

Numerical Methods

Credit Weighting: 5 ECTS

Teaching Period(s): Period 1

No. of Student(s): Min. 5

Pre-requisite(s): Relevant primary honours degree in Engineering or Science

Co-requisite(s): None, although companion course in programming would be of great assistance.

Teaching Methods: 9 x 1 hr lectures in the first term. Supporting documents and notes will be available via web download.

Module Co-ordinator: Prof. Stephen Fahy, UCC

Lecturer(s): Stephen Fahy and Jim Greer, Tyndall National Institute

Module Objectives: Overview of some numerical methods that are widely used in nanoscale simulation and electronic structure applications.

Module Content:

FOURIER TRANSFORM METHODS

Lecture 1

Review: Fourier Series and Integrals
Spatial and Temporal Fourier Series
The Fast Fourier Transform

Lecture 2

Relationship of Fourier transforms to correlation functions
Time Fourier series: Finding normal modes from MD simulation
Solution of Heat Conduction (Diffusion) Equation by Fourier Series

Lecture 3

Spatial Fourier Series:
A. plane-wave (momentum) representation of electronic states
B. Solution of Poisson Equation

LINEAR ALGEBRA AND MATRIX METHODS

Lecture 4

Matrix Diagonalization
Dynamical Matrices and classical normal modes

Lecture 5

Finite basis representation of Schrodinger equation

Transfer Matrix method for transmission problems

Lecture 6

Eigenvalue problem as an optimization problem

Variational method

Lecture 7

Large Sparse Matrix Methods: Conjugate Gradient, Lanczos and Davidson

INTEGRATION

Lecture 8

Grid Integration and Gaussian Quadrature

Examples:

A. tetrahedral method for density of states

B. Integration of Spherical Harmonics

MONTE CARLO METHODS

Lecture 9

Metropolis Method

Importance Sampling

Boltzmann Distribution

Variational Quantum Monte Carlo

Assignments and Assessment:

Exercise: write a simple 1-D Schrodinger-Poisson solver for a periodic semiconductor heterostructure.

Textbooks:

Press *et al.*, "Numerical Recipes", Cambridge University Press