Schedule PHYS476/576 "Computational Physics", Spring 2019

Instructor: Dr. Boris Kiefer

Time permitting, I provide a one-lecture overview to data mining and machine learning at the end of the semester.

DATE	TOPICS	READING ASSIGNMENT	Other
R 01/17	**Introduction** to scientific programming/documentation, scientific visualization (gnuplot), and uses of programming techniques in data recovery.	Ch. 1; 3.5	
T 01/22	Machine numbers and round-off errors. How to compute exp(-x)?	Ch. 2	
R 01/24	**Interpolation**: Lagrange polynomial. Richardson-deferred –extrapolation.	Ch. 3	Pre-reqs due
T 01/29	**Numerical Differentiation**: Finite differences, error estimation, ODE. **Linear algebra**: Gauss/Gauss-Jordan elimination.	Ch. 3	
R 01/31	**Linear algebra**: LU; SVD; Banded Matrices.	Ch. 6	
T 02/05	**Linear algebra**: 2nd order ODE primer. Iterative Methods, Jacobi, Gauss-Seidel, SOR.	Ch. 6	
R 02/07	**Roots**: Secant, bisection, bracketing, Dekker, Brent.	Ch. 4	HW01 due
T 02/12	**Roots:** Newton-Raphson; N>1 dimensions.	Ch. 4	
R 02/14	**Integration**: Trapezoidal, Simpson, open-formulas, error estimation.	Ch. 5	
T 02/19	**Integration**: Quadrature, N>1 dimensions.	Ch. 5	
R 02/21	**Workflow design:** accelerating throughput and scientific discovery.		
T 02/26	**Research Computing:** From microscope to manuscript, benefits of research computing (Dr. Jhamba, UNM).		
R 02/28	**Eigensystems**: (Inverse) Power method; orthogonal subspaces.	Ch. 7	HW02 due
T 03/05	**Eigensystems**: Jacobi method; tridiagonal matrices; QM HOSC; QM Infinite well.	Ch. 7	
R 03/07	**Eigensystems**: QR/QL method.	Ch. 7	
T 03/12	**Ordinary differential equations**: Euler method. Velocity-Verlet. Leapfrog algorithm. Checking results: Conservation of energy.	Ch. 8	
R 03/14	**Ordinary differential equations**: Runge-Kutta method. Time step control. Classical dynamical systems.	Ch. 8	**TAKE HOME MIDTERM**
T 03/19	**Two point boundary value problems:**	Ch. 9	

	"Shooting method".		
R 03/21	**Two point boundary value problems**: Examples.	Ch. 9	HW03 due. **TAKE HOME EXAM DUE**
T 03/26	Spring Break – no class		
R 03/28	Spring Break – no class		
T 04/02	**Partial differential equations:** Elliptical: 1-D Diffusion equation; FTCS; BTCS; Crank-Nicholson.	Ch. 10	
R 04/04	**Partial differential equations:** Parabolic; 1-D Heat equation; Time-dependent Schroedinger equation.	Ch. 10	
T 04/09	**Monte Carlo:** Random number generators. Radioactive decay.	Ch. 11	
R 04/11	**Monte Carlo:** Integration; error estimates.	Ch. 11 + 12	HW04 due
T 04/16	**Monte Carlo:** Fundamental Theorem of sampling; direct sampling; rejection.	Ch. 12 + 13	
R 04/18	**Monte Carlo:** Maxwell's equations and 3D printing of ferromagnets.		
T 04/23	**Min/Max extrema of function.** Brent's algorithm. Steepest descent; Conjugate gradient. Variable metric.		
R 04/25	**Global minimization: Simulated Annealing.** **Fast Fourier Transform:**		
T 04/30	**Sampling theorem: Nyquist frequency; sampling theorem.** **Fourier interpolation.**		HW05 due
R 05/02	**Course summary.**		
R 05/09	**10:30 – 12:30; Final exam; cumulative, covering all lecture material and homeworks; GN 218A Gardiner Hall.**		
T 05/14	**Final Grades are due**		