JML 309_(310) Numerical Methods in Physics (JAN)

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; 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.

8. 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.

Book: Mark Newman, Computational Physics