FF505

Computational Science

Introduction to the course

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a joint course between IMADA and FKF
University of Southern Denmark

Outline

1. Course Organization

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Aims of the course

- To learn to use the computer as a tool for scientific reasoning and discovery
- To learn how to solve numerically problems that can be solved analytically
- To equip you with tools you may need when analytical solutions are not known
- To learn to reason on the meaning of the results found

Organization of the Course

1. Introduction to a numerical computing environment, MATLAB
   (Marco Chiarandini) weeks 5-7
2. Introduction to mathematical tools, Linear Algebra
   (Vincent Drach and Claudio Pica) weeks 5-7
3. Applications in physics
   (Paolo Sibani) weeks 8-12
4. Training sessions
   (Martin Hansen) weeks 5-12

Week	5	6	7	8	910	11	12
Man, 09–12		Training (IMADA Terminalrum)	MATLAB (IMADA Terminalrum)				
Tir, 09–12	MATLAB (IMADA Terminalrum)	LinAlg (IMADA Terminalrum)					
Ons, 10–13				Appl. (IMADA Terminalrum)	Appl. (IMADA Terminalrum)		Appl. (IMADA Terminalrum)
Ons, 12–15	LinAlg (IMADA Terminalrum)	MATLAB (IMADA Terminalrum)	LinAlg (IMADA Terminalrum)				
Tor, 09–12						Appl. (IMADA Terminalrum)	
Fre, 09–12		Training (IMADA Terminalrum)	Training (IMADA Terminalrum)	Training (IMADA Terminalrum)	Training (IMADA Terminalrum)	Training (IMADA Terminalrum)	Training (IMADA Terminalrum)

Contents of the course

Mathematical Tools:

- Matrices and vectors: matrix calculs
- Matrix inversion and determinants
- Eigenvalues and Eigenvectors
- Ordinary differential equations
- Coupled differential equations
- Lattice Laplacian
- Fourier analysis

MATLAB Section

The MATLAB Section will cover

- interactive environment
- vectorized operations
- programming: control structures, script, functions
- data input/output
- graphics

More specifically, it should prepare you to carry out the calculations needed in the other parts of the course and in the project.

Communication tools

- BlackBoard (BB)
  (link to MATLAB Section http://www.imada.sdu.dk/~marco/FF505)
- Announcements in BlackBoard
- Discussion Board in (BB) - allowed anonymous posting and rating
- Write to instructors and to Marco or Paolo
- Ask peers
- You are welcome to visit me in my office in working hours (8-16)

⇝ It is good to ask questions!!

⇝ Please, let us know if you think we should do things differently!

Hands on Experience

The course assumes active participation to classes:

Introductory classes: you will be asked to perform small tasks at the computer.

Training sessions: weekly exercises to be carried out in your study group before the classes.

For the MATLAB part, slides and exercises are available at
http://www.imada.sdu.dk/~marco/FF505

You are also recommended to document your progress in a personal log-book, which contains your thoughts, calculations, figures etc.

Assessment

- Project in the last part of the course
  - similar to those you will do with Paolo
  - to be carried out in groups of two persons
  - hand in a written report, you should attempt to argue your case: Why should the examiner or anybody else trust your results?
- Individual oral exam based on the written report
  - Graded with external censor according to 7-grade scale

Some Practical Stuff

Getting Matlab:

- machines in IMADA terminal room have Matlab R2014a installed (type `matlab` from command line)
- Install the free Trail version in your computer
  see link from MATLAB section page.
- wait for SDU Site-License
- remote connection (see note on web page)
- use a Matlab clone, eg, Octave, SciLab
- use other software for similar purposes: python

- buy the student edition of Matlab: (ca. 600 DDK)
  see link from MATLAB section page.

Who is here?

22 registered, 27 in BlackBoard... how many are here?

Student presentation:

- Name
- Which programme are you attending
  - Physics
  - Applied Mathematics
  - Guest student

Unix Operating System

In Linux and MacOsX. In Windows via CygWin:

- The command shell
- Commands: `ls`, `ls -l`, `cd`, `.`, `..`, `~`, `pwd`
- Manuals: `man ls`
- Commands: `cp`, `mv`, `rm`, `rm -r`
- displaying content: `less`, `more`
- searching content: `grep`
- access rights
- editors: `vi`, `emacs`, `gedit`, others like Sublime Text can be installed.
- plenty of useful command line programs: http://www.gnu.org/software/coreutils/manual/

Exercise:
Create a directory called `FF505` and a file named `hello.txt`. Edit the file and write something inside. Then try to access the file of one of your neighbors.

MATLAB

MATLAB (**ma**trix **la**boratory) is a high-level language and interactive environment to perform computationally intensive numerical computations faster than with low-level programming languages such as C, C++, and Fortran.

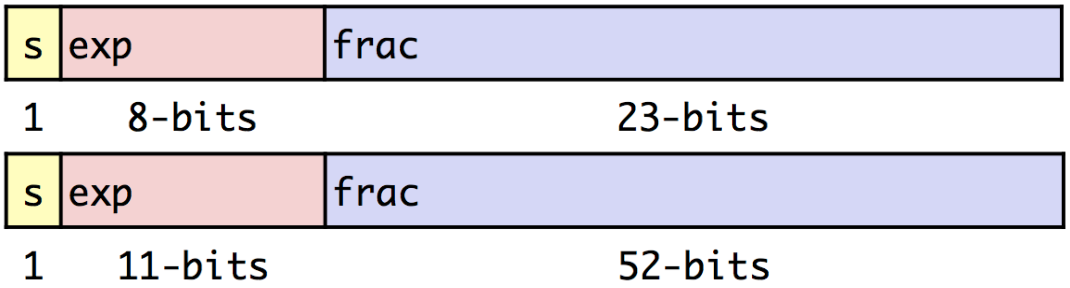
- Developed by a privately held company, MathWorks, 70% located at the company's headquarters in Massachusetts.
- Stable release: 2014b
- Written in C, Java
- License: Proprietary

Other similar numerical computing environments with high-level programming language are:

- Maple www.maplesoft.com (symbolic) – Proprietary
- Mathematica http://www.wolfram.com/mathematica (discrete mathematics) – [Proprietary]
- Octave www.gnu.org/software/octave – [General Public License]
- R www.r-project.org (statistics) – [GPL]
- Sage www.sagemath.org (discrete mathematics) – [GPL]
- SciPy www.scipy.org (based on python) – [GPL]
- ...
- later a comparison

Scientific vs Symbolic Computing

- scientific computing is based on numerical computation with approximate floating point numbers. $(-1)^s M 2^E$



http://www.mathworks.se/help/matlab/matlab_prog/floating-point-numbers.html

- symbolic computation manipulates mathematical expressions and other mathematical objects.
  emphasis on exact computation with expressions containing variables that have not any given value and are thus manipulated as symbols

  $\rightsquigarrow$ Try http://www.wolframalpha.com
  Symbolic computation can be done in MATLAB with the Symbolic Math Toolbox and the MuPAD editor (not installed)