**CME 8990 – Integrated Computational Materials Engineering (ICME): *Multiscale Modeling of Metals*: Syllabus – Fall 2012**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **DATE** | **LSN** | **TOPICS** | **information** | **WHAT'S DUE?** |
|
|  |  | ***Section 1. Background Material*** |  |  |
| 8/17 | 1 | ICME History and Overview | Syllabus, Proj | 4 person team names |
| 8/20 | 2 | Multiscale aspects of materials | Lecture Notes 2 |  |
| 8/22 | 3 | Creating a New Material/Structure/Component | Lecture Notes 3; Book Chapter 9,10 | Literature review topic defined |
| 8/24 | 4 | Case Study: Control arm fracture | Lecture Notes 4; Book Chapter 7 |  |
| 8/27 | 5 | Case Study: Control arm fatigue | Lecture Notes 5:  Book Chapter 8 |  |
| 8/29 | 6 | Constitutive Relations: Definitions | Lecture Notes 6: Book Chapter 1,2 |  |
|  |  | ***Section 2. Basics*** |  |  |
| 8/31 | 7 | Validation and Verification | Lecture Notes 7:  Book Chapter 1,2 |  |
| 9/5 | 8 | Optimization | Lecture Notes 8:  Book Chapter 1 |  |
| 9/7 | 9 | ICME CI overview | Tomasz Haupt/Nitin Sukhija |  |
| 9/10 | 10 | Student presentations of review topic | Students lecture notes |  |
| 9/12 | 11 | Student presentations of review topic | Students lecture notes | Lit Review and Project proposal due |
|  |  | ***Section 3. Quantum Methods*** |  |  |
| 9/14 | 12 | Quantum Theory and Electronics Principles | Lecture Notes 12: Book Chapter 6 |  |
| 9/17 | 13 | QM 2 | Lecture Notes 13: Book Chapter 6 |  |
| 9/19 | 14 | DFT Theory 1 | Lecture Notes 13b: Book Chapter 6 |  |
| 9/21 | 15 | DFT Theory 2 | Lecture Notes 13c: Book Chapter 6 |  |
| 9/24 | 16 | DFT example I -- diamond, H2O | Lecture Notes 16 |  |
| 9/26 | 17 | DFT example II -- surface | Lecture Notes 17 |  |
| 9/28 | 18 | DFT example III -- defects | Lecture Notes 18 |  |
|  |  | ***Section 4. Atomistic Methods*** |  |  |
| 10/1 | 19 | EAM/MEAM potentials: bridging from QM | Lecture Notes 19: Book Chapter 5 |  |
| 10/3 | 20 | Atomistic Plasticity | Lecture Notes 20: Book Chapter 5 |  |
| 10/8 | 21 | Atomistic Damage | Lecture Notes 21: Book Chapter 5 |  |
| 10/10 | 22 | Atomistic Fatigue | Lecture Notes 22: Book Chapter 5 |  |
| 10/12 | 23 | Running MD/MS/MC examples | Lecture Notes 23 |  |
|  |  | ***Section 5. Dislocation Dynamics Methods*** |  |  |
| 10/15 | 24 | Dislocation definitions  (line defect; slip and relation of dislocation to slip; dislocation description: Burgers, plane, line sense; character, sign; core and partials) | Lecture Notes 24: Book Chapter 4 | Homework 1 due |
| 10/17 | 25 | Dislocation Mechanics  (dislocation elastic fields; PK force; equation of motion; plastic strain; dislocation reactions; cross slip, climb) | Lecture Notes 25: Book Chapter 4 |  |
| 10/19 | 26 | Bridging from MD  (mobility; rules for jogs, junction, annihilation, and cross slip) | Lecture Notes 26: Book Chapter 4 |  |
| 10/22 | 27 | Implementation in Dislocation Dynamics  (discretization, stress field computation; time integration; short range interaction rules) | Lecture Notes 27: Book Chapter 4 |  |
| 10/24 | 28 | Running DD examples  (Crystallographic setup and creating initial dislocation structure) | Lecture Notes 28 |  |
| 10/26 | 29 | Running DD examples  (Running the code and postprocessing) | Lecture Notes 29 |  |
|  |  | **Section 6. Crystal Plasticity** |  |  |
| 10/29 | 30 | Crystal Plasticity Theory: kinematics, kinetics | Lecture Notes 30: Book Chapter 3 | Homework 2 due |
| 10/31 | 31 | Bridging from DD and model correlation | Lecture Notes 31: Book Chapter 3 |  |
| 11/2 | 32 | Running rate dependent single CP | Lecture Notes 32 |  |
| 11/5 | 33 | Running rate dependent polycrystalline CP | Lecture Notes 33 |  |
|  |  | **Section 7. Macroscale Continuum Modeling** |  |  |
| 11/7 | 34 | ISV Theory | Lecture Notes 34: Book Chapter 2 | Homework 3 due |
| 11/9 | 35 | ISV Plasticity Model | Lecture Notes 35: Book Chapter 2 |  |
| 11/12 | 36 | MSU DMG Fitting and running model | Lecture Notes 36 |  |
| 11/14 | 37 | ISV Damage Model | Lecture Notes 37: Book Chapter 2 |  |
| 11/16 | 38 | MSF Theory | Lecture Notes 38: Book Chapter 2 |  |
| 11/19 | 39 | MSF Fitting and running model | Lecture Notes 39 |  |
| 11/26 | 40 | Microstructural Image Analysis | Lecture Notes 40 | Homework 4 due |
| 12/3 |  | **Project Presentations** |  | Project due |