MtSE 788
"Applied Computational Methods in Physics and Materials Science "

SYLLABUS

0. Introduction. Matched asymptotes

I. Special functions of mathematical physics

- General overview. Airy functions.
- Bessel and modified Bessel functions. Examples: Fraunhofer diffraction. Diffusion of neutrons.

II. Partial differential equations in Physics

- General classification and physical examples.
- The diffusion equation. Relation between random walk and diffusion.
- Eigenfunction expansions
- Numerical methods of solution

Mid-term exam

III. The stationary Shrödinger equation

- Evaluating the eigenvalues (shooting method, variational, matrix).
- Barrier penetration, scatter. Resonance levels.
- Multidimensional potentials. The hydrogen atom.
- Periodic potential. Bands.

IV. APPLICATIONS

- Deterministic and stochastic (Monte Carlo) methods.
- Simulated annealing.
- The dynamic Ising model - energy, free energy, entropy, specific heat, motion of the interface, nucleation.
- Chaos

FINAL EXAM/PROJECT

PHYS/MtSE 788
"Applied Computational Methods in Physics and Materials Science "

INSTR. Dr. Vitaly A. Shneidman, Rm. 452T, e-mail: vitaly@oak.njit.edu

TIME: Thu. 6:00-9:05 pm
(office hours will be published by the second week of classes)

WEB page: http://web.njit.edu/∼vitaly/788/

Software: The *Mathematica* program will be used. The program is available at NJIT for on-site use (not for download). Alternatively, a student version of *Mathematica* for PC can be purchased from the bookstore or online from wolfram.com (in that case indicate that you are an NJIT student).

Grading. Homework - 15%, mid-term - 40%, final - 45%.

Projects. Students are expected to complete 1-2 small-size computational projects (suggested by the instructor) during the course. In exceptional cases these projects can make up for the Mid-term exam. The topic for a larger final project can be suggested by the student, but must be approved by the instructor no later than by the 8th week of the course. If successfully completed and followed by a presentation, the final project can replace the final exam.

Recommended reading and reference materials:

Special functions, equations of mathematical physics:
Mathematical Methods for Physicists. Arfken and Weber, 5th ed. (Academic Press, 2001).
Handbook of Mathematical Functions by M. Abramowitz and I. Stegun (any edition).

Programming with *Mathematica*:
A Physicist's Guide to Mathematica. Patrick T. Tam. (Academic Press, 2d ed, 2008).
Physics by Computer: Programming Physical Problems Using Mathematica and C. W. Kinzel and G. Reents. (Springer, 1998).

Other:
The UNIX programming environment. B.W. Kernighan and R. Pike. (Prentice-Hall, 1984).
Numerical Recipes in C. W. H. Press and B. P. Flannery and S. A. Teukolsky and W. T. Vetterling. (Cambridge University Press, 1992).

online: http://mathworld.wolfram.com/