MSE 6795

Mathematical, Statistical, and Computational Techniques in Materials Science

A. Statistical Techniques

1. Fundamentals of concepts of probabilities (1 lecture)
2. Poisson process and its application to model nearest neighbor distributions (2 lectures)
3. Random walk and correlated random walk, applications to atomic jumps, diffusion and Brownian motion (2 lectures)
4. Geometric probabilities, Buffon needle, and related problems (1 lectures)
5. Mathematical statistics: Normal distribution, t-distribution, etc. (1 lecture)
6. Central limit theorem, estimation of sampling errors, bias, small sample statistics, applications in materials science (2 lectures)
7. Parameters estimation using maximum likelihood and other methods (1.5 lectures)
8. Hypothesis testing: χ^2 - test and other tests of statistical significance; application to particle coarsening and other experimental data (1.5 lectures)
9. Tutorial on home work problems (1 lecture)
10. Test (1 lecture)

B. Mathematical Techniques

1. Concepts of general directional derivative, gradient, divergence, and curl (1 lecture)
2. Line integrals, point functions and path functions (1 lecture)
3. Green's theorem and Gauss divergence theorem (1 lecture)
4. Application of divergence theorem: derivations of generalized Fick's second law, continuity equation for fluid flow, heat conduction equation (2 lectures)
5. Application: hydrodynamic approach for derivation of governing partial differential equation for evolving particulate distributions (1 lecture)
6. Solutions to partial differential equations for diffusion, heat conduction, stress distributions: infinite systems and initial value problems, finite systems and boundary value problems, moving boundaries, similarity solutions (2 lectures)
7. Calculus of variations, Euler-Lagrange equation: application to thermodynamics of chemically non-uniform systems, spinodal decomposition (3 lectures)
8. Laplace and Fourier transforms, convolution theorems: applications in diffraction, phase transformations, etc. (2 lectures)
9. Tutorial on home work problems (1 lecture)
10. Test (1 lecture)

C. Computational Techniques

1. Ensemble theory and fluctuations (2 lectures)
2. Monte Carlo Methods (2 lectures)
3. Interatomic interactions (1 lecture)
4. Molecular Dynamics simulations (2 lectures)
5. Tensors and matrix operations (1 lecture)
6. Governing continuum equations and constitutive relationships, stress, strain (1 lecture)
7. Displacement-based finite elements approach (1 lecture)
8. Solution methods: Rayleigh-Ritz and Gallerkin methods (1 lecture)
9. Nonlinear problems (1 lecture)
10. Boundary conditions for analysis of ordered and random heterogeneous materials, mesh types, solution convergence (1 lecture)
11. Global system consideration, Jacobian operator for nonlinear problems, implicit and explicit codes (1 lecture)
12. Examples of FE-based analysis: Void growth, plasticity of crystalline materials, deformation of two-phase alloys (1 lecture)