FOUNDATIONS OF COMPUTATIONAL MATERIALS MODELLING

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TYPE OF COURSE : Rerun | Elective | PG
COURSE DURATION : 12 weeks (26 Jul' 21 - 15 Oct' 21)
EXAM DATE : 24 Oct 2021

PRE-REQUISITES : Basic Materials Science Course at the undergraduate level, MATLAB programming, familiarity with LINUX is preferred.

INTENDED AUDIENCE : All Engineering students

INDUSTRIES APPLICABLE TO : None. This course will be useful for students pursuing research requiring molecular simulations of solids.

COURSE OUTLINE :

This course provides the necessary foundations to (a) build computational samples of crystals (b) Introduce statistical mechanics and its connection to Molecular dynamics (c) Provide enough ground in Molecular dynamics using LAMMPS

ABOUT INSTRUCTOR :

The instructor Dr. Narasimhan Swaminathan is an Associate Professor in the Dept. of Mechanical Engineering at IIT Madras. Prior to this, he was a Post Doctoral Research Associate in the Materials Science and Engineering Department at University of Wisconsin, USA. Dr. Narasimhan obtained his Ph.d. from the Georgia Institute of Technology in 2009. His current research areas include molecular simulations to study radiation damage, polymer mechanics,etc. He also studies stress-diffusion interaction in Li-ion battery electrodes using continuum mechanics.

COURSE PLAN :

Week 1**:** Introduction to Computational Modeling

Week 2**:** Introduction to Crystals

Week 3**:** Symmetry in Crystals

Week 4**:** Plane Groups

Week 5**:** Space Groups

Week 6**:** Construction of 2D and 3D crystals in MATLAB

Week 7**:** Statistical Mechanics

Week 8**:** Statistical Mechanics,cont'd

Week 9**:** Introduction to Molecular Dynamics

Week 10**:** Molecular dynamics using LAMMPS – 1

Week 11**:** Molecular dynamics using LAMMPS -2

Week 12**:** Molecular dynamics using LAMMPS -3 and Closure