# MATH661: Scientific Computation I

## Course Info

This graduate course is an introduction to the theory, principles and practice of scientific computation, a third mode of scientific inquiry that complements theory and experiment.

Course goals: students will acquire understanding of the central role of computation in research and design, and proficiency in algorithm formulation, analysis and implementation.

| **Title** | **MATH661: Scientific Computation I** |
|---|---|
| Times | MWF 2:30-3:20 PM, Day 381 |
| Office hours | TuTh 10:00AM-11:00 AM CP451 |
| Instructor | Sorin Mitran |
| Assistant | Yuan Gao |

## Honor Code:

- All work is individual. You may discuss various approaches to homework problems with students, instructors, but must draft your answers by yourself
- All exams are closed book

## Grading

### Required work

- Homework - 8 assignments x (4 1-point exercises + a 4-point computer application) = 64 points
- Midterm - 3 problems x 4 points = 12 points
- Final - 6 problems x 4 points = 24 points
- You will be given the opportunity during the Final Examination to answer one 4-point question from the midterm material (the question will be different from those given during the Midterm Examination). The score from this question will replace your worst score on a problem from the Midterm Examination.
- Undergraduate students taking the course will have a starting award of 20 points

### Extra credit

You may use these extra credit questions to make up for missed homework or points lost on the examinations.

Turn in any of these *before* Fall break to attempt extra credit points:

- EC1 (2 points)
- EC2 (2 points)
- EC3 (2 points)

Turn in any of these *before* end of last class to attempt extra credit points:

- EC4 (2 points)
- EC5 (2 points)
- EC6 (2 points)

### Mapping of point scores to letter grades

| Grade | Points | Grade | Points | Grade | Points | Grade | Points |
|---|---|---|---|---|---|---|---|
| A, H+ *cum laude* | 101-112 | B+,H- | 86-90 | C+,P- | 71-75 | D+,L- | 56-60 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| A,H+ | 96-100 | B,P+ | 81-85 | C,L+ | 66-70 | D,L-- | 50-55 |
| A-,H | 91-95 | B-,P | 76-80 | C-,L | 61-65 | F | 0-49 |

Note: The mapping of points to grades is intended to permit a grade of P (76 points) solely by correct solution of homework and extra credit for graduate students more interested in applications of course methods, and less in the underlying theory. Graduate students aiming for a higher P+ or H grade are expected to demonstrate a good understanding of the theoretical concepts as tested in the midterm and final examinations. Undergraduate students can obtain a grade of B (84 points) by correct solution of the homework problems (64 points) in conjunction with the starting award of 20 points. Higher undergraduate grades require either doing some of the extra credit or dedicating effort to understanding the theoretical concepts of the course.

## Course policies

- This is a graduate-level course. Students are expected to undertake independent work to deepen their understanding of course material
- Due to time limitations, some topics cannot be covered in class. Students are expected to read material on all requested topics (see table below)
- Examination topics may be given from both material covered in class and requested to be read independently
- Students are free to establish their own schedule; there is no need to inform instructor of absences. Course attendance is highly recommended to gain insight into course topics
- Late homework is not accepted
- Homework should be submitted in typeset form (LaTeX, TeXmacs). Handwritten homework is accepted if clearly written. Illegible homework is not graded

## Bibliography

The course text is *Numerical Analysis: Mathematics of Scientific Computing*, D. Kincaid, W. Cheney. Students are encouraged to consult additional numerical analysis books as needed. Recommendations:

- *An Introduction to Numerical Analysis*, K. Atkinson
- *Numerical Methods in Scientific Computing* by G. Dahlquist, A. Bjorck

## Examinations

- Midterm examination: 2:30-3:20 PM, Fr. Oct 9
- Final examination: 4:00-7:00 PM, Fr. Dec 4

## Course materials

### Lectures, reading assignments

The following lecture notes are meant as a synopsis of class discussions. For more details consult the corresponding sections within the textbook.

| Week | Monday | Wednesday | Friday |
|---|---|---|---|
| 1 | | 8/19 Numerical approximation Lesson01.pdf | 8/21 Lesson02.pdf |
| 2 | 8/24 Approximation, polynomial interpolation Lesson03.pdf | 8/26 Newton interpolating polynomial, divided differences Lesson04.pdf | 8/28 Error in polynomial interpolation, Runge function example Lesson05.pdf |
| 3 | 8/31 Chebyshev polynomials Lesson06.pdf | 9/2 Vector spaces and subspaces, left null space Lesson07.pdf | 9/4 Finite difference calculus Lesson08.pdf |
| 4 | 9/7 (Labor Day, no class) | 9/9 Hermite interpolation, piecewise interpolation Lesson09.pdf | 9/11 Spline interpolation Lesson10.pdf |
| 5 | 9/14 Homework 1 solution review | 9/16 B-splines Lesson12.pdf | 9/18 Numerical differentiation Lesson12.pdf |
| 6 | 9/21 Numerical quadrature: Newton-Cotes Lesson13.pdf | (No class) | 9/25 Gauss quadrature Lesson14.pdf |
| 7 | 9/28 Gauss quadrature examples | 9/30 Adaptive quadrature, Romberg | 10/2 Nonlinear equations Lesson16.pdf |

| | | | |
|---|---|---|---|
| | | quadrature Lesson15.pdf | |
| 8 | 10/5 Newton, secant methods Lesson17.pdf | 10/7 Midterm review, typical examination questions | 10/9 Midterm examination |
| 9 | 10/12 Midterm examination solution review | 10/14 Graeffe-Lobachevski | 10/16 (no class, Fall Break) |
| 10 | 10/19 Graeffe-Lobachevski example Lesson18.pdf | 10/21 Functional iteration | 10/23 Nonlinear systems: quasi-Newton, descent methods |
| 11 | 10/26 Numerical ODEs: Taylor series, Runge-Kutta | 10/28 Numerical ODEs: Multistep methods | 10/30 Numerical ODEs: stability, convergence |
| 12 | 11/2 Numerical ODEs: BVPs | 11/4 Numerical ODEs: ODE systems, stiff equations | 11/6 Numerical PDE overview |
| 13 | 11/9 Numerical stochastics: Random number generators | 11/11 Numerical stochastics: Monte Carlo integration | 11/13 Numerical stochastics: Stochastic differential equations |
| 14 | 11/16 Case study 1: Porous medium flow | 10/21 Case study 2: ODE system control | 10/23 Case study 3: Cellular motility |
| 15 | 11/23 Course concepts review | 11/25 (no class, Thanksgiving) | 11/27 (no class, Thanksgiving) |
| 16 | 11/30 Final examination preparation | 12/2 Final examination preparation | - |

## Homework

| Nr. | Issue Date | Due Date | Topic | Problems | Solutions |
|---|---|---|---|---|---|
| 1 | 8/31 | 9/9 | Newton interpolation | Homework1.tm Homework1.pdf | Homework1.tm Homework1.pdf |
| 2 | 9/14 | 9/23 | Spline interpolation | Homework2.tm Homework2.pdf | |
| 3 | 8/31 | 9/9 | Numerical quadrature | Homework3.tm Homework3.pdf | |

## Course topics

- Basic principles of numerical computation
- Univariate approximation
- Applications of univariate approximation:

  1. Root finding
  2. Numerical differentiation
  3. Numerical integration
  4. Numerical solution of ordinary differential equations

- Introduction to functional analysis and applications:

  1. Normed, metric spaces
  2. Orthogonal bases
  3. Linear spaces and applications
  4. General approximation theory

- Introduction to numerical stochastics

  1. Basic probability theory
  2. Stochastic processes
  3. Stochastic approximation and applications:

- Algorithms for parallel computations

## SciComp@UNC Linux environment

Scientific computation is typically carried out in a Un*x environment (e.g. OS/X, various Linux versions). This course uses a customized Linux environment named SciComp@UNC. There are two ways to access the environment:

1. As a virtual machine on your laptop or desktop. This is the recommended procedure. See SciComp@UNC.
2. Through the UNC Virtual Computing Lab. A version of SciComp@UNC with software used in undergraduate classes, but without several additional packages is available. Use your Onyen to log on the UNC VCL site, and make a reservation to use the SciComp@UNCminimal environment VCL Reservation. You will need to have an X-window server installed on your local machine. Under windows use Xwin32. Under OS X use XQuartz

## Lecture notes, homework texts and solutions

Course materials (lecture notes, homework, quizzes) are distributed through the subversion utility, available on all major operating systems. In TarHeel Linux the following will check out an initial copy of course materials:

- mkdir ~/courses
- cd ~/courses
- svn co http://mitran-lab.amath.unc.edu:8082/subversion/courses/MATH661/

Update the course materials before each lecture by:

- cd ~/courses/MATH661
- svn update

Links to course materials will also be posted to the wiki site, but the most up-to-date version is that from the subversion repository, so carry out the svn update procedure prior to each lecture.