



IIT PALAKKAD

**NSM**  
NATIONAL  
SUPERCOMPUTING  
MISSION

# Molecular Simulations

## Using GPU



**Dr. Avisek Das**

Assistant professor, IACS,  
Kolkata, INDIA



hoomdblue

**HOOMD-Blue**



**OpenMM**

**15th Feb 2025**

**9:30 AM to 3:00 PM**

Nila CC Lab, Samgatha, IIT Palakkad,  
Kerala, INDIA

**Register**

**before 13th Feb**



Hands-on workshop on HOOMD-Blue  
and OpenMM: Exploring GPU-based  
molecular simulation tools.

Organisers: Dr. Vishwas V. and Dr. Sandeep Chandran,  
IIT Palakkad.



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MOLECULAR  
SIMULATIONS  
USING GPU

# EVENT PROGRAM

15th February 2025

Nila CC Lab, Samgatha, IIT Palakkad

9:30 AM TO 11:30 AM

- Introduction to Molecular Dynamics
- Parallel Computing CPU vs GPU
- OpenMM
- Hands-on Session

12:00 PM TO 1:30 PM

- Introduction to Monte Carlo
- HOOMD-Blue
- Hands-on Session

2:30 PM TO 3:30 PM

- Q&A and Clarification

## More Information

- OpenMM Tutorials and Examples

<https://openmm.github.io/openmm-cookbook/latest/tutorials.html>

- HOOMD-Blue Tutorials and Examples

<https://github.com/glotzerlab/hoomd-workshop>

<https://github.com/glotzerlab/hoomd-examples>

Organisers: Dr. Vishwas V. and Dr. Sandeep Chandran, IIT Palakkad.



OpenMM



HOOMD-Blue

