MtSE 688 "Mathematical and Statistical Methods in Materials Science"

SYLLABUS

- Introduction to *Mathematica*, graphics; review of algebra and calculus (2 weeks).
- Algebra of Vectors and Matrices (2 weeks): vector algebra, matrices, transformation of coordinates, matrix solutions of linear equations, operations with matrices. Eigenvalues and eigenvectors, diagonalization. Application: rotation and vibration of molecules.
- Fourier and Laplace Transforms (3 weeks):
 Basic definitions and examples in 1 dimension. Delta-function. Three-dimensional generalizations and applications.
- Ordinary differential equations (2 week):
 Classification. Non-linear first-order equations. Linear second and higher order equations. General and particular solutions. Numerical solutions. Application: driven oscillations and resonance.
- Introduction to partial differential equations (2 weeks):

 Physical background, types of equations and boundary conditions. The Laplace operator in 1, 2 and 3 dimensions. Separation of variables and solutions using Fourier expansions. Application of Laplace transformations to diffusion equation.
- Elements of Probability, Statistics and data analysis (3 weeks):
 Basic definitions, mean value. Moments. Discrete and continuous distributions. (Binomial, Poisson, Gaussian, and connection between them). Central limit theorem (no proof). Random walk and connection with diffusion. "Smoothing" of data. Variance, skewness, etc. Comparing two distributions: Kolmogorov-Smirnov and other tests. Correlation between data. Modeling of data.

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

TIME: Mon. 6:00-9:05

(office hours will be published by the second week of classes)

WEB page: http://web.njit.edu/~vitaly/688/

Software: The *Mathematica* program will be used. A personal copy of the program (student version) can be purchased from the bookstore or from the wolfram.com web site (mention that you are a registered NJIT student...). Alternatively, the program is accessible from several locations on campus for on-site use. The first option is more convenient and is strongly recommended, especially if you own a laptop or a PC (and you will find *Mathematica* helpful for your other classes and research).

Grading. Will be determined by cumulative points obtained on the mid-term exam (30%), final exam (40%) and homeworks (30%).

Textbook: Advanced Engineering Mathematics. E. Kreyszig. 9th ed. (John Wiley & Sons, 2005. ISBN: 0471488852 .)

Recommended reference materials:

Mathematica Computer Guide. E. Kreyszig and E. J. Norminton. (John Wiley & Sons, 2006).

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