MS2860: **Computational Methods in Materials Science**

Syllabus:

Computational Linear algebra (Numerical Methods)

- Linear System of Equations (Gauss Elimination, LU Decomposition, etc.)
- Finding roots/Non-linear Equations (Bisection, Newton-Raphson, Secant Method, etc.)

Numerical methods for solving selected Partial Differential Equations (PDE)

- Conservation Equations (Mass Transfer, Heat Transfer, etc.)
- Numerical Differentiation/Finite difference methods
- Boundary conditions

Fourier Spectral Method

- Periodic functions and Fourier Transform
- Concept of Reciprocal space

Computational Methods: Time and length scales

- Solving Schrodinger Equation
- Solving Newton equation of motion
- Monte Carlo Method