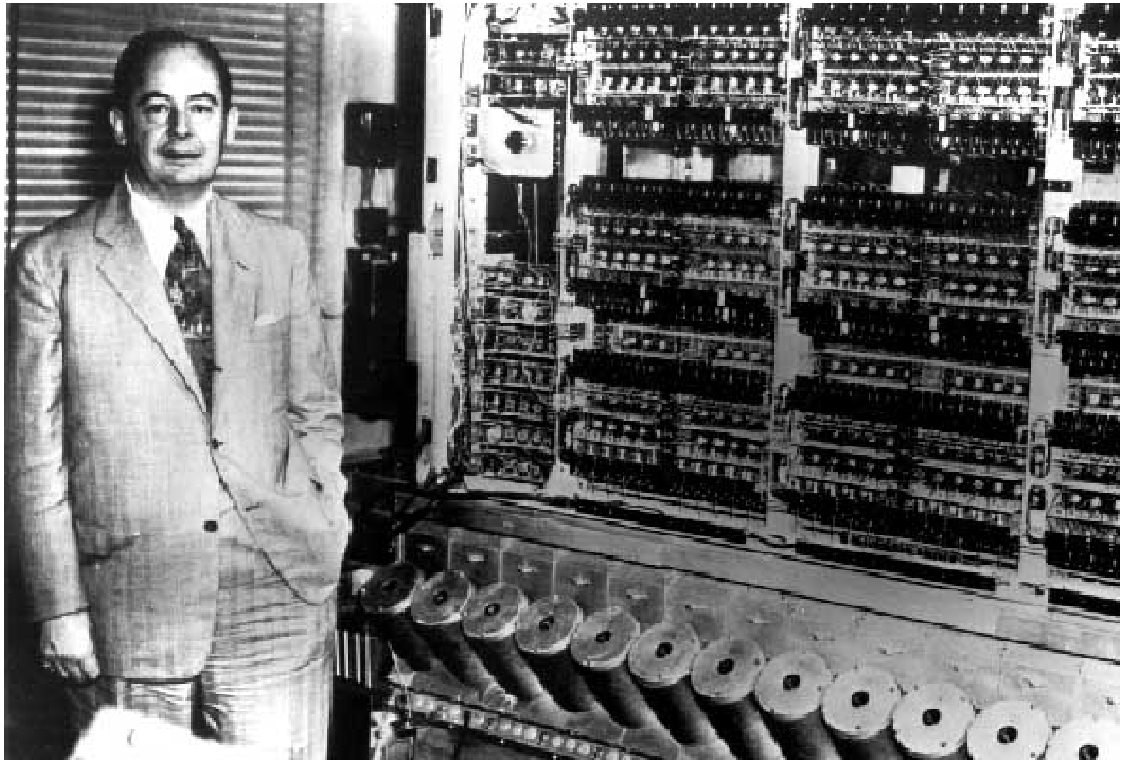
计算物理发展史简述

其中许多图片未征得原作者同意。
仅供教学免费使用。

第一台计算机

- 世界上第一台计算机的思想是由冯·诺伊曼提出,尔后在**1939** 年由**IBM**公司资助,在**1944** 年建成的。与“曼哈顿”计划有关。



Einstein to Roosevelt, Aug.2, 1939

Albert Einstein
Old Grove Rd.
Nassau Point
Peconic, Long Island

August 2nd, 1939

F.D. Roosevelt,
President of the United States,
White House
Washington, D.C.

Sir:

Some recent work by E.Fermi and L. Szilard, which has been communicated to me in manuscript, leads me to expect that the element uranium may be turned into a new and important source of energy in the immediate future. Certain aspects of the situation which has arisen seem to call for watchfulness and, if necessary, quick action on the part of the Administration. I believe therefore that it is my duty to bring to your attention the following facts and recommendations:

In the course of the last four months it has been made probable - through the work of Joliot in France as well as Fermi and Szilard in America - that it may become possible to set up a nuclear chain reaction in a large mass of uranium,by which vast amounts of power and large quantities of new radium-like elements would be generated. Now it appears almost certain that this could be achieved in the immediate future.

This new phenomenon would also lead to the construction of bombs, and it is conceivable - though much less certain - that extremely powerful bombs of a new type may thus be constructed. A single bomb of this type, carried by boat and exploded in a port, might very well destroy the whole port together with some of the surrounding territory. However, such bombs might very well prove to be too heavy for transportation by air.

-2-

The United States has only very poor ores of uranium in moderate quantities. There is some good ore in Canada and the former Czechoslovakia, while the most important source of uranium is Belgian Congo.

In view of this situation you may think it desirable to have some permanent contact maintained between the Administration and the group of physicists working on chain reactions in America. One possible way of achieving this might be for you to entrust with this task a person who has your confidence and who could perhaps serve in an inofficial capacity. His task might comprise the following:

a) to approach Government Departments, keep them informed of the further development, and put forward recommendations for Government action, giving particular attention to the problem of securing a supply of uranium ore for the United States;

b) to speed up the experimental work,which is at present being carried on within the limits of the budgets of University laboratories, by providing funds, if such funds be required, through his contacts with private persons who are willing to make contributions for this cause, and perhaps also by obtaining the co-operation of industrial laboratories which have the necessary equipment.

I understand that Germany has actually stopped the sale of uranium from the Czechoslovakian mines which she has taken over. That she should have taken such early action might perhaps be understood on the ground that the son of the German Under-Secretary of State, von Weizsäcker, is attached to the Kaiser-Wilhelm-Institut in Berlin where some of the American work on uranium is now being repeated.

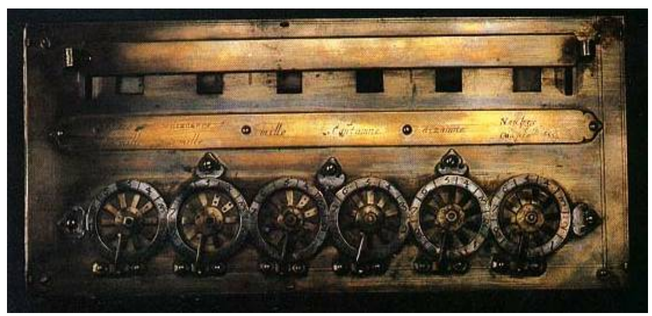
Yours very truly,
A. Einstein
(Albert Einstein)

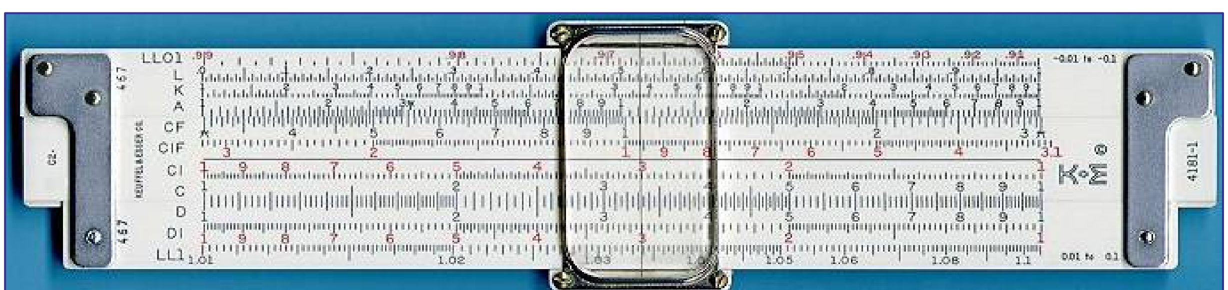
1941年珍珠港事件后 1942年8月“曼哈顿”计划实施

- 在爱因斯坦和一批物理学家的推动下,美国于**1942**年**8** 月开始秘密实施“曼哈顿”计划。早期计算机技术的发展主要是由“曼哈顿”计划 **(The Manhattan Project)**推动的**.**

美国于1944 年大规模建造计算机

- 在研制原子弹和氢弹的过程中，许多物理规律必须通过计算机上的计算摸清楚（原子弹是不能轻易做实验的！），因而计算物理就不知不觉自然地产生了。
- 由于原子弹的研制需要涉及流体动力学、核反应过程、中子输运过程、辐射输运过程和物态变化过程等, 涉及的都是十分复杂的非线性方程组，因此,冯·诺伊曼估计的结果是“曼哈顿”计划研制过程需要的计算量可能超过人类有史以来进行的全部算术运算.





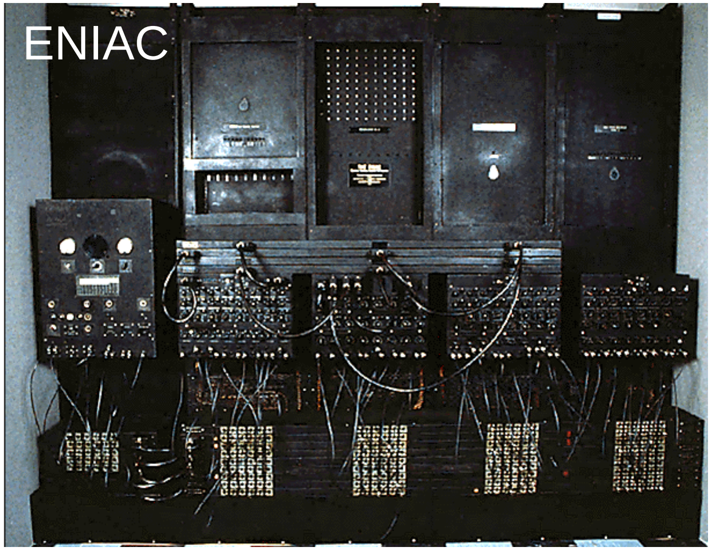
The Harvard Mark I: an electro-mechanical computer

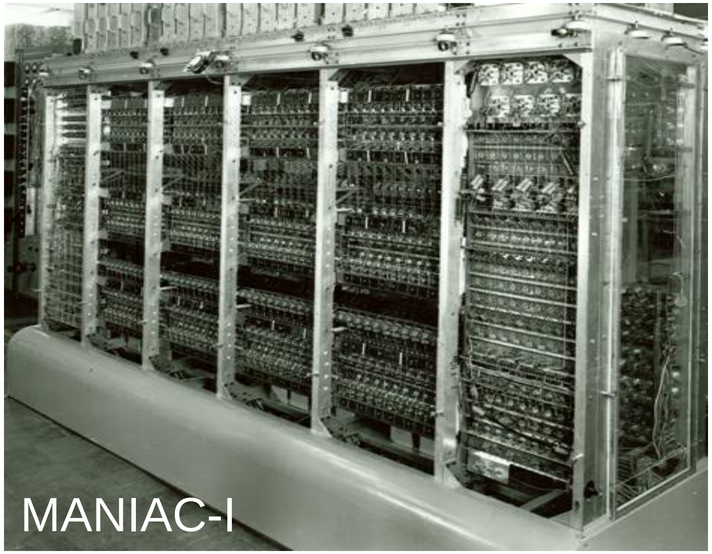
- H. Aiken（1900-1973）在哈佛大学做博士论文时需要计算空间电荷传导问题，于是计划设计一个计算机来求解。1937 年提出方案，1939 年得到 IBM 资助，1944 年建成投入使用。这台计算机在美国原子弹研究设计中立了大功。

随后，电子管计算机，晶体管计算机，集成电路计算机，。。。

ENIAC电子计算机

- J.W. Manchly（1907-1980）是宾夕法尼亚大学物理博士，因从事天气预报需要，计划设计计算机，后接受美国陆军弹道研究所弹道计算任务。1942 年提出方案，1945 年底建成，这就是世界上第一台电子计算机ENIAC 机。被称为计算机之父的J. von Neumann（1903-1956）参与了美国核武器研制，1944 年参与ENIAC 的改进，1945 年提出EDVAC 机设计方案（存储程序计算机），后在普林斯顿研制成**MANIAC** 机(**M**athematical **A**nalyzer, **N**umerical **I**ntegrator **A**nd **C**omputer)，有力地支持了美国的氢弹研制。


ENIAC


MANIAC-I

原子弹带来了极端的恐惧
计算机促进了科学的发展

奥本海默(**R.Oppenheimer**)面对核爆炸的巨大威力，引用了印度古诗中的名句表达自己的感想：
"如果一千个太阳在天空一起放光，
人类就会灭亡，
我似乎成为死神，
成为世界万物的毁灭者！"

If the radiance of a thousand suns
Were to burst at once into the sky
That would be like the splendor of the Mighty One ...
I am become Death,
The Destroyer of Worlds.

—Bhagavad-Gita

曼哈顿计划解密，以“计算物理方法”丛书的名义陆续出版

1959年5月美国总统发布命令，可以揭开曼哈顿计划的内幕，部分内容可以解密。故以“计算物理方法”丛书的名义陆续编辑出版。这套丛书从1963年到1977年共出版17卷，内容涉及到统计物理、量子力学、流体力学、核粒子运动、核物理、天体物理、固体物理、等离子体物理、原子与分子散射、地表波、地球物理、射电天文、受控热核反应和大气环流等方面的物理问题，在计算机上进行计算所需要的计算方法以及反映当时水平的研究成果。这套丛书也大致反映了“计算物理”的概貌。

METHODS IN
COMPUTATIONAL PHYSICS

Advances in Research and Applications

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Volume 3

Fundamental Methods in Hydrodynamics

1964
ACADEMIC PRESS
NEW YORK AND LONDON

计算物理的正式起点：1955年

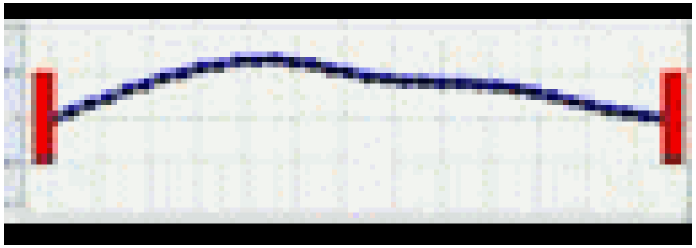
- 计算物理发展的原始动力是美国核武器研制的刺激。计算机最初是为开发核武器以及破译密码之用的，但在20 世纪50 年代初期就部分转为非军事用途。
- 在费米的推动下,洛斯阿拉莫斯实验室于1952 年就将计算机应用于非线性系统的长时间行为和大尺度性质的研究. 1955 年5 月,费米和合作者编写的一个洛斯阿拉莫斯研究报告提出了许多重要问题,很多人把它看成是计算物理的正式起点。

1955年：FPU 模型

STUDIES OF NON LINEAR PROBLEMS

E. FERMI, J. PASTA, and S. ULAM

Document LA-1940 (May 1955).



ABSTRACT.

存在孤波，能量均分不成立，
MD及非线性科学均源于此。

A one-dimensional dynamical system of 64 particles with forces between neighbors containing nonlinear terms has been studied on the Los Alamos computer MANIAC I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted as a function of time.

CHAOS, 15 (2005) 015104

The Fermi-Pasta-Ulam problem: 50 years of progress

G. P. Berman and F. M. Izrailev*

Theoretical Division and CNLS, Los Alamos National Laboratory,

计算机实验的概念

- 1965 年, FH Harlow和JE Fromm 在 Scientific American 杂志上发表了“流体力学的计算机实验”一文,提出计算机实验的概念.

Scientific American **212**, 104 - 110 (1965)
doi:10.1038/scientificamerican0365-104

Computer Experiments in Fluid Dynamics

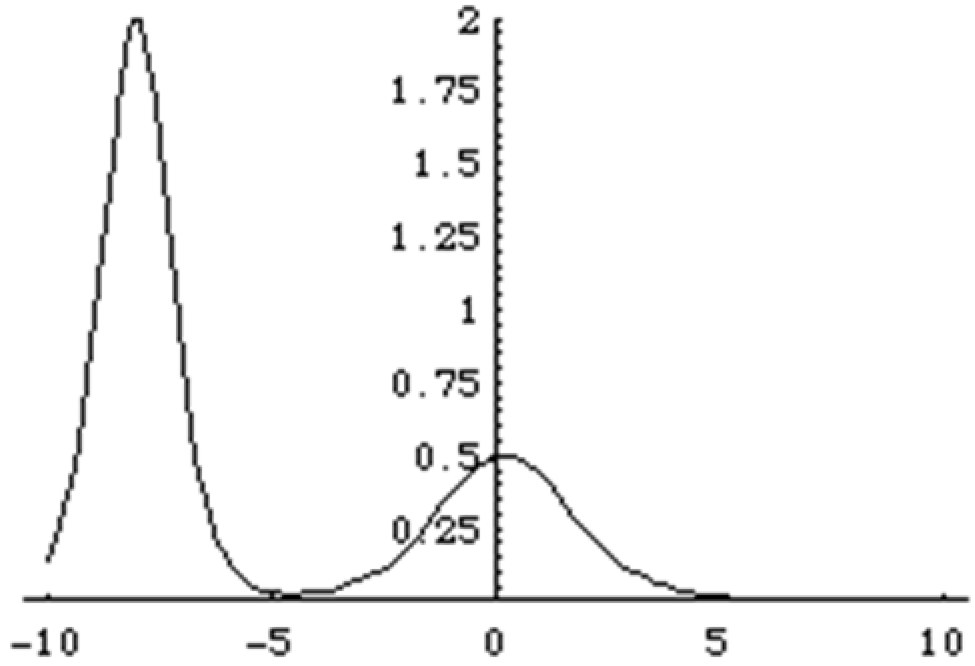
Francis H. Harlow & Jacob E. Fromm

数值实验与KdV 方程孤立波

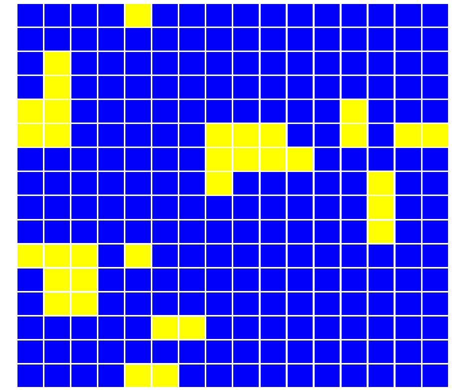
Phys. Rev. Lett. 15, 240–243 (1965)

Interaction of "Solitons" in a Collisionless Plasma and the Recurrence of Initial States

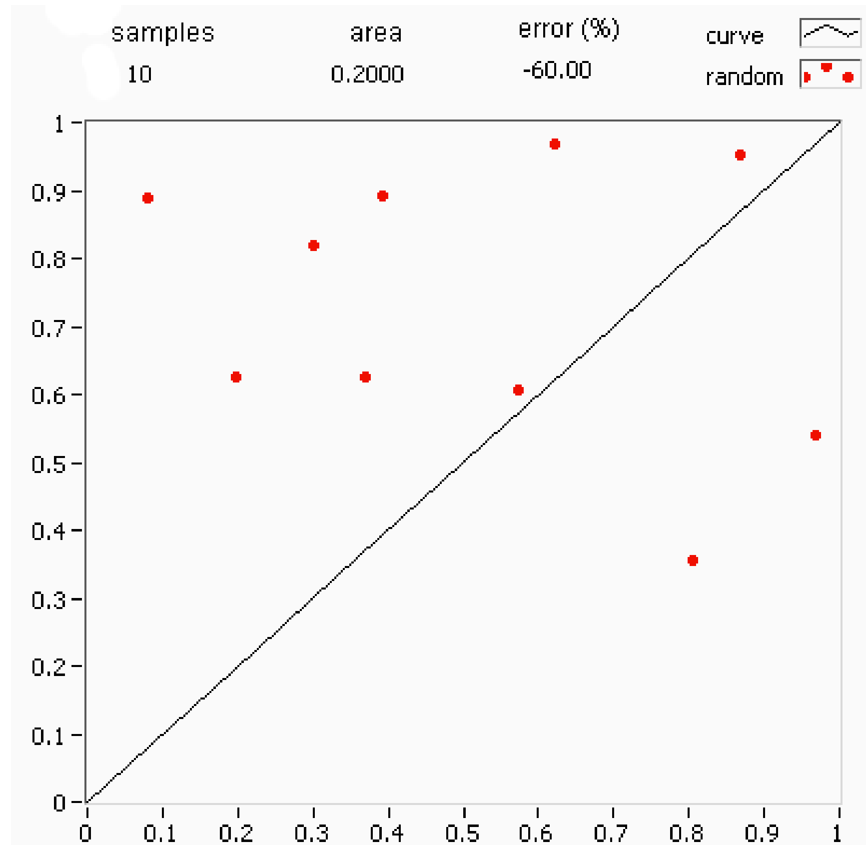
- 1965 年,Zabusky 和 Kruskel 通过数值实验揭示了KdV 方程的孤立波所呈现的守恒性与类粒子性. 利用计算物理技术,人们不断提供一系列新概念,并发现一系列新的物理现象,从而实现了计算物理理解、发现和预言新物理现象的目的.



统计物理是计算物理最早涉足的领域之一

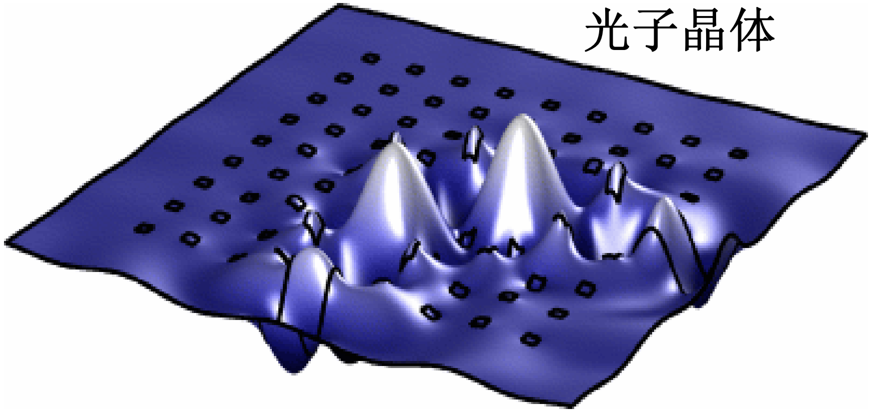


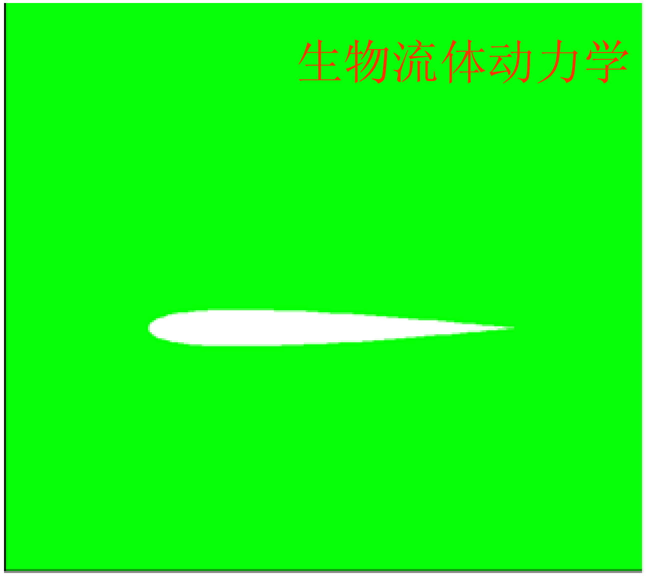
- 计算物理不必大大简化模型,使得它擅长复杂现象的研究. 传统的解析方法使许多问题不能得到解决. 例如,在统计物理学中最简单的伊辛模型,只能在一维和二维找到解析解,具有量子效应的海森伯模型只有一维解. 计算机可以模拟大量微观粒子组成的宏观系统的动力学过程. 目前较成熟的计算机模拟方法就是蒙特卡罗方法。



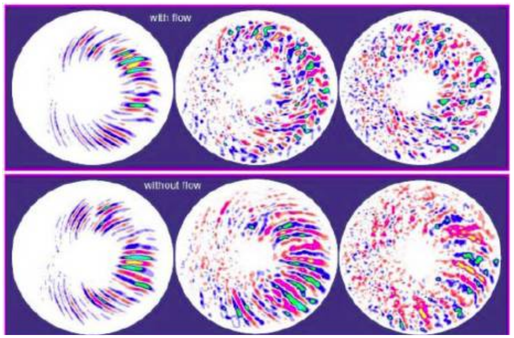
计算物理对电动力学和流体力学领域也大有作为

- 物理问题能够由相当完美的方程组来描述， 但是都是非常复杂的偏微分方程组,传统的分析方法几乎无能为力。然而,如果使用数值计算方法,譬如有限差分方法 **(FDM)** ,有限元方法 **(FEM)** ,傅里叶变换方法 **(FTM)** 和多重网格方法 **(MGM)** 等,计算物理能得出令人满意的结果.

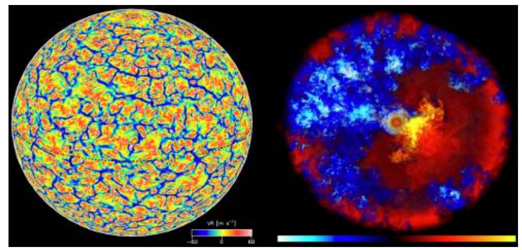




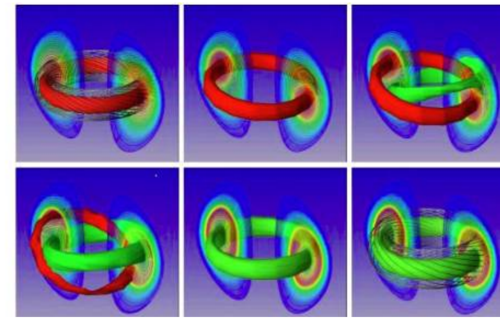
计算物理能模拟实验上不能或很难实现的系统



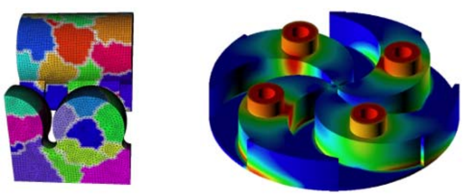
等离子体静电湍流模拟



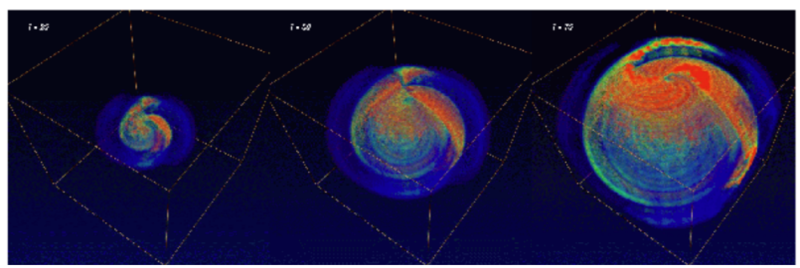
太阳表面对流层速度和温度径向分布模拟



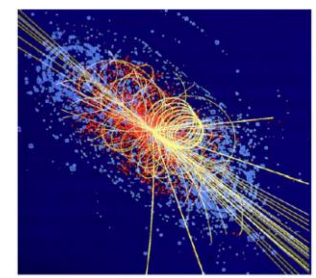
等离子体的多尺度模拟



加速器腔体设计及电流密度模拟



两个黑洞融合产生的引力波模拟



有一个Higgs玻色子的LHC事件模拟

早期宇宙行为、强磁场、极高压、极低温或高温环境下物理系统的行为等往往需要超级计算机进行模拟。

狄拉克在1929 年的著名评论

Dirac, P. A. M.,“Quantum Mechanics of Many-Electron Systems”, Proceedings of the Royal Society A: Math., Phys. and Eng. Sci. 123 (792): 714

量子力学和整个化学所需的所有基本规律都已经给出。然而量子力学方程非常复杂,传统的方法根本无法求解,甚至在使用近似方法的前提下,也很难求解.

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Quantum Mechanics of Many-Electron Systems.

By P. A. M. Dirac, St. John's College, Cambridge.

(Communicated by R. H. Fowler, F.R.S.—Received March 12, 1929.)

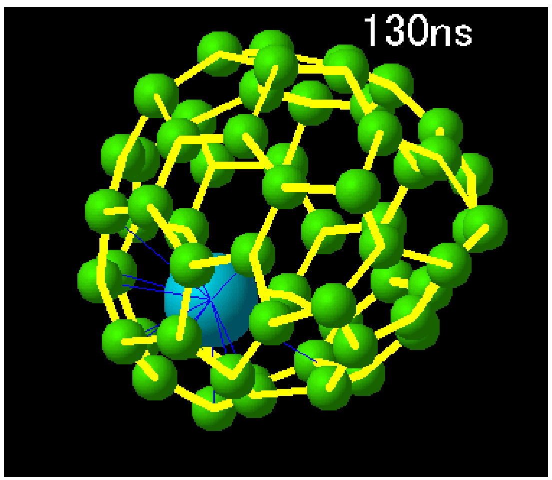
§ 1. *Introduction.*

The general theory of quantum mechanics is now almost complete, the imperfections that still remain being in connection with the exact fitting in of the theory with relativity ideas. These give rise to difficulties only when high-speed particles are involved, and are therefore of no importance in the consideration of atomic and molecular structure and ordinary chemical reactions, in which it is, indeed, usually sufficiently accurate if one neglects relativity variation of mass with velocity and assumes only Coulomb forces between the various electrons and atomic nuclei. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

凝聚态领域代表性的三类方法

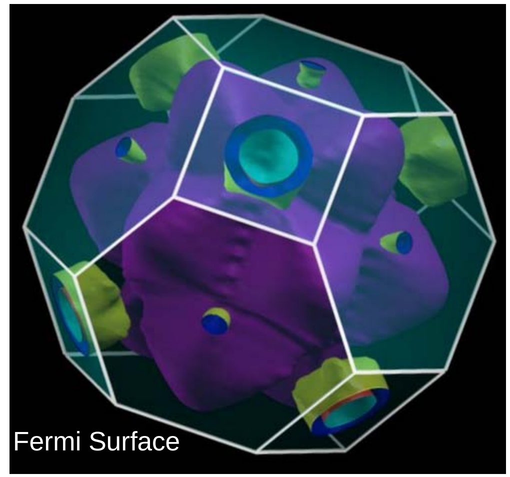
分子动力学(MD)

$$m_i \frac{d^2 R_i}{dt^2} = F_{empirical}$$



量子分子动力学

$$m_i \frac{d^2 R_i}{dt^2} = -\nabla_{R_i} E_{tot}^{DFT}(\{R_j\})$$

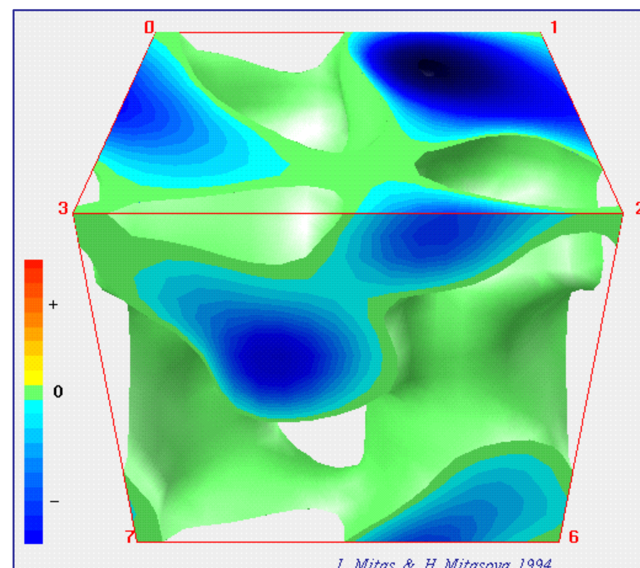


第一性原理(DFT)

[部分能带费米面，XCrsyDen图例]

蒙特卡洛方法(MC)

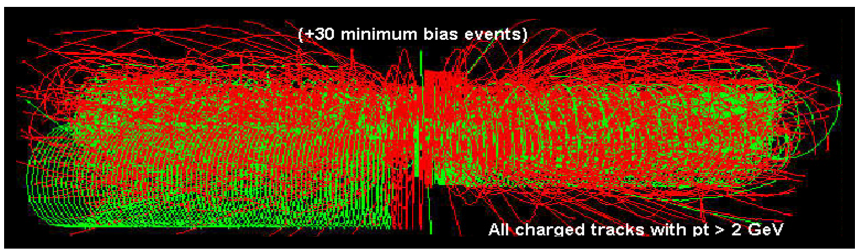
[氮固体59维多电子波函数节点3D截面图]



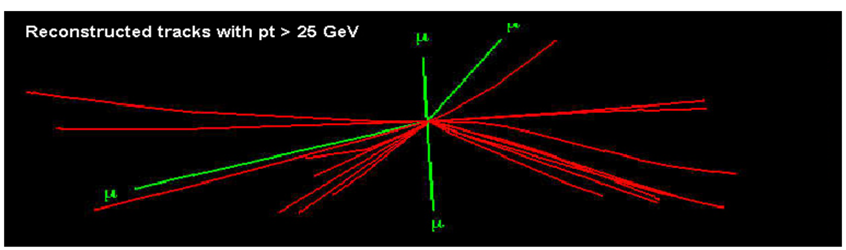
海量实验数据处理

- 计算物理学在海量实验数据的获得、处理和理解等方面发挥着非常重要的作用。

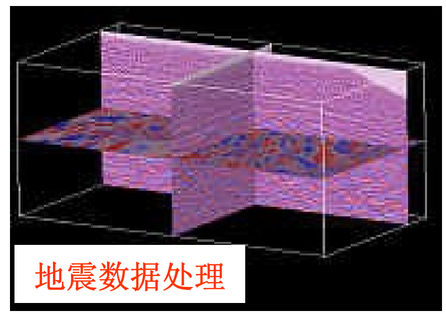
海量数据处理：大海捞针

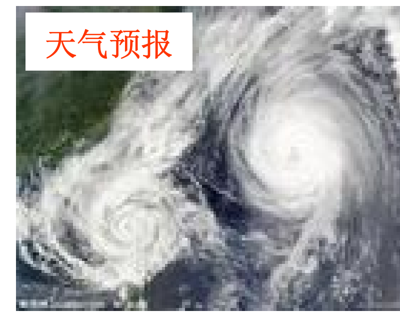


对撞机上产生大量本底过程

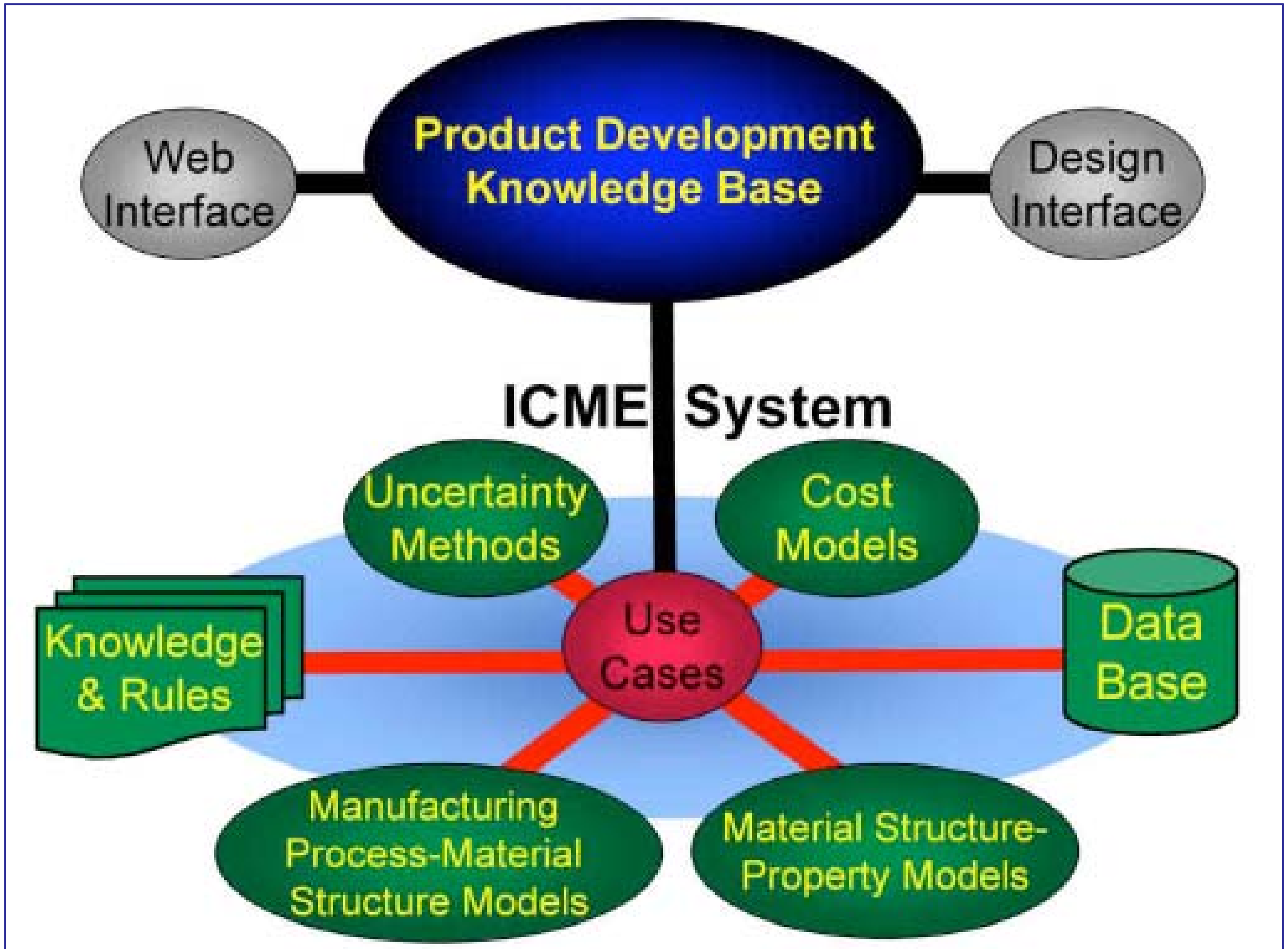


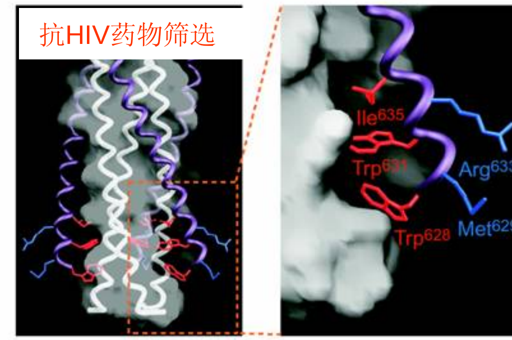
目标寻找的Higgs粒子的特征过程

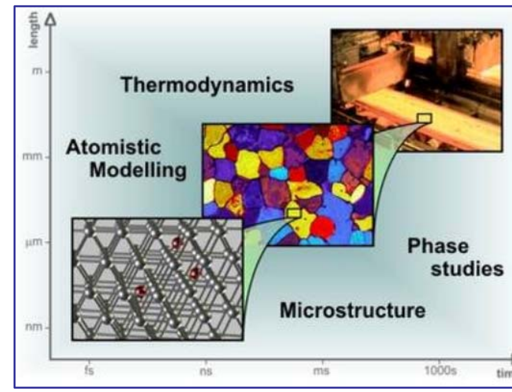


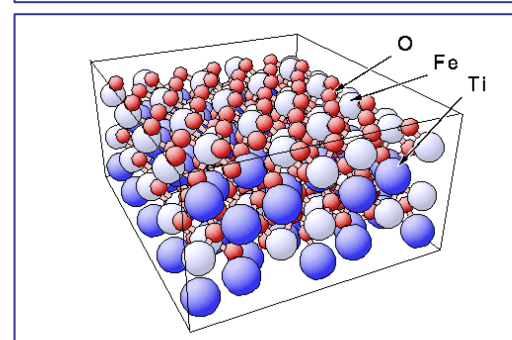


提供设计分子和材料的“虚拟”环境







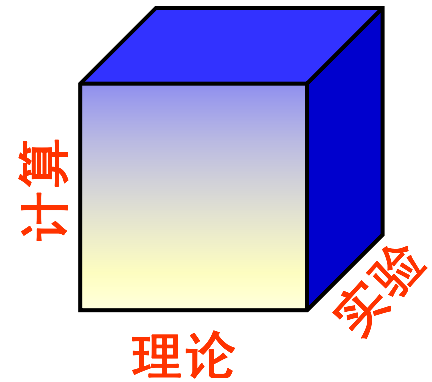


$FeTiO_3$ (ilmenite) lattice

计算物理涉足的领域

- **物理学科：**统计物理学、核物理、高能物理、粒子物理、生物物理、凝聚态物理、地球物理、大气物理、光学、力学、流体力学、电磁学、量子力学、量子色动力学等领域。
- **其它学科：**化学，生物，地球，工程，金融，社会等领域。

实验、理论、计算三足鼎立



计算机生来就是物理学的工具，但已经渗入进各个领域

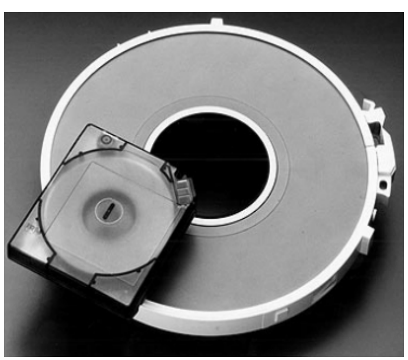
- 计算及计算机影响科学
- 计算及计算机影响经济
- 计算及计算机影响生活
- 计算及计算机影响政治

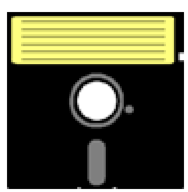
无论你打算做什么，都离不开计算和计算机！

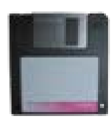
自己用过的计算机

- 1981年，DJS-130机(退役机器)，字长16位，内存32K，穿卡，读卡，algol语言
- 1983年，IBM-360机(8088机器，中型机),Unix系统， fortran语言
- 1984年，TRS-80机(微机), basic
- 1986年，Macintosh机(apple一体机)
- 1988年，兼容PC机（80286）等
- 1992年，自购兼容PC机（80386）
- 1993年，兼容80486机器，mathamatica
- 1995年，IBM-PS2集群,Fortran, C
- 2011年，多核个人机，大型集群

TRS-80







U盘16G

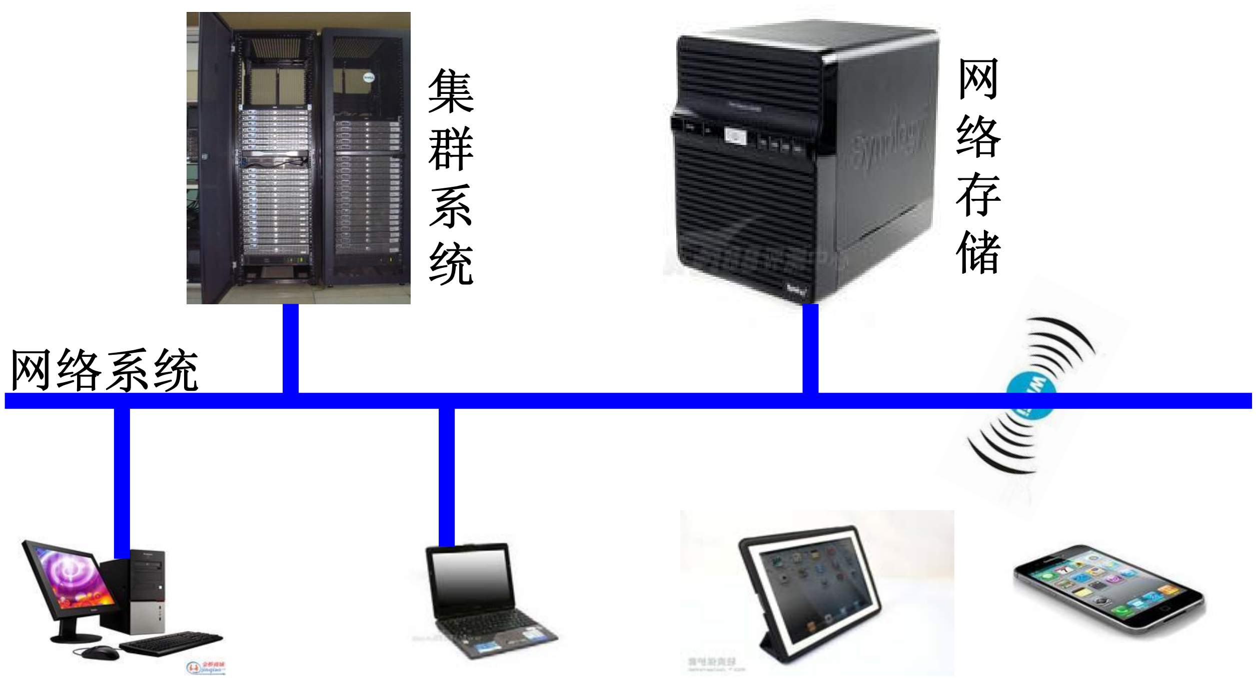
3.5吋盘1.44M

5.25吋盘1.2M

10.5吋磁带150M

计算及计算机知识在不断更新

格点计算，云计算，云存储，**GPU**计算，量子计算机，**DNA**计算机，。。。



后记