Indian Institute of Technology Kharagpur

2021

SHORT-TERM WEEKEND COURSE

on

Molecular Dynamics Simulations in Materials Science & Engineering

3 Weekends (20 hours)

18th September – 3rd October 2021

Metallurgical & Materials Engineering

Civil Engineering

Introduction

Atomistic modeling of materials has become a popular approach to explore the properties of materials from a modern perspective. Here, a material is simulated by directly computing the dynamics of its constituent atoms from first-principle kinematics. Over the last decade, this technique has witnessed tremendous interest with the advent of enhanced capabilities of modern hardware and algorithms. The practical utility of this method spans several traditional engineering and science disciplines, and the potential applications are limitless. Using the same method, one can find the mechanical properties of a material as well as engineer new materials to have better properties.

Program Objectives

This course aims at introducing the fundamental and practical aspects of atomistic simulations. Both theoretical and hands-on practical aspects shall be covered comprehensively. The theory lectures will commence with a gentle introduction to the basic philosophy of molecular dynamics simulations and gradually progress towards the finer details like structural optimization, time-integrators, thermostats and barostats, etc. Finally, the lectures will demonstrate applications of these tools from the standpoint of fundamental research and domains of industrial applications. Apart from the theory classes, there will be a laboratory component, where the participants will implement the algorithms taught in the theory classes.

This course is designed such that it is beneficial to people from various backgrounds including physics, metallurgy and materials engineering, chemical engineering, civil engineering, mechanical engineering, etc. The topics covered span a broad spectrum of interests ranging from purely fundamental research to industrial R&D.

What you will learn

Program Content*

- Introduction to molecular statics and dynamics; length and time scales associated with MD simulations
- Difference between continuum and atomistic mechanics
- Bonding and interatomic forces; models of various interatomic potentials
- Deriving force fields from potentials; creating new potentials
- Applications of optimization algorithms in molecular statics simulations
- Time integration algorithms – Leapfrog, Velocity Verlet, Runge-Kutta; symplectic and non-symplectic algorithms
- Thermostats and Barostats – Nose-Hoover, Nose-Hoover chains, Nose-Poincare, Gaussian isokinetic
- Relationship with classical thermodynamics – different laws of thermodynamics, ergodicity, canonical ensemble, Green-Kubo relations
- Filtering and visualization in atomistic simulations; exploring structural and mechanical behavior
- Computing transport properties – thermal conductivity, viscosity – using molecular dynamics
- Challenges in molecular dynamics simulations
- Applications in fundamental and industrial research

*Additional Content on computing elastic constants and thermal expansion may be taught depending on the interest of the participants

About IIT Kharagpur

Kharagpur - a dusty town tucked away in the eastern corner of India, famous until 1950 as home to the longest railway platform in the world - became the nursery where the seed of the IIT system was planted in 1951. IIT Kharagpur started its journey in the old Hijli Detention Camp in Eastern India, where some of the country's great freedom fighters toiled and sacrificed their lives for India's independence. Spurred by the success of IIT Kharagpur, four younger IITs sprouted around the country in the two following decades, and from these five came thousands of IITians, the brand ambassadors of modern India. It was the success of this one institution at Kharagpur that wrote India's technological odyssey.

The Institute takes pride in its relentless effort to provide the best platform for both education as well as research in the areas of science and technology, infrastructure designs, entrepreneurship, law, management, and medical science and technology. IITKGP is not just the place to study technology, it is the place where students are taught to dream about the future of technology and beam across disciplines, making differences enough to change the world.

Program Features/ Structure

Classroom lectures – **50%**

Numerical / Problem solving, Case study and Activity – **25%**

Hands-on work with molecular dynamics coding and software - **25%**

Program Schedule and Venue

3 weekends, 18 September – 3 October 2021

Venue: Online

Program Fee

For students (UG/PG/PhD) - INR 5,000 (including GST)

For others (Teachers/ Researchers) - INR 10,000 (including GST)

Who will benefit (Eligibility)

1. For faculty/students of Civil, Mechanical, Aerospace, Metallurgy, Chemical, Materials / Nanotechnology, Physics, Chemistry, and any other allied .

2. Industrial researchers

Last day of Registration

14

September 2021

Accommodation

No accommodation will be provided due to the ongoing pandemic.

How to Apply

Use the link: **https://erp.iitkgp.ac.in/CEP/courses.htm** to apply ONLINE.

Signup → Login → Profile Fillup → Choose a Program → Apply Now

Payment if applicable is to be done **ONLINE** after getting short listed for the program.

Contact Us

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About the Faculty

Dr. Amlan Dutta

Dr. Amlan Dutta is an Assistant Professor in the Department of Metallurgical and Materials Engineering, IIT Kharagpur. He has also worked as a scientist at the Dept. of condensed matter physics and material science of the S.N. Bose National Centre for Basic Sciences, Kolkata. His research interests involve atomistic modeling, general scientific computing, data science and materials informatics, theoretical micromechanics of solids, multiscale modeling in materials science, etc. He holds a PhD from the Variable Energy Cyclotron Centre, Dept. of atomic energy, Govt. of India.

Dr. Puneet Kumar Patra

Dr. Puneet Kumar Patra is an Assistant Professor in the Department of Civil Engineering, IIT Kharagpur. Prior to this, he worked as a postdoctoral research scholar in the Department of Biomedical Engineering and Mechanics, Virginia Polytechnic Institute and State University. His research interests include non-equilibrium statistical mechanics, thermodynamics, molecular dynamics simulations and thermal transport characteristics in low dimensional systems. He holds a PhD degree in Mechanics from IIT Kharagpur and a B.Tech. (H) degree in Civil Engineering also from IIT Kharagpur.