<table>
<tr><td>Course Title</td><td>Multiscale Modeling of Materials using Machine Learning</td><td>Course Code</td><td colspan="4"></td></tr>
<tr><td>Dept./ Specialization</td><td>Mechanical Engineering</td><td>Structure (LTPC)</td><td>3</td><td>1</td><td>0</td><td>4</td></tr>
<tr><td>To be offered for</td><td>B.Tech, M.Tech, PhD</td><td>Status</td><td colspan="2">Core ☐</td><td colspan="2">Elective ■</td></tr>
<tr><td>Faculty Proposing the course</td><td>Dr. Arul Kumar Mariyappan</td><td>Type</td><td colspan="2">New ■</td><td colspan="2">Modification ☐</td></tr>
<tr><td colspan="2">Recommendation from the DAC</td><td>Date of DAC</td><td colspan="4"></td></tr>
<tr><td>External Expert(s)</td><td colspan="6">Prof. Alankar Alankar, IIT Bombay, India
Prof. Irene Beyerlein, University of California, Santa Barbara, USA</td></tr>
<tr><td>Pre-requisite</td><td>Consent of Teachers (CoT)</td><td colspan="3">Submitted for approval</td><td colspan="2">___th Senate</td></tr>
<tr><td>Learning Objectives</td><td colspan="6">To provide an opportunity for the students to appreciate how the integration of machine learning with multiscale modeling of materials advances the field to meet rapidly growing industrial demands.</td></tr>
<tr><td>Learning Outcomes</td><td colspan="6">• Understand the concept of multiscale modeling of materials and the basics of machine learning algorithms.
• Ability to develop numerically efficient computational models for engineering applications.</td></tr>
<tr><td>Contents of the course
(With approximate break-up of hours for L/T/P)</td><td colspan="6">Review of Materials Science and Machine Learning concepts (L8+T3)
• Crystal systems/structures, symmetry, anisotropy, tensorial representation of crystal properties
• Multiscale hierarchical microstructure (polycrystals, grains, sub-structures, defects, and atoms) and its effect on properties
• ML algorithms: supervised, unsupervised and reinforcement learning methods
Conventional Multiscale Modeling of Materials (L12+T4)
• Atomistic (density functional theory and molecular dynamics) and micro-scale (defect dynamics) modeling
• Meso-scale (phase field and meso-plasticity) and macro-scale (finite element methods) modeling
• Integration of length and time scales for materials modeling
Machine Learning for Materials Science (L10+T3)
• Materials Data: Source, size, composition, version, and uncertainty
• Materials modeling: Model selection, data scaling and normalization, and model evaluation
• Model development: Calibration, validation, benchmarking, and uncertainty quantification
Machine Learning and Multiscale Modeling of Materials (L12+T4)
• Concurrent and sequential transfer of data, theory, and correlations
• Data-driven and physics-driven machine learning approaches
• Bayesian approach to multiscale modeling of materials: Surrogate models</td></tr>
</table>

Textbook	1. R. J. Asaro and V.A. Lubarda: *Mechanics of Solids and Materials*, Cambridge University Press, 1st edition, 2006. 2. D. Barber: *Bayesian Reasoning and Machine Learning*, Cambridge University Press, 2nd edition, 2012.
Reference Books	1. U.F. Kocks, C. N. Tome, and H. R. Wenk: *Texture and Anisotropy*, Cambridge University Press, 1st edition, 2000. 2. J. Fan: *Multiscale Analysis of Deformation and Failure of Materials*, John Wiley & Sons, 1st edition, 2011. 3. A. C. Mü ller and S. Guido: *Introduction to Machine Learning with Python*, O'Reilly, 1st edition, 2016. 4. Aurelien Geron: *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems*, Shroff/O'Reilly, 3rd edition, 2022.