EPFL

ME-414

Computational multi-scale modeling of solids

Derlet Peter

Cursus	Sem.	Type
Mechanical engineering	MA2, MA4	Opt.

Language of teaching	English
Credits	5
Session	Summer
Semester	Spring
Exam	During the semester
Workload	150h
Weeks	14
Hours	**4 weekly**
Courses	3 weekly
TP	1 weekly
Number of positions	

Summary

This course considers the multi-scale computational modeling of hard-matter systems, with an emphasis on the physical phenomena of matter transport and emergent macroscopic mechanical properties, and how their microscopic origin is coarse grained to the engineering scale of a material component.

Content

Multi-scale modelling of hard-matter systems:

- review of material transport, diffusion and viscous flow theory
- the multi-scale physics of plasticity in metals – from atoms to dislocation line defects to the continuum.
- introduction to the physics and numerics of point particle simulation – molecular dynamics and discrete element methods.
- coarse graining strategies and uncertainty quantification.
- continuum models of transport and plasticity using the finite element method

Computational and simulation frameworks:

- parallel computing computing
scientific modelling frameworks
data analysis and visualization

Keywords

material properties, mass transport, plasticity and strength, multi-scale modelling, numerical algorithms, scientific software and hardware computational frameworks, parallel computing.

Learning Prerequisites

Important concepts to start the course

- Fick’s law of diffusion
- The stress-strain characteristics of hard matter (elasticity, transition to yield, and plastic flow).
- Partial differential equations and their numerical solution.
- Knowledge of a traditional procedural scientific programming language such as Fortran and C.

Learning Outcomes

By the end of the course, the student must be able to:

- Model the key microscopic mechanisms for material transport and plasticity in hard matter, and how such processes can act collectively resulting in emergent macroscopic material properties.
- Choose the key numerical frameworks to model the different time and length-scales
- Differentiate the key advantages and disadvantages of these numerical frameworks
- Explore a variety of simulation methodologies and gain detailed experience in at least one of them.
- Integrate computational simulation tools with an emphasis on open source applications and the use of pyhton
- Formulate a problem and strategies for its solution, as part of a project team

Transversal skills

- Plan and carry out activities in a way which makes optimal use of available time and other resources.
- Set objectives and design an action plan to reach those objectives.
- Assess progress against the plan, and adapt the plan as appropriate.
- Use a work methodology appropriate to the task.
- Communicate effectively with professionals from other disciplines.
- Give feedback (critique) in an appropriate fashion.
- Evaluate one's own performance in the team, receive and respond appropriately to feedback.
- Manage priorities.

Teaching methods

Lectures and practical tutorials will constitute traditional content covering core theoretical concepts and interactive content covering practical use of computational modelling frameworks. It is envisioned that no more than 50% of classroom time, will be spent this way, distributed heterogeneously over the entire semester.
The remaining time will be devoted to project work, involving teams of about four students, focused on a particular engineering/physical problem, and its appropriate numerical solution.

Expected student activities

- Attendance to lectures
- Learning of python and the use of at least one other specialized computational modelling platform
- Team work to solve a problem and present it as a lecture or practical tutorial
- To have an articulated role and responsibility within the team.

Assessment methods

The project work outcome will lead to a student developed and presented lecture or practical tutorial content.
Assessement will be based on this content and the individual's contribution to it.