Lecture 1
Introduction to Computational Physics

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Computational Physics

- Combines physics, computer science and applied mathematics.
- Provides scientific solutions to real-world problems.
- Employs common techniques to areas such as
  - Material design
  - Environmental modeling
  - Nuclear cleanup
  - Energy management
  - Medical imaging
  - Finance
  - …

Computational Physicist

- A computational physicist not only understands the working of computers and the relevant science and mathematics, but also know how to connect them all!
- Computational physicists enjoy careers mixing both high-performance computing and science.

Career Outlook

- Students with a solid platform in physics, computing, and mathematics, as well as valuable skills in complex problem-solving and team work.
- An excellent preparation for
  - high-performance computing in science and engineering areas such as energy and aerospace, chemistry, finance, medicine, environmental science, oceanography, material science, computer science, and applied mathematics, etc;
  - Research in academic, industrial, or national laboratories;
  - Teaching at all levels.

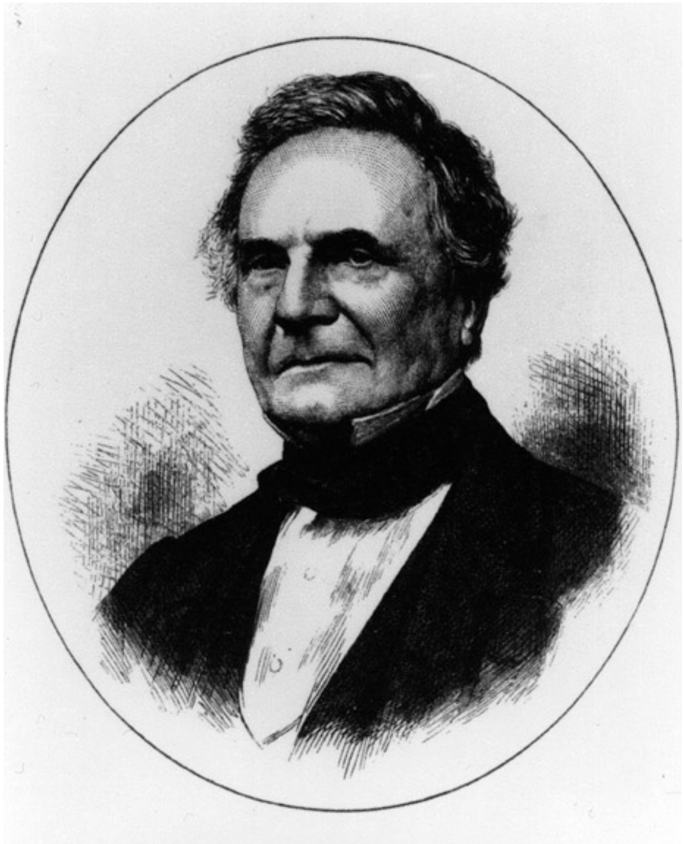
Computational Physics

- Originated from the Manhattan Project during the World War II to study the material state equation and the nonlinear dynamics problem
- **An aid** to theoretical physics in the initial stage
- **An indispensable research tool** in the past few decades
- Combines physics, computer science and applied mathematics.
- Provides scientific solutions to real-world problems.
- Employs common techniques to areas such as: Material design, Environmental modeling, Nuclear cleanup, Energy management, Medical imaging, Finance, AI…

Importance of Computers in Physics

- Affect out thinking and learning process
- The uses of computers
  - Numerical analysis: Solving linear equation, summation and integration, etc. The simplifying physical principles are discovered before computation.
  - Symbolic manipulation: quadratic equation, differentiation, integration, matrix inversion, power series expansion, etc.
  - Simulation: numerical experiments, testing models.
  - Collection and analysis of data: controlling experiments, curve fitting, forecasting, etc.
  - Visualization/Multimedia: important new development.
  - Quantum computing: future generation.

Father of Computer



Charles Babbage

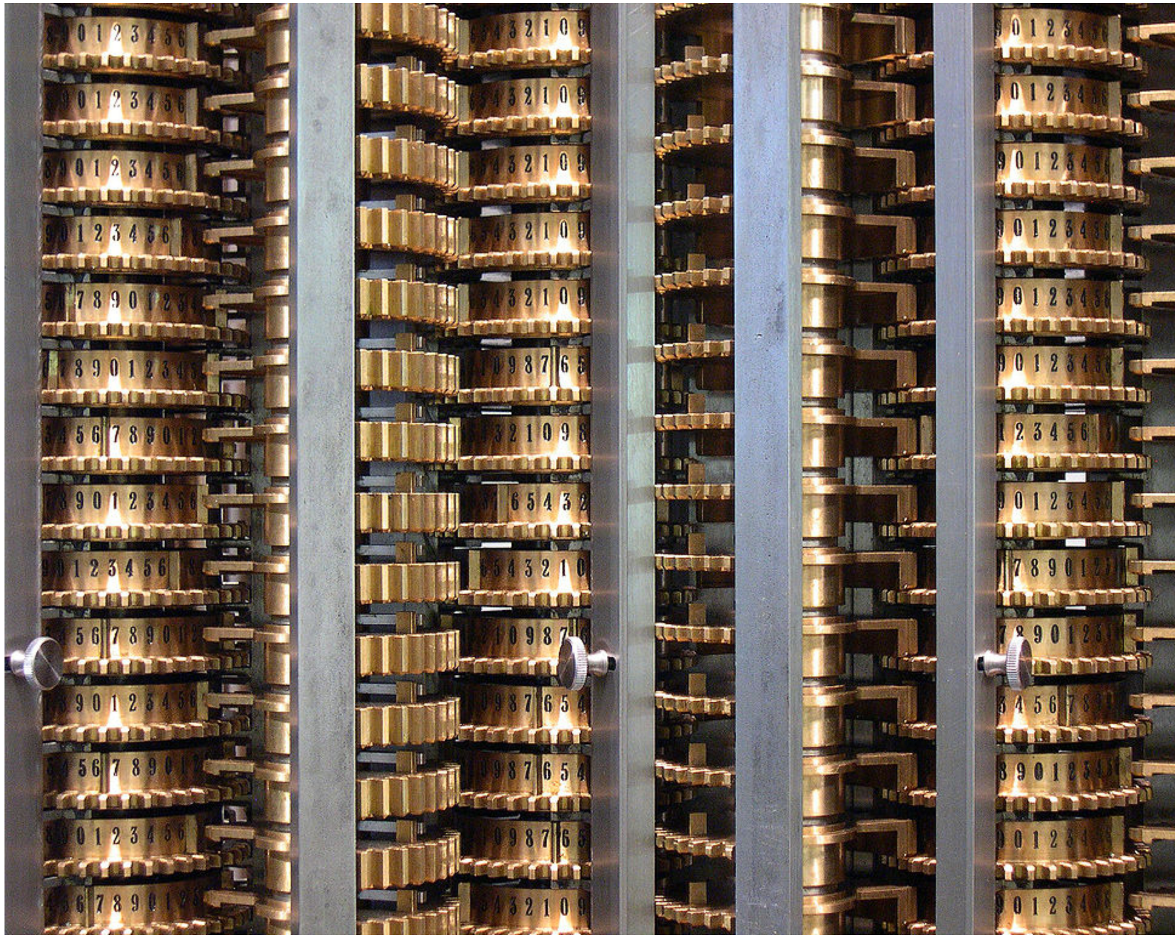
(1791 - 1871), the Analytical invented Engine, a mechanical digital computer which anticipated virtually every aspect of present-day computers.

- 1821, concept of DE1
- 1847, design of DE2

(*fail to construct*)

Babbage's Difference Engine No.1(DE1)

This wood cut depicts a trial piece of the DE1, built in1833.

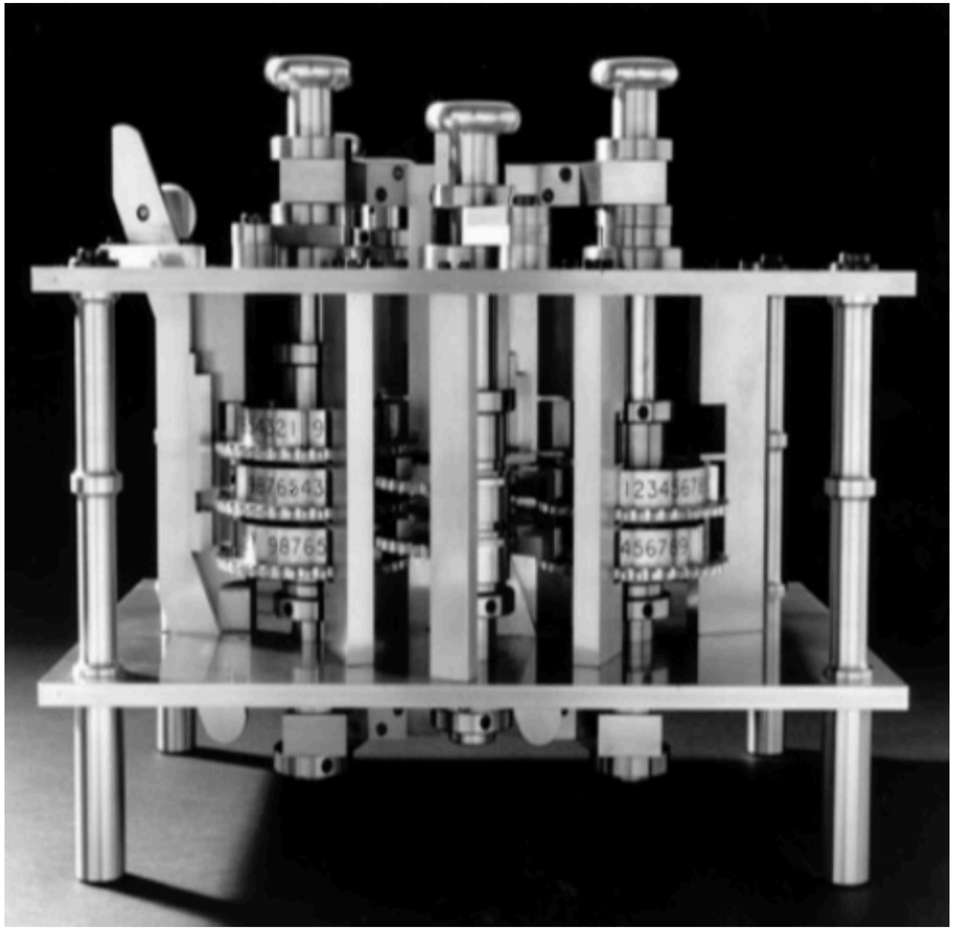


- It was commenced 1823
- put together 1833
- Abandoned 1842.
- The plate was printed in June 1853.
- This portion was in Exhibition 1862.

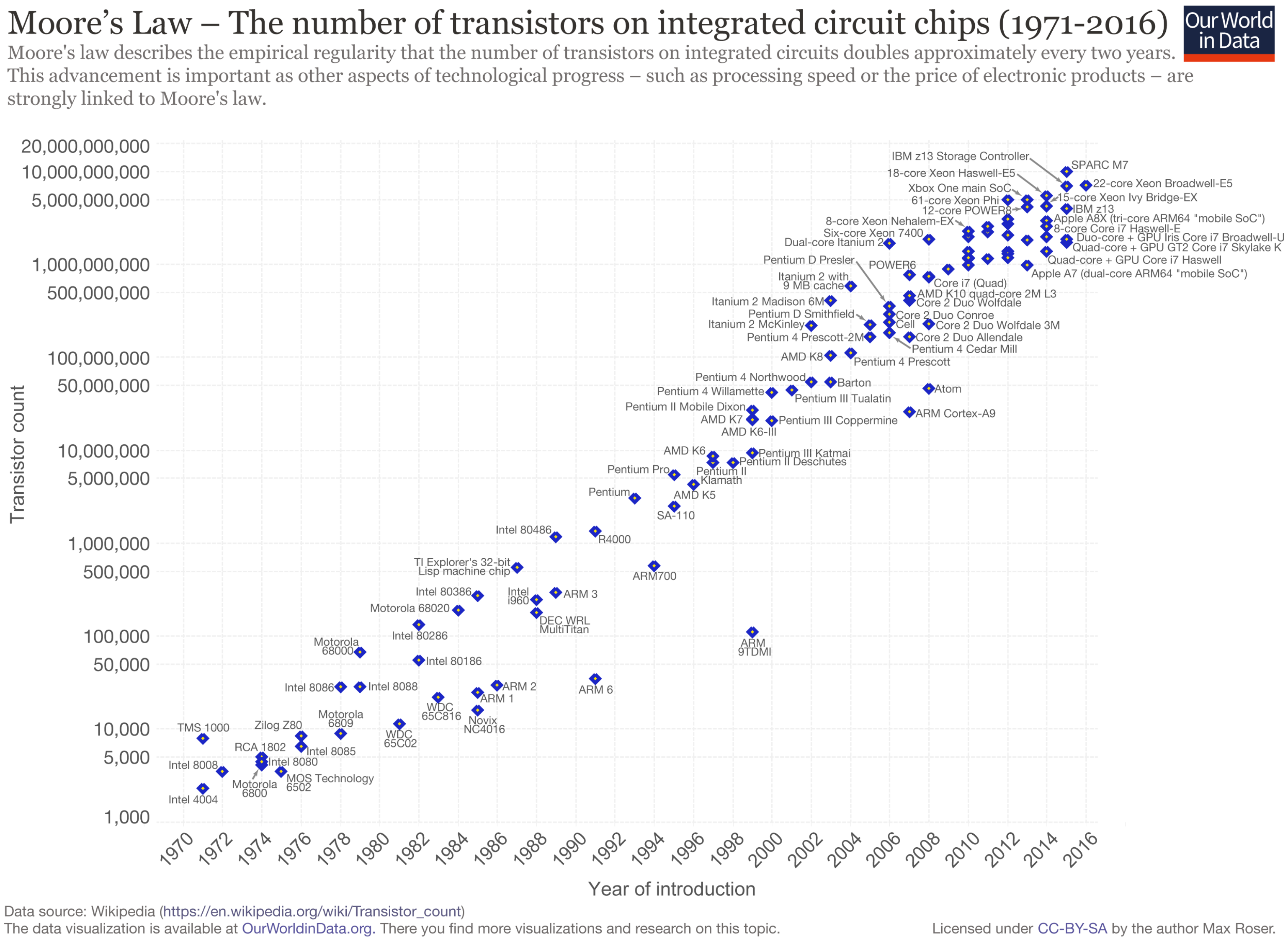
Babbage's Difference Engine No.2(DE2)

Between 1847 and 1849 Babbage designed, but did not build, the DE2. The Science Museum, London, constructed it in 1991, using Babbage's original designs.

(Photograph courtesy of the Science Museum of London.)



Moore's Law



Doubling every two years

A Brief History of Computers

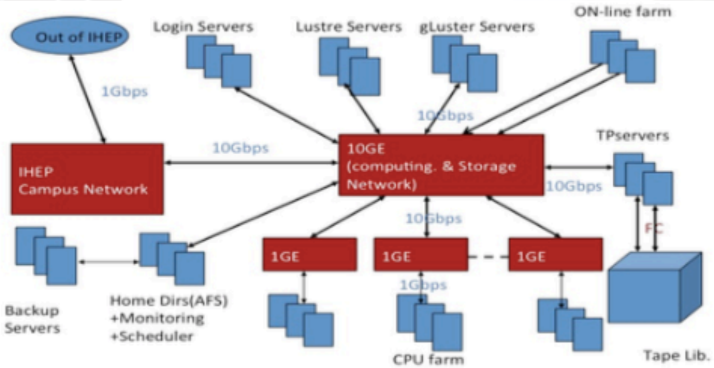
Machine	Year	Speed(in Flops)
ENI-AC	1946	0.36K
IBM 70	1954	12K
CDC 6600	1966	4.6M
CRAY 1	1976	50M
CRAY X/MP, Y/MP, C90, T3E	1983	166M-1.5T
C-2/200, CM-5(1024 nodes)	1989	1.2T
Intel Paragon (128 nodes)	1991	10G
IBM SP-2 (64 nodes)	1994	17G
P6/Sandia (9072)	1996	1.2T
IBM RS/6000 SP 2002	2002	100G
TH2-JK RS/6000 SP	2015	809T*

*Supercomputers at CSRC & CUHK

TH2-JK

809TFlops集群系统
CPU+GPU+Phi(Mic)

14112cores



131.1TB Memory

1440TB disks 2304TB
back-up disks

80Gb/s QDR

First Computers in the World

ENI-AC, U Penn, 1946; 360 Flops

Power: 120 W; 18800 Tubes

Weight: 30 ton

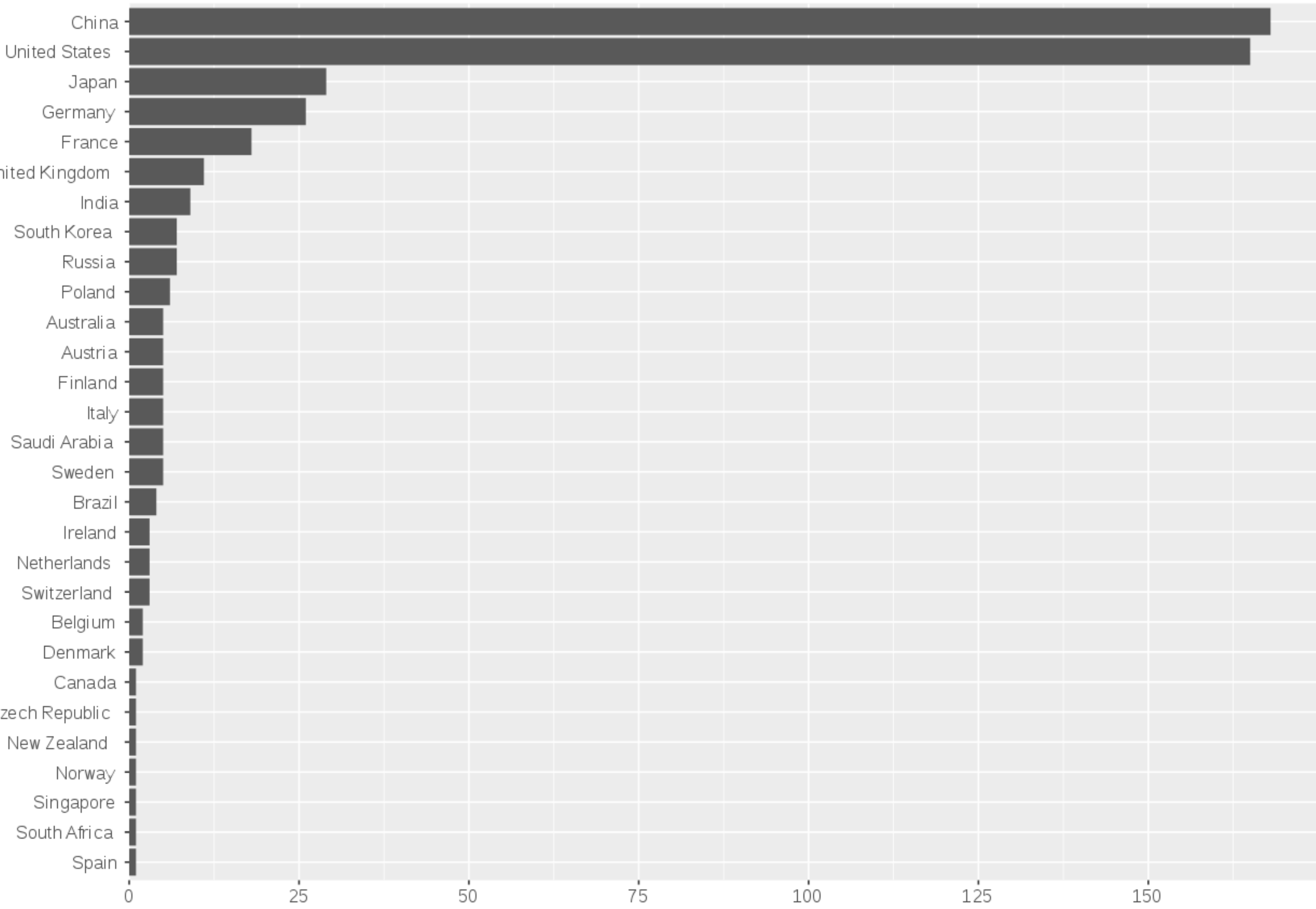
Size: about 3 classrooms

Speed: ~ 360 Flops (* very different from +/-)

Memory: <1000 digits

TOP 10 Sites for November 2018

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	Summit IBM	2,397,824	143,500.00	200,794.90	9,783
2	Sierra	1,572,480	94,640.00	125,712.00	7,438
3	**Sunway TaihuLight**	10,649,600	93,014.60	125,435.90	15,371
4	**Tianhe-2A**	4,981,760	61,444.50	100,678.70	18,482
5	Piz Daint	387,872	21,230.00	27,154.30	2,384
6	Trinity	979,072	20,158.70	41,461.20	7,578
7	ABCI	391,680	19,880.00	32,576.60	1,649
8	SuperMUC-NG	305,856	19,476.60	26,873.90	
9	Titan	560,640	17,590.00	27,112.50	8,209
10	Sequoia	1,572,864	17,173.20	20,132.70	7,890



Distribution of supercomputers in the TOP500 list by country, June 2016.

Country	Top speed (Rmax) (Tflops)	Number of computers in TOP500
China	93014.6	206
United States	122300.0	124
Japan	19880.0	36
United Kingdom	7038.9	22
Germany	6177.7	21
France	5283.1	18
Netherlands	1649.1	9
South Korea	13929.3	7
Ireland	1649.1	7
Canada	4608.0	6

Up to June 20

No. 1 Computer in the World

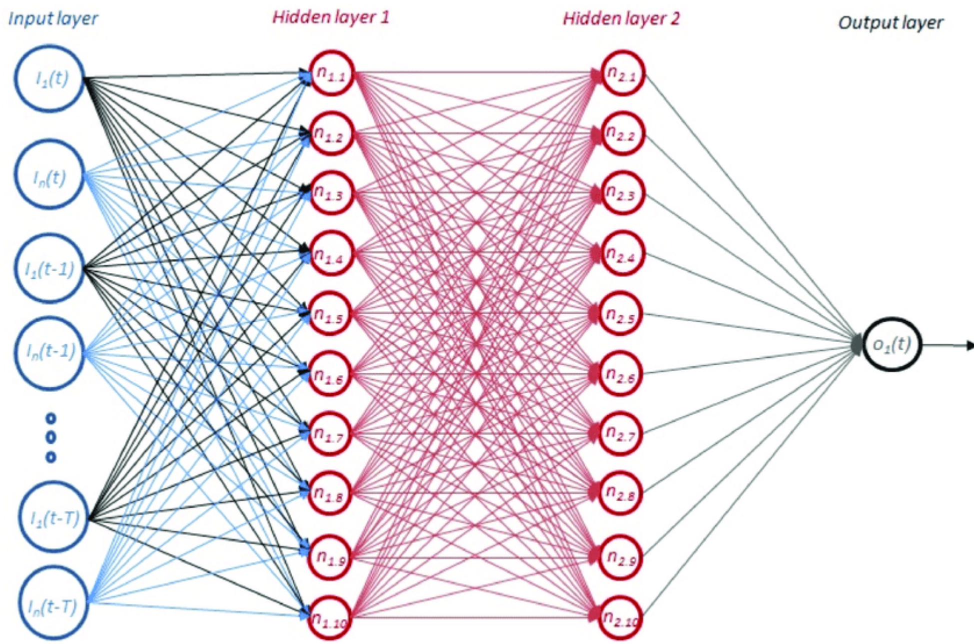
- 2018, Summit, USA/ORNL, 143/200 PFlops
- 2017-2016, Sunway TaihuLight, Wuxi/China, 10,649,600 cores, 93/125 PFlops, 15,371 kW
- 2013-2015, Tianhe-2, Guangzhou/China, 33.86/55 P, 17,808 kW
- 2012, Titan-Cray, ONL/US, 17.59/27.11 P
- 2011, K Computer, Japan, 8 P
- 2010, Tianhe-1, Tianjin/China, 2.57 PFlops

Sunway TaihuLight

- the world's fastest supercomputer for two years, from June 2016 to June 2018
- nearly three times as fast as the previous Tianhe-2, which ran at 34 petaflops.
- 1.45 GHz (3.06 TFlops single CPU, 105 PFLOPS LINPACK, 125 PFLOPS peak)
- 10,649,600 CPU cores
- 20PB storage

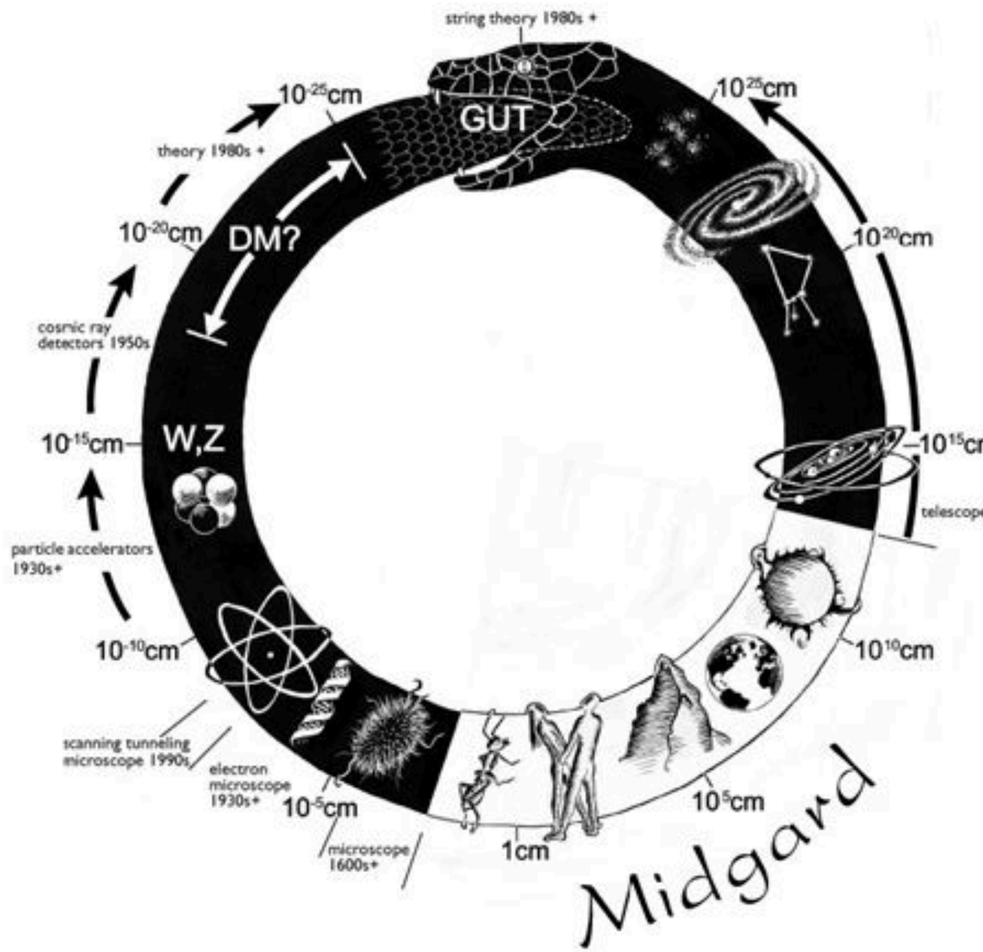
Machine Learning

- Use machine learning methods to design materials and chemical molecules, accelerating the discovery of materials and drugs
- Judge and characterize a phase transition, serve as a quantum many-body wave function or the like.
- The combination of the machine learning methods and traditional methods



Application fields in physics

- Cosmology
- Particle physics
- Nuclear physics
- Plasma physics
- Condensed matter physics
- Optics
- Atomic and molecular physics



Computer Simulation

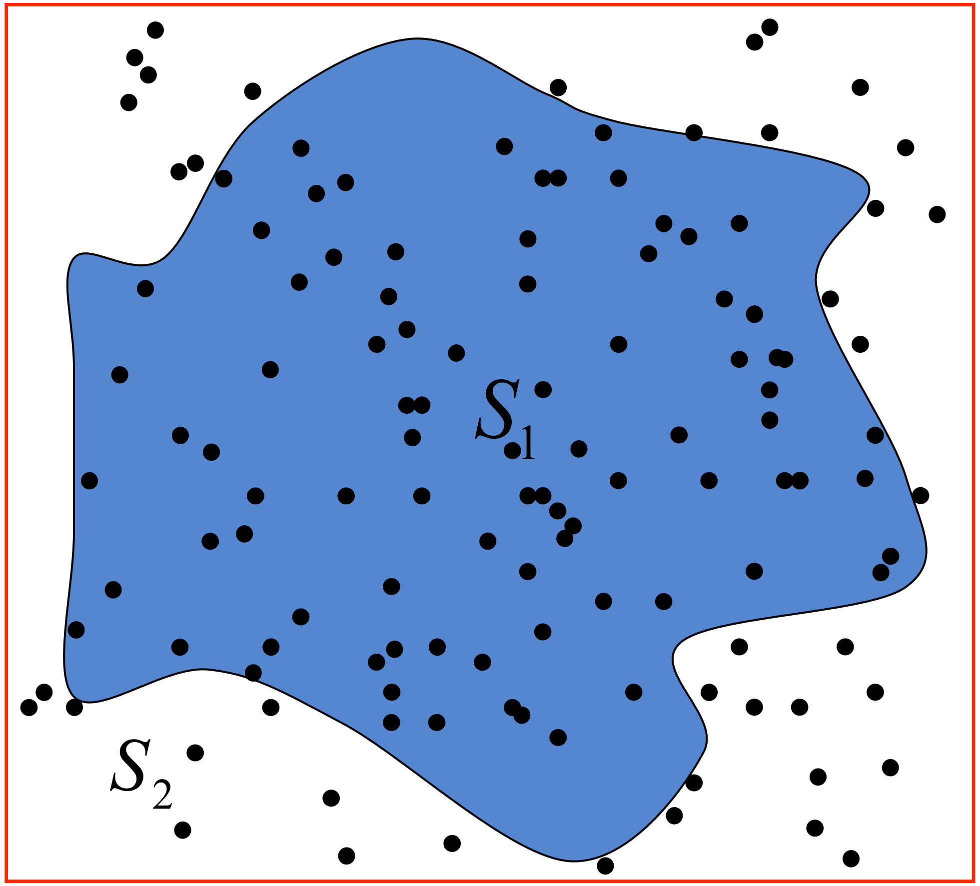
- restore the description and simulation of the nature of objective things.
- no measurement error, systematic error and no interference problem of the test probe
- free selection parameters
- plays a role in matching and even leading experimental physics

Sub-fields

- Statistical physics
- Condensed matter physics
- Soft condensed matter physics
- Atomic and molecular physics
- Nuclear physics
- High energy physics
- Plasma physics

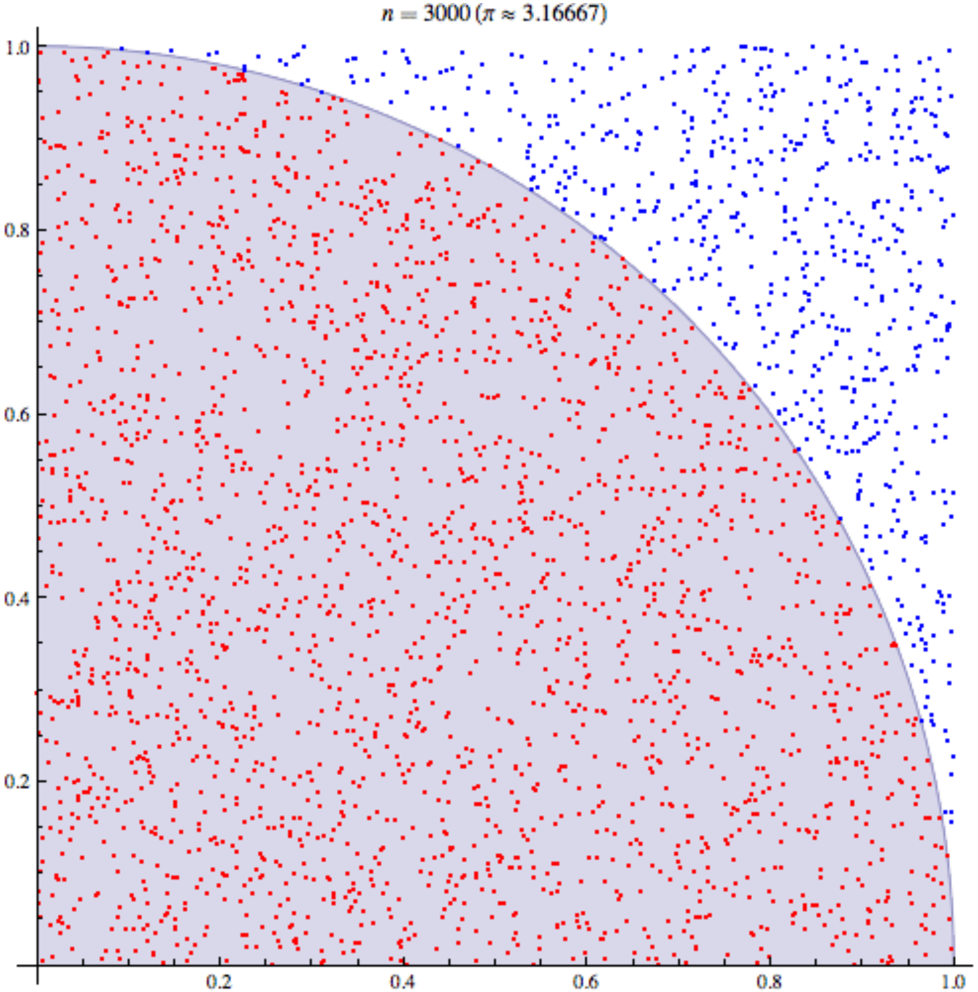
1. Statistical Physics: Monte Carlo method

How to measure the area?



$$\frac{S_1}{S_2} \approx \frac{N_1}{N_2}$$

How to calculate π ?

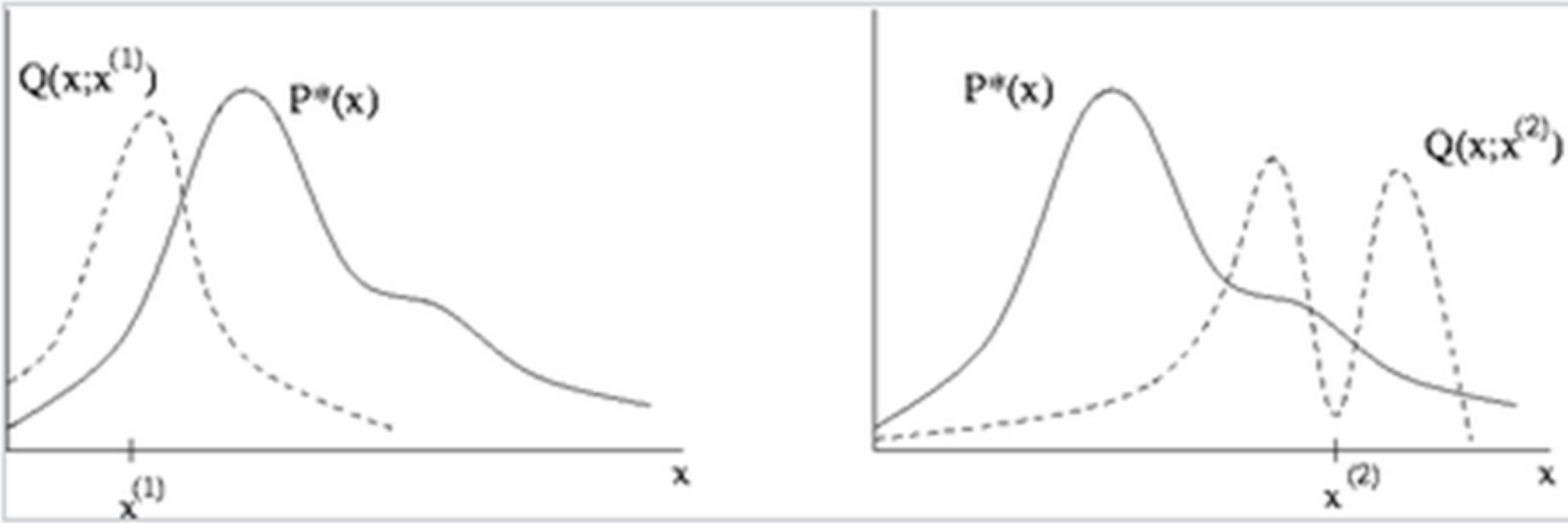


$$\frac{S_1}{S_2} = \frac{\pi/4}{1} = \frac{\pi}{4} \approx \frac{N_1}{N_2}$$

$$\therefore \pi \approx \frac{4N_1}{N_2}$$

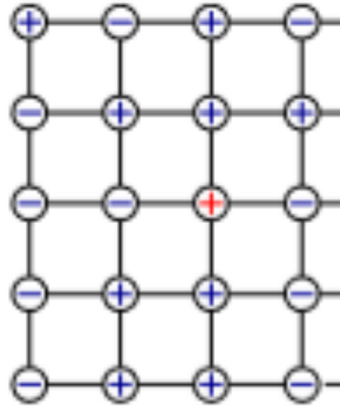
When N_2=30000,
the relative bias of π
is only 0.07%

Metropolis algorithm



The proposal distribution Q proposes the next point to which the random walk might move.

Metropolis algorithm in Ising model

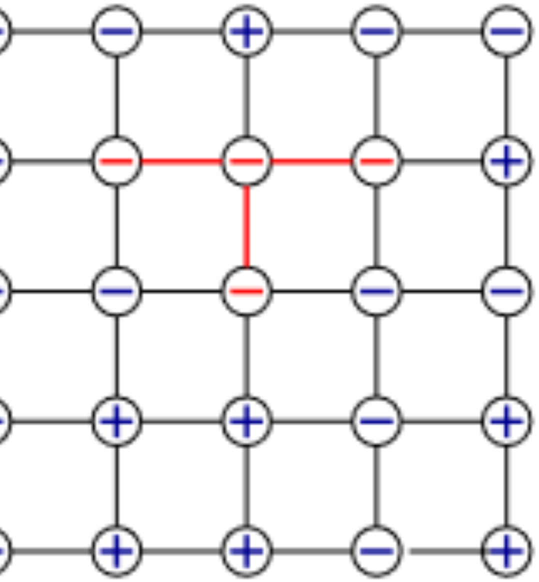


1. Select one of the spins in the form $\Gamma = (s_1, s_2, \cdots, s_i, \cdots, s_N)$, like s_i.
2. Flip it, $\Gamma' = (s_1, s_2, \cdots, -s_i, \cdots, s_N)$. *C*hoose a new configuration according to attempt probability $1/N$
3. Calculate $\Delta E = E(\Gamma') - E(\Gamma)$, and get ratio $W(\Gamma')/W(\Gamma) = e^{-\Delta E/kBT}$
4. Set up $P_{accept}(\Gamma', \Gamma) = min[W(\Gamma')/W(\Gamma), 1]$:
   1) if $\Delta E \leq 0$, accept Γ';
   2) if $\Delta \mathrm{E} > 0$, accept Γ' as probability $e^{-\Delta E/kBT}$;otherwise, reject.
5. back to step 1 to generate enough configuration.

Clustering

- Group a set of objects which are more similar (in some sense) to each other than to those in other groups (clusters).
- A common technique for statistical data analysis used in many fields:
  - machine learning
  - pattern recognition
  - image analysis
  - information retrieval
  - Bioinformatics
  - data compression
  - computer graphics.

Wolff algorithm



Flip a group in one step instead of flipping $N = L^d$ one by one in one step:

1. Choose a spin i arbitrarily
2. Turn $s'_i = -s_i$
3. Do the following for all nearest neighbors of i:
   If $s_k = s_i$, the probability is $1-e^{-2K}$, $K = J/k_BT$
   1) turn $s_k \rightarrow s'_k = -s_k$
   2) Record k to the address list (stack)

   If $s_k = s'_i$, do nothing
4. Read an address l from the stack
5. Perform step 3 on l
6. Remove l from the stack
7. Repeat 4-6 until the stack is empty

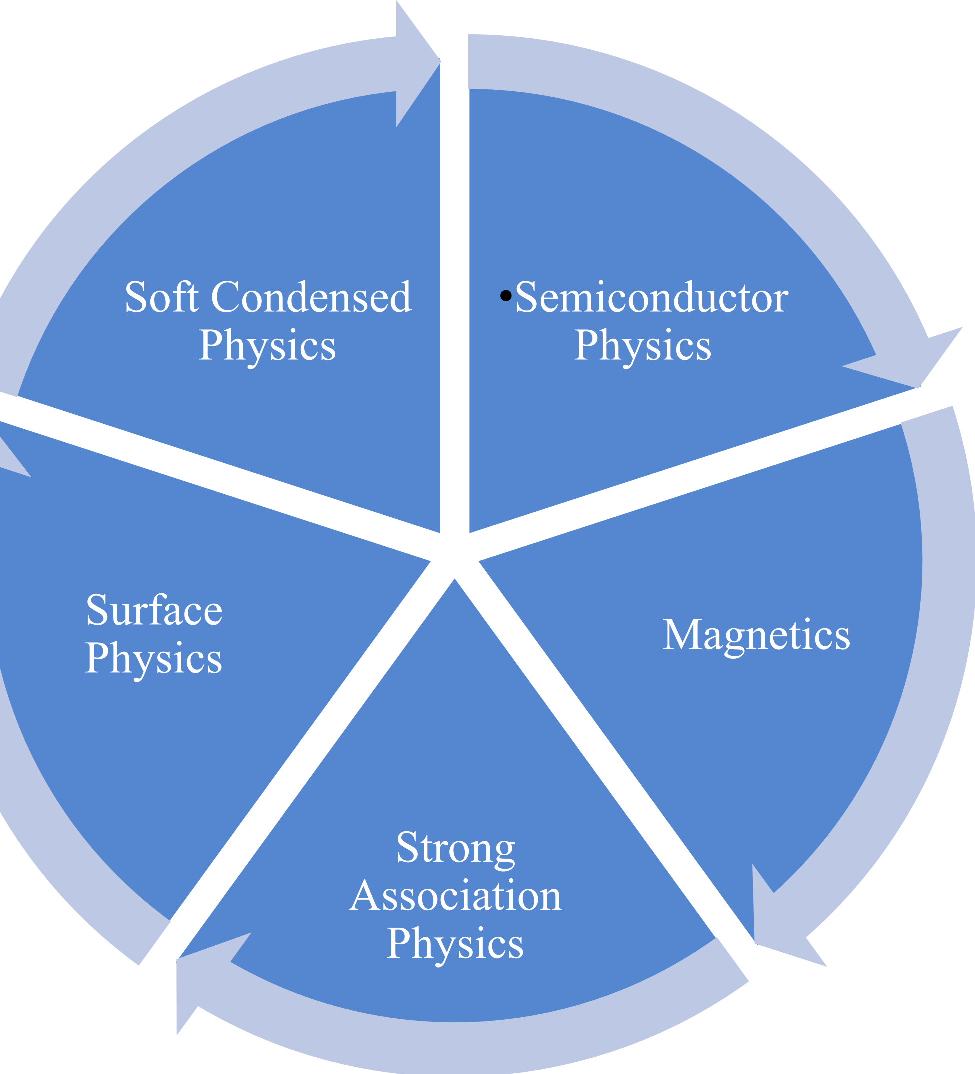
Quantum Monte Carlo

- aim to study complex quantum systems.
- provide a reliable solution (or an accurate approximation) of the quantum many-body problem.
- going beyond mean field theory
- offering an exact solution of the many-body problem in some circumstances.

Other algorithms

- Hybrid algorithm
- Multigrid algorithm
- Monte Carlo renormalization group method

2. Condensed matter physics



Two methods:

- First-Principles method (Condensed matter calculation I)
- Model Hamiltonian method (Condensed matter calculation II)

Condensed matter calculation I

- Based on First-principles Calculation of Electronic structure and dynamic Simulatio

- The description of electronic structure strictly includes density functional theory (Density-Functional Theory, DFT), post-Hartree-Fock method and Quantum Monte Carlo method.

- At present, in the first principle simulation technology of the condensed matter , the method of the electronic structure layer refers to the DFT.

Condensed matter calculation I

➢ The research in this area:

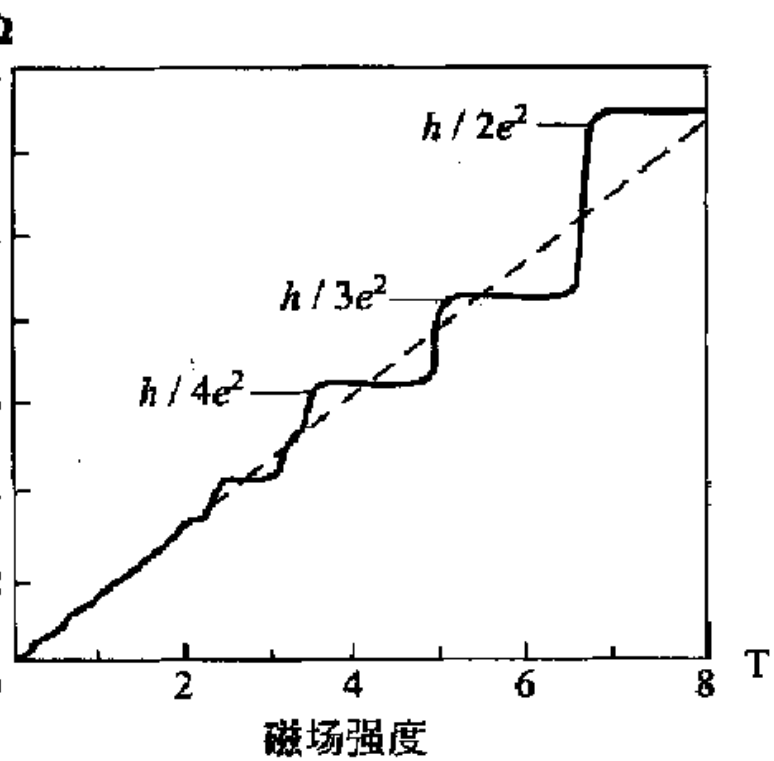
1)the processing of the exchange association interaction of the electronic structure in the development of the method, study on the properties of excite states of electron, the development of algorithms and programs and their possible applications in complex Large-Scale systems, study on dynamics a statistical methods.

2) application level from structural analysis to physical properties prediction, and to material precise design and so on.

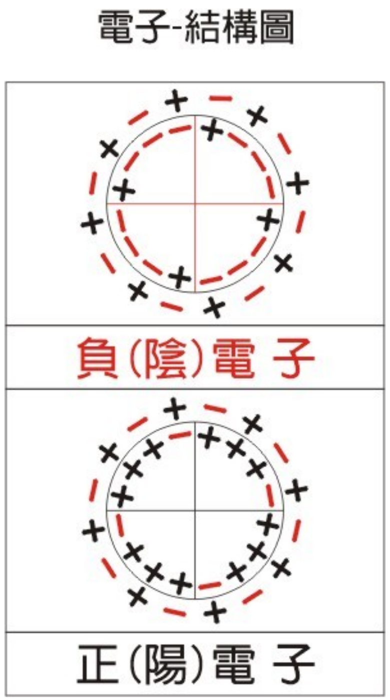
Condensed matter calculation II

- Belong to the category of many-body and strong correlation physics in condensed matter physics
- Explain some novel phenomena：
  Integer and Fractional Quantum Hall effect ； High temperature superconductivit
  Colossal magnetoresistance； Quantum phase transition； Magnetic frustrati
  Kondo effect； Heavy fermion behavior； Giant thermoelectric effect； Giant nonlinear optical effect
- Strong correlation and quantum fluctuation
- Numerical Renormalization Group and Quantum Monte Carlo methed

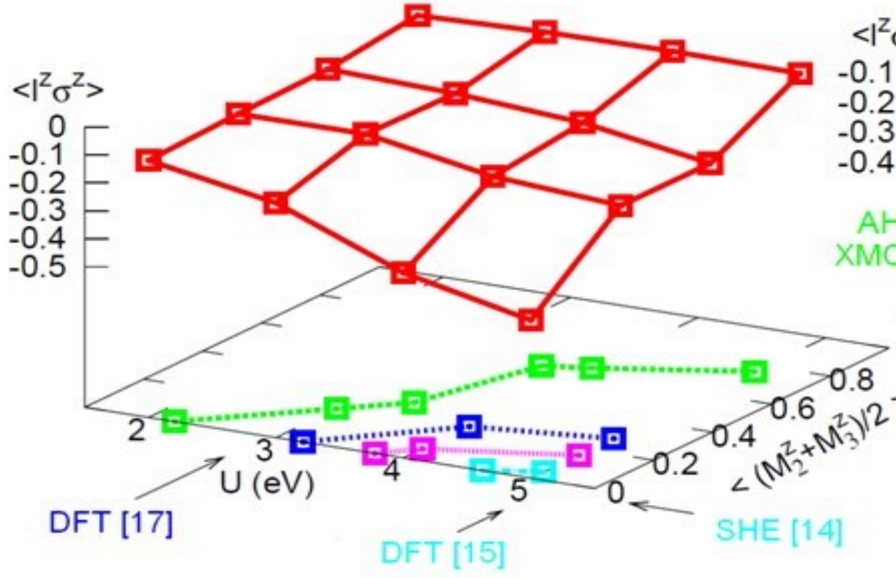
Condensed matter calculation II



[nteger quantum Hall effect]



[Fractional Quantum Hall Effect]



[kondo effect]

Numerical Renormalization Group Methoc

1. proposed by K. G. Wilson in 1970s, and successfully used to solve Kon problem
2. extended to the numerical solution of lattice model in real space in the following years (but the result error increases rapidly with the increase c lattice points)
3. Refined by Xiangtao in 1992 to reduce result error(only one lattice poin was added at a time)
4. Proposed density matrix renormalization group(DMRG) White.
5. DMRG in momentum space, Transport Matrix Renormalization Group, Quantum Chemistry DMRG, Time-dependent DMRG, Dynamic DMRG
6. DMRG in Two-Dimensional Systems.

Difficulties of strongly correlated problem :

1. have no comprehensive understanding of strongly correlated problems
2. lack a complete and accurate description of physical images.
3. Strong interaction between particles is very strong and beyond Perturbat and other methods

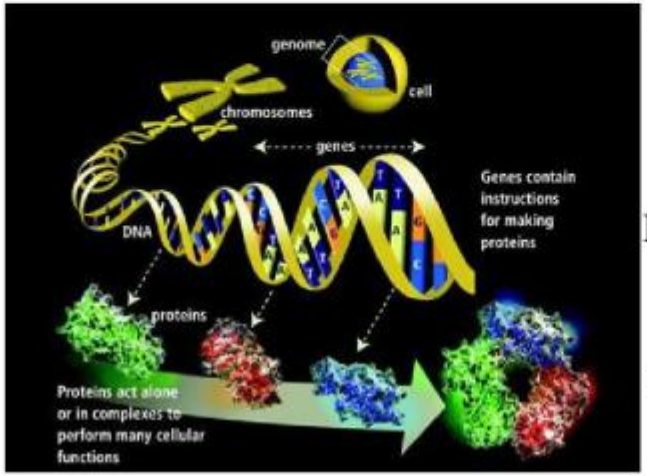
A way to learn:

- master basic knowledge of relevant courses
- master basic computer operations and programming languages, especial can use a computer language programming adroitly
- process data, organize images

3. Soft condensed matter physics

➢Research object：

Complex fluids, liquid crystals, multilayer films, protein folding



DNA sequence
↓
Protein sequence
↓
Protein structure
↓
Protein function

➢Research content:

Low-dimensional nanomaterials, etc.

4. Atomic and Molecular Physics

- Atomic and Molecular Physics is the first research field in Computationa physics