ME806 **Computational Nanotechnology** **4-0-0 4**

Introduction

Advancement in computer technology has brought in new method of scientific investigation, the simulation technique. It can also be termed as computer experiments. Coming to nanotechnology, Computer simulations are important due to two main reasons. One is the difficulty in conducting actual experiments at this length scale. We can achieve time and spatial resolution inaccessible in the experiment. The second reason is that, even though in some cases the conventional theoretical models are valid, the inability to solve these models by incorporating all the complexities has brought in new challenges. So to have a clear understanding of the phenomenon occurring at this domain we need accurate computer experiments. According to *Nature Research,* Computational nanotechnology is a branch of nanotechnology concerned with the development and use of computer-based models for understanding, analysing and predicting the behaviour or properties of systems relevant to nanotechnology. In the present course, student will be introduced to the theory, modeling, and simulation methods for understanding nanoscale systems. This course will also give a brief overview of the interdisciplinary nature of research required at this scale.

Course Objectives

- Students will be introduced to the theory, modeling, and simulation methods for understanding nanoscale systems.
- Students will be able to devise, select and use modern techniques and computational tools needed for analyzing and solving complex problems encountered in nanoscale systems.

Course Outcomes

CO1: To gain knowledge on fundamental topics like classical mechanics and statistical mechanics.
CO2: Have exposure about atomistic simulation techniques and its applications.
CO3: Have exposure about data driven modeling for nanoscale systems.
CO4: To identify, formulate, and solve interdisciplinary problems relevant for nanoscale systems.

Syllabus

MODULE 1
Introduction: Computational simulation, need for discrete computation.
Classical Mechanics: Mechanics of Particles, D'Alembert's principle and Lagrange's equation, variational principles, Hamilton's principle, conservation theorems and symmetry properties, central force problems, virial theorem.
MODULE 2
Statistical Mechanics: Review of probability and statistics, quantum states of a system, equations of state, canonical and microcanonical ensemble, partition function, energy levels for molecules, equipartition theorem, minimizing the free energy, partition function for identical particles, Maxwell distribution of molecular speeds.
MODULE 3
Atomistic Simulation Techniques: Molecular Dynamics (MD), Monte Carlo (MC) Method
Mesoscopic Simulation Techniques: Lattice Boltzmann Method (LBM), Dissipative Particle Dynamics (DPD). Introduction to Multiscale methods and applications.
MODULE 4
Introduction to Intelligent Computational Nanotechnology – Data driven modeling and scientific computation.

References:

1. Bird, G.A., Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Oxford Science Publications, 1994.
2. Goldstein, H., Poole, C., and Safko, J., Classical Mechanics, 3 rd Edn., Pearson Education, 2006.
3. Bowley, R., and Sanches, M., Introductory Statistical Mechanics, 2 nd Edn., Oxford Science Publications, 2007.
4. Ercolessi, F., A Molecular Dynamics Primer, Notes of Spring College in Computational Physics, ICTP, Trieste, June 1997 .
5. Liu, Wing Kam, Karpov, E.G., and Park, H.S., Nanomechanics and Materials, John Wiley & Sons, 2006.
6. Robert, K., Ian, H., Mark, G., Nanoscale Science and Technology, John Wiley & Sons, 2005.
7. Groot, R.D., and Warren, P.B., Dissipative particle dynamics: Bridging the Gap between Atomistic and Mesoscopic Simulation, J. Chem. Phys, 107, 4423 (1997).
8. Kutz, J. N., Brunton, S., Brunton, B., and Proctor, J., Data driven Modeling and Scientific Computation: Method for Complex Systems and Big Data, Oxford University Press, 2013.
9. Kutz, J. N., Brunton, S., Brunton, B., and Proctor, J., Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems. SIAM, 2016.

Course 2: **Microflows and Nanoflows**

Credits: 4

Introduction

Microflows and nanoflows covers the behavior, precise control and manipulation of fluids in micro and nano scale. It has emerged only in the 1990s and is a multidisciplinary field intersecting engineering, physics, chemistry, microtechnology and biotechnology and find wide applications in the development of DNA chips, micro-propulsion, micro-thermal technologies, and lab-on-a-chip technology.

Course Objectives

- Students will be introduced to the behavior, precise control and manipulation of fluids in micro and nano scale.
- Students will be able to devise, select and use theoretical models needed for analyzing and solving complex problems encountered in micro and nano flows.

Course Outcomes

CO1: To gain knowledge on the physics of miniaturisation.
CO2: Have exposure about electrokinetic flows and its applications.
CO3: Have exposure about fabrication techniques for micro and nano flows.
CO4: To identify, formulate, and solve interdisciplinary problems relevant for micro and nano flows.

MODULE 1
Physics of miniaturisation – scaling laws. Microscale fluid mechanics: Intermolecular forces, Continuum assumption, Governing Equations, Gas and liquid flow, Slip Models, Shear driven flows, Pressure driven flow, Separated, internal and external flows.
MODULE 2
Electrokinetic Flows: Electroosmotic flows Applications of electroosmotic flows. Electrophoresis Surface tension Driven flows: Mixers and chaotic advection . Simple Fluids in Nanochannels:

Theories of hydrophobic surfaces. Water in nanochannels: definitions and models (atomistic models).Static behaviors- density distribution and dipole orientation, hydrogen bonding, contact angle. Dynamic behaviors – basic concepts, diffusion transport, filling and emptying kinetics.

MODULE 3

Microfabrication techniques – Materials, Crystallography, Bulk and surface micromachining, LIGA, Packaging of microsystems.

Few Applications of microfluidics: Micro pumps, Micro Valves, Micromixers, Microreactors, NEMS, MEMS, Drug delivery, BioMEMS.

References

1. Karniadakis, G., Beskok, A., and Aluru, N., Microflows and Nanoflows: Fundamentals and Simulation, Springer, 2005.
2. C B Sobhan, G P Peterson, Microscale and Nanoscale Heat Transfer-Fundamentals and Engineering Applications, Taylor and Francis/CRC, 2008.
3. Satish, K., Srinivas, G., Dongqing, L., Stephane, C., and Michael R. K., Heat Transfer and Fluid Flow in Minichannels and Microchannels, First Edition, Elsevier, 2005.
4. Bird, G.A., Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Oxford Science Publications, 1994.
5. Kirby, B.J., Micro- and Nanoscale Fluid Mechanics: Transport in Microfluidic Devices,Cambridge University Press, 2010
6. Tabeling, P., Introduction to microfluidics, Oxford University Press Inc., 2005.
7. Madou, M. J., Fundamentals of Microfabrication, CRC press, 2002.