

MSE 350 - Numerical Methods in Materials Science and Engineering

Designation: Required

2012-2013 catalog description: Fundamentals of high-level scientific and engineering computing using the Python programming language, including a broad introduction to numerical methods with applications to materials science and engineering. [3 units offered in the Fall]

Prerequisites Vector calculus, differential equations.

Textbook: None. Course materials are on the course website, and use is made of the online version of *Dive Into Python*, (M. Pilgrim, CreateSpace, Paramount, CA, 2009.) as well as the documentation and tutorials on SciPy.org.

References: Travis E. Oliphant, *Guide to Numpy*, Trelgol Publishing (online), 2006.
(<http://www.tramy.us/guidetosci.py.html>)

Topics Covered:

- Programming fundamentals
- Overview
- Flow control
- Loops
- Input/Output
- Concepts related to object-oriented programming
- Arrays, array operations, and universal functions (ufuncs)
- Scientific Visualization
- Line and scatter plots
- Contour plots
- Vector plots
- Numerical methods, with case studies in MSE
- Solution of linear systems
- Numerical quadrature
- 1-D interpolation
- Numerical root-finding, including solution of systems of nonlinear systems
- Nonlinear optimization
- Nonlinear curve-fitting and parameter estimation
- Solution of ordinary differential equations
- Solution of partial differential equations using the finite-difference technique

Computer Usage: The entire course focuses on writing computer programs, so computer usage is extensive. Many assignments require internet research to discover existing functionalities.

Contribution to 25 % Math & Basic Sci. 1 credits Math & Basic Sci.

Criterion 5: 15 % Engr. Science 2 credits Engr. Topics
60 % Engr. Design

Person preparing syllabus and date: Robert Erdmann, Feb. 2010