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Enhancing and Supporting Integrated Computational Material Science Engineering Education

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Abstract

In this paper we describe a novel approach for teaching a multi-disciplinary course "Integrated Computational Materials Engineering (ICME) for Metals" aimed to support the generation of future taskforce of engineers. By combining traditional teaching of the theoretical concepts of the ICME paradigm (based on a textbook) with in-class practical training sessions using the resources accessible online through ICME Cyberinfrastructure (CI), the students are motivated to work in dynamic, shared, and collaborative learning environment while learning and utilizing the state-of-art, high-performance computational tools. This course was taught as a part of Fall 2012 and 2013 graduate coursework of Mechanical Engineering Department at Mississippi State University. The paper discusses the rationale for the course, the course description, the grading procedures, and survey-based course assessments. The surveys showed that the students' reaction to the class was very positive. The impact of this course was evident in students learning outcomes that were published online on ICME Wiki. The majority of the students were awarded the top grade for the class, reflecting their performance, interest and effort.

Introduction

Integrated Computational Materials Engineering (ICME) is an emerging discipline that aims to integrate computational material science tools into a holistic system than can accelerate materials development, transform engineering design optimization, and unify product design and manufacturing. The concept of ICME arose from the new simulation-based design paradigm that employs a hierarchical multiscale modeling approach to relate phenomena that occur at different length scales leading to greater accuracy in simulation-based design[1]. Consequently, the application of ICME methods, that is, performing multiscale simulations, requires multidisciplinary expertise in modeling these phenomena using multifarious computational tools.

The realization of the anticipated revolutionary change in material engineering offered by ICME critically depends on the ability to teach the arcana of multiscale modeling[2] to engineering graduate students. To address this challenge, we have developed a new graduate course, entitled "Integrated Computational Materials Engineering (ICME) for Metals" (ME8990). This course is also deployed for online learning in a virtual classroom. The course was taught for the first time during the Fall 2012 semester and is being taught for the second time during the Fall 2013 semester. The course design is based on blended learning approach[3] to facilitate integration of advanced technological resources (ICME Cyberinfrastructure) with traditional pedagogical practices (textbook, Mark F. Horstemeyer, "ICME for Metals"[4]).

The interdisciplinary course curriculum is fragmented into independent learning modules with each module focusing on teaching different material length scales with its respective collaborative student group assignments and learning outcomes[5]. In addition to teaching theoretical concepts of ICME paradigm (based on the textbook), the course lectures are supplemented with in-class practical training sessions using the resources accessible online through ICME Cyberinfrastructure (CI) named Engineering Virtual Organization for

CyberDesign (EVOCD)[6]. The resources enabled though the shared CI include experimental data, material models and constants, computational tools and software artifacts, and the knowledge pertaining to multiscale physics-based models. These resources are used with different modules to investigate experimental procedures for model exploration, model calibration, and model validation as well as failure prevention in the context of a diverse set of real world case studies.

The emphasis of this course is to teach students in a modular fashion[7] the essential concepts of computational tools describing phenomena at different length scales, to perform simulations at different scales, and to bridge all this information together to determine process-structure-properties-performance relations of materials. On successful completion of the assigned collaborative projects, all students are required to update their learning contributions on the ICME CI portal Wiki[8], facilitating easy assessment of student achievements. Moreover, using the example case studies, PowerPoint lectures, computational tools and other resources which are made available via Wiki based EVOCD web portal, academic institutions or industry members can seamlessly deploy and teach this ICME course in real classrooms or virtually through distance learning.

This paper is organized as follows. We start with stating the course objectives, followed by a detailed description of the course organization and curriculum. Next, we present the class grading procedure. Finally, we conclude this paper with the presentation and discussion of the course assessment.

Course Objectives, Design, and Delivery

While ICME is a promising new approach for materials innovation but still is in its infancy and realizing ICME's full potential requires synergy between ICME technologies and pedagogical practices. In a recent survey, ICME education is mentioned as one of the cross-cutting issues that must be addressed simultaneously with development of ICME demonstration projects based on Foundational Engineering Problems[9]. Additionally, the National Academy of Engineering Report clearly indicates the lack of adequate expertise in overall computational engineering tools among current workforce of material science researchers and engineers and embraces ICME as a discipline, which in order succeed mandates changes in education, research, and information sharing[1]. Moreover, for advancing new materials discovery the Genome Initiative for Global Competitiveness [10] laid emphasis on establishing new course curricula at undergraduate and graduate levels in academic institutions for training and educating next generation of engineering workforce with a more integrated approach for materials development.

Consequently, our primary goal was to develop a course to support the generation of future taskforce of engineers who would be motivated to work in dynamic, shared, and collaborative learning environments and would use the materials knowledge and the computational tools leveraged through the shared CI for new materials discovery and development. The result is the course named "ICME for Metals" that was designed as an effort to address the above mentioned issues by integrating ICME directly into the traditional educational curricula and was deployed as a part of fall 2012 and 2013 graduate coursework in mechanical engineering department at Mississippi State University. There were two pre-requisites required for this course: 1) Strength of Materials, and 2) Material Science Fundamentals. While the course was deployed at the mechanical department, the course was aimed to also be appropriate for interested students from any other discipline, in that it will assist in integrating ICME with other STEM disciplines by raising awareness of new potential issues and technologies and igniting an innovative thought process among students in different science fields for utilizing ICME in practice.

More specifically, this course aims that the students are exposed to the state-of-the-art computational tools which will enables them to gain strong practical insight of the multidisciplinary interactions involved in multiscale modeling and bridging methodologies among different length scales. This includes the understanding of the upscaling[2] and downscaling[2] techniques required to fully characterize the properties of the materials of their interest. In this course, the students learn to use collective intelligence to execute the team assignments which would prepare them to work in future collaborative corporate learning environments for materials research and development. Another significant expected outcome of this course is to make students to learn, integrate and utilize the high end technological resources offered by ICME CI (EVOCD) and overcome the challenges of using them with both experiencing and implementing bridging simulations at multiple materials length scales.

The course curricula discussed in this work was a fifteen-week program and was divided into independent modules to effectively educate students in basic ICME skills along with the practical, real world case studies involving multiscale simulations and bridging procedures for determining the structure-properties-performance relationships among multiple material length scales. The course was delivered both in-class and online in virtual classroom.

The lectures were intended to strike a balance between the traditional and modern approaches for teaching the multidisciplinary nature of multiscale modeling by fostering an interactive outcome-driven learning environment enabled through ICME cyberinfrastructure (EVOCD). The course lectures: 1) covered the basic examples and principles pertaining to each material length scales (atomic, molecular, dislocation, crystal-plasticity, macro-scale FEA); 2) described and demonstrated the use of state-of-the-art computational tools and technologies provided via ICME CI to perform simulations at different length scales; 3) provided hands-on training sessions for blending all the expertise and information gained through exploratory experiments, calibration of material models, and validation of models to determine structure-property-performance relationships of materials.

One of the novel aspects of this course is that each module culminates with a collaborative homework assignment where the students were motivated to publish, validate, and visualize their multiscale modeling learning outcomes on Wiki based EVOCD web portal[8] with an anticipation of sharing and defending their research findings with other class members, thus facilitating easy assessment of students accomplishments. Through this exercise students demonstrated how the knowledge attained and exchanged from ICME wiki resulted in practicing and publishing the potential impact of adopting the multiscale modeling paradigm in their diverse research areas related to their Master/PhD dissertations.

Course organization and curricula

The interdisciplinary course curriculum described here was designed in a modular way with the goal of integrating new pedagogical approaches with ICME education such as teamwork, technology enhanced in-class practical training sessions. The course was divided in five modules inherently supporting blended learning[3] where traditional module lectures pertaining to the multidisciplinary aspects of ICME based on the book entitled "ICME for Metals"[4] are supplemented with an interactive collaborative environment enabled by ICME CI (EVOCD)[8] for improving graduate student educational experience by engaging them in their own learning processes. The course was taught as three 50 minute sessions per week for 15 weeks where each module consisted of four to seven lectures depending on the needs of the topic covered in that corresponding module. The course was taught for the first time during the fall 2012 semester and for the second time during the fall 2013 semester. The course was attended by students not only from mechanical engineering but also from aerospace engineering, biochemistry, biological engineering, chemical engineering, computer science, geosciences, and industrial engineering.

The following subsections describe the learning modules which were delivered in this course.

(i) Multiscale Modeling Methodology:

This module was focused on providing students an understanding of ICME paradigm that employs a hierarchical multiscale modeling methodology, and its major advantages for designing new materials in comparison with conventional design and optimization processes often based on trial and error. More details on topics and learning objectives of this module are summarized in Table 1.

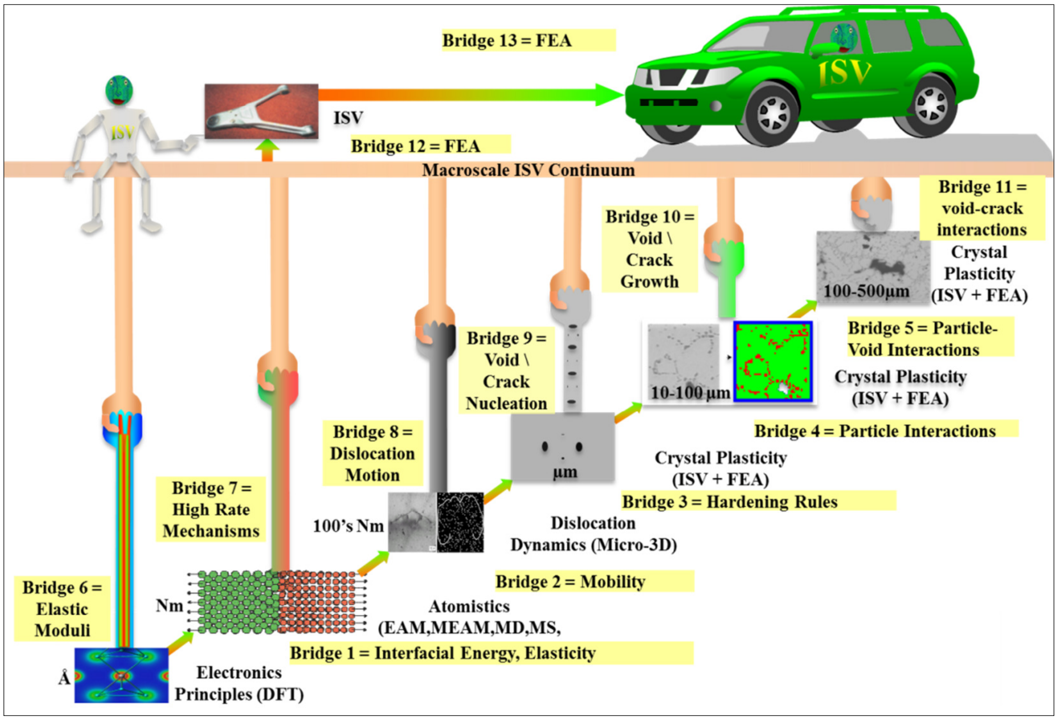

Figure 1. Multiscale modeling example of a metal alloy. The example illustrates different length scales analysis methods used and various bridges needed[4].

The module was started with an overview of ICME methodologies and its advantages in design, such as reduction in the product development time and cost, and increase in increase product quality and performance. The second topic covered provided a brief background about the usage of multiscale materials modeling to capture the process-structures-properties-performance of a material[2]. The third topic covered demonstrated upscaling[2] and downscaling[2] requirements of hierarchical multiscale modeling required to perform multiscale bridging. The guidelines for multiscale bridging were demonstrated to the students with an example of a bridging model illustrated in Figure 1.

Then in this module two real world case studies were described to students. The control arm fracture[11] and the control arm fatigue[12] case studies based on the "From Atoms to Autos" modeling philosophy[12] to enable students to learn the relationship between requirements, process-structure-property modeling, and the associated history for solving complex engineering problems.

Table 1. Topics and learning objectives used in Module 1.

	Topics	**Learning Objectives**
1	ICME History and Overview	Introduce Advantages of Employing ICME in Design. Social, Economical, and Political Driving Forces for ICME.
2	Multiscale Aspects of Materials	Classify Eight Guidelines for Multiscale Bridging . Multiscale Modeling Disciplines: Hierarchical and Concurrent, Multiscale Experiments (Exploratory exps, Model Correlation exps and Model validation exps). Process-Structure-Property Modeling and the Associated History. Illustrate Multiscale Concrete Modeling example. Identify Multiscale Modeling issues related to Concrete. Multiscale Polymer Modeling example.
3	Creating a new Material/Structure/Component	Illustrate Cradle-to-crave modeling: stamping example. Downscaling and upscaling Requirements.
4	Case Study: Control Arm Fracture	Investigate Physical Observations of Ductile Fracture and the Role of Pore/Void Coalescence. Materials Processing Influence on Ductile Fracture. Pore Coalescence Definitions. Pore Coalescence Bridging to the Macroscale.
5	Validation and Verification	Consider the comparison between a simulation result and experimental data. Definition of Verification, Validation and Uncertainty (Error). Types of Uncertainty Analysis. Model Calibration Example Under Uncertainty. Uncertainty Quantification and Propagation. Uncertainty and Sensitivity Analysis of Damage.
6	Optimization	Explain Conventional Design Methodology. What is optimization? Unconstrained minimization. Constrained minimization. Global-Local Approaches. Multi-Objective Optimization. Optimization software. Structural optimization. Surrogate optimization (Metamodeling).
7	Constitutive Relations: Definitions	Explain Relationship of Manufacturing Process, Defect, and Ductile Fracture Mechanisms. Relationship of Manufacturing Process, Defect, and Fatigue Mechanisms

The module culminated in an individual class assignment where each student was required to perform a literature review of papers pertaining to mutiscale modeling aspects of ICME paradigm. Additionally, each student was required to choose a research topic of their interest and to present in class a 30 minute presentation demonstrating his/her understanding of downscaling and upscaling requirements to create "bridges" between different material length scales (electronic scale, nanoscale, microscale, mesoscale, macroscale, and structural scale). By performing this exercise the students examined the importance of integrating multiscale modeling methodology in their chosen research topic.

(ii) Basic Skills and ICME CI (EVOCD):
As mentioned earlier the students enrolled in this class widely vary with respect to their engineering disciplines. Moreover, not all of the students were skilled and confident with basic skills, such as running Linux/Unix scripts and submitting jobs on clusters. Additionally, some students were also new to the concept of cyberinfrastructure and were not equipped with knowledge of using it. For this reason we designed this module aiming at introducing ICME CI to the students, along with providing students with hands-on tutorials on the basic computational skills required to use various software artifacts utilized in other modules.

Table 2. Topics and learning objectives used in Module 2.

	Topics	**Learning Objectives**
1	ICME CI (EVOCD)	Discuss Need for ICME CI. Discuss Webportals such as nanoHub[13], 3D Material Atlas[14], MatDL[15], NIST Data Gateway[16], EVOCD[8].
2	EVOCD Components	Illustrate Knowledge management Wiki. Repository of Data. Online Model Calibration Tools. Repository of codes.
3	Knowledge Management: Wiki	Introduce Wiki. What is Wiki? Knowledge managed by EVOCD Wiki: different Classes of Materials, Material Models of behavior at various length scales, and design issues.
4	Repository of Codes	Discuss Installation instructions, User manuals, theoretical background, and examples of various codes. Computational and Visualization tools such as MATLAB[17], VASP[18], ABAQUS[19], LAMMPS[20], OVITO[21], OpenGL[22], Xmgrace[23] and others
5	Online model calibration tools	Discuss Intuitive user interface for using Calibration Models, such as the Plasticity-Damage model[24] , MultiStage Fatigue model[25] , and Thermoplastic model[26.] Microstructure Image Analyzer for Material Charaterization[8].
6	Basic computation skills	Discuss Basic Unix/Linux commands. Working with the PBSworks[27] software job resource manager for submitting jobs to cluster environments (HPC systems). Compiling and writing shell scripts, Examples :interactive jobs, batch jobs

In the beginning of the module (see Table 2) students were demonstrated various components of EVOCD[8] which are the knowledge management Wiki, the repository of codes, experimental data repository, and the online model calibration tools. Following the introduction students were given a hands-on training on EVOCD components in which students learned (1) to upload/modify/delete knowledge on ICME Wiki pages (2) to use model calibration tools along with the repository of data such that the students can upload the experimental data, perform model calibration using the models provided, and then store the derived material constants back into the repository of data (3)to utilize state-of-the-art simulation, optimization, and material modeling codes for materials manufacturing process and design (4) Running simulations code the retrieved from repository of codes along using the knowledge gained from ICME Wiki with the experiment data obtained from repository of code on the university HPC clusters (Talon and Raptor). Two important aspect of this module was that the learning provided in this module was interwoven with the other modules and the module learning was not graded.

(iii) Bridging Electronic to Atomistic scale:

The foremost objective of this module was to present students with an approach to evaluate properties of an aluminum material at the electronic principles scale using Density Functional theory (DFT)[28] and to train them about the bridging these DFT calculations to the higher atomic scale simulations, demonstrating how the atoms and electrons react with one another. The module curricula (see Table 3) covered the quantum mechanics approach, density functional theory (DFT) to compute the ground-state properties (electronic structure) of aluminum metal which are required to perform molecular dynamic (MD) simulations at the atomistic scale. This module also aimed at describing students the preferred techniques for material modeling in metals at the atomistic level, which are Modified Embedded-Atom Method (MEAM) [29] and the embedded atom method (EAM) [30].

Table 3. Topics and learning objectives used in Module 3.

	Topics	Learning Objectives
1	Quantum Theory and Electronics Principles	Describe Evolution of wave-particle duality. Schrödinger equation. Heisenberg's Uncertainty Principle. Postulates and Interpretations of quantum mechanics.
2	Density Functional Theory (DFT)	Discuss DFT methodology. Class of approximations to the exchange correlation (XC) energy functional: local density approximation (LDA)[31] and generalized gradient approximation (GGA)[31] .
3	Introduction to DFT simulations	Determine Thermodynamic and Elastic properties for an aluminum system. Use a first principles method based on Density Functional Theory (DFT) (using VASP). Determine the elastic constants, vacancy formation energies, interstitial formation energies, and extrinsic/intrinsic stacking fault energies[32].
4	EAM/MEAM Potentials	Discuss Methods of Calculating Atomistic Interactions. Methodology to calculate Modified Embedded-Atom Method (MEAM) potentials based on the embedded atom method (EAM). Determination of Atomic Stress Tensor
5	Atomistic Plasticity, Damage, Fatigue and MEAM Fitting	Identify Void growth and Void nucleation and hydrogen effects. Fatigue crack growth in single crystals. Design Map methodology[33]: Potential Space evaluation, Potential Space Sampling, Analytical Model Generation, Potential Design Map Development, and Potential Design Map Validation. Sensitivity analysis and calibration of a MEAM potential (using LAMMPS).

The practical element of this module was a hands-on introduction to use Vienna ab initio simulation (VASP) package for determining first order properties as well as energy versus volume/interatomic distance curves. This data was then used to ascertain optimized MEAM potential parameters such that the potentials can reproduce several materials or mechanical properties as accurately as possible. Moreover, LAMMPS tool was also used to demonstrate the sensitivity of specific parameters (e.g, lattice constant, bulk) as well as the uncertainty related to those parameters. At the end of this module students were given a group assignment to simulate a FCC aluminum at the electronic and nano scale and use VASP tool to determine first principle calculations based on density functional theory (DFT) such as cohesive energy, equilibrium lattice constant, and bulk modulus. Then students were required to perform convergence studies on the parameters obtained from DFT simulations and then use those parameters to calibrate the MEAM model and generate a new MEAM potential for aluminum. Students were required to document the results into a report

(iii) Bridging Atomistic to Microscale:

This module focused on second bridge for upscaling from atomistic simulations to the dislocations dynamics (DD) length scale. The module presented an approach for evaluation of aluminum at the nano and micro scale by using molecular dynamics (MD) and dislocation dynamics (DD)[34]. Various topics covered in this module are summarized in Table 4.

Table 4. Topics and learning objectives used in Module 4.

	Topics	**Learning Objectives**
1	Dislocation fundamentals	Discuss Line defect Continuum concept, Dislocations & Slip in Crystalline materials. Mixed Dislocation.
2	Dislocation Dynamics (DD) Theory	Describe Kinematics and Geometric aspects. Kinetics and Interaction forces. Investigate the FCC single crystals response under high strain rate loading using Multi-scale Dislocation Dynamics Plasticity Model. Study the effect of different parameters on the deformation patterns and dislocation microstructures. Burgers vector direction. MEAM and EAM. Molecular dynamics (MD), molecular statistics (MS), Monte Carlo (MC) methods to study the effects of different temperatures and strain rates.
3	Introduction to MD and DD Simulations	Calibrate MEAM/EAM potentials using MD. Investigate inelasticity of a material. Study Peierls stresses, dislocation velocities of edge and screw dislocations. Examine different crystal orientation effects on the dislocation mobility. Frank Read source (FRS) [35], as an example with Multiscale Discrete Dislocation Plasticity (MDDP) [36], FCC data, and BCC data codes for providing drag stress coefficients and their mobility effects.

At the beginning of the module students were demonstrated to use MD simulations of an edge dislocation of aluminum using LAMMPS to obtain the dislocation mobility that was used to study the effect on stress strain curve and dislocation density of aluminum at the microscale. Then DD fundamentals were introduced to provide students' knowledge of how DD aids in accurately model material behavior at the microscale by appropriately capturing the effects of dislocation motion and interactions between dislocations and other microstructural features.

Overall this module provided an insight of DD simulations used for directly observing *in situ* dislocation mechanisms and interactions, stress-strain curves, and dislocation structures resulting from deformation. Practically, the students were given hands-on experience with atomistic simulations to calculate calibrated MEAM potential parameters to be used in dislocations mobility calculations. Next, students experienced Multiscale Discrete Dislocation Plasticity (MDDP)[36] simulations using Frank Read Source (FRS) [35] type scenario to gain crucial information about the plasticity response aluminum material.

This module concluded with the second assignment where students were required to conduct atomistic length scale calculations using the modified embedded atom method (MEAM) for molecular dynamic dynamics simulation utilizing LAMMPS software. Then students were required to obtain four different sets of MEAM parameters to determine the dislocation mobility at the nanoscale. The dislocation mobility's obtained were then bridged to the microscale to conduct DD simulations. Next, students finally conducted the comparative simulations for each estimated mobility in order to determine their effect on the materials stress-strain relationship (using TecPlot[37]) and the entire dislocation structure (visualized using OVITIO software).

(iv) Bridging Microscale to Mesoscale:

This module focused on investigating the third bridge for upscaling from the dislocations dynamics (DD) to crystal plasticity length scale by using the ICME approach. The module curricula (shown in Table 5) involved examining the method for bridging the Internal State Variable (ISV) model[38] at the dislocation length scale to the crystalline length scale for aluminum in a face centered cubic crystal structure.

In the beginning of this module, the crystal plasticity theories were introduced to the class and then students were described how crystal plasticity models forms the basis of grain-level (mesoscale) approaches to materials modeling using multiscale strategies. Next the kinetics of crystal plasticity and the use of DD simulations to obtain the parameters included in the hardening rules in the kinetics were described to the students.

Table 5. Topics and learning objectives used in Module 5.

	Topics	**Learning Objectives**
1	Crystal Plasticity (CP) Theory	Discuss Basic elements of the theory: Kinematics, Kinetics and intergranular constraint laws.
2	Crystal Orientation and Elasticity	Identify Different Crystalline materials: FCC, BCC, HCP. Orthogonal slip system vectors and elastic moduli for each crystalline lattice. Rate dependent vs Rate independent implementations of crystal plasticity
3	Upscaling bridges	Explore Upscaling for plasticity, for plastic spin, for the texture, for yield surfaces, for damage/fracture and for fatigue.

The first practical component of this module was the hands-on experience with the MDDP code and FRS code to create dislocations. Consequently, use these dislocation dynamics calculations to determine hardening constants which can then be used as upscale bridging for crystal plasticity calibration. In a second practical component students were demonstrated the use of the UMAT user subroutine of ABAQUS with the crystal plasticity finite element method (CPFEM) code to run the crystal plasticity finite element simulations.

This module culminated with the third group assignment where each team was required to run DD simulations at the microscale to create stress-strain curves. Then using the Voce equation each team was required to determine the hardening parameters (needed at the crystal plasticity level) from the post-yield (working-hardening) portion of the stress-strain curve. The hardening parameters were then used to calibrate the crystal plasticity model. Next, teams were required to perform one-element finite element simulation using ABAQUS software to ascertain a stress-strain response.

(v) Bridging Mesoscale to Macroscale Continuum:
This module presented an approach to bridge the crystal plasticity to polycrystalline continuum length scales which involved evaluating aluminum at both scales by use of crystal plasticity finite element analysis and internal state variable (ISV) [11] plasticity model calibration.

Table 6. Topics and learning objectives used in Module 6.

	Topics	**Learning Objectives**
1	Internal State Variable (ISV) Theory	Discuss Kinematics of Deformation and Strain. Continuum theory constitutive equations. Thermodynamics and Kinetics of the ISV constitutive equations. Continuum theory ISV constitutive equations with discrete structures/defects. Guidelines for the development of ISV
2	ISV Plasticity Model	Discuss Kinematics in the continuum damage mechanics Framework. Kinematics in the continuum damage mechanics Framework. BCJ internal state variable plasticity model.
3	MSU Damage (DMG) Model	Demonstrate the Usage of DMGfit tool. Graphical user interface for entering experimental data. Initial model parameters, and solution settings. Explanation of 55 constants that are fitted, using DMGfit, from stress-strain data from experiments on the samples. Optimization and plot module.

In this module (see Table 6), the students were described the importance and the usage of the ISV model in capturing the mechanical history of a material and in predicting mechanical properties such as strength and failure of a material.

The practical component of this module was to perform a multigrain crystal plasticity analysis using ABAQUS on aluminum to garner stress-strain curves for continuum scale modeling. Then the model calibration tool, DMGfit, was used to calibrate the macroscale plasticity-damage ISV model[12] to the meso-scale plasticity stress strain curve. Then a macroscale continuum ISV model was selected which had capability to capture yield and hardening effects in aluminum. The obtained model was then used in a single element FEA calculation to validate the model capability. At the end of this module fourth assignment was given to the groups, where each team was required to perform the bridging exercise in which the stress-strain curves obtained by running single element crystal plasticity simulations were used to calibrate the ISV plasticity-damage model. Then the constants supplied by this calibration were verified by their use in the proprietary fitting UMAT routine (written in MATLAB along with ABAQUS) and single element simulation. This verified that the plasticity-damage model accurately captured the material behavior.

Class Grading

Our grading approach was to assign each of the four group assignments 15% weight of the total class grades except for two individual assignments each of which were assigned 10% weight of the total grades. The remaining weight of 20% was assigned to a final exam covering all the learning modules. To objectively assess student's ability, four scoring rubrics were used:

1) **Scoring rubrics specific to the four group assignments**
   This rubric was used only by instructor/TA covering technical content, writing (spelling/grammar), organization (flow) and quality benchmarks' to assess group assignments
2) **Scoring rubrics specific to project presentation and literature review (individual assignment)**
   This rubric was used not only by instructor/TA but also by the in-class or online students covering benchmarks, such as, motivation behind choosing the research topic, significance of the research work and richness of the content presented with respect to multiscale modeling to critically assess presentation given by each student.
3) **Scoring rubrics specific to ICME Wiki contributions (individual assignment)**
   This rubric was also used both by instructor/TA and in-class or online students to assess the preliminary web pages developed by each student in ICME web Wiki. The following benchmarks were considered to evaluate individual ICME Wiki contribution: 1) Clear and meaningful titles; 2) Relevance of the content; 3) Organization and coverage of the information; 4) Design and appearance; 5) Ease of navigation; 6) Text based alternatives such as images and multimedia files convey essential information; 7) References clearly defined; 8) Balanced Layout
4) **Scoring rubrics specific to peer evaluation (group assignment)**
   This rubric was used only by in-class or online students where each member of the team assessed other members in terms of their motivation, communication, sharing, leadership skills, involvement in the assignments, and the accuracy and significance of their ICME Wiki contributions.

The scoring rubrics mentioned above were completed by instructor/TA/students by giving ratings from 1 through 5 on a set of criteria's specific to each rubric, where 5 is the most desirable rating. All the assessments (using the above mentioned rubrics) received from students were combined with the assessments performed by instructor/TA to deliver final class grades.

Course Assessment

To evaluate student response to the course structure, a formal course assessment based on the standard University survey was being performed for the both offerings of this course. This survey was designed as an open-ended questionnaire to assess how well the class was received by the students. In this survey students complete course evaluations by giving ratings from 1 through 5 on a set of criteria listed in the survey, where 5 infer as strongly agree and 1 as strongly disagree. In the fall semester of 2012, the course received an average rating of 4.6 and during the fall semester of 2013 it received a 4.7 rating; these ratings indicate that students were satisfied with the course (strongly agreed or agreed with all statements in the questionnaire). Additionally, a pre- and post-survey were also administered to identify key student experiences about their gains in understanding ICME technologies, in using computational tools, and in conducting multiscale simulations and about the future perspectives of the course. As in the first survey, the students were asked to rank the inquiries listed in the both the surveys on a scale of 1 to 5, where 5 infer as excellent and 1 as very poor. The results of the pre- and post - surveys performed at the beginning and at the end of the class are shown in Figure 2.

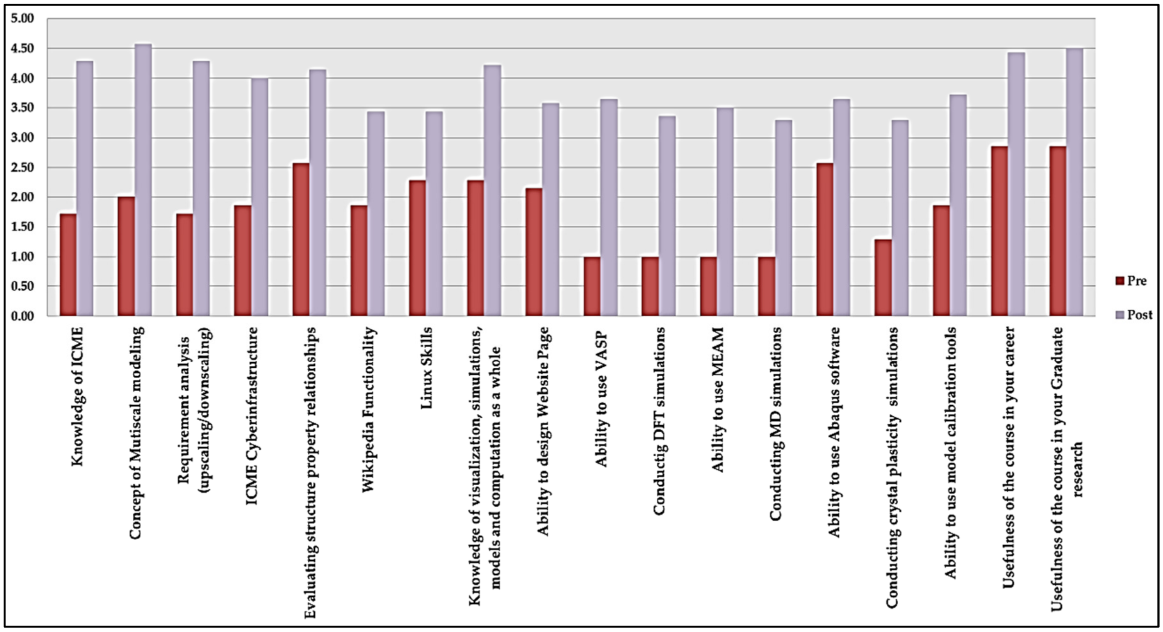

Figure2: Pre- and Post-Survey results of the addition course evaluation performed by the students; shows the mean ranking of the inquiries on a scale of 1 (very poor) to 5 (Excellent)

Results of the pre- and post- surveys illustrate a significant percentage increase in gains of students in terms of understanding ICME paradigm and their ability to conduct multiscale simulations using various computational tools. Furthermore, results also indicate that student's intention to use this course in their graduate studies or in their future career increased by a percentage of more than 50%. To conclude, the combined results of all three surveys established the fact that students were strongly satisfied that this class proved to be an enriching experience for them.

Conclusion

ICME entails cradle-to-grave history modeling and multiscale modeling of a material through its manufacturing process and in-service life; however, the tech transfer and knowledge sharing from the few researchers who have conducted ICME studies has not occurred, placing a limit in harnessing full potential of ICME. The formulated self-contained course described in this work is the first step in creating multidisciplinary curricula for diffusing the ICME technologies into academia. During both semesters the course was taught, students' reaction to the class was very positive proving that augmenting the traditional method with interactive and collaborative Cyberinfrastructure is both efficacious and attractive. The impact of this course was evident in students learning outcomes that were published online on ICME Wiki. The majority of the students were awarded the top grade for the class, reflecting their performance, interest and effort. One important aspect of this modular course is that all the material pertaining to teaching the course modules is available on-line through EVOCD portal. Therefore, by using the examples case studies, PowerPoint lectures and ICME tools available through EVOCD portal, any academic institutions or industry members can seamlessly deploy this ICME learning course in virtual classroom or in-class sessions, thus supporting ICME education.

In future, we would like to engage a project centric learning teaching approach that will involve ICME related projects from industry along with the resources provide by CI to be a part of this course. Consequently, these industry projects can be considered as a part of capstone design courses of the academic institutions.

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