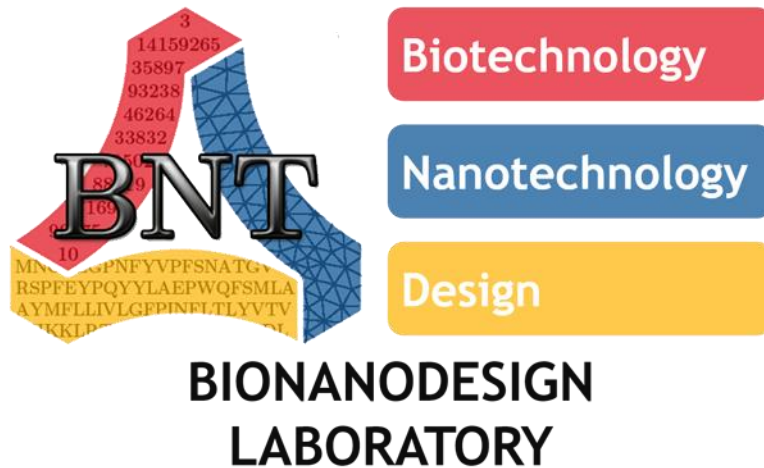


MBN 310

Numerical Methods in Materials Science & Engineering

Introduction to Numerical Methods



Dr. Ersin Emre Ören

Bionanodesign Laboratory

Department of Biomedical Engineering

Department of Materials Science & Nanotechnology Engineering

TOBB University of Economics and Technology

Ankara - TURKEY

eeoren@etu.edu.tr

<http://eeoren.etu.edu.tr>

2018-2019 Fall Semester:

	Monday	Tuesday	Wednesday	Thursday	Friday
08:30-09:20					
09:30-10:20					
10:30-11:20					
11:30-12:20					
12:30-13:20				MBN 310	
13:30-14:20				MBN 310	
14:30-15:20	MBN 310				
15:30-16:20	MBN 310				
16:30-17:20					
17:30-18:20					



TOBB ETÜ TM

MBN 310 Course Description:

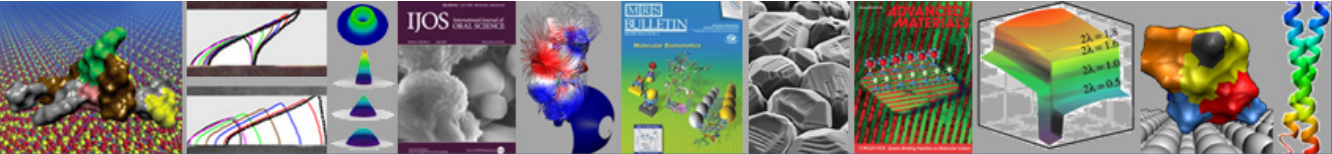
Computational materials science is one of the fastest growing disciplines in materials science. The simulation of materials at a range of scales, from the quantum and molecular, via the mesoscale to continuum level, can provide various scientific advances. MBN 310 course will cover both the theoretical 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 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
6	Numerical Methods for Ordinary Differential Equations / Applications
7	Numerical Methods for Partial Differential Equations / Diffusion
8	Numerical Methods for Partial Differential Equations / Diffusion 2D
9	Numerical Methods for Partial Differential Equations / Wave Equation
10	Molecular Dynamics
11	Molecular Dynamics
12	Molecular Dynamics

Evaluation Criteria

	Adet	Impact (%)
Midterm Exams	1	25
Quiz+Homework	5+	25
Projects	1	15
Final	1	35



MBN 310

Numerical Methods in Materials Science & Engineering

Assist. Prof. Dr. ERSIN EMRE OREN

MAIN	SYLLABUS	LECTURE NOTES	HW	PROJECTS	GRADES	ANNOUNCEMENTS	TURKISH
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Numerical Methods in Materials Science & Engineering

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.

Students are required to bring their laptops to classes.

Lecture Hours


- Tuesday: 10:30 - 12:20 (TOBB ETU Technology Center 218)
- Friday: 14:30 - 16:20 (TOBB ETU Technology Center 218)

Course Outline

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

Teaching Assistants

- Büşra Demir
- Çağlanaz Akın



Bionanodesign Laboratory

SEARCH www TOBB ETÜ

E-Mail Library CV

Address: Sogutozu Cad. No: 43, Sogutozu, Ankara, 06560 TURKEY /// Phone: +90 (312) 292-4514 Fax: +90 (312) 292-4091 eoren@etu.edu.tr

Lecture Plan

2020-2021

Eylül							Ekim							Kasım									
Pt	Sa	Ça	Pe	Cu	Ct	Pz	Pt	Sa	Ça	Pe	Cu	Ct	Pz	Pt	Sa	Ça	Pe	Cu	Ct	Pz			
36		1	2	3	4	5	6	40			1	2	3	4	44						1		
37	7	8	9	10	11	12	13	41	5	6	7	8	9	10	11	45	2	3	4	5	6	7	8
38	14	15	16	17	18	19	20	42	12	13	14	15	16	17	18	46	9	10	11	12	13	14	15
39	21	22	23	24	25	26	27	43	19	20	21	22	23	24	25	47	16	17	18	19	20	21	22
40	28	29	30					44	26	27	28	29	30	31	48	23	24	25	26	27	28	29	
															49	30							

Aralık							Ocak								
Pt	Sa	Ça	Pe	Cu	Ct	Pz	Pt	Sa	Ça	Pe	Cu	Ct	Pz		
49		1	2	3	4	5	6	53				1	2	3	
50	7	8	9	10	11	12	13	1	4	5	6	7	8	9	10
51	14	15	16	17	18	19	20	2	11	12	13	14	15	16	17
52	21	22	23	24	25	26	27	3	18	19	20	21	22	23	24
53	28	29	30	31				4	25	26	27	28	29	30	31

October 05, 2020

Add/drop
(Ekle/Sil)

November 09, 2020

Withdraw
(Dersten Vazgeçme)

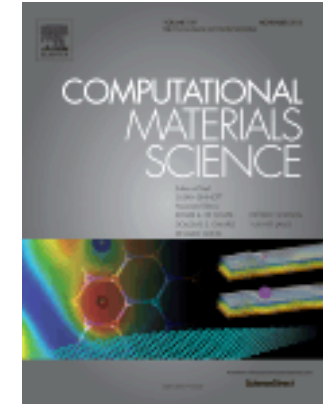
Aims and Scope

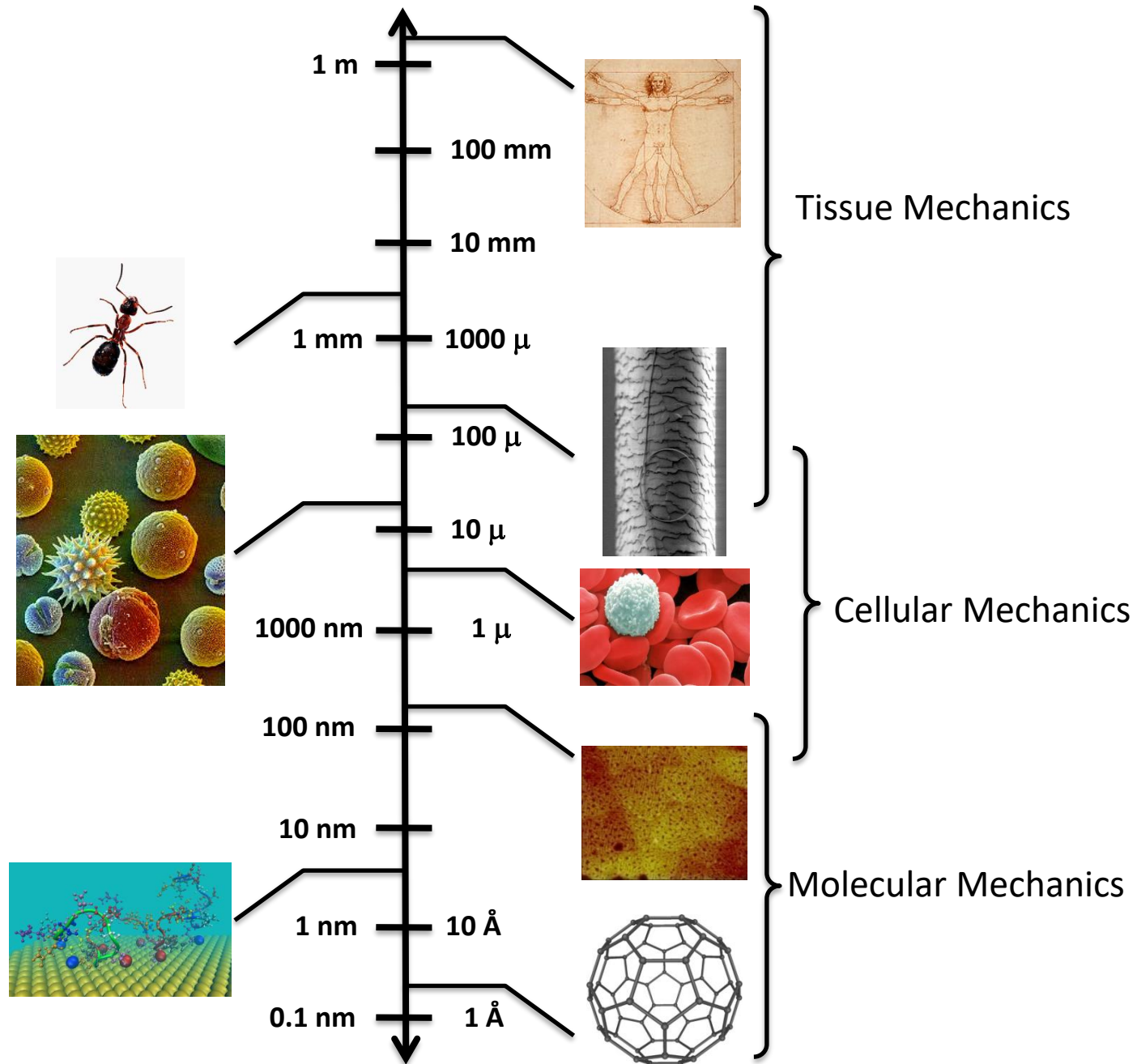
[Computational Materials Science](#) and [International Journal of Computational Materials Science](#) are international journals which publish both full length and short refereed papers describing significant developments in numerical methods and their application to materials science & engineering problems.

Contributions are encouraged in all areas of materials modeling, such as:

- *quantum chemical methods,*
- *density functional theory,*
- *semi-empirical and classical approaches,*
- *statistical mechanics,*
- *atomic-scale simulations,*
- *mesoscale modeling,*
- *phase-field techniques,*
- *finite element methods,*

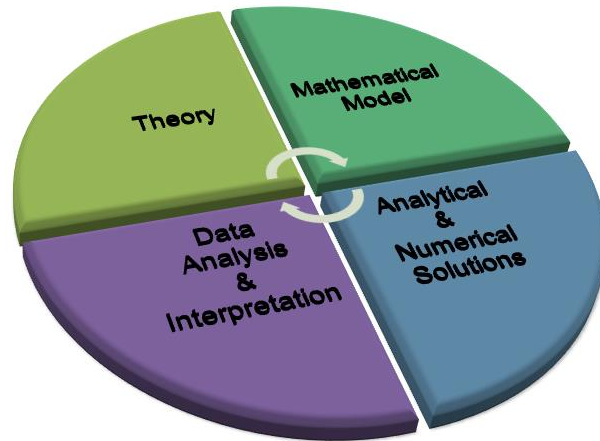
These journals aim to promote international exchange of new knowledge and recent developments in all aspects of computational materials science and engineering, featuring the most advanced mathematical modeling and numerical methodology developments. It includes all classes of materials (metals, polymers, ceramics, composites, biomaterials, nanomaterials, etc.) and their structures (functional solids, soft matter, multiphase materials, coatings, etc.). Of specific interest are the underlying physics and chemistry governing the functional elements of the materials, and these functions include (but are not limited to) structural, electronic, thermal, chemical, magnetic, optical, or a combination of any of these.





Theoretical & Computational Materials Science

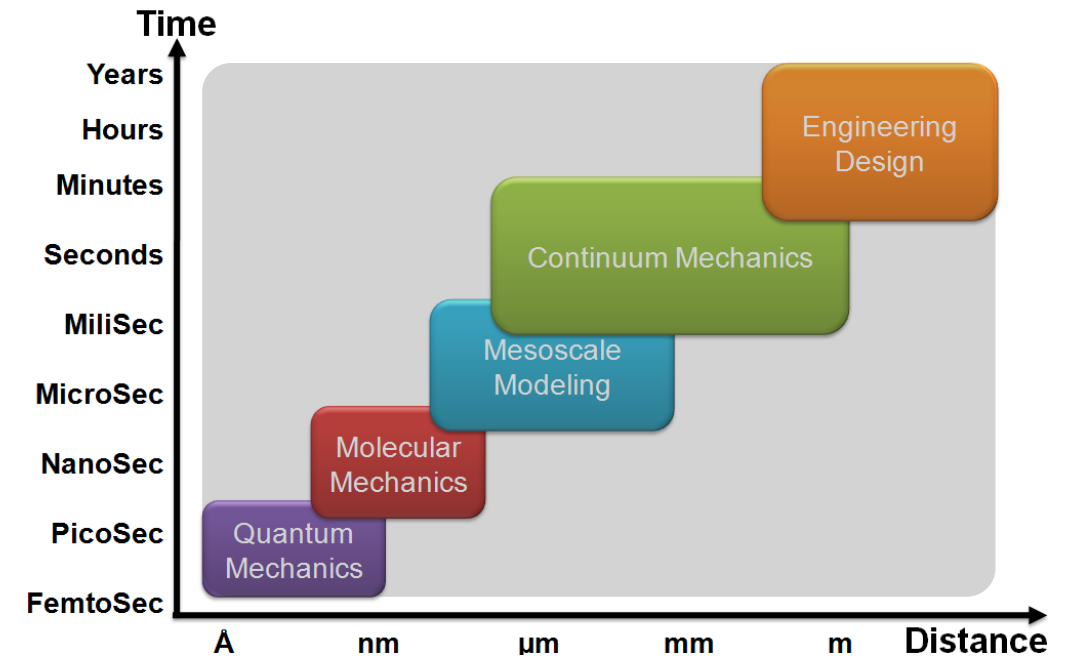
constructs theories, mathematical models and quantitative analysis techniques and uses computers to analyze and solve scientific problems.



one of the fastest growing disciplines.

crucial for characterizing, predicting and simulating physical events and systems.

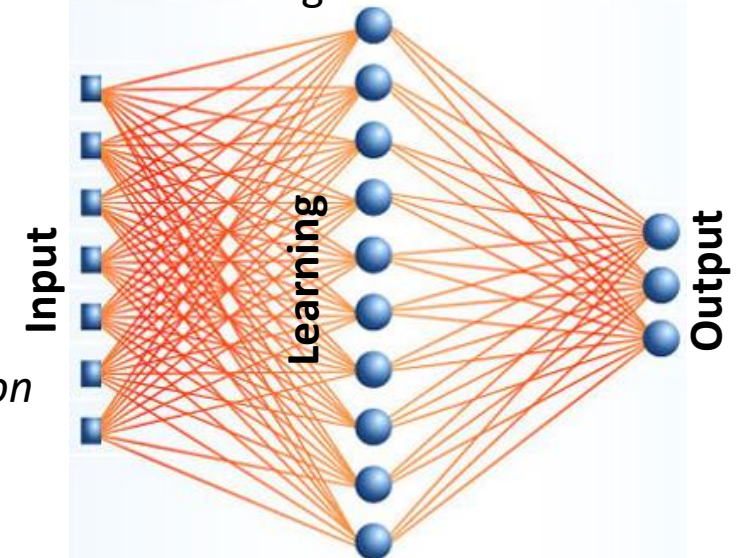
simulate the behavior of materials across various time and length scales.



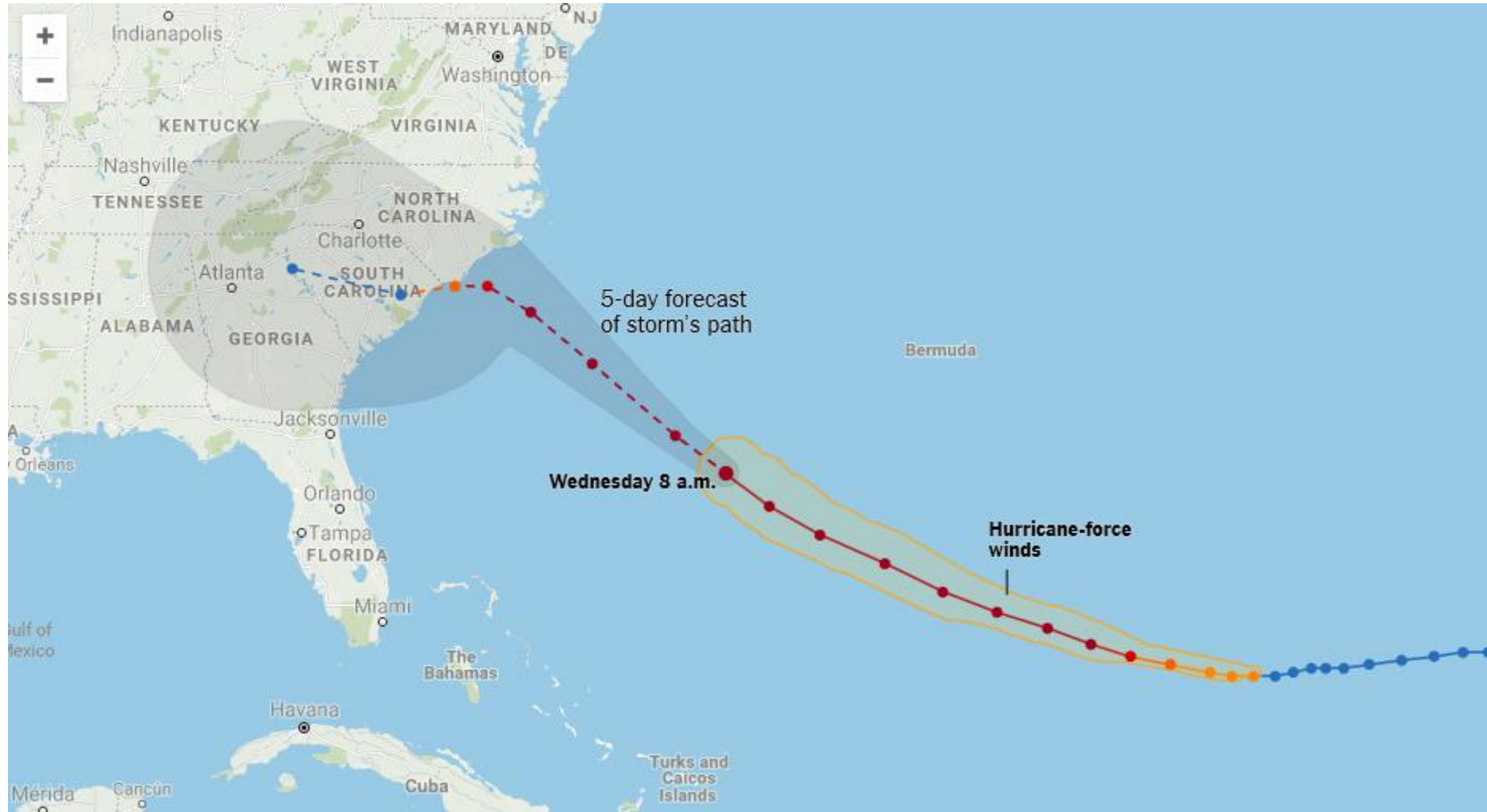
Data Analysis / Statistical Learning Methods

- Bioinformatics*
- Machine learning*
- Network analysis*
- Neuroinformatics*
- Neural Networks*
- Weather forecast*
- Pattern recognition*

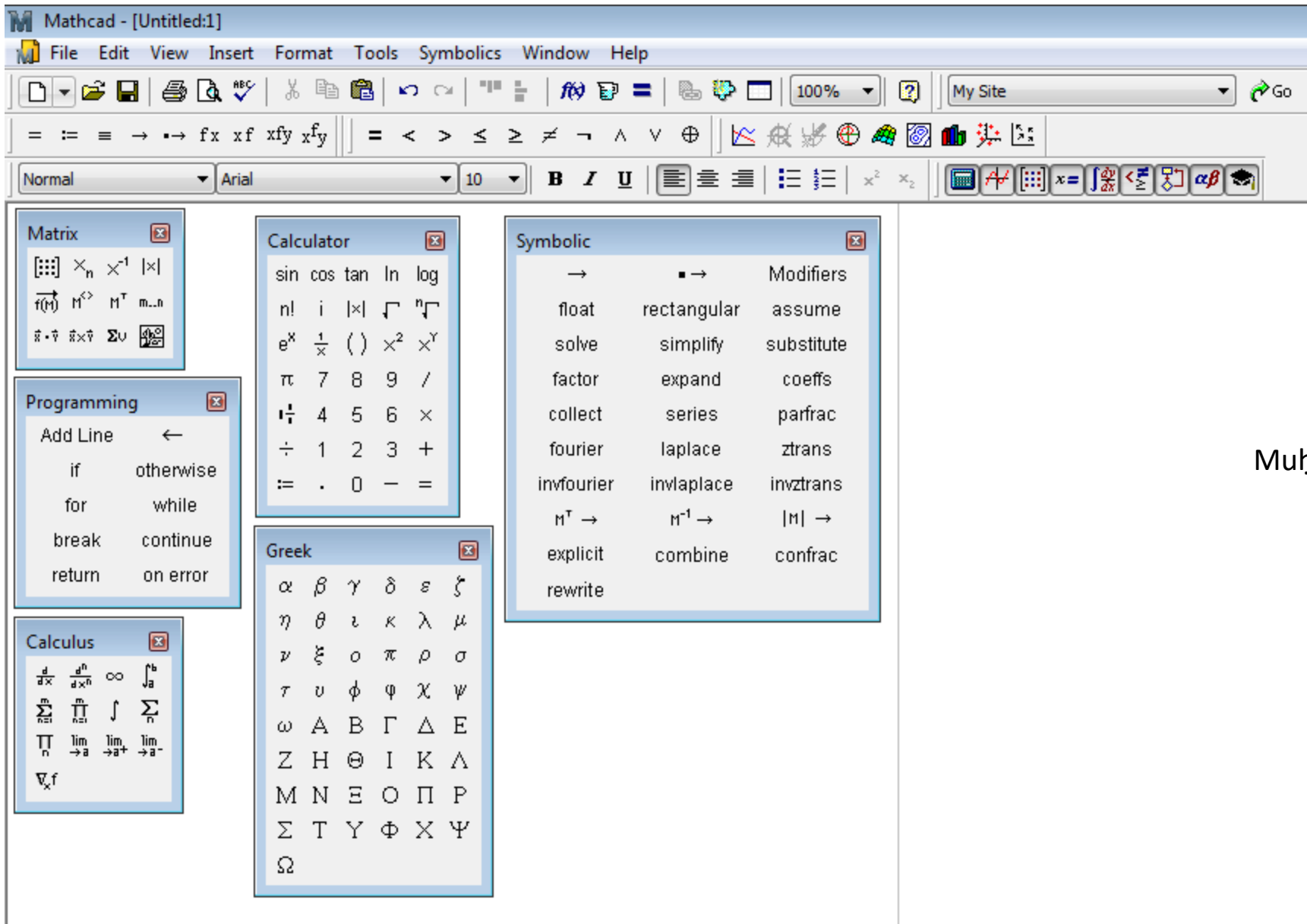
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Hurricane FLORENCE



Programming & Algorithm



780-850

Muḥammad ibn Mūsā al-Khwārizmī

