Introduction to Scientific Computing

PHYS 2500

Lecture 1

Introduction

Introduction to Scientific Computing

PHYS 2500

Class Administration
and
Syllabus

Introduction to Scientific Computing

PHYS 2500

Class:	M	3:30 - 6:20	SER 005
Instructor:	Robert Call		SER 222D
		R.Call@aggiemail.usu.edu	
Office Hours:			
Faculty Instructor:	J.R. Dennison		SER 222D
	797-2936	JR.Dennison@usu.edu	
Class Web Site:	http://www.physics.usu.edu/		
	Go to Classes/Class Websites		

Introduction to Scientific Computing

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Syllabus for PHYS 2500 Introduction to Computer Methods in Physics *Fall 2011*	
Date	**Assignments**
8/29/11	**Chapters 1-2** Overview of *Introduction to Scientific Computing* and *Mathcad Basics.* Required problems: Section 2.3 of **Modern** handbook.
9/12/11	**Chapter 3** *Variables and Units of Measure.* Required problems: Sections 3.3 and 3.5 of **Modern** handbook.
9/19/11	**Chapter 4** *Solving Equations.* Required problems: Section 4.3 of **Modern** handbook.
9/26/11	**Chapter 5** *Graphing.* Required problems: Section 5.3 of **Modern** handbook.
10/3/11	**Chapter 6** *Arrays and 3D Graphing.* Required problems: Section 6.3 of **Modern** handbook.
10/10/11	**Chapter 7** *Symbolic Processing and Numerical Analysis.* Brief introduction to *Mathematica* software. Required problems: Section 7.3 of **Modern** handbook.
10/17/11	**Chapter 8** *Data Analysis I: Descriptive Statistics & Linear Regression.* Required problems: Section 8.3 of **Modern** handbook..
10/24/11	**Chapter 9** *Data Analysis II: Non-Linear Curve Fitting* continued.
10/31/11	Required problems: Section 9.3 of **Modern** handbook.

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11/7/11	**Chapter 10** *Mathcad Capstone Project.* Required problems: Section 10.1 of **Modern** handbook and prepare a separate *Mathcad* report in your own words.
11/14/11	**Chapter 11.Bibliographic Databases.** Brief exercise in the use of Google Scholar and EndNote Web to locate reference materials and prepare citations. Continue work on Mathcad Capstone Project Required problems: Bibliographic assignment.
11/21/11 **Meet in SER 132 (VERY IMPORTANT: You must be in class for the lab)**	**DataStudio and LabVIEW** lab (session 1) Learn to use the *DataStudio* program and take data with the Pasco probes. Analyze the data with *Mathcad*, *Excel* and *MatLAB*. Required work: Separate analysis files in *Mathcad*, *Excel* and *MatLAB*.
11/28/11 **Meet in SER 132 (VERY IMPORTANT: You must be in class for the lab)**	**DataStudio and LabVIEW** lab (session 2) A brief introduction to *LabVIEW*. Continue work from previous week. Required work File from previous week.
12/5/11	**Make Up Session.** Make up missed assignment by advanced arrangement with instructor.

*Any changes to the syllabus will be announced in class.

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Save files to a memory stick.

- **Transfer assignments to the instructor via a memory stick or e-mail.**
- **Files handed in should be saved in this format:**
  last name_section.
- **For example, if I were to hand in the assignment from section 3.3, I would name the file Dennison_3-3.**

BACKUP YOUR WORK OFTEN!!!

- **Files may not transfer properly or be lost via e-mail.**
- **If for some reason your work does not reach me glitch-free, you will need to re-submit it.**
- **If you don't have a backup copy, you will have to re-do the assignment.**

Intermediate Lab

PHYS 3870

Grading:

160 Points	20 Points for each of 8 weekly assignments
60 Points	for Mathcad capstone project
60 Points	for total for the 3 Data Acquisition and Analysis sections
280 Points	Total for Class

The main reason student do not do well in this class is that they get behind and cannot easily catch up.

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Texts:

MathCAD Version 15, (Mathsoft, Cambridge, MA, 2007).
REQUIRED COMPUTER ANALYSIS PROGRAM
Available for purchase at bookstore for ~$100
or in SER 005 or Engineering Computer Labs
or as USU cite license from Physics Office in SER 250.

Introduction to Scientific Computing Electronic Workbook
Distributed free

Additional Mathcad Handbooks
Distributed free

Additional references are listed in the attached *Annotated Bibiliography*.

Introduction to Scientific Computing

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Mathcad CD File Listing

The following files are included in this CD:

Handbooks

Datapack—Data analysis Extension Pack
EMag—Schaum's Outline of Electromagnetism (Sophomore Level)
EThermo—Schaum's Outline of Thermodynamics (Sophomore Level)
Images—Creating Amazing Images with MAthcad
Improc—Image Processing with Mathcad
Intro—Introduction to Problem Solving with Mathcad (Algebra Based) for PHYX 2500
Intro6—Introduction to Problem Solving with Mathcad (Algebra Based) for PHYX 2500 (Mcad Ver. 6)
Int_Lab—Intermediate Lab with Mathcad for PHYX 3870-80
Modern—Introduction to Problem Solving with Mathcad (Calculus Based) for PHYX 2500
Modern6—Introduction to Problem Solving with Mathcad (Calculus Based) for PHYX 2500 (Mcad Ver. 6 V)
ODEblock—Ordinary Differential Equations Solve Blocks Handbook
Physics—Schaum's Outline of College Physics (Freshman Level)
Phyx2110—Problem Solutions for Physics for Life Sciences PHYX 2110 (Freshman Level)
Signal—Signal Processing Handbook
Solve—Solving and Optomizing Extension Pack
Visualem—Visual E&M (Junior Level)
Visqm—Visual Quantum Mechanics (Senior Level)
*Wavelets*Wavelets Extension Pack
Waves—Introduction to Wave Phenomena with Mathcad for PHYX 2750
Waves6—Introduction to Wave Phenomena with Mathcad for PHYX 2750 (Mathcad 6 Version)

Other Files

Ancona Mathcad Numerical Methods Book—A full advanced graduate-level text on numerical methods. Included are Mathcad 2001i versions and the text in PDF format.
Drumhead—Calculations of the standing wave solutions on a drumhead
Miscellaneous Mathcad Files—Additional useful physics files

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Foundations of Wave Phenomena

by
C. G. Torre

Mathcad Electronic Handbook

by
J.R. Dennison and D. Mark Riffe
Utah State University

- Go to the Table of Contents

Table of Contents

Introduction to Scientific Computing

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How is Physics Done?

What is Physics?

"Study of the basic nature of matter and the interactions that govern its behavior."

BORING!!!

"How Stuff Works."

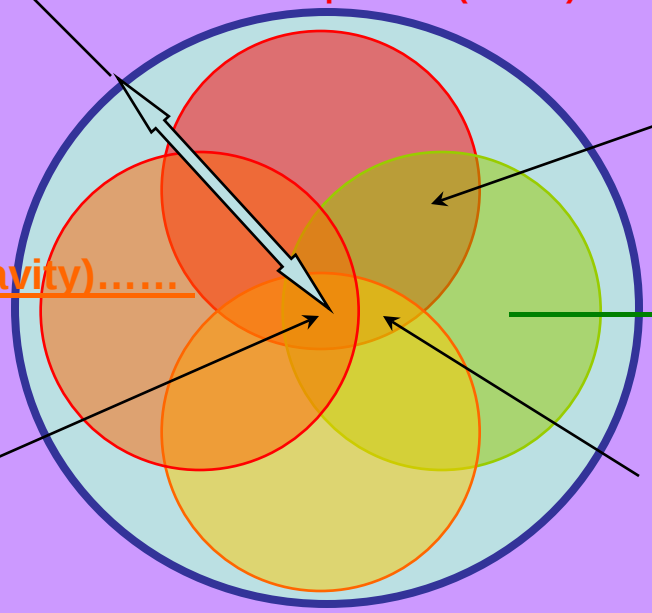
True, but vague.

"Common Sense Approach to How Things Work" (with units!)

Common Sense—A minimal set of simple, straightforward guides.

Units—Predictions on a quantitative level

Current State of Physics *cira* 2009



Statistical Mechanics
- Physics of many particles
- Fermions and Bosons
- Partitioning of Energy
- Thermodynamics
- Time and Entropy

Conservation Laws
- Energy
- Linear & Angular Momentum
- Charge, Spin
- Lepton and Baryon Number

Electricity & Magnetism
Maxwell Equations (c 1880)

Weinburg-Salom Model
- QED
- Unites E&M, Weak NF

Mechanics (Gravity)……
General Relativity
Space and time

Weak Nuclear Force
Radioactivity

Quantum Mechanics
- Schrodinger/Dirac Equation
- Probabilistic approach

Standard Model
- QCD
- Unites E&M, Strong NF, Weak NF

Strong Nuclear Force
Composition of subatomic particles

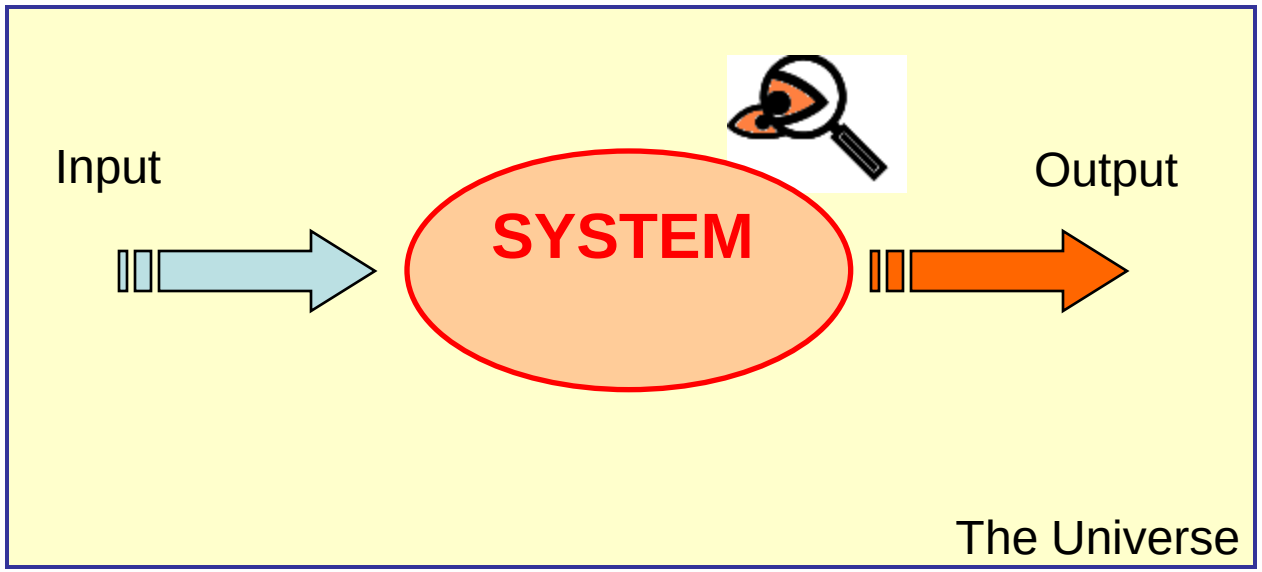
What is Experimentation?

Baird defines experimentation as the process of:

- **Identifying a portion of the world to study (the system)**
- **Obtaining information from this system**
- **Interpreting this result**

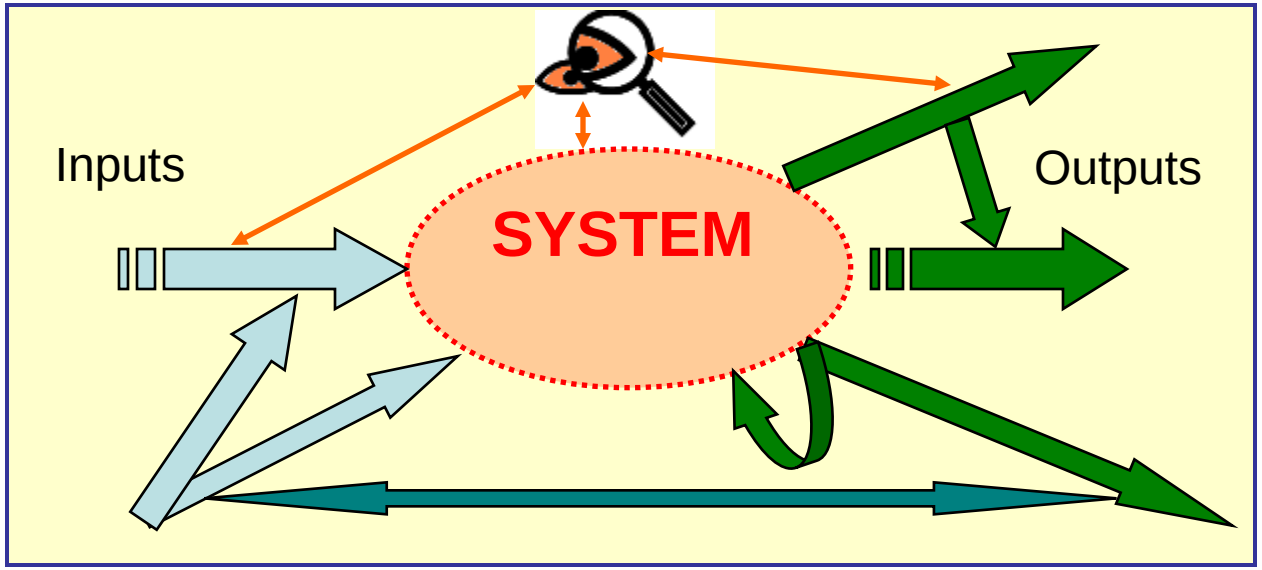
Observations of the Physical World

The Simplest (Ideal) System



- **The system (portion of the world being studied) is well defined**
  - **Single input (things we can control) affects system**
  - **Single output (things we cannot control directly) results from interaction of system with inputs**
  - **Observations characterize the system to within the uncertainty of the measurements**

A Complex System



- Complex (or ill defined) system and system boundaries
- Multiple inputs
- Multiple output
- Possible complicating interactions:
  - Between inputs
  - Between outputs
  - Between inputs and outputs
  - Between outputs and inputs
  - Between outputs and system
  - Between observations and system, inputs and outputs

What is Science?

The scientific method goes further in:

- Developing a description (model) of the system behavior based on observation

- Generalizing this description (model) to other behavior and other systems

- That is to say, the scientific method is experimentation and modeling intertwined

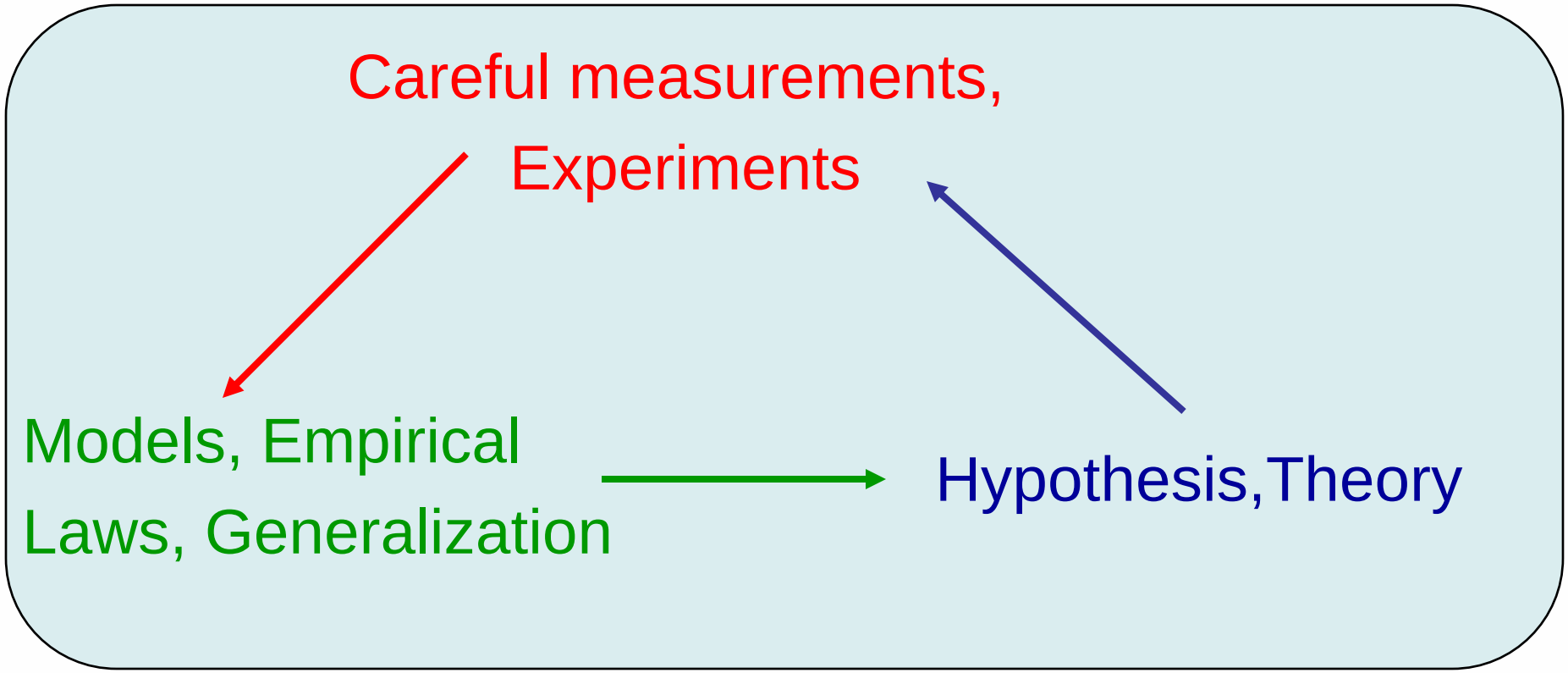
- It is the scientific method that distinguishes science from other forms of endeavor

As Neils Bohr famously said,

"All science is either physics or stamp collecting."

Scientific Method:

Leads to ***new discoveries*** → how scientific progress is made!



What is a Model?

1. A model:
   a) Describes the system
   b) Proposes how input variables interact with the system to modify output variables

2. Models versus systems
   a) A system is real. Information about the system can be known incontrovertibly.
   b) Models are not real.
      (1) Models are mankind's descriptions of reality
      (2) Models can never be fact (period), though they can be very good descriptions of how real systems behave.
      (3) Neither Newton's Law's, nor Special Realitivity, nor Einstein's Equations for General Relativity, nor TOE (Theory of Everything) are the final answer; Nature is!

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What Is the Role of Scientific Computing?

What Is the Role of Scientific Computing?

Definition: Using computer hardware and software to facilitate experimentation, modeling and merger of these two:

- **Increased speed and complexity is data acquisition**
- **Enhanced data management and presentation**
- **Increased speed, accuracy and precision in computations**
- **Automation of tasks (including symbolic math and data acquisition!)**
- **Enhanced dissemination of results**

What Is the Role of Scientific Computing?

Experimentation

Data Acquisition
Data Organization
Data Visualization
Data Analysis

Modeling

Model Definition
Model Development
Model Visualization
Model Computation

Overlap of Experimentation and Modeling

Qualitative Comparison of Data & Models
Quantitative Comparison of Data & Models
Dissemination of Results

What are Required Scientific Computing Capabilities?

Experimentation		Modeling	
Data Acquisition & Inst. Control	Data Acquisition	Model Definition	Symbolic Math
Spreadsheets, Databases	Data Organization	Model Development	Symbolic Math
Graphing, Tables	Data Visualization	Model Visualization	Graphing, Tables
Computation, Num. Meth, Stats	Data Analysis	Model Computation	Computation, Num. Meth.

Overlap of Experimentation and Modeling

Computation, Graphing	Qualitative Comparison of Data & Models
Computation, Num. Methods, Stats	Quantitative Comparison of Data & Models
Technical WP, Graphing, Tables	Dissemination of Results

Required Computation Capabilities

Data Acquisition & Instrument Control
Spreadsheets, Databases
Graphing, Tables
Computation
Numerical Methods
Statistics
Symbolic Math
Technical Word Processing
Bibliographic Databases

Introduction to Scientific Computing

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Specific Software for Scientific Computing?

Data Acquisition and Instrument Control

Definition: Using computer hardware and software to facilitate experimentation:

- Increased speed and complexity is data acquisition
- Automation of tasks (including symbolic math!)

- Instrument Specific
  - Calculator (TI)
  - USB-to-Spreadsheet Macros
  - DataStudio (Pasco Interface)*
  - I-Phone, Android
- For General Instruments
  - Labview#
  - Labview clones
- Programming Languages (C++, Visual Basic, etc)

*** Class emphasis** **# Introduction in class**

Spreadsheets and Databases

Definition: Management of large lists of data:

- Enhanced data management and presentation
- Automation of tasks
- Enhanced dissemination of results

- Primary Software
  - Spreadsheets (Excel* and clones)
  - Databases (Access and clones)
- Related Software
  - Matlab#
  - Graphical software (Igor, Origin and others)
  - Computational Software (Mathcad*, Mathematica#, etc)
- Programming Languages (C++, Visual Basic, Fortran, etc)

*** Class emphasis # Introduction in class**

Graphing and Tables

Definition: Graphical and Tabular presentation of data.

Animations:

- Enhanced data management and presentation
- Increased speed, accuracy and precision
- Automation of tasks
- Enhanced dissemination of results

- Primary Software
  - Graphical software (Igor, Origin and others)
  - Graphical calculators
- Related Software
  - Computational Software (Mathcad*, Matlab#, Mathematica#, etc)
  - Spreadsheets (Excel* and clones)

- Programming Languages (C++, Visual Basic, Fortran, etc)

*** Class emphasis** **# Introduction in class**

Computation

Definition: Calculating numerical results from numerical inputs:

- Increased speed and complexity is data acquisition
- Increased speed, accuracy and precision in computations
- Automation of tasks
- Enhanced dissemination of results

- Primary Software
  - Graphing calculators
  - Spreadsheets (Excel* and clones)
  - Computational Software (Mathcad*, Matlab#, Mathematica#, etc)

- Related Software
  - Graphical software (Igor, Origin and others)
  - Programming Languages (C++, Visual Basic, Fortran, etc)

*** Class emphasis** **# Introduction in class**

Numerical Methods

Definition: Calculating numerical results with symbolic inputs. Advanced calculation methods:

- Increased speed, accuracy and precision in computations
- Automation of tasks

- Primary Software
  - Computational Software (Mathcad*, Matlab#, Mathematica#, etc)
  - Programming Languages (C++, Visual Basic, Fortran, etc)

- Related Software
  - Graphing calculators
  - Spreadsheets (Excel* and clones)
  - Graphical software (Igor, Origin and others)

*** Class emphasis** **# Introduction in class**

Statistical Methods

Definition: Calculating numerical results with numeric or symbolic inputs. Advanced statistical methods:

- Increased speed, accuracy and precision in computations
- Automation of tasks

- Primary Software
  - Statistical Software (SISTAT, etc)
  - Computational Software (Mathcad*, Matlab#, Mathematica#, etc)

- Related Software
  - Graphing calculators
  - Spreadsheets (Excel* and clones)
  - Graphical software (Igor, Origin and others)
  - Programming Languages (C++, Visual Basic, Fortran, etc)

*** Class emphasis** **# Introduction in class**

Symbolic Math

Definition: Symbolic manipulation of mathematical (non-numeric) symbols, including algebra, calculus and geometry:

- Increased speed, accuracy and precision in computations
- Automation of tasks (including symbolic math!)

- Primary Software
  - Symbolic Math Programs (Mathematica#, Maple)
- Related Software
  - Computational Software (Mathcad*, Matlab#, etc)

*** Class emphasis** **# Introduction in class**

Technical Word Processing

Definition: Using computer hardware and software to facilitate experimentation, modeling and merger of these two:

- Enhanced data management and presentation
- Automation of tasks
- Enhanced dissemination of results

- Primary Software
  - Word Processor (Word, Wordstar, Open Office and clones)
  - Presentation software (Powerpoint, Open Office and clones)
  - Bibliographic databases and bibliographies (Google Scholar, Web of Science, EndNote Web, Zotero)
- Related Software
  - Computational Software (Mathcad*)

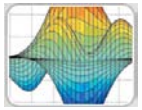
*** Class emphasis** **# Introduction in class**

Scientific Software Used in this Class

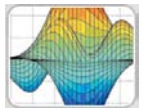
Data Acquisition & Instrument Control

Spreadsheets, Databases

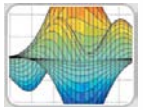
Graphing, Tables



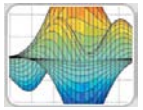
Numerical Methods



Computation



Statistics



Symbolic Math

Technical Word Processing

zotero

Google scholar

Scientific Software Used in Other Classes

PHYS 2500: Introduction to Computer Methods in Physics

USU Curricula Related to Scientific Computing

The following is a partial list of classes and other curricula used at USU that provide experience with scientific computing software. Course descriptions are copied from the USU General Catalog. Software used in these classes is noted in red; this is subject to change from semester to semester.

Computer & Information Literacy

The ability to use computers to access and present information is an important basic skill that you will build on during your time at USU. For this reason, Computer & Information Literacy (CIL) is a general education requirement that should be completed your first year at USU. Information is available at the web site http://cil.usu.edu/ .

Study Materials

- Electronic Presentations (Powerpoint)
- Spreadsheets (Excel)
- Information Law & Ethics
- Document Processing (Word)
- Information Resources (Google Search)
- Computer Systems

Computer Science (CS)

CS 1020 Campus Computing and Beyond 1
Hands-on laboratory for CS 1030. Introduces the campus network and the Internet. Emphasizes general problem-solving strategies and skills associated with computer and application software use.

of the concept of concurrency as it applies to operating system design and application. (JAVA)

CS 3410 DSC/QI Computational Science: JAVA/Internet 3
Introduces computational science for algorithm development in JAVA-based applications. Examines information representation, storage, retrieval, and transmission in quantitative Internet-based environments. (JAVA)

CS 4700 Programming Languages 3
Theories of programming design and implementation. Introduction to variety of programming languages, showing how they represent trade-offs with respect to these theories. (C++, JAVA, Perl, others)

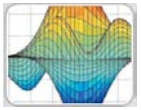
Chemistry and Biochemistry (CHEM)

CHEM 3080 CI Physical Chemistry Laboratory I 1
Experimental work to accompany CHEM 3060. (Excel)

CHEM 3090 CI Physical Chemistry Laboratory II 1
Continuation of CHEM 3080. Experimental work to accompany CHEM 3070. (Excel)

Civil and Environmental Engineering (CEE)

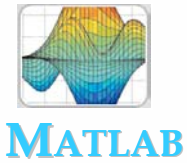
Scientific Software Used in this Class



Scientific Software Used in Other Classes

Computer-Aided Mathematics

ENGR 2450.
PHYS 2500, 3750, 3870, 3800.



ENGR 2450.
PHYS 2500.

ENGR 2450.
CEE 1880,3030.

Click on symbol to access home web site.

Scientific Software Used in Other Classes

Numerical Programming Languages

C++

CS 1400, 1405, 1410, 2420, 4700.
ENGR 2450.

Fortran

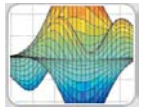
PHYS 5350.
MAE 2200, 2450.
ENGR 2450.

Visual Basic

ENGR 2450.

JAVA

CS 3100,3400, 4700.



MATLAB

ENGR 2450.

MATHEMATICA

MATHCAD

ENGR 2450.

Click on symbol to access home web site.

Scientific Software Used in this Class

Data Acquisition & Instrument Control

PHYS 2110, 2120, 2210, 2220, 2500, 3870, 3880.

PHYS 2500, 3870, 3880.

Scientific Software Used in Other Classes

Technical Word Processing

MATHCAD

ENGR 2450.
PHYS 2500, 3870, 3880.

Computer Literacy
CEE 1880.
MAE 2200, 2450.
ENGR 2450.
PHYS 3870, 3880.

Computer Literacy

Google scholar

USU Library Tutorials
PHYS 2500, 3870, 3880.

EndNote

PHYS 2500, 3870, 3880.

DataThief

PHYS 2500, 3870, 3880.

Scientific Software Used in Other Classes

A Real Gem—Urroz Software Resource Page

Webpage Screenshot

UtahState UNIVERSITY

Home
Classes
Calculators
Software
Useful links
CEE Department
Water Research Lab
Engineering College

USU Directories
USU Calendar
USU Libraries
QUAD
USU Webmail
Engineering Mail
USU Webcams
Giving to USU

HP 50G
TI 89
Scilab
Maple
Mathcad
Matlab
R
OpenOffice.org
Excel

My favorite SOFTWARE

Gilberto E. Urroz - ph. 435-797-3379 - gurro@cc.usu.edu - ENGR 223 - fax 435-797-1185

These are links to my favorite software. - Some links lead you directly to my own web pages on the subject, others to their main web pages.

Software for my classes

- Excel - commercial spreadsheet program
- Maple - Commercial symbolic environment
- Matlab - Commercial matrix-based numerical environment (similar to SCILAB).
- Mathcad - Commercial math worksheet
- Maxima - Free computer algebra system
- OpenOffice - Free, open source office suite
- R - Free statistical and graphics software, similar to S.
- SCILAB - Free matrix-based numerical environment (similar to Matlab)
- Smath Studio - free math worksheet
- VBA & Excel - Macro language for Excel spreadsheets
- Visual Basic 6.0 - Commercial programming language

Other software

- F language - a subset of Fortran 90
- FreeZip - Free, windows zip/unzip program
- FORTRAN 77
- FORTRAN 90/95 - Modern FORTRAN compilers
- Java - Free, portable programming language (from Sun Microsystems)
- Mathematica - Commercial symbolic environment
- MuPad - Commercial symbolic environment
- Visual Basic .NET - Object-oriented programming

Web software

- Frontpage - for creating web pages
- JavaScript - Web scripting language supported by most web browsers
- PERL - Web scripting language
- TCL - Web scripting language

http://www.neng.usu.edu/cee/faculty/gurro/Software_Calculators/Calculators.htm

Scientific Software Used in Other Classes

Where to Go From Here?

Computer skills are one of the best things to study to enhance your employment opportunities after graduation.

Programming Skills

C++ CS 1400, 1405, 1410, 2420, 4700. ENGR 2450.
Fortran PHYS 5350. MAE 2200, 2450. ENGR 2450.
Visual Basic ENGR 2450.
JAVA CS 3100,3400, 4700.

Numerical Methods

C++ ENGR 2450.
Matlab ENGR 2450.
Fortran PHYS 5350. MAE 2200, 2450. ENGR 2450.
Mathcad ENGR 2450. PHYS 2500.
Visual Basic ENGR 2450.

Instrument Control & Data Acquisition

Labview PHYS 2500, 3870, 3880.
Datastudio PHYS 2500 3870, 3880.