SCHOOL ON SCIENTIFIC AND ENGINEERING SIMULATION:

Theory and applications

Applications in the field of Physical, Chemical, Biotechnology, Nanotechnology and Engineering

22nd - 27th May, 2019

Organized by: Division of Research and Development
Lovely Professional University
MOTIVATION

Computers have been used to solve various science and engineering problems. It even provides solution to complex problems with high computational processing power which were almost impossible to resolve earlier. Due to rapid technological advancements, the demand for scientific programming is enhancing every day in the field of academic as well as industrial research. Growing popularity for intelligent computational systems is creating an enormous demand for scientific software developers. The research domain requires very intense knowledge of programming, mathematics, science, and engineering. This workshop aims to teach different levels of programming, from basic to advance and its applicability in scientific modeling. To make the complex theories and algorithms easy to understand both theory and hands-on will go simultaneously. Practical demonstrations from various aspects of basic science, biotechnology, and engineering will be included. It will be useful for novice and expert researchers who are pursuing research work in the field of computational science and want to become a scientific software developer. We encourage people from biology, physics, chemistry, material science, chemical engineering and all other related fields to participate.

TOPICS OF INTEREST

- Introduction to simulation in the field of Physical, Chemical, Biotechnology, Nanotechnology and Engineering
- Introduction to programming
- Stochastic Simulations
  - Introduction to stochastic simulations
  - Random number generators
  - Monte Carlo and Kinetic Monte Carlo Simulations
  - Metropolis method, Detailed balance
  - Important sampling
  - Markov chain
  - The Gillespie algorithm
- Molecular Dynamics
  - Introduction to molecular dynamics
  - Force Calculation
- Integrating the equation of motion
- Molecular dynamics on various ensembles
- Quantum mechanical simulation
  - Introduction to quantum mechanics
  - Hartree Fock theory and application to simple molecules
  - Density Functional theory and application to simple molecules
- Parallel programming.
  - Parallel programming with multi-threading
  - Implementation of parallel programming to various examples
LEARNING OUTCOMES:
After this short term course, the participants will be able to:
- Write and debug code
- Formulate new hypothesis and test algorithms
- Develop parallel programing
- Test and critically analyze real time scientific projects
- Identify future research possibilities

WHO CAN ATTEND:
- Research scholar’s eager to refine & improvise on their research projects
- Any science and engineering students (M.Sc, M.Tech, PhD, and Postdoc)
- Faculty members of any discipline having interest in establishing research credentials and Improving upon academic competence

WORKSHOP PREREQUISITES
- Personal laptop is compulsory

PEDAGOGY
- A mix of pedagogical tools will be used i.e. lectures, discussions, presentations and experiential exercises
- Hands on experience will be given on C, C++ and python (for Equation Modeling)
- Participants will be provided

experiential learning through simulation.

Examples from natural science, biotechnology and engineering will be used

IMPORTANT DATES AND REGISTRATION FEE:

<table>
<thead>
<tr>
<th>Participant Type</th>
<th>Registration Fee per participant</th>
<th>Registration Closes</th>
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<tbody>
<tr>
<td>Internal Participants</td>
<td>Rs. 2450/-</td>
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<tr>
<td>External Participants</td>
<td>Rs. 2950/-</td>
<td>May 15th 2019</td>
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**WORKSHOP SCHEDULE:**

<table>
<thead>
<tr>
<th>Days</th>
<th>Session 1</th>
<th>Session 2</th>
<th>Session 3</th>
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<tbody>
<tr>
<td>Day 1</td>
<td>Introduction to simulation in the field of Physical, Chemical, Biotechnology, Nanotechnology and Engineering. Basic programming</td>
<td>i/o statements</td>
<td>Object oriented programming</td>
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<td>Day 2</td>
<td>Random number generators, Monte Carlo and Kinetic Monte Carlo Simulations, Metropolis method, Detailed balance</td>
<td>Interactions</td>
<td>Markov chain, the Gillespie algorithm</td>
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<td>Day 3</td>
<td>Introduction to molecular dynamics Force Calculation, Integrating the equation of motion</td>
<td>Interactions</td>
<td>Molecular dynamics on various ensembles</td>
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<td>Day 4</td>
<td>Introduction to quantum mechanics, Hartree Fock theory and application to simple molecules</td>
<td>Interactions</td>
<td>Density Functional theory and application to simple molecules</td>
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<td>Day 5</td>
<td>Introduction to Parallel programing, implementation of multi-threading</td>
<td>Interactions</td>
<td>Summary of content</td>
</tr>
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<td>Day 6</td>
<td>Future research possibilities</td>
<td>Networking and collaborations</td>
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**NOTE:**
- Online payment will be accepted up to 15th May 2019.
- Cash payment will be accepted for registered participants latest by 15th May 2019 up to 4 p.m., subject to the availability of seats.
- Fee once paid is non-refundable.
- Accommodation can be arranged on request at subsidized rates.

**HOW TO REGISTER:**

**Step1:** https://www.lpu.in/academics/research.php

**Step2:** Click on the heading “Scientific and Engineering Simulation Training”

**Step3:** As a New user enter your particulars to Register

**Step4:** Select the Payment mode and make payment accordingly.
MODE OF PAYMENT:

**Online Payment:** Net Banking/Debit Card/Credit Card

**Cash Payment:**

**Step 1:** Register for Scientific and Engineering Simulation Training;

**Step 2:** Download the offline form

**Step 3:** Submit the Form and Cash in Division of Accounts Block 32-103 Window no. 1 from 09.00 am - 04.00 pm

VENUE:

Division of Research and Development, Lovely Professional University Campus, Jalandhar-Delhi G.T. Road, National Highway, Phagwara, Punjab 144411.

CERTIFICATION:

Participation certificates will be awarded all the attendees.

RESOURCE PERSONS:

**Dr. Pinku Nath,** PhD in Computational Chemistry from IIT-Kanpur and has 5 years of research experience as material scientist and scientific software developer at Duke university, NC, USA. He is currently working as an assistant professor in the department of Chemistry at Lovely Professional University. His current research area: Developing high throughput ab initio methodologies, Lattice dynamics, ab initio thermodynamics, high temperature superconductors.

**Dr. Aman Singh,** PhD in Computational Biology from Lovely Professional University and has 7 years of teaching and research experience. He is currently working as an assistant professor in the department of computer science and engineering at Lovely Professional University. His current research areas are computational biology, cyber security, healthcare systems and machine learning.

ORGANIZING COMMITTEE

Program Convener

Dr. G. Geetha, Professor and Head of Department (HD), Division of Research and Development, Email: geetha.15484@lpu.co.in

Program Coordinator

Dr. Ajit Kumar Sharma, Associate Professor, Division of Research and Development, Email: ajit.24338@lpu.co.in, M: +91-7400249029, +91-7355155514.
ABOUT THE HOST INSTITUTION:
Lovely Professional University has a mammoth ultra-modern high-tech campus sprawling along the National Highway No.1 at the entry of Jalandhar City. Lovely Professional University is acclaimed for academic excellence, range of programme offerings, the inspiring quality and breadth of its academic programmes and research initiatives. It has established uniqueness through its world class pedagogy, creative work, leadership skills, nurturing faculty and providing support needed in achieving career goals. Human Resource Development Center (HRDC) is an entity established under the aegis of Lovely Professional University for professional development of staff. The Center is responsible for planning, organizing, implementing, monitoring and evaluating the staff development programs as per the desired standards of quality intended to be delivered. A variety of Faculty Development Programs are conducted to enhance the quality of teaching and research. The Programs are specifically designed to master state of the art developments in course content, pedagogy and research methods. Training Programs are conducted by eminent resource persons from nationally and globally reputed institutions. LPU is the Local Chapter for National Programme on Technology Enhanced Learning (NPTEL), offered by seven premier IITs and IISC Bangalore with support from Ministry of HRD, Govt. of India. LPU has been awarded AAA rating by NPTEL, a status accorded to the top ten chapters. LPU has MOU with reputed institutions specializing in the area of Training and Development like National Institute of Technical teachers Training and Research (NITTTR), Chandigarh.