

Indian Institute of Technology  
Kharagpur

2023

ONLINE WORKSHOP  
(weekend basis)  
on

# MATLAB Programming for Physical & Chemical Sciences

3 Weekends (20 hours)

18<sup>th</sup> June – 3<sup>rd</sup> July, 2023

## Introduction

Modern science curriculum is deemed incomplete without a significant component involving scientific computing. All domains of natural sciences require computer programming to augment theoretical and experimental progresses. Furthermore, this aspect has laid its footprints on modern industries in addition to the academia. Unfortunately, a lack of exposure to relevant courses and training is a serious shortcoming in most of the B.Sc./M.Sc. programmes across India. **Having realized this issue after interacting with numerous students, we have carefully designed this workshop to cater to the needs of the students of natural sciences.** Here the participants shall have an opportunity to obtain a hands-on introduction to scientific programming using MATLAB/Octave. In addition to gaining basic familiarity with the language, the students will get interesting demonstrations from the fields of physical and chemical sciences.

## Program Objectives

This workshop aims at providing a gentle introduction to the fundamental and practical aspects of scientific computing with MATLAB. As many users do not have access to MATLAB, which is a proprietary software, the workshop shall also cover Octave programming that has a syntax similar to MATLAB and can be used as an open-source alternative. Both theoretical and hands-on practical aspects shall be covered comprehensively. Besides demonstrating the implementations of numerical algorithms from scratch, the workshop will also include built-in tools for higher-level usage.

**This workshop is specifically designed such that it is beneficial to the students with Physics, Chemistry, and Materials Science majors.** Handpicked case studies from quantum mechanics, classical mechanics, spectrum analysis, diffusion, chemical kinetics, etc. shall be covered with live demonstrations.

## What you will learn

### Program Content\*

Introduction to MATLAB, OCTAVE, and scientific computing; matrix as the elementary data-type in MATLAB; accessing matrix elements through indices; Index-slicing and special matrices; matrix operations and element-wise operations.

Mathematical functions in MATLAB/OCTAVE; Loops and conditional statements; logical statements.

Input and output; Creating 2-D and 3-D plots.

Creating functions and sub-functions.

File handling in MATLAB/Octave.

Interpolation and curve fitting in MATLAB/OCTAVE; Numerical differentiation and integration.

Solutions of linear & nonlinear equations; Eigenvalues and Eigenvectors

Solution of differential equations.

Demonstrations of problems related to natural sciences.

\*Additional content such as numerical approximation of boundary value problems may be discussed depending on time availability and interest of 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 Hijili 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

Theory sessions – 50%  
Demonstration - 50%

### Program Schedule and Venue

3 weekends, 18 June –  
3 July 2023

Venue: Online

Platform:  
MS Teams

### Programme Fee

UG/PG/Ph.D. candidates-

INR 1800(Application Fee  
Waived)

Professionals - INR 4500 +  
INR 500 (Application Fee)

### Who will benefit

1. UG, PG, and PhD students of Physics, Chemistry, Materials Science, & Geo Science.
2. Working professionals.

Last day of  
Registration

# 15

June 2023

Certificates will be  
provided to successful  
candidates on  
completion of the course

## How to Apply

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



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

## Contact Us

**Dr. Sankha Mukherjee**, Co-ordinator,  
Department of Metallurgical and Materials  
Engineering, Indian Institute of Technology  
Kharagpur Phone: +91-3222-283260  
Email: [matlab.mmeiitkgp@gmail.com](mailto:matlab.mmeiitkgp@gmail.com)

## About the Coordinators



### 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. Sankha Mukherjee

Dr. Sankha Mukherjee is an Assistant Professor in the Department of Metallurgical and Materials Engineering, IIT Kharagpur. Prior to this, he worked as a postdoctoral research scholar in the Department of Materials Science and Engineering, at the University of Toronto (Toronto, Canada). His research interests include ab-initio modelling of nanomaterials for electronic and energy storage applications, molecular dynamics simulations of mechanical properties and heat transport at the nanoscale. He holds a PhD degree in Mechanical Engineering from McGill University (Montreal, Canada).