



Course Syllabus: Computational Science and Engineering - AMCS 330

Division	Computer, Electrical and Mathematical Sciences & Engineering
Course Number	AMCS 330
Course Title	Computational Science and Engineering
Academic Semester	Spring
Academic Year	2016/2017
Semester Start Date	01/22/2017
Semester End Date	05/18/2017
Class Schedule (Days & Time)	16:00 - 17:30 Mon Wed

Instructor(s)				
Name	Email	Phone	Office Location	Office Hours
Gabriel Wittum	Gabriel.Wittum@kaust.edu.sa		Bldg 1, Rm 0117	By appointment as needed.

Teaching Assistant(s)	
Name: Dmitry Logashenko	Email: Dmitry.Logashenko@kaust.edu.sa

Course Information	
Comprehensive Course Description	This course is an advanced introduction to computational science and engineering. The main topic is modelling and simulation based on first principles. After a short presentation to the basic ideas of computational science and engineering, we introduce the major methods used in numerics of partial differential equations such as discretization, solvers and sensitivity analysis. In what follows, we discuss solving several relevant problems from different areas, mainly from life sciences. Modelling geometry and processes is discussed in detail, as well as the selection of appropriate numerical methods. First, we model and compute diffusive transport through mammalian skin. This is a highly interesting problem for dermatology, pharmacy and pharmaceutical as well as cosmetics industry. Next, we discuss problems from neuroscience. First, we introduce methods to reconstruct neuron morphology. Using these recovered morphologies, we model signal transduction in neurons.
Course Description from Program Guide	This course is an advanced introduction to computational science and engineering. The main topic is modelling and simulation based on first principles. After a short presentation to the basic ideas of computational science and engineering, we introduce the major methods used in numerics of partial differential equations such as discretization and solvers. In what follows, we discuss solving several relevant problems from different areas, mainly from life sciences.
Goals and Objectives	Students completing this course will be able to: (1) derive advanced, partial differential equation-based models for problems from empirical sciences, (2) apply basic as well as advanced methods to discretize and solve the discrete equations, (3) identify main influence sources and parameters, (4) derive solutions to problems from empirical sciences.
Required Knowledge	Basic Mathematics, in particular Analysis, Linear Algebra and differential equations. Furthermore, basic programming skills in C/C++.

Reference Texts	A script will be distributed during the course.
Method of evaluation	100.00% - Homework /Assignments
Nature of the assignments	Assignments will involve analytical work, computer programming, and implementation of open source software.
Course Policies	Course materials and homework submission will be communicated via email.
Additional Information	

Tentative Course Schedule

(Time, topic/emphasis & resources)

Week	Lectures	Topic
1	Mon 01/23/2017 Wed 01/25/2017	Introduction: Basic ideas of CSE, derivation of models, properties of partial differential equations.
2	Mon 01/30/2017 Wed 02/01/2017	Numerical methods
3	Mon 01/30/2017 Wed 02/01/2017	Numerical methods
4	Mon 02/13/2017 Wed 02/15/2017	Numerical methods
5	Mon 02/20/2017 Wed 02/22/2017	Numerical methods
6	Mon 02/27/2017 Wed 03/01/2017	Numerical methods
7	Mon 03/06/2017 Wed 03/08/2017	Numerical methods
8	Mon 03/13/2017 Wed 03/15/2017	Modeling diffusive transport through mammalian skin.
9	Mon 03/20/2017 Wed 03/22/2017	Modeling diffusive transport through mammalian skin.
10	Mon 03/27/2017 Wed 03/29/2017	Modeling diffusive transport through mammalian skin.
11	Mon 04/03/2017 Wed 04/05/2017	Modeling diffusive transport through mammalian skin.
12	Mon 04/10/2017 Wed 04/12/2017	Modeling diffusive transport through mammalian skin.
13	Mon 04/17/2017 Wed 04/19/2017	Modeling diffusive transport through mammalian skin.
14	Mon 04/24/2017 Wed 04/26/2017	Reconstruction of cell geometries from microscopic data
15	Mon 05/01/2017 Wed 05/03/2017	Reconstruction of cell geometries from microscopic data
16	Mon 05/08/2017 Wed 05/10/2017	Reconstruction of cell geometries from microscopic data
17	Mon 05/15/2017 Wed 05/17/2017	Reconstruction of cell geometries from microscopic data
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Note

The instructor reserves the right to make changes to this syllabus as necessary.