Proposal for Add-On Course: Advanced Computational Methods

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Title of the Course: **Advanced Computational Methods**

Course Instructors:

* Dr. Rashmi Patowary, HOD, Assistant Professor, Dept. of Physics, Digboi College.
* Dr. Kanchan Konwar, Assistant Professor, Dept. of Physics, Digboi College.
* Dr. Deep Kumar Kuri, Assistant Professor, Dept. of Physics, Digboi College.
* Sanat Kumar Gogoi, Assistant Professor, Dept. of Physics, Digboi College.

Course co-ordinator: Sanat Kumar Gogoi, Asst. Prof., Dept of Physics, Digboi College.

Hosting Department: Department of Physics, Digboi College, Digboi, Assam 786171.

Course Objective: The objectives of the course are –

1. To learn powerful methods, tools, and techniques for solving advanced scientific problems.
2. To develop practical computational problem-solving skills.

Course Outcome: After completion of the course -

1. Students will be able to solve scientific problems using different numerical techniques.
2. Students will be able to write codes using any of the following languages
   (a) Python (b) Fortran (c) Scilab (d) C, C^{++}

Description of the course:

This is an advanced course for B.Sc and M.Sc. level students. The course is designed to help the students in solving various scientific problems numerically. This course will improve the ability of the students in handling data-sets, plotting in 2D, 3D and transforming an analytic problem into a numerical one. This course is intended to give a flavour of the numerical problems that one will face in pursuing research oriented education.

TABLE I. Course Details

Serial No.	Category	Description
1	Title of the course	Advanced Computational Methods
3	Nature of the course	Programming Simulation Numerical problem solving Data-handling
4	Total Teaching-Learning period	37.5 hours
5	Programming Language to be used	Python Fortran Scilab C, C^{++}
6	Prerequisite	Basic knowledge of computer and secondary level mathematics.
7	Webpage	https://digboicollege.edu.in https://sanatgogoi.github.io/ The lecture notes and assignments will be uploaded here.
8	Enrollment fee.	Rs. 200 (two hundred) per student only.
9	Credit assigned	6 (Assignments – 4, Seminar/Project – 2)
10	Course duration	6 months

The course is open to all B.Sc. and M.Sc. students. There will be continuous evaluation based on Assignments and Seminar (no exam).

Textbooks:

1. Mark Newman, *Computational Physics,* CreateSpace Independent Publishing Platform (2013).

2. Forman Acton, *Real computing made real: Preventing Errors in Scientific and Engineering Calculations,* Dover Publications.

3. Lloyd N. Trefethen and David Bau, *Numerical Linear Algebra,* SIAM.

4. William H. Press, Saul A. Teukolsky, William T. Vetterling and Brian P. Flannery, *Numerical Recipes 3rd Edition: The Art of Scientific Computing*

SYLLABUS

1 Introduction to computational physics, computer architecture overview, tools of computational physics (3 hours)

What is computational physics? Why do we need it?; Computer hardware: basic computer architecture, hierarchical memory, cache, latency and bandwidth; Moore's law, power bottleneck; Software: compiled (Fortran, C) vs. interpreted languages (MATLAB, python); software management.; Parallelization: MPI; OpenMP.

2 Machine representation, precision and errors (1.5 hours)

Representation on a computer: Integer representation; floating-point representation; Machine precision; Errors: round-off; approximation errors; random errors; errors of the third kind; Quadratic equations; Power series; Delicate numerical expressions; Dangerous subtractions; Preserving small numbers; Partial Fractions; Cubic equations; Sketching functions;

3 Quadrature and Derivatives (6 hours)

Direct fit polynomials; Quadrature methods on equal subintervals; Newton-Cotes formula; Romberg Extrapolation; Gaussian quadrature; Adaptive step size; Special cases;

4 Solutions of linear and non-linear equations (9 hours)

Simultaneous linear equations: Gauss elimination (pivoting, scaling); LU factorization; Calculating inverse; Tri-diagonal systems; Eigenvalues and Eigenvectors: QR Factorization; Gram-Schmidt Orthogonalization; Real roots of single variable function; Relaxation method; qualitative behavior of the function; Closed domain methods (bracketing): Bisection; False position method; Open domain methods: Newton-Raphson, Secant method; Complications; Roots of polynomials; Roots of non-linear equations;

5 Fourier methods (3 hours)

Fast Fourier transform; Convolution; Correlation; Power spectrum;

6 Random numbers and Monte-Carlo (6 hours)

Random number generators; Monte-Carlo integration; Non-uniform distribution; Random Walk; Metropolis algorithm;

7 Ordinary differential equations (9 hours)

Initial value problems: First order Euler method; Second order single point methods; Runge-Kutta methods; Multipoint methods; Boundary value problems: Shooting method; equilibrium boundary value method.

Note: The syllabus can be downloaded from `https://sanatgogoi.github.io/`

BASIC INFRASTRUCTURAL REQUIREMENT:

There are a few basic infrastructural requirements to carry out this course, which are listed below –

TABLE II. Infrastructural requirement

Serial No.	Requirements	No. of assets required
1	A computer laboratory	Equipped with minimum 30 working machines
2	Internet log in credentials	An internet access account with minimum 5GB data per day or Equivalent number of log in credentials having 1 GB data per day
3	Pojector	One

ACKNOWLEDGMENT

The course instructors acknowledge Dr. Dip Saikia, Principal, Digboi College for inspiring us to initiate this advanced level course. The course instructors also acknowledge IQAC of Digboi College for providing basic infrastructural needs to conduct the course smoothly.

CONFLICT OF INTEREST

The course instructors declares no conflict of interest.

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Dept of Physics	Dept of Physics	Dept of Physics	Dept of Physics

APPENDIX

In the 21^{st} century, people have advanced a lot in the field of modeling problems with graphics and showcasing it through visual representations. The advancement in computational capacity and coding skills is exemplary. Through this course we are trying to jump start our students in this regard. In this course students will be playing with various tools using which a mathematical solution can be represented visually which gives more insight to the real world. For example, *we*

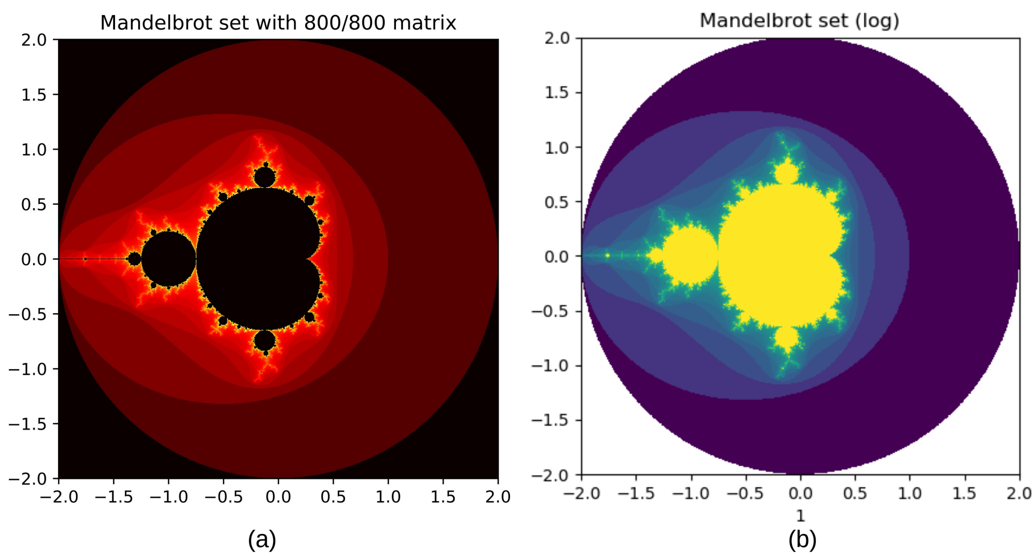

FIG. 1. Mandelbrot set

*can consider the **Mandelbrot set**. For a given complex value of c, start with $z = 0$ and iterate repeatedly. If the magnitude $|z|$ of the resulting value is ever greater than 2, then the point in the complex plane at position c is not in the Mandelbrot set, otherwise it is in the set.* If we plot those numbers than we get the nice looking figure as shown in Fig.1. Students will be solving these kinds of problems and represent them visually. Students will also use different color-maps and different plotting functions to make their figures more attractive.

Students will also get some idea how the computer works. For example we can edit our photos using software available in our devices. But, we have no idea how this works. In this course we are trying to give some basic idea about digital data processing as shown in Fig.2. There are two images, one is the blurry raw image in Fig2(a) and the other is the clear image. Using mathematical tool the raw image can be made clear which is shown in Fig.2(b).

Furthermore, the students need to realize that, in any experiment we do not get the final result

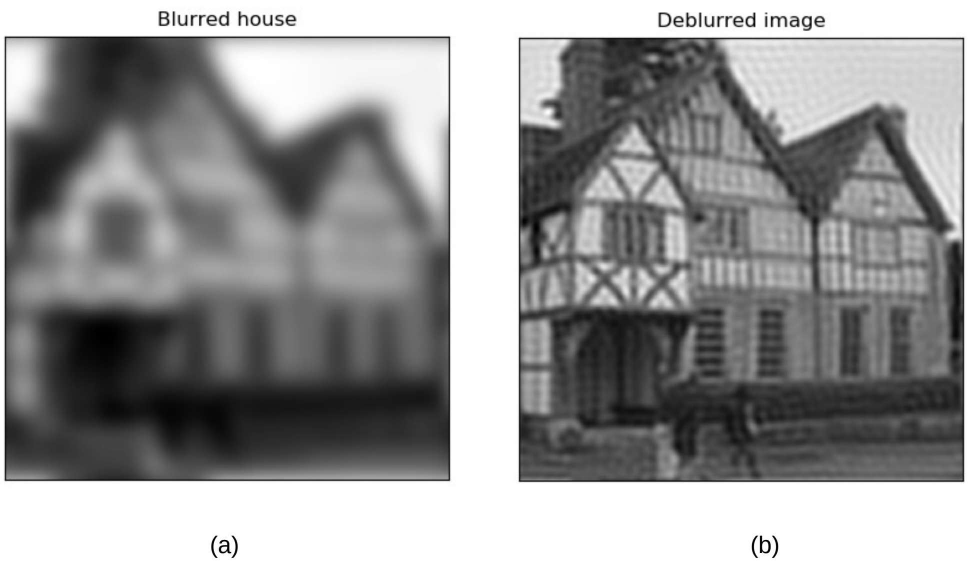

FIG. 2. Blurry and clear image processing

directly. The raw data that we get from the experiments need to be analyzed and processed. For example we can consider the STM image of Si surface as shown in Fig.3(a). Similarly, sometimes the 3D representation of a topic make us understand more about it. The Fig.3(b) shows the band structure of a bulk material. In general we see only 2D lines for band structures and students often struggle to connect into it. Maybe showing a 3D plot will help them understand it more clearly and it will inspire them to know more about these ideas.

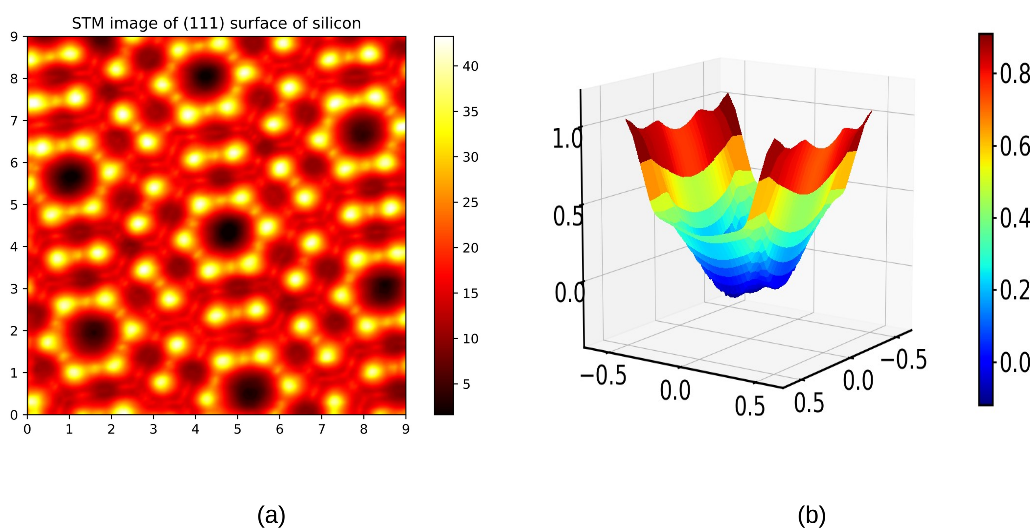

FIG. 3. Experimental raw data to final image