# Teaching computational physics to undergraduates in Kolkata

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- ► The experience at IISER-Kolkata.

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- Course structures.
- Student responses.

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- Course structures.
- Student responses.
- Future directions.

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Students were encouraged to *think* about the physical reasons once simulations gave them results.

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- At that time, it was affiliated to the Calcutta university.
- CU had started a computational course for physics undergraduates.
- Motivation apparently increasing student employability!
- No practical examination students just had to write 10 programs over the duration of the course.

Current syllabus for Paper VIIB

- Sorting.
- Mean, median and mode of *n* numbers.
- Sum of a G.P. series.
- Solution of simple algebraic equations.
- Sum of an infinite series.
- Integration by Simpsons rule.
- Linear least squares fit.

Apart from executing the eight programmes prescribed in the syllabus, students should be encouraged to execute other problems of physics particularly associated with practical with the help of a computer, using available software packages (e.g. graph plotting etc.)

#### CNB: 5, Viva - 10, Experiment : Computer-20

# The St. Xavier's course then - a glimpse

Some problems that were tackled were :

- Motion of a particle under gravity and drag.
- Study of a harmonic oscillator.
- Forced oscillations and resonance.
- Study of an anhramonic oscillator.
- Coupled oscillations.
- Bifurcation and chaos in nonlinear maps.
- Laplace's equation
- Radioactive decay
- ...
- As well as plotting and data analysis using a plotting program.

Students were asked to simulate the motion of a pair of coupled oscillators obeying

$$\ddot{x}_1 = -2x_1 + x_2, \qquad \ddot{x}_2 = x_1 - 2x_2$$

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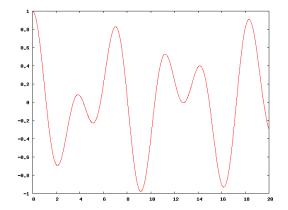
$$\ddot{x}_1 = -2x_1 + x_2, \qquad \ddot{x}_2 = x_1 - 2x_2$$

They were asked to do this for four different initial conditions :

$x_1 = 1, x_2 = 0$	$v_1 = v_2 = 0$
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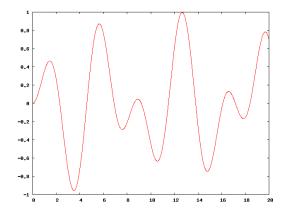
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$$x_1 = 1, x_2 = 0$$



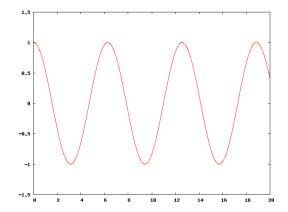
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$$x_1 = 0, x_2 = 1$$

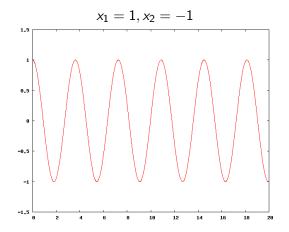


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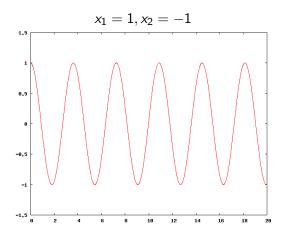
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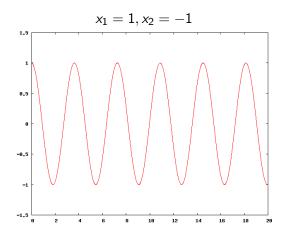
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The discovery of normal modes!!!

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- Especially to nonlinear dynamics.
- A few students even went on to do independent projects.
- However, once the exams neared, student enthusiasm dropped.

The fact that there were no marks to be obtained from this course took its toll.

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- The ultimate aim is to extend this to a full semester course.
- There is a proposed Advanced computational physics course as an elective in the fourth year.

Free and open source operating system

## Free and open source operating system Linux

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Open source and powerful graph plotting tool

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# Open source and powerful graph plotting tool gnuplot

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Simplest possible algorithms

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- Simplest possible algorithms
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Python!

#### Course structure for CS111

- No separate lectures.
- Lab classes used worksheets which had both the background as well as problems.

- Some handouts provided on the (internal) course website.
- Total marks : 100
  - Continuous evaluation : 70
  - Final examination : 30

#### Course structure for PH221

- ▶ 1 lectures per week last year, but none this year.
- Handouts (mostly last years course notes) provided on the course website.
- Lab classes used worksheets which had problems to be worked out in the lab, as well as homework problems.
- Total marks : 50
  - Continuous evaluation : 20
  - Final examination : 15
  - Project : 15
- The final exam is takehome (with a duration of 1 week) and a viva.
- Students are encouraged to choose their own projects.

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- Procedural, object oriented and functional programming.
- ► Allows reuse of legacy software by wrapping.

#### Why not python ? The cons :

► Less popular ?

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- Interpreted and hence slow.
  - Runs at about 80% the speed of C.
  - Program developement is a lot faster, though!
  - Except for very computation intensive application, the latter more than compensates for the former!

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```
sum = 0.0
for i in range(1,10001):
    sum += 1.0/n**2
print sum
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#### The python one liner

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#### The python one liner

print sum([1.0/n\*\*2 for n in range(1,10001)])

```
Produces the list [1,2,...,10000]
```

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sum = 0.0
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print sum([1.0/n\*\*2 for n in range(1,10001)])

List comprehension : produces a new list [1.0,.25,...,1.e-10]



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#### The python one liner

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print sum([1.0/n**2 for n in range(1,10001)])
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Sums up the list.



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#### The python one liner

print sum([1.0/n\*\*2 for n in range(1,10001)])

Prints out the sum.

#### An example program

```
# A program for studying motion under drag
# Uses the Euler algorithm
f = open('drag.out', 'w')
m,g,k = 1.0,10.0,0.1  # parameters
xi,vi = 10.0,0.0 # initial conditions
ti, tf, dt = 0.0, 10.0, .001
t,x,v = ti,xi,vi
while t<tf:
    a = -g - k * v/m
    v += a*dt
    x += v*dt
    t += dt
    if x<0.0:
        x = 0.0
        v = -v
    print >>f, t,v,x
f.close()
```

## The 4th Semester course at IISER

• A course geared towards solving physics problems.

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- More attention paid to numerical methods and errors in computation.

• Exposure to more advanced programming techniques.

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Scrodinger equation by the shooting method - anharmonic oscillators.

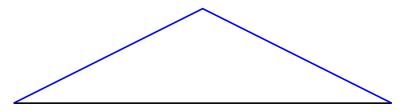
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- ► Simple Monte Carlo methods radioactive decay, Ising model.

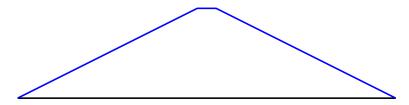
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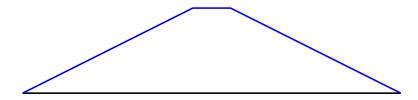
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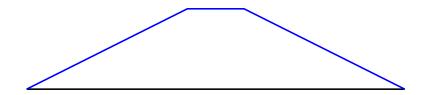
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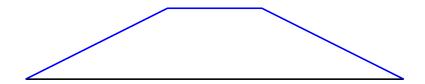
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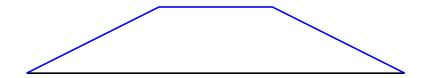
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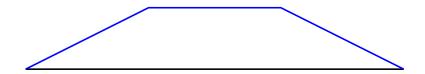


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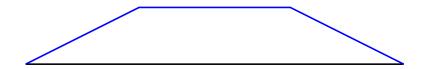


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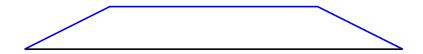
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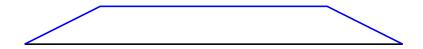
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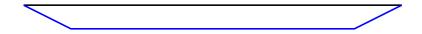
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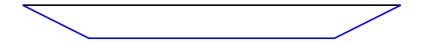
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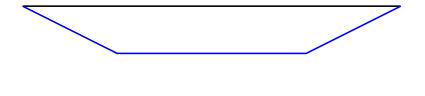
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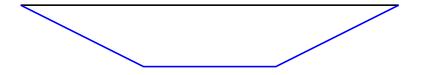
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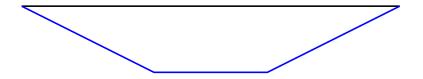
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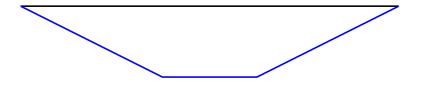
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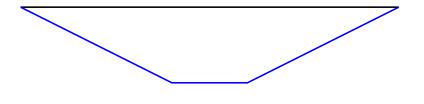
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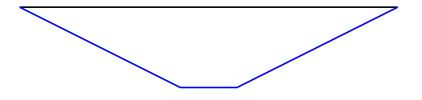
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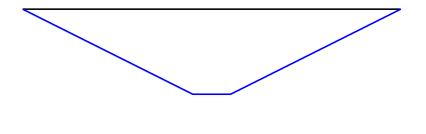
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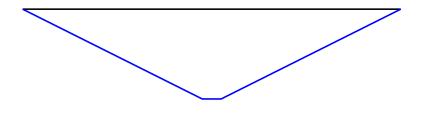
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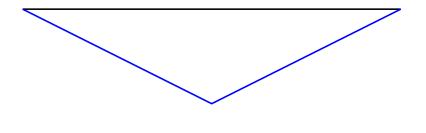
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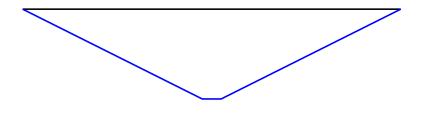
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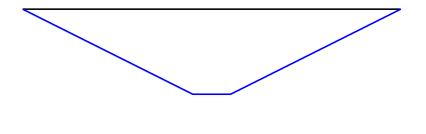
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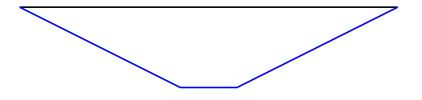
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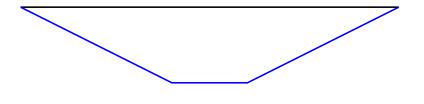
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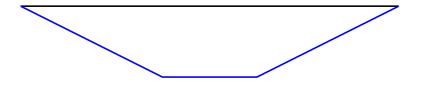
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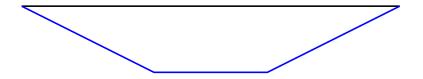
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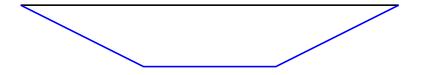
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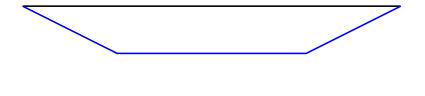
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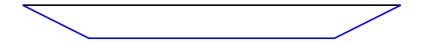
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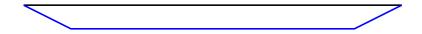
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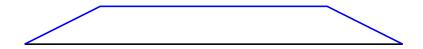


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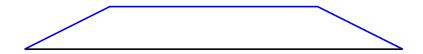
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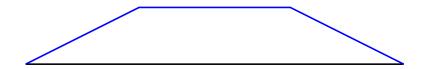
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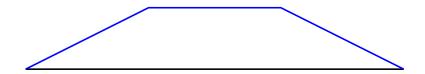


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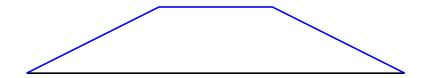


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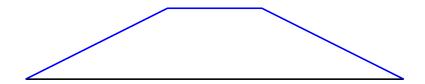


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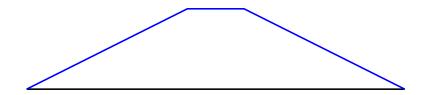
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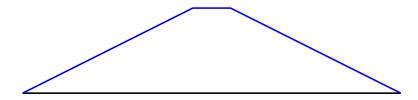
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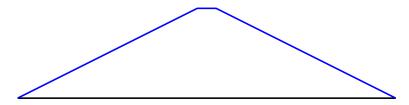
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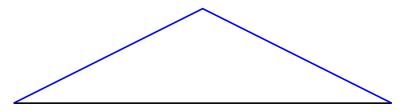
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• Lack of previous exposure.

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There is a proposal to shift the course to the second semester - with one project each to be done over the next two semesters.

► Much more positive.

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- A fraction of students were very excited about some of the problems.

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- ▶ It is a bit early to tell whether the course is a really successful!

This course is still to come and has not been fully fleshed out yet.

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► Introduction to FORTRAN95 and a CAS.

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- Introduction to FORTRAN95 and a CAS.
- A set of nonlinear dynamics problems.

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- Introduction to FORTRAN95 and a CAS.
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- Use of python as a first coding language allows the students to focus on the logic, rather than the details of the language.
- The language, combined with appropriate modules is sufficiently powerful for most applications.
- Once the art of coding has been mastered by the student, picking up another language is relatively easy.

## Acknowledgements

► Dr. Shibaji Banerjee (SXC).



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- Dr. P. A. Sreeram (IISER-K).
- ► Students of SXC and IISER-K.

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