

Event details

Activities	Time	Deliverables
FEB 10, 2024		
Inauguration	9:00AM-9:15 AM	Welcome address and Introduction to the workshop
Lecture 1 By Prof. P.K. Chattaraj	9:20AM 11:00 AM	Introduction to Molecular Simulations (Quantum and Statistical mechanical Concepts)
Tea break	11:00AM-11:15 AM	
Hands-on Session 2 By Dr. Debdutta Chakraborty	11:20AM-1:00 PM	Introduction to Electronic Structure Calculations using Gaussian
Lunch Break	1:00PM-2:00 PM	
Lecture 2 By Dr. Saikat Bhattacharjee Tea Break	2:15PM-3:00 PM 3:00PM-3:15 PM	Basics of Pipe Flow Simulation
Hands-on Session 2 By Dr. Saikat Bhattacharjee	3:15PM-4:00PM	Flow simulation through a pipe bend using COMSOL Multi-Physics
FEB 11, 2024		
Lecture 3 By Dr. Sangram Roy	10:00AM-11 AM	Application of CFD in Simulating Multiphase Reactors Using Ansys Fluent
Hands-on Session 3 By Dr. Sangram Roy Lunch Break	11AM-1PM 1PM-2PM	Simulation of Gas-Solid Fluidized Bed Reactor
Lecture 4 By Dr. Debasree Ghosh	2:15PM-3:30PM	Introduction to "Modern Phase Change and Energy Storage Processes"
Tea Break	3:30PM-3:45PM	
Hands-on Session 4 By Dr. Debasree Ghosh	3:45PM-4:30PM	Heat and Flow analysis of Phase Change using Enthalpy Porosity Model using ANSYS Fluent
Closing Remarks and Vote of Thanks	4:30PM-4:45PM	

Patron

Prof. I. Manna, Vice Chancellor, BIT, Mesra

Chairman

Prof. A. K. Sen

HOD Chemical Engg.

Convenor

Dr. Debasree Ghosh (Chemical Engineering)

Co Convenor

Dr. Saikat Bhattacharjee (Chemical Engineering)

Dr. Sangram Roy (Chemical Engineering)

Organizing Secretary

Dr. Debdutta Chakraborty

Registration Committee

Dr. P Datta (Chemical Engineering)

Dr. B C Ruidas (Chemical Engineering)

Accommodation and Food

Dr. A Tiwari (Food Engineering and Technology)

Dr. J Sudeepan (Chemical Engineering)

Dr. G T Mohanraj (Chemical Engineering)

Press, Web, Media:

Dr. A Mondal (Chemical Engineering)

Venue Management:

Dr. A Karmakar (Chemical Engineering)

Dr. A Bharti (Chemical Engineering)

Dr. Y N Prajapati (Chemical Engineering)

Members:

Prof. P K Chattaraj (Chemistry)

Prof. A Saran (Chemistry)

Dr. S Mishra (Chemistry)

Prof. G Sarkhel (Chemical Engineering)

Prof. S Goswami (Chemical Engineering)

Dr. G T Mohanraj (Chemical Engineering)

Dr. A Choudhury (Chemical Engineering)

Dr. S K Jana (Chemical Engineering)

Dr. A Roy (Food Engineering and Technology)

Dr. R Chatterjee (Food Engineering and Technology)

Workshop

on

MULTISCALE SIMULATION TECHNIQUES IN CHEMICAL ENGINEERING APPLICATIONS

February 10th - 11th, 2024



Organized by

Department of Chemical Engineering

&

Centre for Food Engineering and
Technology

&

Department of Chemistry

Birla Institute of Technology

Mesra - 835215, Ranchi, Jharkhand, India

Website: www.bitmesra.ac.in

IMPORTANT DATES

Last Date for Registration: 8th Feb 2024

To register send e-mail to dghosh@bitmesra.ac.in



About the Chemical Engineering Department



The Department of Chemical Engineering with well qualified faculty provides high standard of education in the diversified fields of Chemical Engineering. The department has immense strength in Polymer Engineering. The department received national recognition by winning the Gold Trophy for Plasticon Award 2012 in the category of Best Educational Institution Contributing to Plastics. The Plasticon Award was conferred on 1st February 2012, at 8th International Plastics Exhibition and conference. The programme was supported by Ministry of Chemicals and Fertilizers, Department of Chemicals and Petrochemicals, Government of India. Faculty members are working on sponsored projects and collaborative research with various organizations. The Department is also recognized under DST-FIST.

The Department has modern and sophisticated laboratories and workshop facilities such as Chemical Engineering Unit Operation laboratory, Chemical Reaction Engineering Laboratory, Process Control Laboratory, Synthesis Laboratory, Energy Engineering Laboratory, Polymer Characterization Laboratory etc. The students are trained in various CAE applications in the field of product and process design with various software such as ASPEN PLUS, MATLAB, PRO/ENGINEER, ANSYS, CATIA, POLYFLOW, and MOLDFLOW.

There are several Projects sponsored by DST, CSIR, ICMR, DRDO, Ministry of New and Renewable Energy, Coir Board etc. to the credit of the Department. Major research areas are: Nanotechnology, Advanced Polymer Composites, Alternative Energy, Energy storage, Bio-resources Utilization, Pollution Control, Water Treatment Technologies, Polymer Blends and Interpenetrating Polymer Networks, Nano filtration Membrane, Recycling of Polymer Waste, Specialty Polymer, Colloids and Interfacial Science, Tissue Engineering, Sensors, Fuel Cell Membrane.

About the speakers

Prof. Pratim Kumar Chattaraj was an Institute Chair Professor at the Indian Institute of Technology (IIT) Kharagpur and a Distinguished Visiting Professor of IIT Bombay. He is presently working as a Distinguished Visiting Professor at BIT Mesra. Prof. Chattaraj has been actively engaged in research in the areas of density functional theory, ab initio calculations, nonlinear dynamics, aromaticity in metal clusters, hydrogen storage, noble gas compounds, machine learning, confinement, fluxionality, chemical reactivity and quantum trajectories. He is a Fellow of The World Academy of Sciences (TWAS), Italy; Royal Society of Chemistry, UK; Indian Natl. Science Academy; Indian Academy of Sciences; National Academy of Sciences, India; West Bengal Academy of Science and Technology; and FWO, Belgium. He is a Sir J. C. Bose National Fellow. He is on the Editorial Board of a number of journals published by the American Chemical Society, Elsevier, etc. Several of his papers have become hot/most accessed/most cited/cover/Editors' choice articles.

Dr. Debdutta Chakraborty is working in the Chemistry Department at BIT Mesra as an Assistant Professor. He worked in Prof. P. K. Chattaraj's research group and received his PhD from IIT Kharagpur. Subsequently, he has worked with Prof. W. L. Hase (deceased) at Texas Tech University, USA and Prof. J. N. Harvey at KU Leuven, Belgium, for his postdoctoral studies. He is interested in employing electronic structure calculations, direct dynamics simulations, statistical rate theories and quantum trajectories in order to understand thermal and photochemical processes.

Dr. Saikat Bhattacharjee is an Assistant Professor in the department of Chemical Engineering BIT Mesra. He has done his PhD from Indian Institute of Technology Kharagpur. Later he worked as a Post Doctoral Fellow in Israel Institute of Technology. He has his research interests in areas like Advanced Transport Phenomena, Microfluidics, and Membrane Separations.

Dr. Debasree Ghosh, an accomplished Assistant Professor in the Department of Chemical Engineering at Birla Institute of Technology, She completed her PhD from Jadavpur University, Dr. Ghosh's research focuses on CFD Modelling & Simulation, Solidification & Melting, and Thermal Energy Storage. Her work in these areas has not only expanded the frontiers of knowledge but also offered practical solutions to challenges in the field of Chemical Engineering. In addition to her academic and research roles.

Dr. Sangram Roy is an Assistant Professor in the Department of Chemical Engineering at BIT Mesra. Prior to that, he was a post-doctoral researcher at the Laboratory for Chemical Technology at Ghent University, Belgium. His research area pertains to the application of CFD in multiphase reaction engineering and process intensification. Sangram has a PhD from IIT Delhi and an M.S. (By Research) from IIT Madras.

About the event

This workshop envisages raising awareness about multiscale simulation and its application in modern Chemical Engineering applications. Over the decades Chemical Engineering has gone through a sea change, the discipline which once was known as "process engineering" has now marked its presence from nano to ultra large-scale applications. Different simulation tools to analyze multiscale phenomena - from molecular to full-scale CFD and process simulation have become the heart of this discipline. This workshop will thus provide a unique opportunity for the students to learn multiscale simulation techniques using:

- (i) Gaussian
- (ii) COMOSOL MULTI PHYSICS
- (iii) ANSYS FLUENT

This will give basic understanding of multiscale simulation techniques and their potential application in modern Chemical engineering problems.

Who can apply:

Interested PGs and research scholars are encouraged to register by filling their details below. It should be e-mailed to dghosh@bitmesra.ac.in

Workshop
on
Multiscale Simulation Techniques in Chemical Engineering Applications
February 10th - 11th, 2024

Name:

Roll Number:

Department:

PG/RS: