# PHY 318 Spring 2017

# Methods of Computational Science

TR 11:00-12:15 PM in Moulton 307B

## Instructor

Rainer Grobe
Office: Moulton Hall 216
Phone: 438-5470
Office hours: MWF 10-11 AM, by appointment, or just walk in.
Email: grobe@ilstu.edu

## Texts

There are no textbooks for the course. You will be provided with course lecture notes written by the instructor.

## References

Recommended references include the following:

Paul L. DeVries, "A First Course in Computational Physics," John Wiley & Sons, Inc.

Rubin H. Landau and Manuel J. Páez, "Computational Physics," John Wiley & Sons, Inc.

Alejandro L. Garcia, "Numerical Methods for Physics," Prentice Hall.

Harvey Gould and Jan Tobochnik, "Computer Simulation Methods, Applications to Physical Systems, Part 1 and Part 2," Addison-Wesley.

Steven E. Koonin and Dawn C. Meredith, "Computational Physics *Fortran Version*," Addison-Wesley.

Nicholas J. Giordano, “Computational Physics,” Prentice Hall.

Ward Cheney and David Kincaid, "Numerical Mathematics and Computing," Brooks-Cole.

William H. Press, Brian P. Flannery, Saul A. Teukolsky, and William T. Vetterling, "Numerical Recipes - The Art of Scientific Computing," Cambridge University Press.

## Homework

A total of eight homework assignments, each worth 50 points, will be distributed throughout the semester. The approximate timing of these assignments is listed in the course outline.

The homework assignments will consist of some theoretical problems and some computer-based problems. The computer-based problems will generally require that you write computer programs in order to solve the problems. Though we will give examples in class using the Fortran programming language, you are welcome to work the problems in any programming language that you are comfortable with. Please consult one of your instructors to discuss the use of compilers for other languages.

In order to encourage students to work together to solve homework problems, homework solutions will be turned in from groups of two students. Therefore, each member of the group will receive the same grade for that homework assignment.

Homework assignments will have specific due dates. *A late penalty of 25% per week will be assessed if a homework assignment is turned in after the due date.*

## Exams

There will be one mid-term exam and a final exam given in this course:

| | |
|---|---|
| Mid-term exam (200 points): | possibly Tuesday, March 21, 2017 |
| Final exam (300 points): | to be announced |

Make-up exams will not be given unless you can present a legitimate excuse. *An arrangement for a make-up exam must be made within one week after the exam.* If you fail to do so, you will not be able to take a make-up exam.

## Grades

| | |
|---|---|
| 8 homework assignments (50 points each) | 400 points |
| Mid-term exam | 200 points |
| Final exam | 300 points |
| **TOTAL** | **900 points** |

Your final letter grade will be determined as follows:

| | |
|---|---|
| A | 90 – 100 % |
| B | 80 – 89 % |
| C | 70 – 79 % |
| D | 60 – 69 % |
| F | 59 % and below |

# PHY 318 Course Outline
## Spring 2017

**The lecture schedule is based on a total of at most 24 classes, each 75 minutes in length.**

## I. Computer representation (3 classes, 1-3)

- 1.1 What is computational science?
- 1.2 Available software - commercial vs. writing programs
- 1.3 Programming - structured Fortran
- 1.4 Writing programs, using graphics packages, etc.
- 1.5 Computer representation of numbers
  - 1.5.1 Bits and bytes
  - 1.5.2 Fixed-point number representation
  - 1.5.3 Floating point notation
  - 1.5.4 Machine precision
- 1.6 Round-off errors
- 1.7 Truncation errors

***Homework #1***

## II. Numerical discretization (roughly 2 classes, 4-5)

- 2.1 Intro to numerical differentiation
- 2.2 Taylor series
  - proof, error estimate
- 2.3 Three formulas
  - 2.4.1 Forward difference
  - 2.4.2 Backward difference
  - 2.4.3 Symmetric 3-point
  - 2.4.4 Graphical illustration
- 2.4 Generalization to higher derivative formulas

***Homework #2***

## III. Numerical integration (roughly 4 classes, 6-9)

- 3.1 Different types
- 3.2 Rectangular methods
- 3.3 Trapezoidal method
  - 3.3.1 Local method
  - 3.3.2 Composite method
  - 3.3.3 Local and global error estimates
  - 3.3.4 Alternate derivation
  - 3.3.5 Derivation of local error
- 3.4 Simpson method
- 3.5 Interpolating polynomials
- 3.6 Gaussian integration
  - 3.6.1 Equidistant grid points
  - 3.6.2 Gaussian nodes and weights
  - 3.6.3 Theorem on Gaussian nodes and weights
  - 3.6.4 Other Gaussian quadrature formulas
- 3.7 Comparison of various integration formulas

***Homework #3***

## IV. Ordinary differential equations (roughly 7 classes, 10-16)

- 4.1 Introduction
- 4.2 Taylor series method, first and second order
- 4.3 Runge-Kutta method
- 4.4 Predictor-corrector methods
- 4.5 Verlet algorithm
- 4.6 Verlet algorithm example
- 4.7 Appendix: Amber force field

***Homework #4***

- 4.8 ODE Examples
  - 4.8.1 Pendulum dynamics
    - 4.8.1.1 Equations of motion
    - 4.8.1.2 Linear plane pendulum
    - 4.8.1.3 Introduction to phase space
    - 4.8.1.4 Nonlinear plane pendulum
    - 4.8.1.5 Numerical solution of nonlinear plane pendulum
  - 4.8.2 Chemical kinetics
    - 4.8.2.1 General chemical reactions
    - 4.8.2.2 Reaction rates
    - 4.8.2.3 Rate laws
    - 4.8.2.4 Elementary reactions
    - 4.8.2.5 Example mechanisms
    - 4.8.2.6 Oscillating reactions: Lotka-Volterra model
    - 4.8.2.7 Oscillating reactions: Belousov-Zhabotinsky reaction
    - 4.8.2.8 Oscillating reaction demo: Briggs-Rauscher reaction
  - 4.8.3 Molecular vibrations
    - 4.8.3.1 A model of an ABA triatomic molecule
    - 4.8.3.2 Potential energy of the ABA triatomic molecule
    - 4.8.3.3 Kinetic energy of the ABA triatomic molecule
    - 4.8.3.4 Equations of motion for stretching dynamics
    - 4.8.3.5 Solution of equations of motion
    - 4.8.3.6 Connection with quantum mechanics
    - 4.8.3.7 Connection with experiments

***Homework #5***

## V. Fourier transforms (roughly 5 classes, 17-22)

- 5.1 Review and introduction
- 5.2 Analytical properties of Fourier transformations
- 5.3 Properties of Fourier transformations
  - 5.3.1 Linearity
  - 5.3.2 Scaling relation
  - 5.3.3 Shifting relations
  - 5.3.4 Symmetry relations
  - 5.3.5 Fourier transformations of derivatives
  - 5.3.6 Orthogonality relation
  - 5.3.7 Parseval's identity
  - 5.3.8 Generalization to N dimensions
- 5.4 Discrete Fourier transformation
  - 5.4.1 Introduction
  - 5.4.2 Fast Fourier transformation
  - 5.4.3 Aliasing
  - 5.4.4 Leakage
  - 5.4.5 Graphical examples of discrete Fourier transforms

        - 5.4.5.1 DFTs of simple periodic time series
        - 5.4.5.2 Examples of DFTs illustrating aliasing
        - 5.4.5.3 Examples of DFTs illustrating leakage

- 5.5 Examples of the use of Fourier transforms
    - 5.5.1 Introduction to nuclear magnetic resonance (NMR)
    - 5.5.2 Analysis of NMR signals using Fourier transforms
    - 5.5.3 Signal processing

***Homework #6***

## VI. Monte Carlo simulations (at least 3 classes, 23-25)

- 6.1 Introduction to random numbers
- 6.2 Generation of random numbers
    - 6.2.1 Clock method
    - 6.2.2 Middle-square method by von Neumann
    - 6.2.3 Linear congruence method
- 6.3 Probability theory
    - 6.3.1 Averages
    - 6.3.2 Probability distributions and histograms
    - 6.3.3 Mean, most probable and median value
    - 6.3.4 Standard deviation and variance
    - 6.3.5 The scaling of the variance
    - 6.3.6 The central limit theorem

***Homework #7***

- 6.4 Monte Carlo integration in one dimension
- 6.5 Monte Carlo integration in many dimensions
- 6.6 Monte Carlo simulations
    - 6.6.1 Neutron shielding
    - 6.6.2 One-dimensional random walk simulations
    - 6.6.3 Two- and three-dimensional random walk simulations
- 6.7 Monte Carlo simulations: The Ising model
    - 6.7.1 Introduction
    - 6.7.2 Magnetization
    - 6.7.3 Interaction energy
    - 6.7.4 2x2 lattice example
    - 6.7.5 Special case of magnetization and interaction energy
    - 6.7.6 Boltzmann probability weighting
    - 6.7.7 Monte Carlo simulations of the Ising model
- 6.8 Monte Carlo simulations: Diffusion-Limited Aggregation and Cluster Growth
    - 6.8.1 Introduction
    - 6.8.2 Examples of Diffusion-Limited Aggregation
        - 6.8.2.1 DLA in Electrodeposition
        - 6.8.2.2 DLA Cluster Growth in Minerals
    - 6.8.3 Random Walk Model for DLA Cluster Growth
    - 6.8.4 Fractal Dimension by the Mass-Counting Method

***Homework #8***