BIL 108E

Introduction to Scientific Computing and Engineering

Assist Prof. Dr. F. Aylin Konuklar

- Course attendance : Required
- Course Grading : Curve
- Lab attendance is required
- Lectures:

- Labs:

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Book :

- Engineering Problem Solving with Matlab, Ettet,D.M.,2nd ed. Prentice Hall, 1997
- References & Supplementary Materials
  - MATLAB programming for engineers / Stephen J. Chapman
  - MATLAB programming / David C. Kuncicky
  - MATLAB 6 for Engineers, A Biran, M Breiner, Prentice Hall, 2002
  - www.mathworks.com
  - R. Otto and J.P. Denier, An Introduction to Programming and Numerical Methods in MATLAB, Springer-Verlag, London, 2005. (pdf format is available online on //bil.be.itu.edu.tr)

Tentative Schedule

Lecture	Date	Topics
1		Introduction to Scientific and Engineering Computing
2		Introduction to Matlab Computing Environment
3		Variables, Operations and Simple Plot
4		Errors and Source of Errors, Algorithms and Flow Control
5		Functions
6		Linear Algebra **Exam 1**
7		Solving Equations
8		Polynomials
9		Curve Fitting, Interpolation
10		Least-Squares Method (**Exam 2**)
11		Numerical Integration
12		Symbolic Mathematics
13		ODE Solutions
14		Review

Course Objectives

- To familiarize students with the fundamentals of scientific computing concepts
- To develop problem solving skills
- To develop skills in constructing an algorithm,
- To train students how to use Matlab in scientific and engineering calculations
- To train students to visualize their results and prepare written reports

TOOLS USED TO ACHIEVE THE OBJECTIVES:

- Lecturing, laboratory sessions held in the computer labs, homework problems requiring computer and software use, two midterms and final exam (limited access to internet)

- **Homework:**Six homework assignments will be announced on the web of the course, one week before they are due and they will be due 18:00, the same day of the next week. Five of them will be taken into consideration.

Exams & Grading

- First Midterm ->
- Second Midterm ->
- Final -> will be annouced by ITU

1st Mid : 15 pts

2nd Mid : 15 pts

Final : 40 pts

Homeworks: 5*6=30 pts

TOTAL =100 pts

- **Laboratory Sessions:** Laboratory sessions will be based on the material covered in the lectures. Attending the class is required

- **Exams:** All exams have limited access to internet and will be held in computer labs unless otherwise stated.

COURSE OUTCOMES:

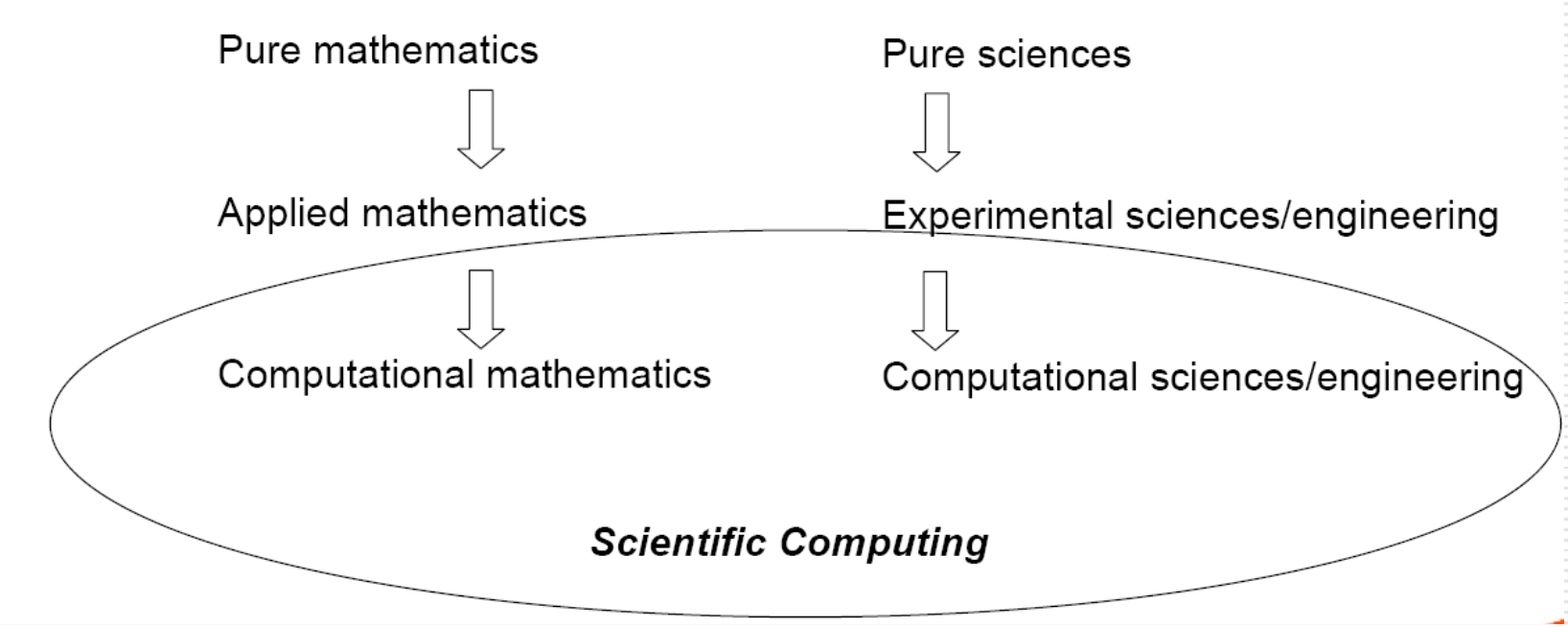
- Students will be able to,
- Analyze a problem and develop an algorithm
- Test, debug, and verify the program
- Understand and do both pre- and post-processing of raw data (input) and produced data (output) for scientific and engineering problems
- Prepare scientific report

What is scientic computing?

- Design and analysis of algorithms for solving
- mathematical problems in science and engineering numerically

- Traditionally called
  - numerical analysis

Evolution of scientific computing from other sciences and engineering disciplines



Interdisciplanary!!!

Why scientific computing?

- Mathematical problems that do not have closed form solutions.
- Example Solve $33x^5 + 3x^4 - 17x^3 + 2x^2 + 4x - 39 = 0$
- Even if solution formula exist, it may be difficult to compute.
- To replace expensive experiments with computer simulations

Objectives depend on concrete task of simulation:

– reconstruct and understand known scenarios (natural disasters)

– optimize known scenarios (technical processes)

– predict unknown scenarios (weather, new materials)

Grand Challenge Problems include

- climate research
- combustion
- automobile development
- aircraft design
- electronic design automation
- biology and medicine
- chemistry and physics
- material science
- financial engineering
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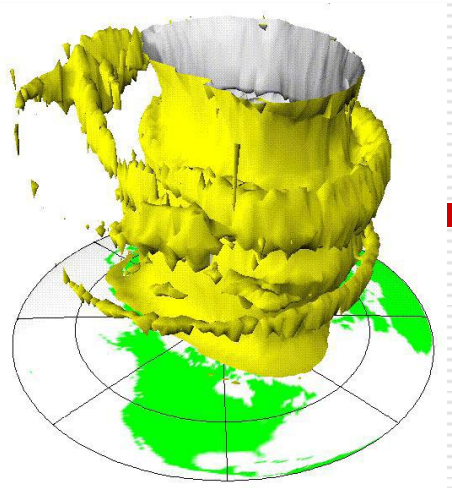
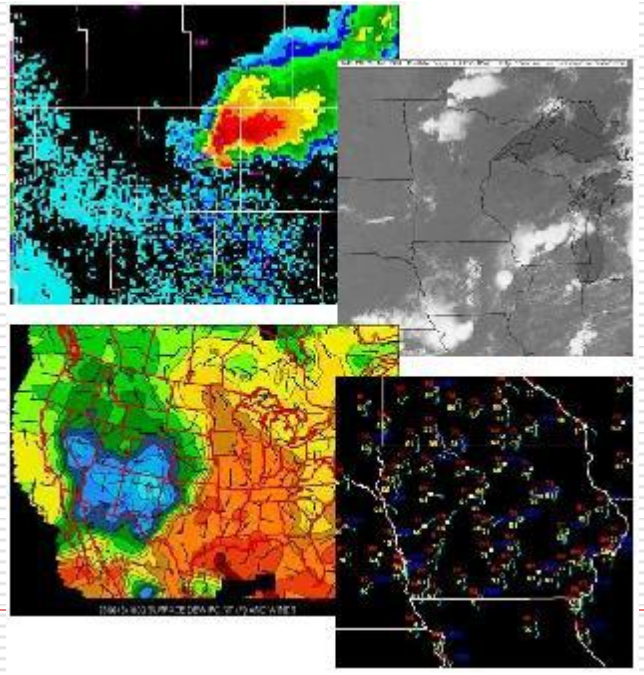
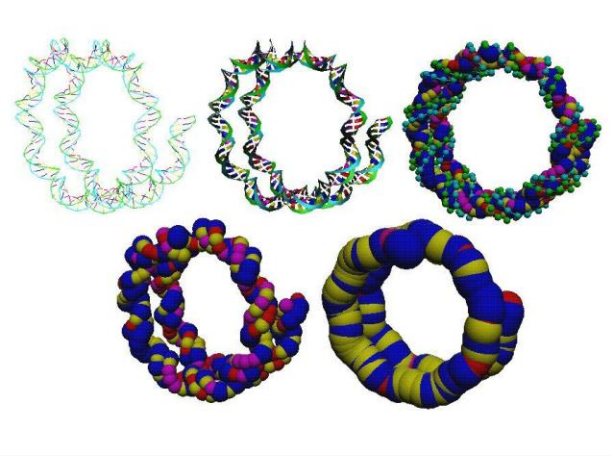


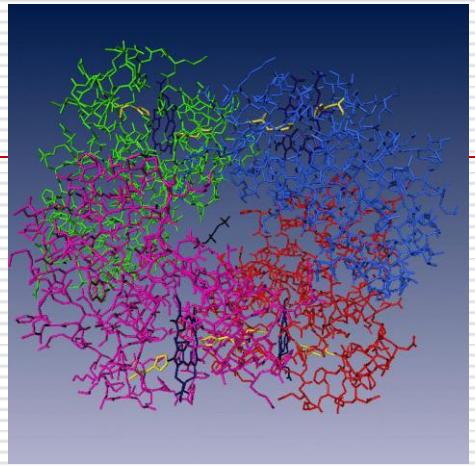
• climate research: Gulf Stream, greenhouse effect etc.



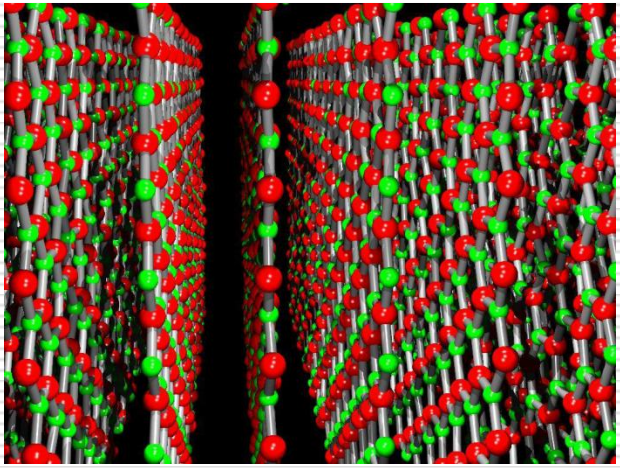
•weather forecast: tornadoes – where, when, and how strong?



genetics



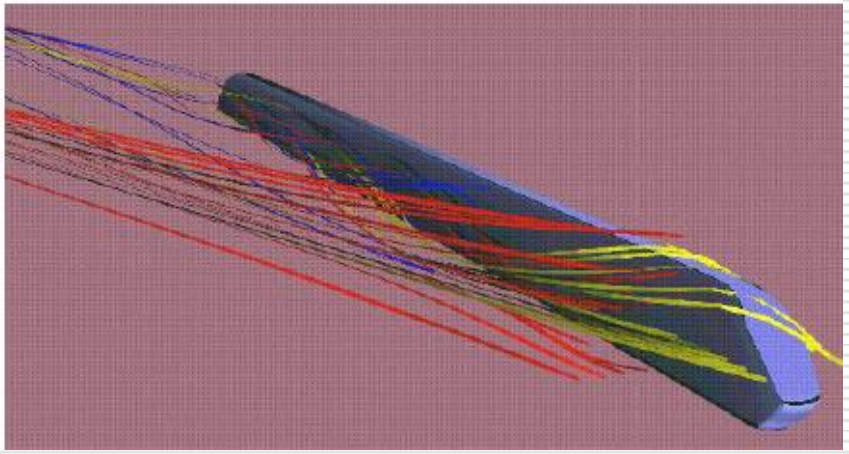
proteins



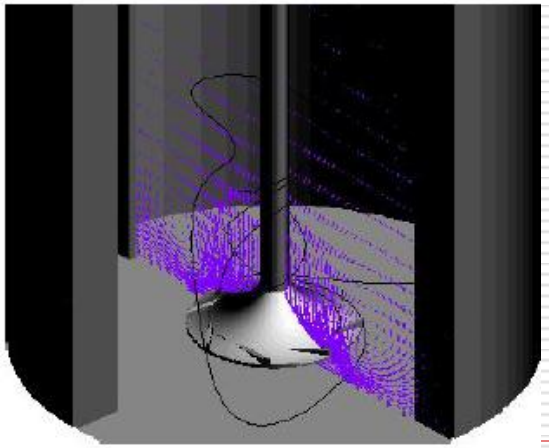
Crystal structures &macromolecules

since simulations are sometimes just cheaper or faster,

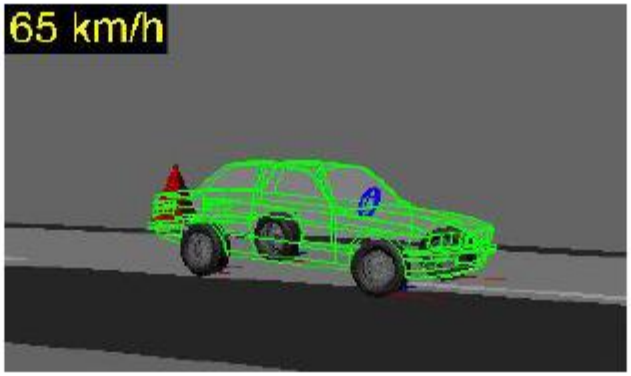
- aerodynamics, turbulence: objects in a wind tunnel and so on



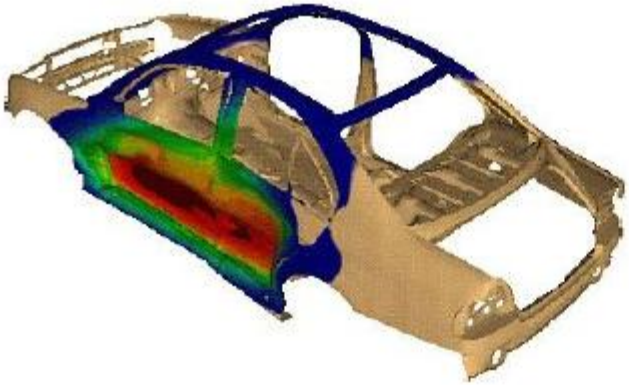
- process engineering: stirring and mixing processes

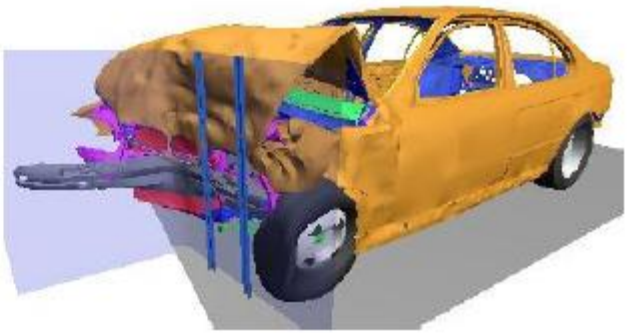


- car industry: vehicle dynamics, elk test



- car industry: crash tests



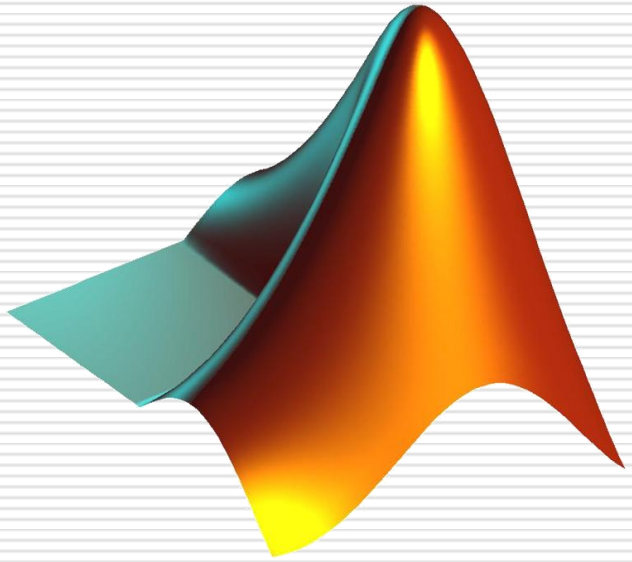


Computer Tools

- Spreadsheet applications
- Matlab (Octave, Scilab), Mathematica (Mupad), Maple, Matcad
- High level programing languages Fortran, C, C++

Why MATLAB?

- **Advantages**
  - Interpreter
  - Many many toolboxes
  - Visualization
  - Friendly environment
  - Wide usage
- **Disadvantages**
  - Slower than C and Fortran
  - Not freeware/open source



Other than MATLAB

- SciLab
- Distributed freely and open source

  http://scilabsoft.inria.fr/

  Scilab works on most Unix systems (including GNU/Linux) and Windows (9X/NT/2000/XP).

- Octave
- It is easily extensible and customizable via user-defined functions written in Octave's own language, or using dynamically loaded modules written in C++, C, Fortran, or other languages.
- GNU Octave is also freely redistributable software.

  http://www.octave.org/

Matlab/Mathematica/Maple

- Matlab is designed to solve problems numerically, that is, in finite-precision arithmetic.
- It produces approximate rather than exact solutions,
- It should not be confused with a symbolic computation system (SCS) such as Mathematica or Maple..

Useful Links

- www.mathworks.com
- http://www.mathtools.net/
- http://www.math.utah.edu/lab/ms/matlab/matlab.html
- http://www.owlnet.rice.edu/~ceng303/Matlab/MatCont.html
- And many other

Historical Facts about Matlab

- Matrix-based numeric computation
- - **MAT**rix **LAB**oratory
- The language was invented by Cleve Moler in the late 1970s
- He designed it to give his students access to LINPACK and EISPACK without having to learn Fortran.
- MATLAB is rewritten in C and founded The Mathworks is founded in 1984 to continue its development by Cleve Moler and Steve Bannert.