematical analysis of numerical algorithms (numerical analysis) and practical problem solving. This is not a programming course but programming in homework projects with Matlab (Python, Fortran, C/C++, or other language of your choice) is an important part of the course work.

### Textbooks

*Required (primary)*
***Scientific Computing with MATLAB and Octave***, Alfio M. Quarteroni & Fausto Saleri, Springer, ***any*** *edition*. The second edition is available in PDF form through the library, and a paper copy is available on 2h reserve in the Courant Library.

*Optional (secondary)*
Draft of an upcoming book Principles of Scientific Computing by my colleagues Jonathan Goodman and David Bindel, see course webpage for links.

*Additional* Some suggestions are on the course webpage, and of course lots of free online materials.

### Prerequisites

A good background in linear algebra (review it *before* the first class), and experience with writing computer programs (in Matlab, Python, Fortran, C, C++, or other language). Prior knowledge of Matlab is not required, but it will be used as the main language for the course. If you have experience with compiled languages (Fortran, C, C++), Matlab will be easy to learn and use, and comes with a great help facility.

This course will be challenging and lots of material will be covered in a short period of time! Some background review will be done at the end of each class, but this will assume you have already been exposed to the material.

### Assignments and Grading

There will be regular (biweekly) *challenging* assignments and a take-home final project. The assignments will be mostly computational but some will be theoretical problems. You will be expected to submit a PDF of your solutions, as explained in more detail in the course webpage. The grade will be 70% based on assignments and 30% on the final, and the grading scale can be found on the course webpage. Solutions of assignments will be posted after the deadline so no late submissions will be accepted.

Academic integrity policies will be strictly enforced for homework assignments. Each student must write the solutions independently. Copying of any portion of someone else's solution or allowing others to copy your solution is considered cheating. Code sharing is not allowed. You must type (or create from things you've typed using an editor, script, etc.) every character of code you use.

### Computing

Computing on your own will form an essential part of the learning process and you will be expected to learn and use Matlab. Please become familiar with MATLAB and gain access to a running version (e.g., via a Courant computer account, student version from computer store) *before* the first class. Learning how to apply the methods we discuss in class in practice is a critical part of this course and the main component of your grade. You will also be expected to present your results effectively, e.g, using clearly-annotated figures.

### Tentative Schedule

This is only a tentative agenda for the lectures.

- Jan 26th: *Numerical Computing*: Well posedeness, numerical conditioning, stability, and scientific software (MATLAB, compiled languages, GPUs, etc).
- Feb 2nd: *Sources of Error*: Truncation and floating-point roundoff error and their analysis. IEEE floating point standard.
- Feb 9th: *Dense Linear Systems*: Conditioning, Gaussian elimination, LU factorization, Cholesky factorization, pivoting.
- Feb 16th: *Symmetic, Overdetermined and Sparse Linear Systems*: Banded systems, sparse factorizations and reordering.
- Feb 23rd: *Eigen and Singular Values*: diagonalization, QR and SVD decompositions. Power method. Applications such as principal component analysis.
- Mar 1st: *Nonlinear Equations*: One dimensional root finding (bisection, secant), fixed-point iteration, Newton's method, safeguarded Newton, higher dimensions.
- Mar 8th: *Unconstrained optimization*: steepest descent, conjugate-gradient, Quasi-Newton methods.
- **Mar 15th**: No class, **spring break**
- Mar 22nd: *Interpolation*: Polynomial interpolation (Newton, Lagrange) in one dimension. Piecewise polynomial interpolation. Least squares approximation. Extensions to two and three dimensions.
- March 29th: *Numerical Integration*: One-dimensional quadrature (midpoint, trapezoidal, Simpson, Newton-Cotes, Hermite methods, etc.), Richardson extrapolation, automatic integration, extensions to two and three dimensions and the curse of dimensionality.
- Apr 5th and 12th: *Monte Carlo Methods*: Pseudo-random numbers (uniform, normal, and other distributions). Numerical integration in high dimensions and sampling variance.
- Apr 19th: *Ordinary Differential Equations*: Euler and Heun's method. Runge-Kutta schemes. Implicit integrators.
- Apr 26th: *Partial Differential Equations*: Heat and Black-Scholes equations. Stability and local truncation error analysis.
- May 3rd: TBD: No lecture or guest lecture on
  *Fourier Transforms*: Trigonometric polynomials and Discrete Fourier Transforms (DFT). Fast Fourier transforms (FFT). Convolution. Filtering/smoothing.
- **May 10th**: **Take-home final** due! Final will be posted on April 27th.