Introduction to Computational Physics

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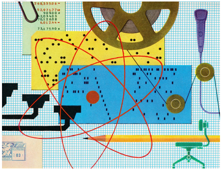


计算物理

课程访问量(PV值)：23346

主讲教师：顾斌
教师团队：共 4 位

Computational physics is an applied science, that uses computers as tools and numerical calculation as methods and takes the advantage of program deigning to solve complex physics problems. It is one of the three pillars of modern physics, alongside theoretical physics and experimental physics. As a bilingual course, it is designed for third-year undergraduates majoring in physics and related subjects.

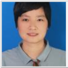
学校：南京信息工程大学
开课院系：物理与光电工程学院
课程英文名称：Computational Physics
编号：0900819
学分：2
课时：32

目录

- 教师团队
- 课程内容
- 教学效果
- 参考教材

教师团队

顾斌
职称：教授
单位：南京信息工程大学
部门：物理与光电工程学院



杨翠红
职称：教授
单位：南京信息工程大学
部门：物理与光电工程学院

Robert Wieser
职称：教授（校聘）
单位：南京信息工程大学
部门：物理与光电工程学院

于洋
职称：讲师
单位：南京信息工程大学
部门：物理与光电工程学院

课程章节

- Introduction to Computational Physics
- Python programming for physicists
- Graphics and visualization
- Accuracy and speed
- Integrals and derivatives
- Solution of linear and nonlinear equations
- Ordinary differential equations
- Partial differential equations
- Random processes and monte carlo methods

Click here! The invitation code: **91325719**.

Outline:

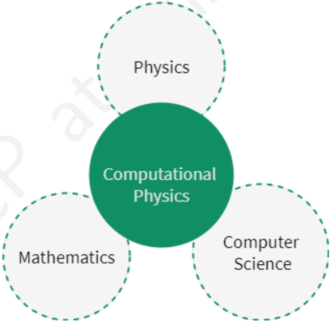
1. What is Computational Physics?
2. Why should we learn Computational Physics?
3. What we will learn in this course?
4. How to learn Computational Physics?

1. What is Computational Physics?

Q1.1: What tasks do your computer perform everyday?

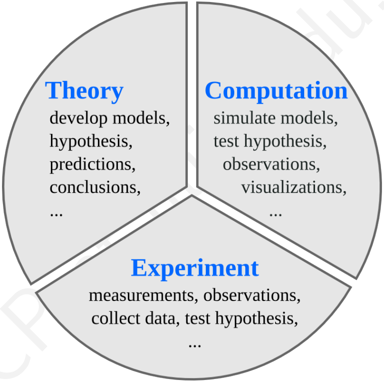
As a computer of a physicist: calculates; simulations; visualizations.

- **Computational physics** is the **subject** to study scientific (physics) problems based on mathematics and using computational methods.



1. What is Computational Physics?

- **Computational physics** complements the areas of theory and experimentation in traditional scientific investigation.



1. What is Computational Physics?

A short history:

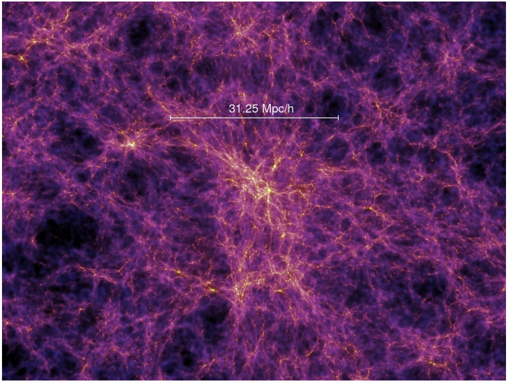
- **Early developments** (1940s-1950s): WWII, ENIAC, $\cdots$
- **Rise of simulation methods (1960s-1970s):** fluid dynamics, quantum mechanics, and astrophysics.
- **Advancements in algorithms and computing power (1980s-1990s):** more accurate and faster simulations.

- **Multidisciplinary applications (2000s-present):** materials science, biophysics, climate modeling, and cosmology.
- **High-performance computing (HPC) and machine learning/AI (present and future):**

  Q1.2: AI Paradox: Physics is the collection of beautiful and useful models of our universe. However, with the development of AI technology, physic is disappearing $\cdots$

1. What is Computational Physics?

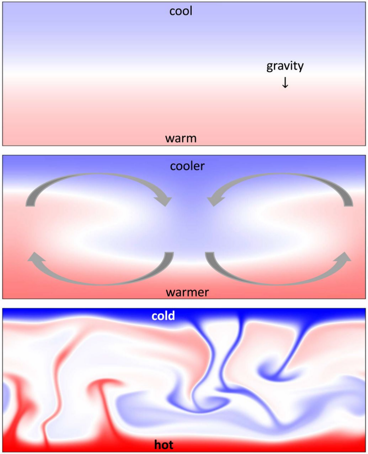
Case 1: Simulations of the formation, evolution and clustering of galaxies and quasars.



A visualization of the density of **dark matter** in a simulation of the evolution of the universe on scales well above the size of a galaxy. ***Nature*** **435**, 629 – 636 (2005)

1. What is Computational Physics?

Case 2: Turning up the heat in turbulent thermal convection.



Snapshots of the temperature field in 2D Rayleigh – Bénard convection simulations.

Top: For suitably weak temperature drops (ΔT) the fluid remains at rest, and heat transfers via conduction.

Middle: Sufficiently large ΔT destabilizes the conduction state and coherent convection rolls actively increase the heat flux.

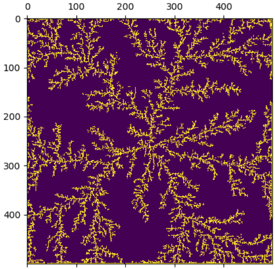
Bottom: Convective turbulence sets in at larger ΔT.

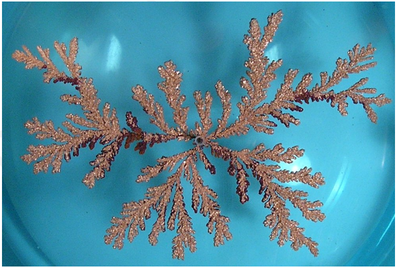
***PNAS* 117**,18, 9671-9673 (2020)

1. What is Computational Physics?

Case 3: Diffusion-Limited Aggregation (DLA) [PhysRevB.27.5686] is the process whereby particles undergoing a random walk due to Brownian motion cluster together to form aggregates.

DLA and DLE erosion





Left: a DLA simulation consisting of 33,000 particles obtained by allowing random walkers to adhere to a seed at the center. Right: observation of DLA of copper sulfate in the electroplating bath.

2. Why should we learn Computational Physics?

In a nutshell: Computational physics will allow you to tackle realistic problems in practically every field of science and engineering.

"**You think you know** when you can learn, are more sure when you can write, even more when you can teach, but certain **when you can program.**"
— Alan Perlis

After-class Reading: R. F. Martin, "Undergraduate Computational Physics Education: Uneven History and Promising Future," *Comput. Sci. Eng.*, vol. 19, no. 2, pp. 70–78, 2017, ISSN: 15219615. DOI: 10.1109/MCSE.2017.24

3. What we will learn (syllabus)?

Topics:

1. Program with Python, or Modern Fortran
2. Plotting and visualization with Python, Gnuplot
3. Numerical fundamentals: numbers, errors
4. Differentiation and Integration
5. Ordinary differential equations (ODE)
6. Integration of equations of motion
7. Root finding and optimization
8. Partial differential equations (PDE) e.g. Poisson's equation, diffusion equation, wave equation
9. Monte Carlo methods (importance sampling, Ising model)

3. What we will learn?

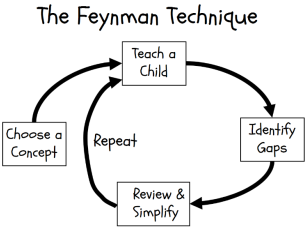
Outcomes by the completion of the course:

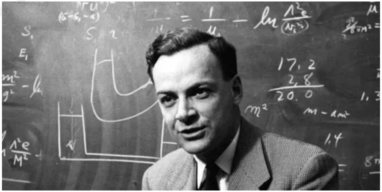
1. Be able to program with Python, in order to solve physical problems.
2. Be able to quickly apply your knowledge to problems in experimental and theoretical research projects, and even in your future career either as a STEM teacher or in big companies.
3. Learn how to solve problems in teams and to communicate clearly and effectively.

4. How to learn Computational Physics?

- Read: books and materials!
- Practice: Python programming [With IDE such as Jupiter-lab]
- Summarize: Method+results [Latex]

Peer Instruction and collaboration





4. How to learn Computational Physics?

E-learning online!

Scores: Class 20%, Exercises/homework 40%, Projects/test 40%

4. How to learn Computational Physics?

Reference books:

1. M. E. Newman, *Computational physics*. Createspace Seattle, 2013. [Online]. Available: http://www-personal.umich.edu/~mejn/cp/

2. R. H. Landau, M. J. Páez, and C. C. Bordeianu, *Computational physics: Problem solving with Python*. John Wiley & Sons, 2015

3. B. A. Stickler and E. Schachinger, *Basic Concepts in Computational Physics*. Addison-Wesley, 2016

4. A. Scopatz and K. D. Huff, *Effective computation in physics: Field guide to research with python*. O'Reilly Media, 2015

Further reading: What Computational Physics Is Really About, Rhett Allain 2015

Any question?

Office time: Oufang 523, Tuesday, 14:00-18:00.

Thank you for your attention!