PH354 Jan. 3:0

Computational Physics

Instructor

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Teaching Assistant

Email:

Department: Physics

Course Time:

Lecture venue:

Detailed Course Page:

Announcements

Brief description of the course

This course is a very hands-on course which has two main objectives:

1.Learning basic methods, tools, and techniques of computational physics.

2.Developing practical computational problem-solving skills.

The course will have a project as well as biweekly assignments.

Prerequisites

None (masters level physics)

Syllabus

1 Introduction to computational physics, computer architecture overview, tools

of computational physics (1.5 hours)

2 Machine representation, precision and errors (1.5 hours)

3 Tools of the trade (6 hours)

Quadratic equations; Power series; Delicate numerical expressions; Dangerous subtractions; Preserving small numbers; Partial Fractions; Cubic equations; Sketching functions;

4 Roots of equations (6 hours)

Real roots of single variable function; iterative approach; qualitative behavior of the function; Closed domain methods (bracketing): Bisection; False position method; Open domain methods: Newton-Raphson, Secant method; Mullerâ€™s method; Complications; Roots of polynomials; Roots of nonlinear equations;

5 Quadrature (6 hours)

Direct fit polynomials; Quadrature methods on equal subintervals; Newton-Cotes formula; Romberg Extrapolation; Gaussian quadrature; Adaptive step size; Special cases;

6 Random numbers and Monte-Carlo (6 hours)

Random number generators; Monte-Carlo integration; Non-uniform distribution; Random Walk; Metropolis algorithm;

7 Fourier methods (3 hours)

Fast Fourier transform; Convolution; Correlation; Power spectrum;

8 Ordinary differential equations (9 hours)

Initial value problems: First order Euler method; Second order single point methods; Runge-Kutta methods; Multipoint methods; Boundary value problems: Shooting method; equilibrium boundary value method;

9 Numerical Linear algebra (9 hours)

Matrix Factorizations: QR Factorization; Gram-Schmidt Orthogonalization; Householder Triangularization; LU and Cholesky factorization; Schur factorization; Direct elimination methods: Gauss elimination (pivoting, scaling); Tri-diagonal systems; Iterative methods: Jacobi iteration; Conjugate Gradients; Eigenvalue problems: Rayleigh Quotient; Arnoldi and Lanczos methods;

Course outcomes

Learn basic programming and applying it to physics problems.

Grading policy

50% Project and 50% Assignments

Assignments

7/8 assignments (biweekly) and project. The project will be decided in consultation with the instructor (and research advisor)

Resources

Textbooks:

1. Mark Newman, Computational Physics, CreateSpace Independent Publishing Platform (2013).

2. Rubin H. Landau, Manuel J. Paez and Cristian Bordeianu, Computational Physics, 3rd Ed Problem Solving with Python, Wiley (2015).

3. A. Klein and A. Godunov, Introductory Computational Physics, Cambridge University Press (2006).

4. Forman Acton, Real computing made real: Preventing Errors in Scientific and Engineering Calculations, Dover Publications.

5. Lloyd N. Trefethen and David Bau, Numerical Linear Algebra, SIAM.