

# Computational Physics

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# **Contact Information**

Instructor: Pablo Laguna

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Class MWF 13:05-13:55 Howey N210

Hours:

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Office Hours: MWF 14:00-15:00 or by appointment

A First Course in Computational Physics, 2nd Edition, Paul L. DeVries and Javier E. Hasbun (Jones and Barlett,

References: 2011)

Numerical Recipes, 3th Edition, by William H. Press, Saul A. Teukolsky, William T. Vetterling and Brian P. Flannery

(Cambridge University Press 2007)

Software: Matlab

# **Objective**

Applications of numerical methods and computer programming to condensed matter; astrophysical hydrodynamics, gravitational physics, black holes and cosmology.

Pablo Laguna: School of Physics, 837 State Street, Georgia Tech, Atlanta, GA 30332-0430 | Phone: (404) 385-3907 | Office: 1-63 Boggs



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# **Topics**

#### Introduction

## **Solving Non-linear equations**

- · Bisection method
- · Linear interpolation
- · Newton-Raphson Method
- Programs: findroot.m froot.m dfroot.m d2froot.m

#### Solving systems of equations

- Gaussian elimination
- · Iterative methods
- Matrix inversion
- Eigenvalues and Eigenvectors
- Non-linear systems

## Interpolation and curve fitting

- Polynomials
- Cubic Splines
- · Least Squares Fitting

#### **Numerical Integration**

- Trapezoidal rule
- Simpson rule
- Romberg integration
- · Splines and Integration

## **Numerical Approximations to Derivatives**

- · Finite Differences
- Truncation Errors & Convergence
- Richardson Extrapolation
- Programs: deriv.m

## **Ordinary Differential Equations**

# Initial-value Problems

- Euler Method: ode euler.m
- Runge-Kutta Methods
- Stellar Models: stellar.m, stellar rhs.m, chandra.m

#### **Ordinary Differential Equations**

## Boundary-value Problems

- Tri-diagonal Solver
- Shooting method: shooting.m, shooting rhs.m

#### **Partial Differential Equations**

- · PDEs examples
- Advection Equation: advect.m, advect rhs.m, euler.m, rk2.m, rk4.m
- von Neumann Stability Method
- · Method of Lines
- Burgers Equation: burgers.m, burgers rhs.m

#### **Time-dependent Partial Differential Equations**

- Hyperbolic Equations
- · Cosmological Inflation
- Domain Walls: inflation.m

# **Time-dependent Partial Differential Equations**

- Diffusion Equations
- · Proto-planetary disks

# **Schrodinger Equation**

- Time dependent using Crank Nicholson
- Time dependent using Iterative Crank Nicholson
- Stationary Solutions

# **Time-independent Partial Differential Equations**

- Successive Over-relaxation
- Poisson Equation

## **Monte Carlo Methods**

- Simple Monte Carlo integration
- Von Neumann Rejection Method
- Maxwell-Boltzmann distribution
- · 2D Ising Model

# **Fourier Analysis**

- Fast Fourier Transform
- · Convolution and Correlation

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# **Policies**

**HOMEWORK:** There will be THREE homework assignments during the semester. Homework problems will typically require writing computer programs based on the numerical algorithms discussed in class. Computer programs MUST be written completely from scratch, with the essential steps fully commented. The structure of the program can, however, be based, if necessary, on programs written or discussed by the instructor. The instructor reserves the right to request the student the reproduction of results submitted in homework assignments. Delays in the submission of homework sets will be penalized 2 points per day.

**TEAM PROJECT:** 2/5 of the course grade is assigned from a project. The project consists of two parts. One of them is an oral presentation the week before dead week. The second part is a written report, between 3 and 5 pages in length, due the day of the final exam. The teams for the projects could have a minimum of 3 and maximum of 5 members. The research project should clearly require the use of numerical methods. All members of each team participate in the oral presentation. At the end of each presentation there will be a Q&A session involving fellow classmates and the instructor. Both, the final report and oral presentation must include:

- 1) description of the nature of the problem,
- 2) the numerical techniques used,
- 3) code testing,
- 4) results, using scientific visualization where applicable, and
- 5) scientific implications.

**GRADES**: The homework assignments are computed on a 0-100 point scale. Their weights are:

Homework 1 (PDF) 20 % Due February 10, 2012

Homework 2 (<u>PDF</u>) 20 % Due March 16, 2012

Homework 3 (<u>PDF</u>) 20 % Due April 18, 2012

magnetic.m magnetic plot.m

Project Presentation 20 % Due

Project Report 20 % Due

Total 100 %

The final letter grade is assigned using the following conversion table. Plus/minus letter grades are used only for borderline cases.

A 100 - 85

B 84 - 75

C 74 - 65

D 64 - 55

F 55 - 0



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#### **Honor Code**

The policy on academic integrity as stated in the <u>GIT Honor Code</u> will be fully enforced during this course. In particular: Collaboration during in-class activities is permitted and encouraged unless your instructor explicitly indicates otherwise. Collaboration on homework assignments is permitted and encouraged unless your instructor explicitly indicates otherwise. Such collaboration should have the purpose of sharing an understanding of the principles and general solution techniques, not simply the sharing of answers. Collaboration is NOT permitted during exams. Violations of these rules will be prosecuted as violations of the GIT Honor Code.

Note that the Honor Code formally defines academic dishonesty as ...any act that does or could improperly distort student grades or other student academic records. If you should have any question regarding the propriety of a particular behavior, you are encouraged to discuss the matter with the instructor.

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