Proposals for Interdisciplinary PG courses to be offered by Centre for Theoretical Studies

Course 2: Nanomechanics (2-1-0-3)

Instructors

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Justification

There is a growing interest in nanoscale devices and processes in various branches of science and engineering. At the length scale of about one to 100 nanometers, some key assumptions and simplifications in continnum mechanics begin to break down. At this scale, discreteness in matter and structure cannot be ignored, surface effects become comparable to those within the bulk, and fluctuations in states may begin to dominate the mean. This course in nanomechanics is intended to highlight the limitations of continuum approaches, and to equip the student with the concepts and tools necessary to model and interpret mechanical behaviour at the nanoscale.

Syllabus

1. *Review of elementary continuum mechanics and how mechanics at nanoscale can be different:* Lagrangian vs. Eulerian. Tensors. Displacement. Stress – Cauchy, Piola Kirchhoff. Strain small, large. Equilibrium, constitutive laws, surface stresses. Cauchy-Born rule.
2. *Basic statistical mechanics:* Review of probability distributions, laws of thermodynamics, entropy, temperature, free energy. Ergodic hypothesis, statistical ensembles. Liouville's equation. Maxwell-Boltzmann statistics.
3. *Classical molecular dynamics:* Hamiltonian, equations of motion, microscopic reversibility, integration schemes,periodicity. Thermostatting. Elastic and fracture properties of crystals using MD simulations.
4. *Linear atomic chains:* Binary molecule, three atom chains,N atom linear chain. Modes of vibration. Phase and group velocity, boundary conditions. Phonons.
5. *Fluctuations:* Dissipation and noise in mechanical systems, Brownian Ratchet and why it is not feasible. Green-Kubo relations. Second law and its statistical nature. Fluctuation theorems.

Lecture-wise split-up

Lectures 1 - 2: Review of elementary continuum mechanics: Lagrangian vs. Eulerian, Tensors, displacement, strain - small and large. Cauchy-Born rule.

Lectures 3 - 4: Review of continuum mechanics (contd.): Cauchy and Piola Kirchhoff stresses, equilibrium, surface stresses.

Lectures 5 - 6: Basic thermodynamics: Laws of thermodynamics, entropy, temperature, free energy. Thermodynamics of elasticity, constitutive laws.

Lectures 7 - 8: Basic statistical mechanics: Review of probability distributions, Ergodic hypothesis, statistical ensembles. Liouville's equation. Maxwell-Boltzmann statistics.

Lectures 9 - 10: Classical MD: Hamiltonian, interatomic potential functions. Equations of motion, microscopic reversibility, integration schemes, periodicity.

Lectures 11 - 12: Classical MD (contd.): Thermostatting. Virial theorem and virial stresses. Elastic and fracture properties of crystals using MD simulations.

Lectures 13 - 14: Classical MD (contd.): Elastic and fracture properties of crystals using MD simulations.

Lectures 15 - 16: Phonons: Linear atomic chains – Binary molecule, three atom chains, N atom linear chains. Modes of vibration, boundary conditions.

Lectures 17 - 18: Phonons (contd.): Lattice structure and lattice vibrations. Phase and group velocity, dispersion relations.

Lectures 19 - 20: Brownian motion. Dissipation and noise in mechanical systems. Brownian Ratchet and why it is not feasible. Green-Kubo relations.

Lectures 21 - 22: Second law and its statistical nature.

Lectures 23 - 24: Fluctuation theorems and computation of free energy differences for nanoscale systems.

In addition to lectures there will be one tutorial every week discussing problems and assignments.

Texts and References

1. Weiner, J.H. *Statistical Mechanics of Elasticity*, Dover Press
2. Cleland, A.N. *Foundations of Nanomechanics: From Solid-State Theory to Device Applications*, Springer
3. Huang, K. *Introduction to Statistical Physics*, CRC Press
4. Hoover, W.G. *Time Reversibility, Computer Simulation, Algorithms, Chaos*, World Scientific
5. Evans, D.J. and Moriss, G. *Statistical Mechanics of Nonequilibrium Liquids*, Cambridge University Press

Exam and evaluation:

Mid-semester: 15% (in hall exam) + 15% (term paper 1)
End-semester: 25% (in hall exam) + 25% (term paper 2)
TA: 20% (home work, class interaction etc.)

Pre-requisites: Consent of the instructors

Maximum number of students allowed to register: 30

Semester in which the course will be offered: Spring