MBN 310 Numerical Methods in Materials Science Engineering		Department of Materials Science & Nanotechnology Engineering	
Semester	**Credit**		
	Theory	**Practice**	**Laboratory**
2015/2016 Fall	3	0	0
Compulsory / Elective	Compulsory		
Prerequisites	-		
Instructors	Assist. Prof. Dr. Ersin Emre Ören		
Course Description	Computational materials science is one of the fastest growing disciplines in materials science. The simulation of materials at a range of scales, from the quantum and molecular, via the mesoscale to continuum level, can provide various scientific advances. MBN 310 course will cover both the theoretical and practical studies in the computational materials science and nanotechnology. Within the framework of this course, students will learn numerical methods and algorithms in general. This course will provide information about diffusion, kinetics, and molecular dynamics; and give hands-on information about state of the art computer software to adapt the students into this rapidly developing field.		
Course Objectives	Students who complete this course will be able to: 1. have a general knowledge about the computational materials science; 2. develop an understanding of the assumptions/approximations, involved in the modeling frameworks at the various time and length scales; 3. learn how to use computational modeling, and how to present and interpret the results of simulations.		
Course Outcomes	Key areas of achievements will be obtaining essential information about the basic principles of computational materials science and nanotechnology, and applying this know-how for the solution of engineering problems.		
Textbook	• -		
Other Resources	• Advanced Engineering Mathematics, P.V. O'Neil, PWS Publishing Company, 2002. • Numerical Solution of Partial Differential Equations: An Introduction, K.W. Morton and D.F. Mayers, Cambridge University Press, 2005. • Ashby, M.F., Ferreira P.J., Schodek D.L., *Nanomaterials, Nanotechnologies and design*, Elsevier Academic Press, 2009. • Related up-to-date articles.		

Evaluation Criteria		**Number**	**Impact (%)**
	Midterm Exams	1	25
	Quiz	8+	25
	Homework		
	Projects	-	-
	Term Paper	1	20
	Laboratory	-	-
	Others	-	-
	Final	1	30

Distribution of Course Content into Basic Fields (%)		
	Mathematics and Basic Sciences	20
	Engineering Sciences	40
	Engineering Design	40
	Social Sciences	-

COURSE OUTLINE	
Week	**Subject**
1	Basic Programming and Algorithms
2	Matrix Operations and Root finding
3	Matrix Operations and Numerical Integration
4	Random Numbers and Random Walk
5	Numerical Methods for Ordinary Differential Equations / Eulers & Heun Methods
6	Numerical Methods for Ordinary Differential Equations / Applications
7	Numerical Methods for Partial Differential Equations / Diffusion
8	Numerical Methods for Partial Differential Equations / Diffusion
9	Numerical Methods for Partial Differential Equations / Wave Equation
10	Molecular Dynamics
11	Molecular Dynamics
12	Molecular Dynamics / Project Presentations

RELATIONSHIP BETWEEN THE COURSE AND THE DEPARTMENT PROGRAM				
	Program Outcomes	**1**	**2**	**3**
1	Ability to apply mathematical, scientific and engineering knowledge			√
2	Ability to design and conduct experiments, analyze and interpret the experimental results		√	
3	Ability to design systems, components or process as desired/required			√
4	Ability to work in interdisciplinary teams			√
5	Ability to identify, formulate and solve engineering problems			√
6	Ability to communicate effectively in English and Turkish		√	
7	Comprehensive training necessary to understand the impact of the engineering solutions on globe and society			√
8	Knowledge of contemporary issues			√
9	Ability to use modern tools, techniques and skills necessary for engineering practice			√
	Course Contribution: 1: None 2: Partial 3: Full			