Advanced Computational Methods
Syllabus

November 22, 2021

This is a very hands-on course which will involve a lot of programming assignments. The main aims of the course are two fold:
1. Learning methods, tools and techniques for solving advanced scientific problems.
2. Developing practical computational problem solving skills.
Textbooks:

1. Mark Newman, *Computational Physics,* CreateSpace Independent Publishing Platform (2013).
2. Forman Acton, *Real computing made real: Preventing Errors in Scientific and Engineering Calculations,* Dover Publications.
3. Lloyd N. Trefethen and David Bau, *Numerical Linear Algebra,* SIAM.
4. William H. Press, Saul A. Teukolsky, William T. Vetterling and Brian P. Flannery, *Numerical Recipes 3rd Edition: The Art of Scientific Computing*

1 Introduction to computational physics, computer architecture overview, tools of computational physics (3 hours)

What is computational physics? Why do we need it?; Computer hardware: basic computer architecture, hierarchical memory, cache, latency and bandwidth; Moore's law, power bottleneck; Software: compiled (Fortran, C) vs. interpreted languages (MATLAB, python); software management.; Parallelization: MPI; OpenMP.

2 Machine representation, precision and errors (1.5 hours)

Representation on a computer: Integer representation; floating-point representation; Ma- chine precision; Errors: round-off; approximation errors; random errors; errors of the third kind; Quadratic equations; Power series; Delicate numerical expressions; Dangerous subtractions; Preserving small numbers; Partial Fractions; Cubic equations; Sketching functions;

3 Quadrature and Derivatives (6 hours)

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

4 Solutions of linear and non-linear equations (9 hours)

Simultaneous linear equations: Gauss elimination (pivoting, scaling); LU factorization; Cal- culating inverse; Tri-diagonal systems; Eigenvalues and Eigenvectors: QR Factorization; Gram-Schmidt Orthogonalization; Real roots of single variable function; Relaxation method; qualitative behavior of the function; Closed domain methods (bracketing): Bisection; False position method; Open domain methods: Newton-Raphson, Secant method; Complications; Roots of polynomials; Roots of non-linear equations;

5 Fourier methods (3 hours)

Fast Fourier transform; Convolution; Correlation; Power spectrum;

6 Random numbers and Monte-Carlo (6 hours)

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

7 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;