AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Code:	int.courses-047	Module name:	Multi scale numerical modelling in metallurgy and materials science

Academic year:	2019/2020	Semester:	Spring, Fall	ECTS credits:	6

Programme: AGH UST International Courses

Course homepage:	https://intcourses.agh.edu.pl/	Lecture language:	English

Responsible teacher: Madej Łukasz (lmadej@agh.edu.pl)

Description of learning outcomes for module

MLO code	Student after module completion has the knowledge/ knows how to/is able to	Method of learning outcomes verification (form of completion)
Social competence		
M_K001	Can appreciate the advantages of the use of multiscale modeling techniques to develop new technologies that can be useful for the society.	Participation in a discussion
Skills		
M_U001	Has the ability to analyze and interpret obtained results from the implemented model.	Report, Participation in a discussion
M_U002	Has the ability to develop and implement a model that is based on knowledge about analyzed physical phenomenon.	Participation in a discussion, Execution of a project
Knowledge		
M_W001	Has general knowledge about the advantages and possibilities of application of multiscale modeling techniques in engineering.	Examination, Test
M_W002	Has general knowledge on selection of appropriate methods of macro, meso, micro and nano scale analysis to solve problem under consideration.	Examination, Test

Number of hours for each form of classes

Suma	Form of classes										
	Lectures	Auditorium classes	Laboratory classes	Project classes	Conversation seminar	Seminar classes	Practical classes	Fieldwork classes	Workshops	Prace kontrolne i przejściowe	Lektorat
56	28	0	28	0	0	0	0	0	0	0	0

FLO matrix in relation to forms of classes

MLO code	Student after module completion has the knowledge/ knows how to/is able to	Form of classes										
		Lectures	Auditorium classes	Laboratory classes	Project classes	Conversation seminar	Seminar classes	Practical classes	Fieldwork classes	Workshops	Prace kontrolne i przejściowe	Lektorat
Social competence: is able to												
M_K001	Can appreciate the advantages of the use of multiscale modeling techniques to develop new technologies that can be useful for the society.	+	-	+	-	-	-	-	-	-	-	-
Skills: he can												
M_U001	Has the ability to analyze and interpret obtained results from the implemented model.	-	-	+	-	-	-	-	-	-	-	-
M_U002	Has the ability to develop and implement a model that is based on knowledge about analyzed physical phenomenon.	-	-	+	-	-	-	-	-	-	-	-
Knowledge: he knows and understands												
M_W001	Has general knowledge about the advantages and possibilities of application of multiscale modeling techniques in engineering.	+	-	-	-	-	-	-	-	-	-	-
M_W002	Has general knowledge on selection of appropriate methods of macro, meso, micro and nano scale analysis to solve problem under consideration.	+	-	-	-	-	-	-	-	-	-	-

Student workload (ECTS credits balance)

Student activity form	Student workload
Udział w zajęciach dydaktycznych/praktyka	56 h
Preparation for classes	70 h
Realization of independently performed tasks	24 h
Summary student workload	150 h
Module ECTS credits	6 ECTS

Additional information

Module content

Lectures

Multi scale numerical modelling in metallurgy and material science

Multi scale modeling has recently become very popular in various disciplines. The number of applications of these models is increasing rapidly and the variety of approaches to multi scale problems is large. Industry is also paying a lot of attention to the multi scale modeling methods as they provide new possibilities in description of modeled systems that are in their nature of multi scale character. Therefore, there is a need for broad review and classification of the available methods and systematization of their applications.
The lecture will be focused on the role of multi scale numerical modeling in today's science and manufacturing engineering. It will be divided into three parts.
The first one is focused on the basic definitions of the finite element method as one of the most commonly used tools in industry. Advantages and limitations of the FE models will be discussed. Modification to the FE methods e.g. Multi scale Extended Finite Element Method will be discussed as well. Basics of other macro scale modeling techniques (Finite Difference Method, Finite Volume Method, Boundary Element Method, Mesh Free Methods) and differences between them will be discussed.
The second one is focused on the description of micro scale modeling methods Cellular Automata (CA), Monte Carlo (MC), Molecular Dynamic/Static (MD). Basic definition of the CA, MC and MD methods (e.g. CA space, neighborhood, transition rules etc.) and its various applications are presented. Possibilities in application of mentioned methods to digital material representation (DMR) approach will be highlight. The DMR is particularly interested as it give the possibility to model specific structure of the metallic, ceramic or composite materials.
The third part is on combination of the micro and macro scale modeling techniques. Basis of the multi scale upscaling and concurrent method will be discussed. Examples of applications and possibility provided by these method in industrial applications will be presented.

Laboratory classes

Basis of commercial finite element software 1

Basis of commercial finite element software 2

Development of a macro scale numerical model based on commercial finite element software 1

Development of a macro scale numerical model based on commercial finite element software 2

Development of a macro scale numerical model based on commercial finite element software 3

Development of a macro scale numerical model based on commercial finite element software 4

Basis of in-house cellular automata software 1

Development of a micro scale numerical model based on in-house cellular automata software 1

Development of a micro scale numerical model based on in-house cellular automata software 2

Development of a micro scale numerical model based on in-house cellular automata software 3

Basis of in-house Monte Carlo software 1

Development of a micro scale numerical model based on in-house Monte Carlo software 1

Development of a micro scale numerical model based on in-house Monte Carlo software 2

Development of a micro scale numerical model based on in-house Monte Carlo software 3

Teaching methods and techniques:

Lectures: Treści prezentowane na wykładzie są przekazywane w formie prezentacji multimedialnej w połączeniu z klasycznym wykładem tablicowym wzbogaconymi o pokazy odnoszące się do prezentowanych zagadnień.
Laboratory classes: W trakcie zajęć laboratoryjnych studenci samodzielnie rozwiązują zadany problem praktyczny, dobierając odpowiednie narzędzia. Prowadzący stymuluje grupę do refleksji nad problemem, tak by otrzymane wyniki miały wysoką wartość merytoryczną.

Warunki i sposób zaliczenia poszczególnych form zajęć, w tym zasady zaliczeń poprawkowych, a także warunki dopuszczenia do egzaminu:

Nie określono

Zasady udziału w poszczególnych zajęciach, ze wskazaniem, czy obecność studenta na zajęciach jest obowiązkowa:

Lectures:
– Attendance is mandatory: No
– Participation rules in classes: Studenci uczestniczą w zajęciach poznając kolejne treści nauczania zgodnie z syllabusem przedmiotu. Studenci winni na bieżąco zadawać pytania i wyjaśniać wątpliwości. Rejestracja audiowizualna wykładu wymaga zgody prowadzącego.
Laboratory classes:
– Attendance is mandatory: Yes
– Participation rules in classes: Studenci wykonują ćwiczenia laboratoryjne zgodnie z materiałami udostępnionymi przez prowadzącego. Student jest zobowiązany do przygotowania się w przedmiocie wykonywanego ćwiczenia, co może zostać zweryfikowane kolokwium w formie ustnej lub pisemnej. Zaliczenie zajęć odbywa się na podstawie zaprezentowania rozwiązania postawionego problemu. Zaliczenie modułu jest możliwe po zaliczeniu wszystkich zajęć laboratoryjnych.

Method of calculating the final grade

Weighted average: 0.5 • grade from classes + 0.5 • grade from exam

Sposób i tryb wyrównywania zaległości powstałych wskutek nieobecności studenta na zajęciach:

Nie określono

Prerequisites and additional requirements

Basic knowledge of materials science

Recommended literature and teaching resources

1.O. C. Zienkiewicz, R. L. Taylor, The Finite Element Method Set, Butterworth-heinemann, 2005.
2.Fries T.P., Matthies H.G., Classification and overview of meshfree methods, Scientific Computing, Informatikbericht, 2003-3, Brunswick, 2004.
3.R. Wit, ,,Metody Monte Carlo – wykłady", Wydawnictwo Politechniki Częstochowskiej, 2004.
4.Tao Pang, Metody obliczeniowe w fizyce, PWN, 2001.
5.S. Wolfram, A New kind of science, Wolfram Media, 2002.
6.K. Kułakowski, Automaty komórkowe, Ośrodek Edukacji Niestacjonarnej, Kraków, 2000.
7.Madej L., Hodgson P.D., M. Pietrzyk, Development of the Multi-scale Analysis Model to Simulate Strain Localization Occurring During Material Processing, Archive of Computer Methods in Engineering, 16, 2009, 287 – 318.

Scientific publications of module course instructors related to the topic of the module

1. Madej L., Wang J., Perzynski K., Hodgson P.D., Numerical modelling of dual phase microstructure behavior under deformation conditions on the basis of digital material representation, Computational Material Science, 95, 2014, 651–662.
2. Madej L., Sieradzki L., Sitko M.,Perzynski K., Radwański K., Kuziak R., Multi scale cellular automata and finite element based model for cold deformation and annealing of a ferritic-pearlitic microstructure, Computational Materials Science, 77, 2013, 172–181.
3. Halder C., Madej L., Pietrzyk M., Chakraborti N., Optimization of cellular automata model for the heating of Dual Phase steel by Genetic Algorithm and Genetic Programming, Materials and Manufacturing Processes, 30:4, 2015, 552-562.
4. Szyndler J., Madej L., Numerical analysis of the influence of number of grains, FE mesh density and friction coefficient on representativeness aspects of the polycrystalline Digital Material Representation – plane strain deformation case study, Computational Material Science, 96, 2015, 200–213.
5. Perzyński K., Madej L., Wang J., Kuziak R., Hodgson P.D., Numerical investigation of influence of the martensite volume fraction on DP steels fracture behavior on the basis of digital material representation model, Metallurgical and Materials Transactions A, 45, 2014, 5852-5865.

Additional information

None