SCIENTIFIC COMPUTATION (SC)

671. Computational Methods in Science. Credit 3 hours. Prerequisites: PHYS 331 or MATH 350 or CHEM 395 or permission of the Dean. Computational methods for solving practical problems arising in science. Topics include numerical methods for solving equations, systems of equations, ordinary differential equations, partial differential equations, polynomial integration and least square approximation. Each numerical method will be learned by solving various examples of scientific problems using programming languages such as C or C++.

672. Monte Carlo Simulations. Credit 3 hours. Prerequisites: PHYS 321 or MATH 350 or CHEM 396 or permission of the Dean. Statistical simulation of the thermodynamic properties of atomic/molecular system using Monte Carlo methods. Topics include force fields, statistical ensembles, introductory and advanced techniques in solving simple scientific problems using programming languages such as C or C++.

673. Computational Statistics. Credit 3 hours. Prerequisites: MATH 201 and MATH 380. A survey of computational methods used to analyze data collected from real world settings. Computational methods such as Monte Carlo methods, estimation methods of probability density functions, methods for random number generation, methods for identification of data structure and bootstrap methods will be studied. An emphasis will be on the understanding of the critical role that computational techniques plays in statistical research and the application of statistical methods to real life situation.

674. Scientific Visualization. Credit 3 hours. Prerequisites: MATH 360 and CMPS 390, or permission of the Dean. This course covers a variety of topics in computer graphics using OpenGL with the focus on visualizing scientific and engineering data. Computer graphics emphasizing converting geometry to a display, visualization emphasizing converting data into geometry, and various data visualization techniques and methods will be introduced.

675. Molecular Dynamics Simulations. Credit 3 hours. Prerequisites: PHYS 331 or MATH 350 or CHEM 395 or permission of the Dean. Credit 3 hours. Prerequisites: PHYS 331 or MATH 350 or CHEM 395 or permission of the Dean. Simulation of the dynamic and thermodynamic properties of atomic/molecular systems using molecular dynamics simulations. Topics include the intermolecular forces, statistical mechanics, introductory and advanced techniques of molecular dynamics simulations. A number of projects will be performed throughout the course applying the numerical techniques in solving simple scientific problems using programming languages such as C or C++.

676. Finite Element Method. Credit 3 hours. Prerequisites: MATH 201 or MAT 409, or permission of the instructor. This course introduces the numerical solution of linear problems using finite element methods (FEM). Topics include formation of stiffness matrix, assembly, constraints, solution techniques, and post-processing. How the principles of FEM can be applied to solve physical problems such as stress analysis, heat transfer, acoustics, fluid dynamics, MEMS, and electrical-magnetic fields will be discussed as well.

677. Ab Initio Quantum Chemistry. Credit 3 hours. Prerequisites: PHYS 351 or CHEM 395 or permission of the Dean. A course on numerical methods for solving the electronic Schroedinger equation. Topics include self consistent field methods for molecular orbitals, discretization of partial differential equations using Gaussian basis sets, semi-empirical molecular orbital methods, methods for going beyond self-consistent fields: density functional methods and many-body theory. Students will write programs to compute semi-empirical molecular orbitals.

678. Computational Optimization. Credit 3 hours. Prerequisites: MATH 312, MATH 350, and MATH 360. This is a course on continuous and discrete optimization. Several standard optimization problems along with their numerical and idea solutions will be discussed. Possible topics include unconstrained optimization using vector calculus, Lagrange multipliers, Kuhn-Tucker conditions, Conjugate Gradient Methods, Hilbert space methods in optimization, Linear Programming (simple and interior point methods), quadratic programming shortest path problems, minimal spanning trees, and stochastic optimization.