



**Indian Institute of Technology  
Kharagpur**

presents

**One – day webinar  
on**

*Scientific computing  
in materials  
engineering*

25<sup>th</sup> September 2021

**Department of Metallurgical  
& Materials Engineering**



**IIM**

**Metallurgy Materials Engineering**

The Indian Institute of Metals, Kharagpur Chapter

## About the webinar

With the recent advancements in scientific computing on the fronts of both hardware and software technologies, the field of computational materials engineering has attracted significant attention from academia and industries alike. Scientific computing applications in materials engineering include gaining insights into the physical mechanisms, discovery, design, and characterization of the materials. This has allowed for rapid virtual screening and analysis, thereby saving costs and resources.

The modern theme of computational materials science involves many tools and techniques like ab-initio computations, classical molecular dynamics, mesoscale simulations, finite element methods, phase-field modeling, materials informatics, etc. Because of this diversity of topics and themes, it has become more important than ever to facilitate and encourage exchanging ideas and experiences amongst peers belonging to various branches of this ever-expanding field.

Aiming to achieve the goal mentioned above, the metallurgical and materials engineering department of IIT Kharagpur is organizing a one-day webinar on “Scientific computing in materials engineering”. This event is in honor of Prof. Nirupam Chakraborti\*, who is presently an Emeritus Professor at the department and is known for his globally recognized contributions in the field of materials informatics. This webinar will provide a platform to foster the cross-pollination of ideas from various sub-domains of computational materials science and engineering. We, therefore, extend our invitation to all the researchers, teachers, students, and professionals to attend this event and make it a grand success.

## List of speakers

**Prof. Nirupam Chakraborti\***  
*Indian Institute of Technology Kharagpur*

**Dr. Manoj Warriar**  
*Homi Bhabha National Institute, Mumbai*

**Prof. Shubhabrata Datta**  
*SRM Institute of Science and Technology,  
Kattankulathur*

**Prof. Anirban Patra**  
*Indian Institute of Technology Bombay*

**Prof. Amrita Bhattacharya**  
*Indian Institute of Technology Bombay*

**Prof. Dibakar Datta**  
*New Jersey Institute of Technology*

**Prof. Božidar Šarler**  
*University of Ljubljana*

**Prof. Matthew Daly**  
*University of Illinois at Chicago*

**Prof. Michael Valášek**  
*Czech Technical University in Prague*



*\*Prof. Nirupam Chakraborti is educated in India and USA, receiving his B.Met.E from Jadavpur University, followed by an MS from New Mexico Tech, USA and PhC, PhD degrees from University of Washington. He joined IIT, Kanpur in 1984 and switched to IIT, Kharagpur in 2000, where he is still continuing.*

*Internationally known for his pioneering work on evolutionary computation in the area of Metallurgy and Materials, globally, Professor Chakraborti is among the top 2% highly cited researchers in Materials, as per Scopus records. A former Docent of Åbo Akademi, Finland, former visiting Professors of Florida International University and POSTECH, Korea, he also taught and conducted research at many other academic institutions in Austria, Brazil, Finland, Germany, Italy and the USA. An international conference was organized in Poland honoring him and an issue of a prominent Taylor of Francis journal was dedicated to him as well.*

## 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.

## Scheduled talks

Speaker	Title	Indian standard time	Speaker's local time
Prof. Nirupam Chakraborti	Evolutionary Data-driven algorithms development for materials research.	10:00 am	10:00 am
Prof. Shubhabrata Datta	Designing Hybrid Nanosystems - An AI-based approach	10:35 am	10:35 am
Prof. Anirban Patra	Modeling Microstructure-Mechanical Property Correlations in Multiphase Materials for Accelerated Materials Design	11:10 am	11:10 am
Prof. Manoj Warriar	Development of computational tools to study irradiation induced changes in the micro-structure of materials	11:45 am	11:45 am
Prof. Michael Valášek	Efficient scientific computing for advanced engineering design	03:05 pm	11:30 am
Prof. Božidar Šarler	Mutiscale and multiphysics meshless solution methods for through-process modelling of metallurgical processing	03:40 pm	12:10 pm
Prof. Amrita Bhattacharya	Combining statistical learning with first principles to predict the physical properties of solid state materials	06:00 pm	06:00 pm
Prof. Dibakar Datta	Understanding interfacial chemo-mechanics of two-dimensional materials-based electrochemical systems	06:35 pm	09:05 am
Prof. Matthew Daly	Deformation mechanisms in concentrated FCC solid solutions	07:10 pm	08:40 am

### How to Join

MS Teams: <https://teams.microsoft.com/l/meetup-join/19%3acHibJu3Z40YsfEIV4oIRt5i6xk3gkH5pXd-NZ8FwJog1%40thread.tacv2/1631860776802?context=%7b%22id%22%3a%2271dbb522-5704-4537-9f25-6ad2dcd4278d%22%2c%22oid%22%3a%22cb432564-912e-4d63-8dc1-c1773da1221d%22%7d>

YouTube Live: <https://youtu.be/HRWaQgvNDcA>

***\*The webinar shall commence at 9:30 am on September 25, 2021.***

### Contact Us

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