**Indian Institute of Technology Kanpur**

**Proposal for a new course**

1. **Course No.:**
2. **Course Title:** Introduction to Integrated Computational Materials Engineering
3. **Credits: 3-0-0-27; Duration of Course: Full Semester (Total of ~40 Lectures)**
4. **Proposing Department: Materials Science and Engineering**
   Other Departments which may be interested in the proposed course: CHE, ME, MSP
5. **Proposing Instructor: Krishanu Biswas**

   **Other Instructors interested in taking this course**: Dr. Shikhar Misra, Dr. Shikhar Krishn Jha, Dr. Somnath Bhowmick, Dr. Rajdip Mukherjee, Dr. Shivam Tripathi, Dr. Tanmoy Maiti, Dr. A.K.Singh
6. **Course Details**

**Objectives**:

In this course, we will learn about basic principles of materials design as well as modeling tools at multiple length and timescales. The major objective lies in finding their applications in linking processing-structure-property-performance relations in materials engineering to address the issues related to the product design and applications. This is intended to provide in-depth knowledge on materials and product design, materials discovery with applications using large-scale multiscale modeling with the ultimate goal to speed up the design process and implement prototyping.

| Sl. No | Broad title | Topics | Lectures |
|---|---|---|---|
| 1 | **Introduction to the Course on ICME** | Need to learn ICME. Approach to design products and materials with associated materials processing methods, Historical perspectives | **1** |
| 2 | **Length and time scales in ICME** | Concepts of multiscale modelling- From atomic scale (sub nanometer to) to component scale (meter). The effect of these length scales on the material behaviour and manufacturing. | **3** |
| 3 | **Macroscale models** | Some Constitutive equations at continuum level. | **4** |
| 4 | **Mesoscale models** | Continuum crystal plasticity, dislocation dynamics, homogenization, structure-property relations; relationship between microstructural morphology, crystallography, and mechanisms to the material response at different scales. | **5** |

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| 5 | **Computational Thermodynamics and** | Tools for computational thermodynamics, CALPHAD, Thermodynamic databases and their utilization. | **4** |
| 6 | **Microscale methods** | Phase-field models of microstructure evolution, process-structure relations. | **4** |
| 7 | **Atomistic nanoscale methods and Electronic structure methods** | Molecular Dynamics/Kinetic Monte Carlo methods<br><br>Density functional theory (DFT) model | **5** |
| 8 | **Modeling tools at various length and time scales** | MATLAB, FiPy, NumPy, SciPy, PRISMS, MOOSE | **5** |
| 9 | **Data analytics** | Database management systems, data pre-processing, algorithms, clustering, and text mining. Analysis of images, voxel data, dynamical data, and graphs, language and symbolic methods. | **6** |
| 10 | **Optimization tools** | Basic optimization tools: Bayesian optimization. Hyperparameter optimization, Gradient Descent and Gradient Descent and its variants etc. | **4** |
| **Total** | | | **41** |

**Prerequisites: Basic Materials courses on structure, processing, characterization of materials; mechanical and functional behaviour of materials.**

8. **Short summary of the course content:**

ICME, popularly known as Integrated Computational Materials Engineering, involves the integrating computational framework that aims at designing new materials, products, or structures to meet specific performance criteria. The purpose of this course is to teach the students an accelerated approach to design materials and products concurrently and synergistically. We intend to provide an interdisciplinary education where the students are expected to gain expertise in various ICME techniques and tools, multiscale modeling of materials, computing, optimization, data analytics to learn accelerated design of materials and processes. The course will involve numerous examples and case studies, hands-on tutorials, computational thinking as well as problem-solving. Emphasis will be on linking these models and materials databases for structure-property relationships at multiple length and time scales to address problems relevant to specific products and applications. The students are expected to obtain knowledges on the basic principles of materials design, modeling tools at multiple length-scales and timescales as well as applications.

9. **Text and Reference Books**


1. Introduction to Computational Materials Science, Richard LeSar, MRS (2013)
2. Computational Materials System Design – Dongwon Shin, James Saal (editors) – Springer (2018)
3. Integrated Computational Materials Engineering (ICME): Advancing Computational and Experimental Approaches- Somnath Ghosh, Christopher Woodward, Craig Przybyla, Springer (2020)
4. Integrated Computational Materials Engineering (ICME) for Metals: Concepts and Case Studies, Mark F. Horstemeyer (ed.) Wiley (2013)


Date: 31/12/20224 Proposer (Krishanu Biswas)

Date: DUGC/DPGC Convener: