PEP 345 Modelling and Simulation

Week	Topic
Week 1	C++: types, declarations, loops, functions; editing and compiling.
Week 2	Euler method simulation of LHO; exporting and plotting the data.
Week 3	Leapfrog method and conservation of energy. RK-methods.
Week 4	Damped LHO; phase space. Orbital motion.
Week 5	*Eigen* library. Basic matrix operations. Coupled LHOs.
Week 6	Simulation of coupled oscillators with matrix algebra. Vibrational modes of CO_2 and other simple molecules.
Week 7	Tight binding model. Calculating energy levels and absorption spectra of long chains and aromatic rings using matrix algebra.
Week 8	*Random* library. Pseudorandom numbers. Markov chain.
Week 9	Simulating random walk and Brownian motion.
Week 10	Simulating epidemics using random numbers and matrix algebra.
Week 11	Ising model. Monte-Carlo methods, Markov chain Monte Carlo.
Week 12	Simulating Ising model with Metropolis-Hastings algorithm.
Week 13	Discretization of derivatives. Crank-Nicholson method. Introduction to heat and diffusion equation.
Week 14	Simulating heat and diffusion equation.

Course outcomes:

1. Choose the appropriate approximation scheme for the given problem.
2. Simulate the damped harmonic oscillator and illustrate it using position vs. time and phase space plots.
3. Find the natural frequencies of the system of harmonic oscillators using matrix algebra package.
4. Write the nearest neighbor tight binding Hamiltonian matrix for the polycyclic aromatic compounds (e.g. naphthalene or anthracene).
5. Simulate random walk with and without drift.

Text:

Arieh Iserles, *A First Course in the Numerical Analysis of Differential Equations (2nd ed.)*, Cambridge University Press, 2009.

Jack Simons*, Advanced Theoretical Chemistry*, LibreTexts, https://chem.libretexts.org/@go/page/11538

Grading:

      Homework   -- 55%
      Canvas quizzes – 15%
      Final Project -- 30%

Catalog description:

Development of deterministic and non-deterministic models for physical systems, engineering applications, simulation tools for deterministic and non-deterministic systems, case studies and projects