Physics 381: Winter 2014

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room SB 537
office hours:
    Tuesdays --> 11:00 am-12:00 pm (Room ***SB 504***)
    Thursdays --> 11:00 am-12:00 pm (Room ***SB 504***)

Main webpage for lecture notes:

http://www.pjl.ucalgary.ca ***(follow 381 link)***

Important note: these lecture notes will be available on-line. They do not contain everything that has been or will be presented during the lectures. It is important that you also make your own notes during the lectures.

General information: weekly dates

Schedule: Lectures&Labs are on
Tuesdays & Thursdays

Start at Noon (12:00-14:00 - ***15 minutes***) in **ST 026**

Start of lectures/labs: Thursday, January 9
End of lectures/labs: Thursday, April 10

See course outline

Phys381: Important Dates

- Tuesday, Feb. 25, 12:00-14:00 pm: Midterm
- Thursday, Apr. 10, 12:00-15:00 pm: Final

- Reading days : Feb. 16-23

- *Attendance at the exams is absolutely mandatory*.

Always check the course URL
http://www.pjl.ucalgary.ca ***(follow 381 link)***

Phys 381: Textbook

Textbook:
Ouyed&Dobler,
Computational Physics (1st Ed.)

For Physics 381:

Chapter 1: Numbers&Error Analysis
Chapter 2: Arrays&Matrix Analysis
Chapter 3: Evaluation of functions
Appen. A: Fortran 95
Appen. B: Makefile(s)
Appen. C: Gnuplot
Appen. E: Latex

Can be donwloaded @
http://www.pjl.ucalgary.ca

Phys 381: Marking & Exams

12 week course:

The final mark is calculated as follows:

Assignments (2)/Labs (~6)	20%/20% (40%)
ONE 2-hrs term test	20%
Final Exam (3-hrs)	40%

Phys 381: Marking & Exams

Labs.: 20%

Your report in PDF format should summarize your findings, and should include a copy of your code (use the Latex command [\begin{verbatim}..\end{verbatim}]) and its output. You should also review your results in a discussion section.

Each lab. would require ~**2-3 sessions**. Labs/Assignments are to be emailed in on time.

* Delays are NOT acceptable.

Phys 381: Marking & Exams

Assigns.: 20%

Your report in PDF format should summarize your findings, and should include a copy of your code (use the Latex command [\begin{verbatim}..\end{verbatim}]) and its output. You should also review your results in a discussion section.

Assignments be handed in (emailed) on time.

* Delays: a **10% penalty** per day

Phys 381: The Labs

The Labs

Gnuplot	1 (Appendix C)
Fortran	1 (Appendix A
Makefiles	1 (Appendix B)
Error Analysis	1 (chapter 1)
Matrices	1 (chapter 2)
Functions	1 (chapter 3)

Phys 381: Labs & Assigns

Labs/Assig

Lab 1 (Jan 16) : Latex+Gnuplot
Lab 2 (Jan 30) : Gnuplot+Fortran
Lab 3 (Feb 13) : Fortran

Assign. #1 (Feb. 16th)

February 17-24 (reading week)

Midterm: Feb. 25th (2 hours)

Lab 4 (Mar 11) : Error Analysis
Lab 5 (Mar 25) : Matrice Analysis
Lab 6 (Apr 8) : Evaluation of functions

Assign. #2 (Apr. 8th)

Final: April 10 (3 hours)

Phys 381: Labs & Assigns

Lab #1

Computational Physics I (**Phys381**)
R. Ouyed
Due January 24, 2012 (at the end of class)

(i) Use Latex to prepare your report; Include your codes (Fortran, Gnuplot scripts) in appendices (using the *verbatim* command); (ii) When I refer to *lecture notes* it means the Ouyed&Dobler notes; (iii) If applicable, animations should be shown to the teacher and/or TA before handing in the lab report. The animation should be well documented and contains necessary information (student name, assignment number, run time etc ...). Basically, the information should be included in each frame before they are put together.

→ The latexed report (as a PDF file) is worth **20%** of the total mark. Only well documented and neatly presented reports will be worth that much! It is not sufficient to give only numerical results and show plots. You should include complete figure captions, discussion section and conclusion.

→ Create a tar file which should include your PDF file, your codes (F90 and gnuplot) and any related animations. Name the tar file: *student1-student2-phys381-lab#.tgz*. Then email your tar file to:

rouyed@ucalgary.ca and Cc it to jpulwick@ucalgary.ca [Julia Pulwicki]

To tar all of the necessary files into a tar file named foo.tgz use:

```
tar cvzf foo.tgz file1 file2 file3 ...
```

This creates (c) a compressed (z) tar file named foo.tgz (f) and shows the files being stored into the tar file (v). The .tgz suffix is a convention for gzipped tar files.

1 Introduction

The last method of integration discussed in class was Gauss-Quadrature, by far the simplest and most powerful of the integration techniques. Shown in this document as a tool to evaluate the energy corrections in a vibrating hydrogen molecule to an energy level n. Method of rearanging and solving using nodes and weights of Hermite polynomials is used. Two methods of differentiation of ODE's is also performed when determaning the driving force EOM of a oscillating pendulum and compared to analytical solutions to evaluate the effectiveness of the methods, Euler and forth-order Runge-Kutta.

2 Integration: The Hydrogen Molecule

To determine the vibrational energies of a hydrogen molecule a more accurate potential needs to be determined by the following equation 3. To evaluate the integral, Gauss-Hermite method is used.

Potential of a lowest order vibrating hydrogen molecule

$$V_{harm}(x) = \frac{\mu\omega_0^2}{2}x^2 = \frac{\mu\omega_0^2}{2a^2}(ax)^2 \qquad (1)$$

Where $\mu = 8.37E-28Kg$, $\omega_0 = 8.29E14s^{-1}$, $x = r - r_{eq}$, and $a = 2.01E10m^{-1}$

Approximated by the Moorse potential

$$V_M(x) = \frac{\mu\omega_0^2}{2a^2}(1-e^{-ax})^2 \qquad (2)$$

Equation of the first order energy levels described above

$$E_n^{(1)} = \frac{\int_{-\infty}^{\infty} e^{-k^2x^2}H_n^2(kx)[V_M(x) - V_{harm}(x)]dx}{\int_{-\infty}^{\infty} e^{-k^2x^2}H_n^2(kx)dx} \qquad (3)$$

2.1 Re-writting $\delta V(x) = V_M(x) - V_{harm}(x)$ as a taylor series around $x = 0$

$$\delta V(x) = -\frac{\mu\omega_0^2}{2a^2}a^3x^3 + \frac{7}{12}\frac{\mu\omega_0^2}{2a^2}a^4x^4 \qquad (4)$$

Phys 381: Tools

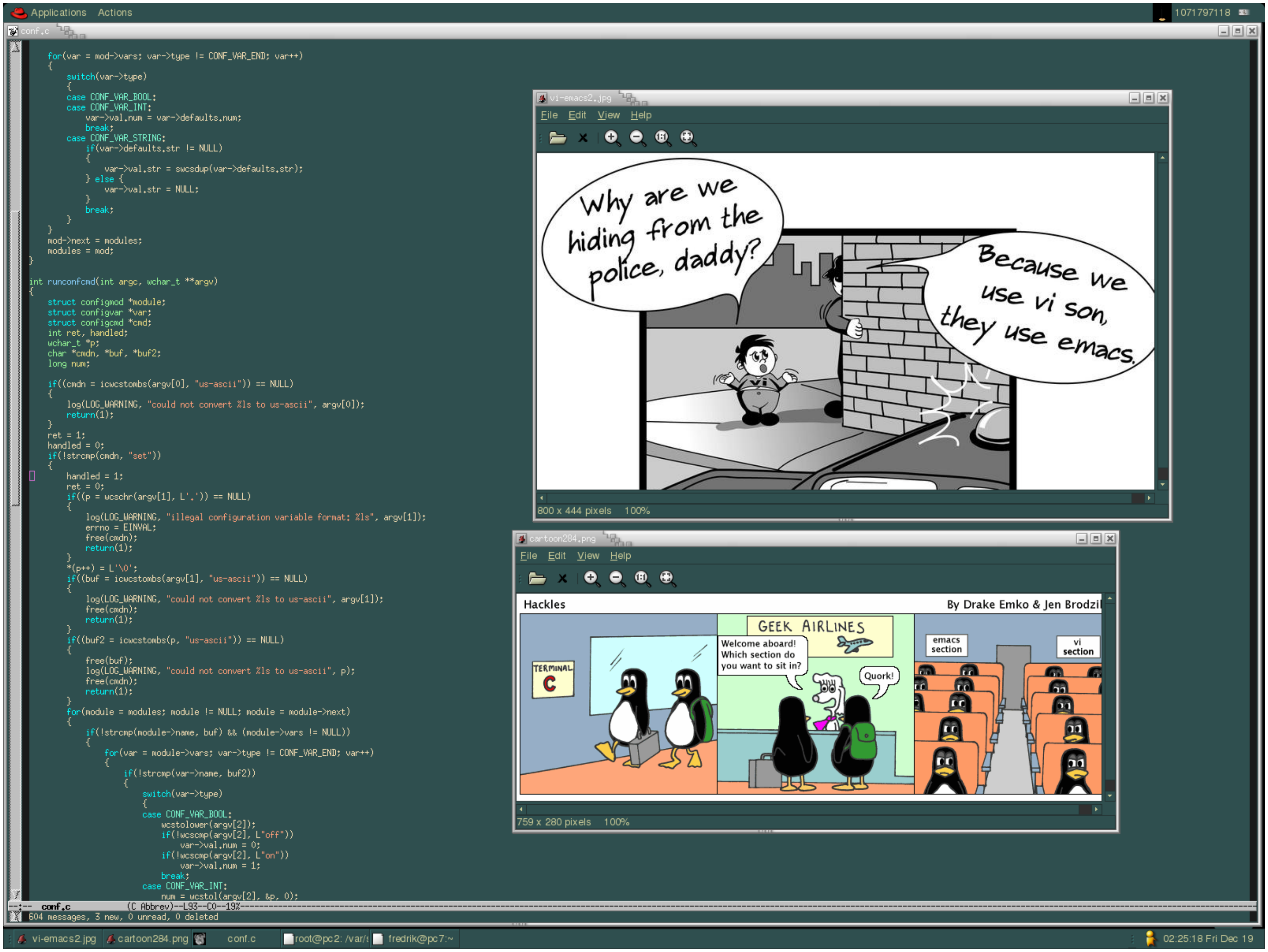
EMACS ← **Text Editor**

GNUPLOT (& Scripts) → Myfile.***gp***

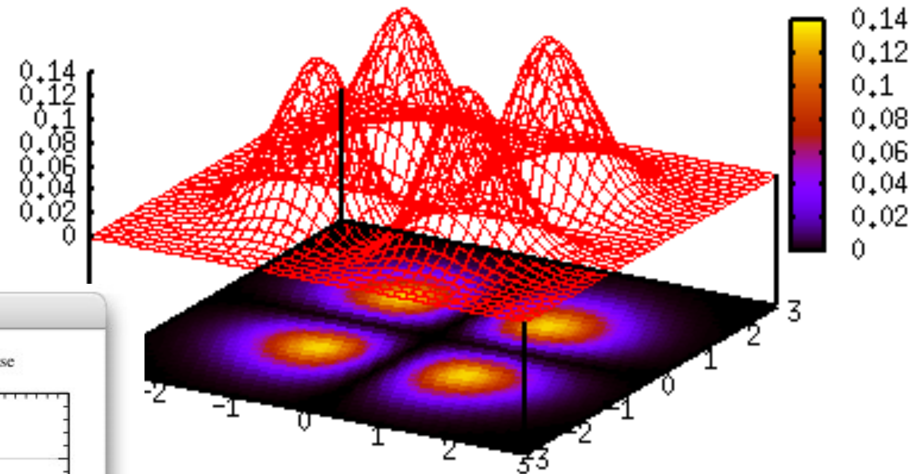
FORTRAN 90
(& Makefiles) → Myfile.***f90***

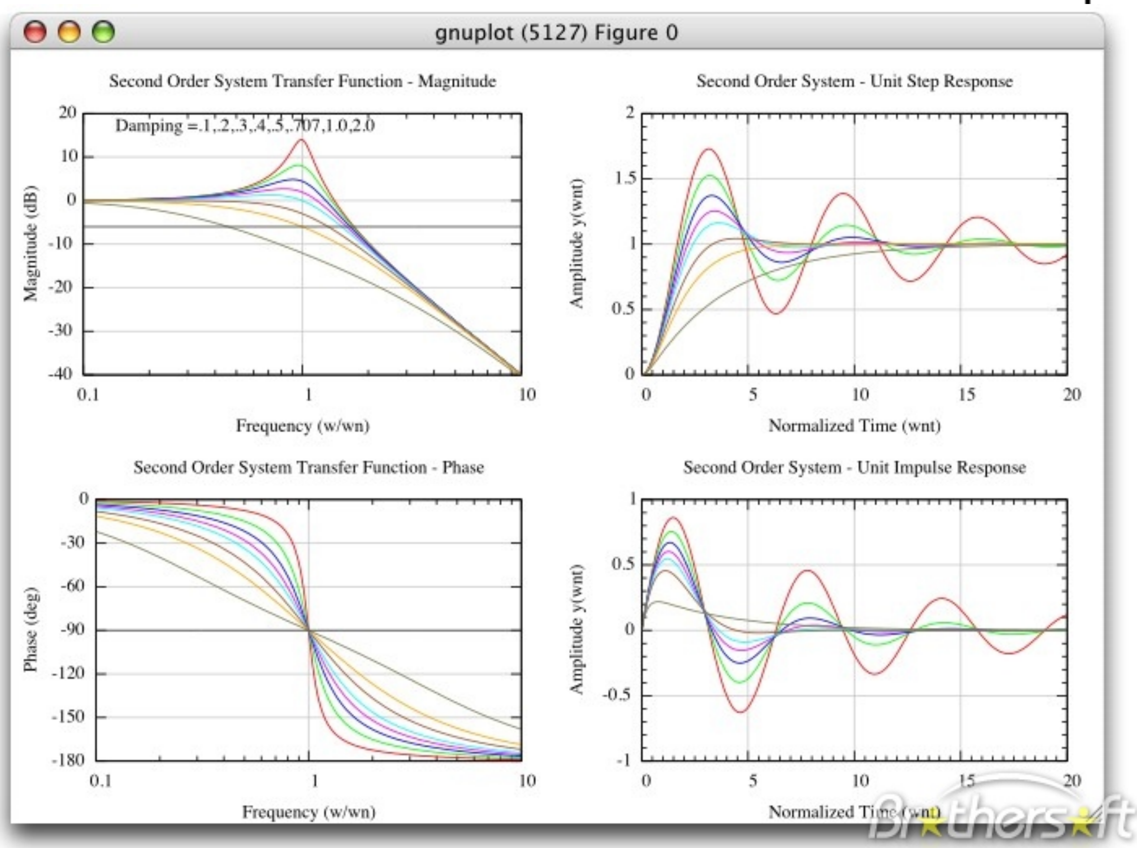
LATEX (& AucTex) → Myfile.***tex***

EMACS

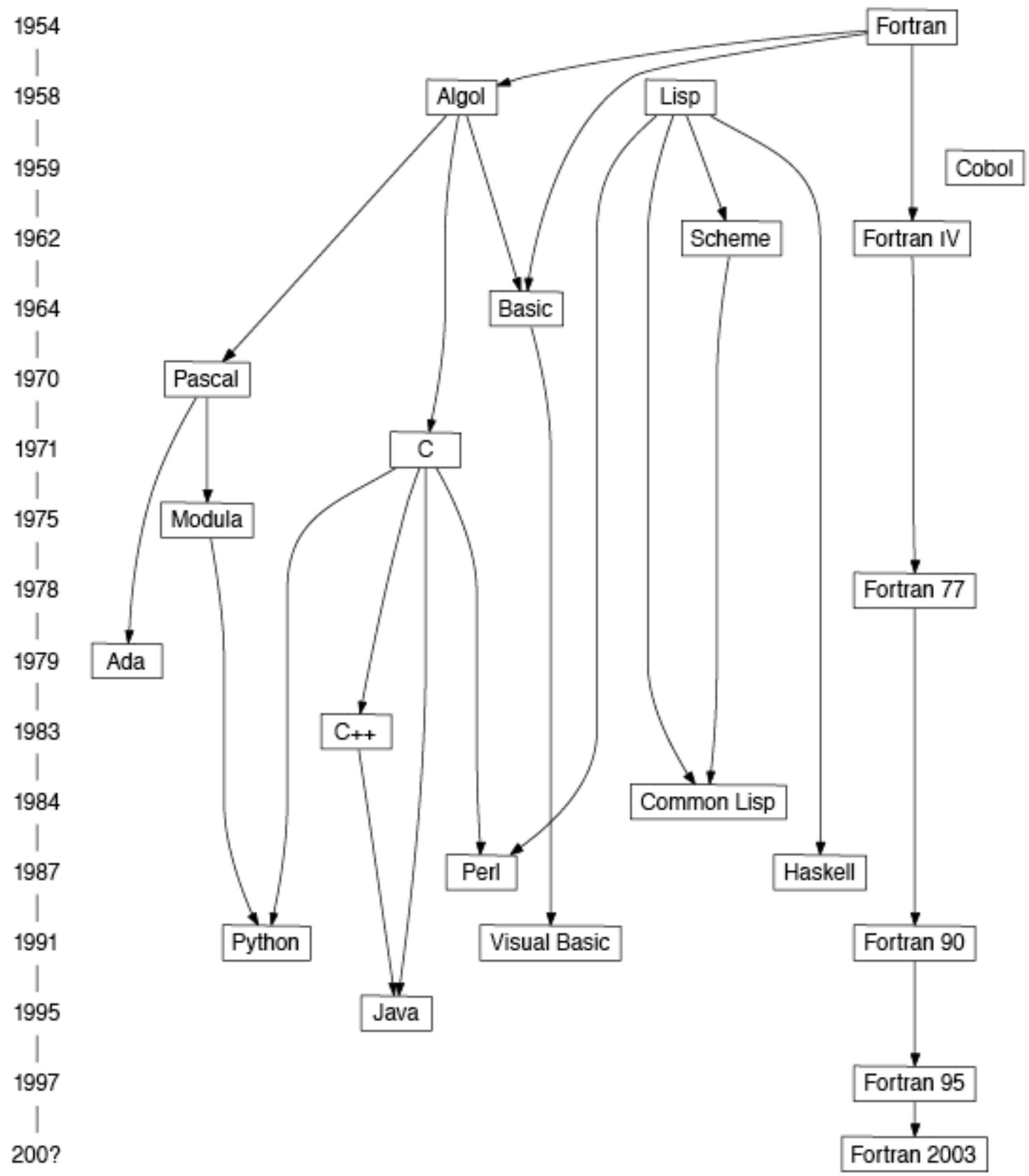

Applications
Actions
Why are we hiding from the police, daddy?
Because we use vi son, they use emacs.
800 x 444 pixels 100%
Hackles
By Drake Emko & Jen Brodzi
GEEK AIRLINES
TERMINAL C
Welcome aboard! Which section do you want to sit in?
Quork!
emacs section
vi section
759 x 280 pixels 100%
02:25:18 Fri Dec 19

GNUPLOT
(& Scripts)

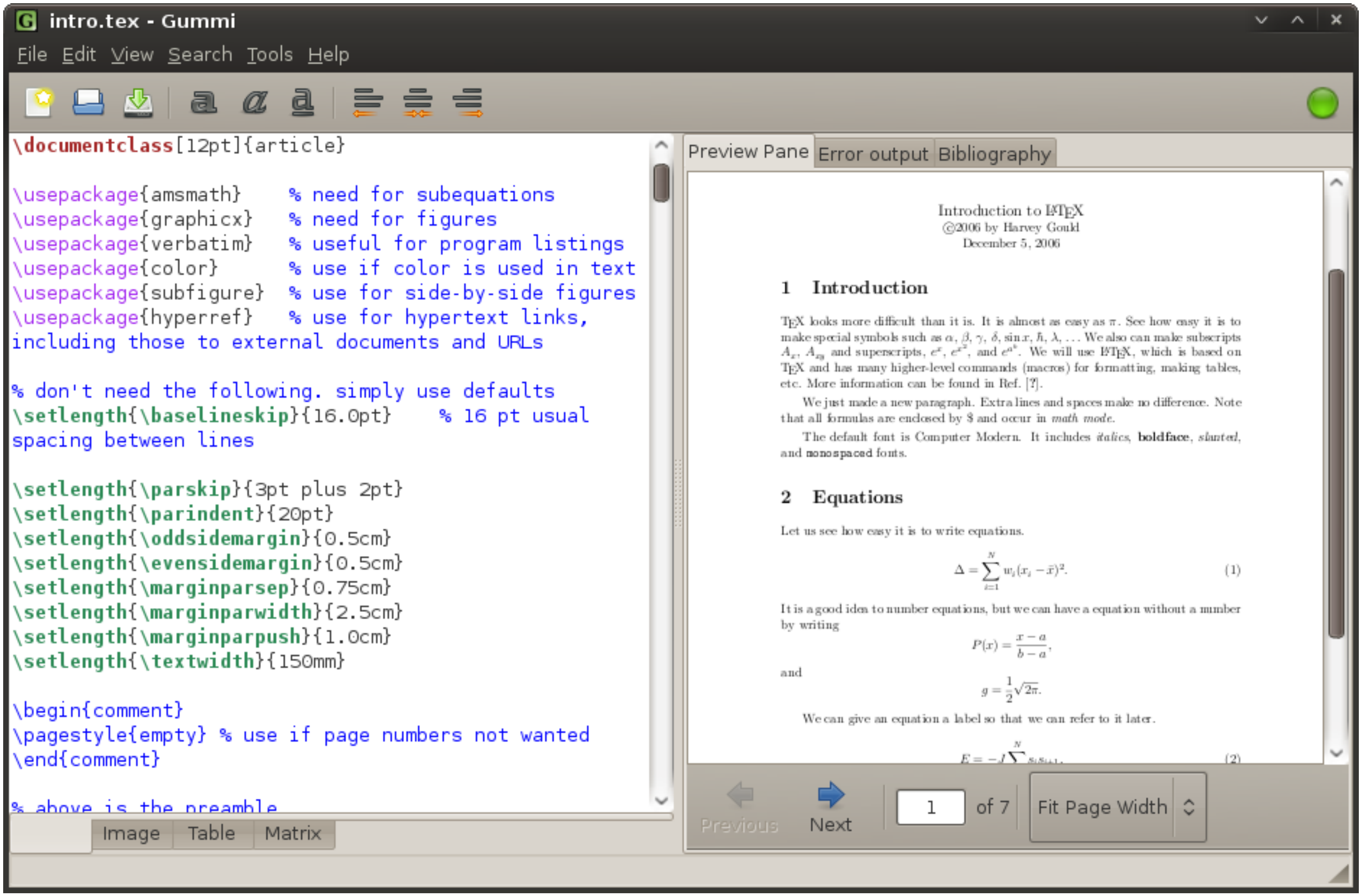




FORTRAN 90 (& Makefiles)



LATEX (& AucTex)



From 381 to 581

(the Journey)

Phys 381/481/581

CONTENT

Phys 381: Description
Phys 381: Outline

Phys 481: Description
Phys 481: Outline

Phys 581: Description
Phys 581: Outline

Phys 381

- Phys 381 deals with the basics of computing: algorithms, precision, efficiency, and verification. The student is introduced to some necessary numerical analysis and its associated approximation and round-off error. Physical applications are used in simple context.

- The students learn Gnuplot and how to program in Fortran 95 in the first few weeks. During this learning stage they are given notebooks or codes to run and then modify (or debug) them as they follow along through worksheets. Eventually in later chapters, students will have to write their own Fortran routines, making Gnuplot figures using scripts, and presenting their assignments and exams in postscript or PDF format using Latex.

Phys 381 content

- Introduction to Emacs (file editor)
- Basic programming (Fortran 95, Makefiles)
- Introduction to Gnuplot (Graphics and Datafiles handling)
- Introduction to Latex (report preparation and formatting)
- Programming guidelines and Philosophy
- Design and construction of a working code
- Numbers (errors and loss of accuracy)
- Scalars, vectors, and matrices (matrix operations)
- Evaluation of functions

Phys 481

- Phys 481 deals with the basic mathematical, numerical, and conceptual elements needed for using a computer as a virtual physical science laboratory. Each element will be studied in the context of physics projects, thus permitting the students to work independently and to understand at their own rate each element's virtues, areas of applicability, and limits. Physical applications are used, including interpolation, extrapolation, least square fitting, cubic spline fitting, Runge-Kutta etc ....

Phys 481 content

(main tool is Mathematica)

- Introduction to Mathematica
- Interpolation/Extrapolation
- Finding Roots and Maxima
- Numerical Integration
- Ordinary Differential Equations
- Runge-Kutta Methods

Phys 581

- Phys 581 focuses on more complex physics and astrophysics problems which apply and extend the techniques learned in the preceding courses (phys 381 and phys 481).

- The students are exposed to the concept of random numbers in physics and computation before introducing them to the world of Monte-Carlo techniques. We follow with more detailed learning of differential equations with specialization on finite differences.

In Phys 581 the students will be asked to develop and write their own codes and use the IDL (Interactive Data Language) tool which is crucial for visualization of Monte Carlo simulation results and Finite-difference simulations.

Phys 581 content

(main tool is IDL)

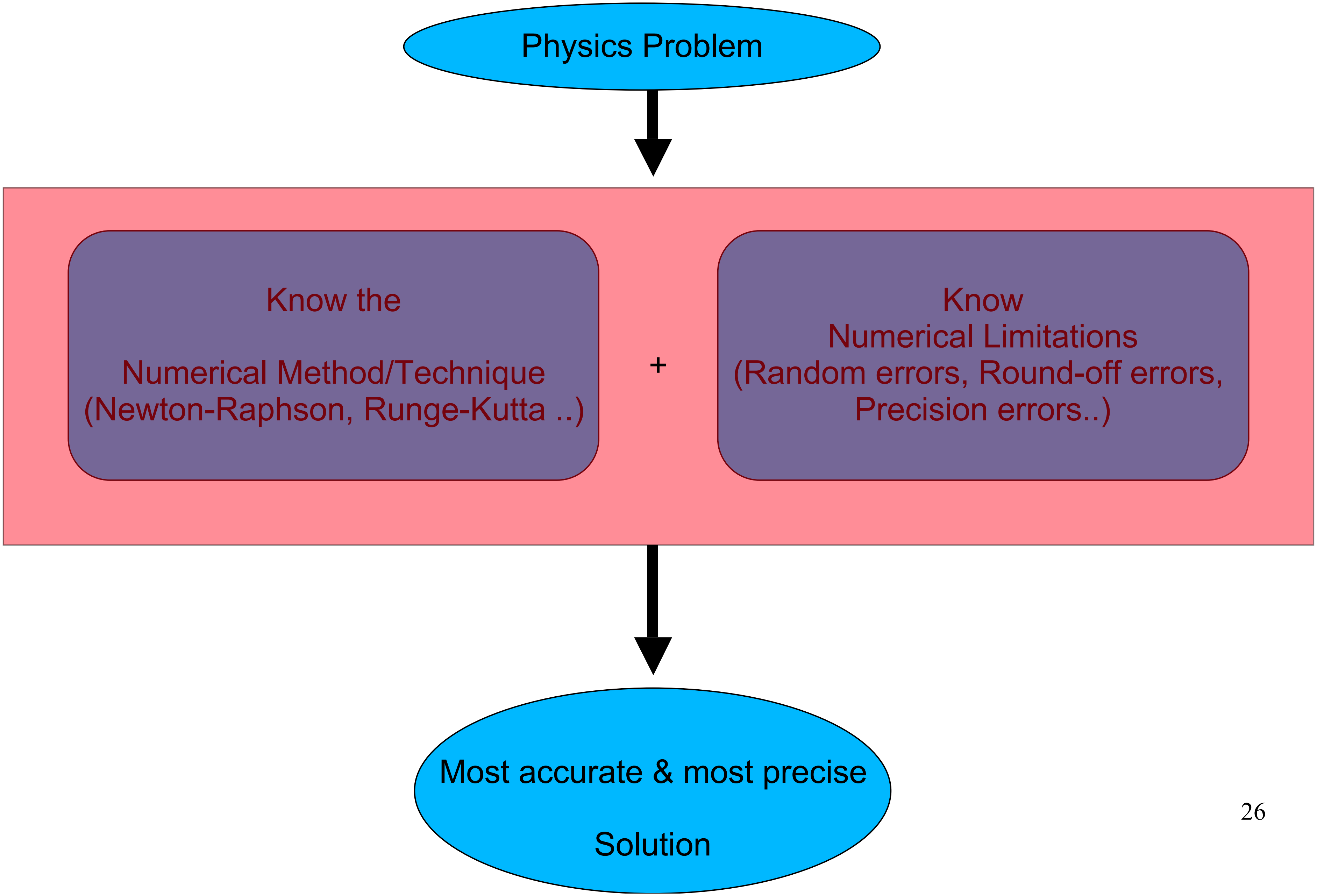
- Introduction to IDL
- Predictor-corrector methods for ODEs
- Random numbers and Monte Carlo methods
- Optimization
- The Fast Fourier Transform
- Partial Differential Equations
- Finite-differences
- Econo-Physics

Phys 381: by the end of the course

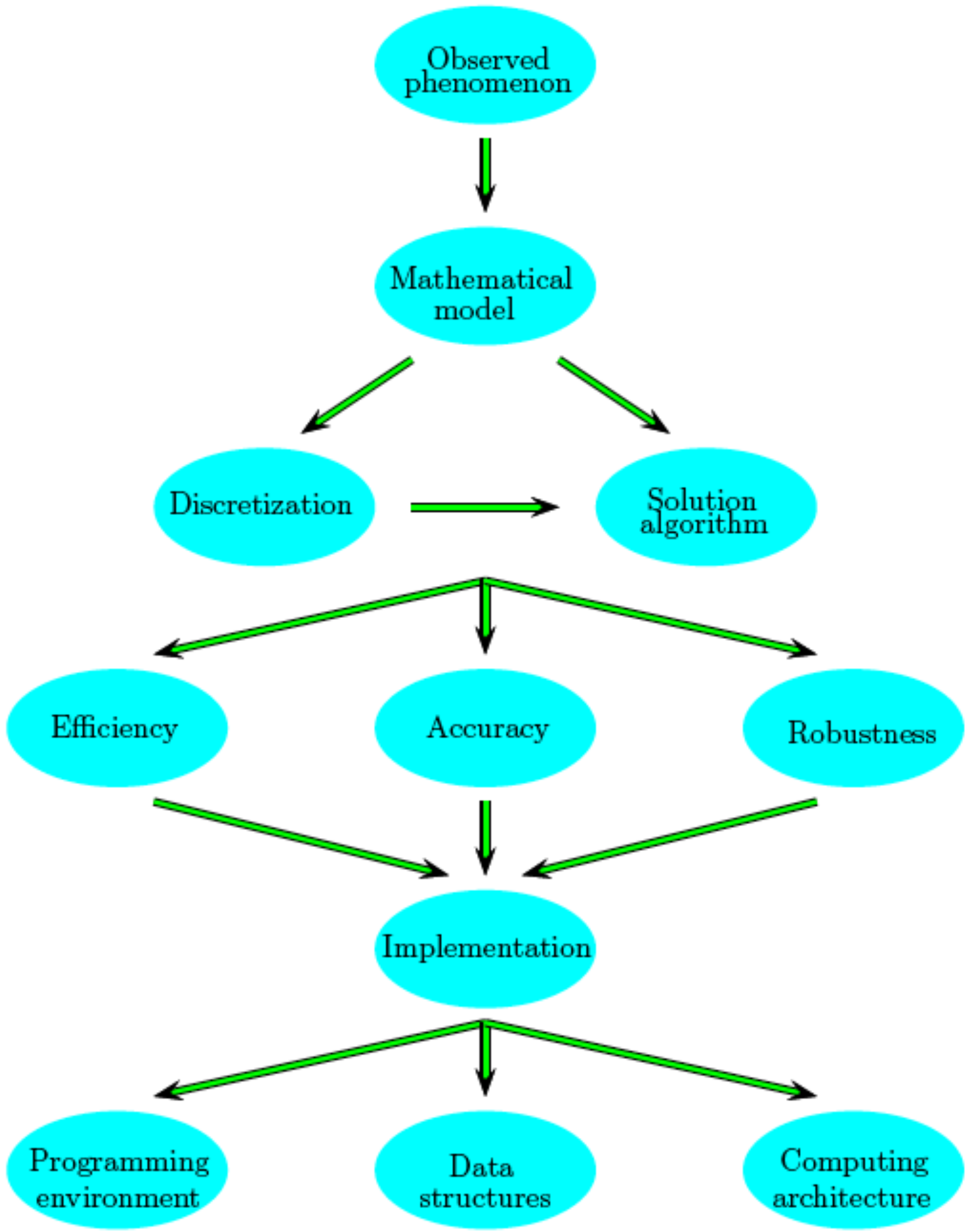
What can you do with

Phys 381?
Phys 481?
Phys 581?

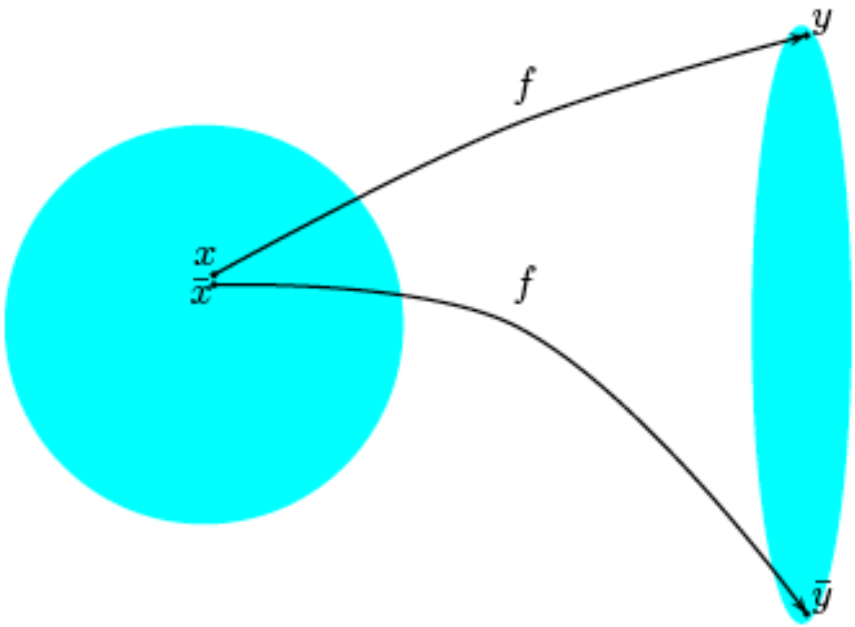
Phys 381: The game



Phys 381: The game in detail



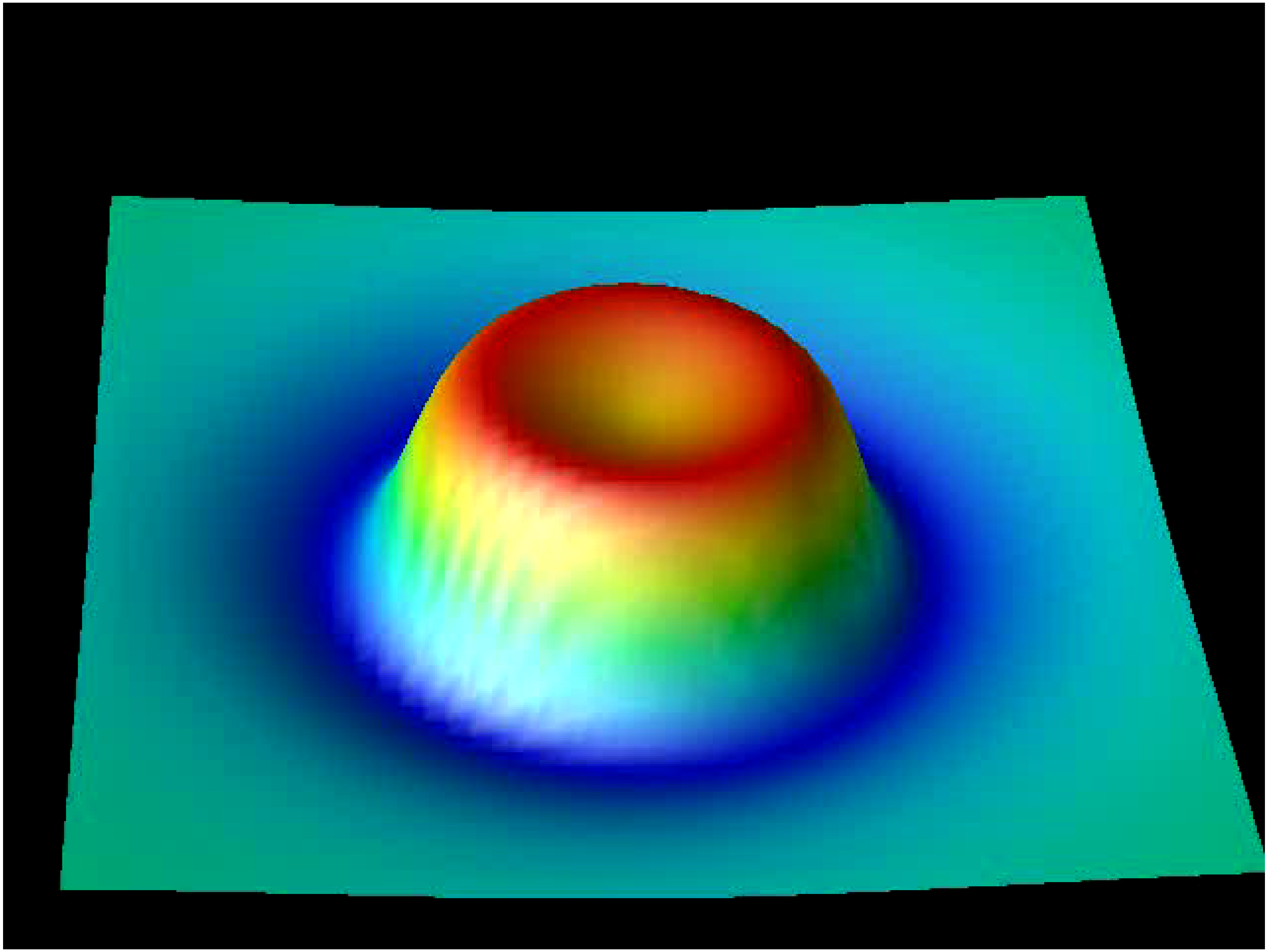
Phys 381: Il-conditioned problem



Conditionning

An ill-conditioned problem of computing $y = f(x)$: When the input x is slightly perturbed to $\bar{x}$, the result $\bar{y} = f(\bar{x})$ is far from y. If the problem were well-conditioned, we would be expecting the distance between y and $\bar{y}$ to be more comparable in magnitude to the distance between x and $\bar{x}$.

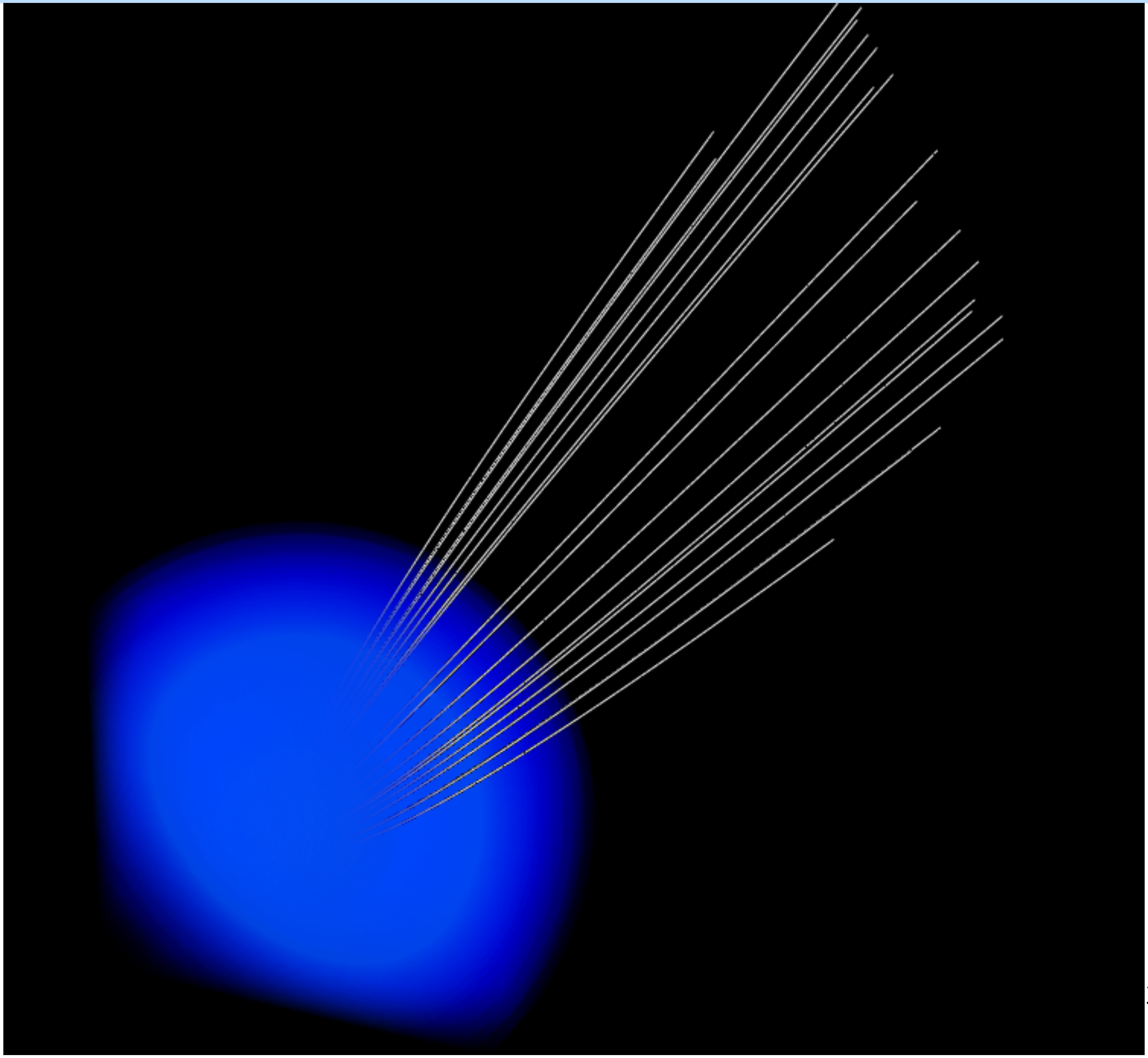
Phys 381: by the end of the course



Wave Packet

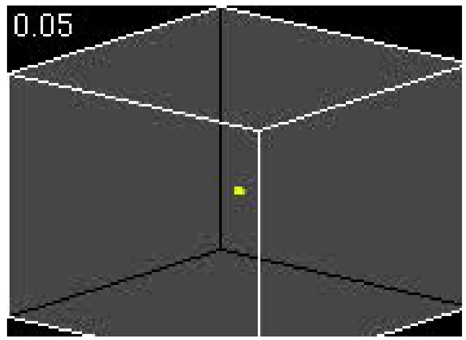
Phys 481/581: by the end of the course

Magneto-Hydro-Dynamic Jet From A Black Hole

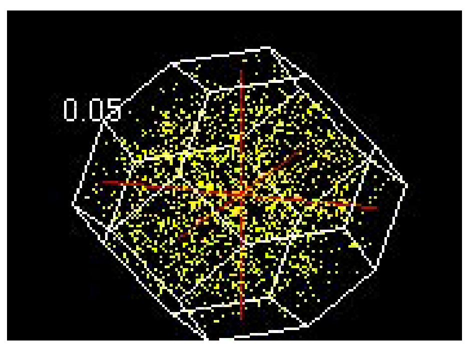


Phys 581: by the end of the course

Monte Carlo simulation of electron transport in a pure silicon crystal at 300 Kelvin (real-space).



Monte Carlo simulation of electron transport in a pure silicon crystal at 300 Kelvin (reciprocal-space).



Thank You!