Condensed matter physics: More is different! (and how to study it by high-performance computing)

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Outline

What is condensed matter physics?
Emerging phenomena and the axis of complexity
Current projects

High-performance computing in scientific research
Pegasus cluster
Monte Carlo simulations

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What is condensed matter physics?

Condensed Matter Physics:
field of physics that deals with the macroscopic properties of matter; in particular ... the “condensed” phases that appear whenever the number of constituents in a system is large and their interactions ... are strong.

Traditionally: Physics of solids and liquids

• What is the structure of crystals?
• How do solids melt or liquids evaporate?
• Why do some materials conduct an electric current and others do not?

Today: all systems consisting of a large number of interacting constituents

• biological systems: biomolecules, DNA, membranes, cells
• geological systems: earthquakes
• economical systems: fluctuations of stock markets, currencies
Why condensed matter physics?

Applications: "Helps you to make stuff."

- semiconductors, transistors, microchips
- magnetic recording devices
- liquid crystal displays
- plastic and composite materials

Magnetic read head, based on Giant Magneto-resistance effect (Physics Nobel Prize 2007)

Maglev train using levitation by superconducting magnets, can go faster than 350 mph
Why condensed matter physics II

Directions of fundamental physics research:

Astrophysics and cosmology: increasing length and time scales

Atomic, nuclear and elementary particle physics: decreasing length and time scales

Particle accelerator at Fermilab

What direction does condensed matter research explore?
Emerging phenomena and the axis of complexity

Emerging phenomena:
When large numbers of particles strongly interact, qualitatively new properties of matter emerge at every level of complexity.
Superconductivity

- zero electrical resistance below a certain temperature
- electrons form Cooper pairs

ferrromagnetic superconductors
Quantum magnetism

Transverse-field Ising model

\[ \hat{H} = -J \sum_{\langle i,j \rangle} \hat{S}_i^z \hat{S}_j^z - h_x \sum_i \hat{S}_i^x \]

transverse magnetic field induces spin flips via \( \hat{S}_i^x = \hat{S}_i^+ + \hat{S}_i^- \)

⇒ Quantum phase transition

dilution of lattice leads to percolation
⇒ quantum magnets on percolating lattices
Many-particle physics meets neuroscience

Serotonergic fibers in vertebrate brains:
- serotonergic fibers: special neurons that transport serotonin
- form inhomogeneous random network

What causes varying fiber densities?
Computational Science

Application of computational and numerical techniques to solve large and complex science problems

3rd independent scientific methodology has arisen over the last 30 years or so
shares characteristics with both theory and experiment
requires interdisciplinary skills in science, mathematics, computer science

Computational Science ≠ Computer Science
Cluster computing

Cluster:
group of connected computers that work together as one machine

- diverse purposes (high availability, fault tolerance, high performance)
- many different cluster architectures

Recipe for cluster supercomputer:

1. Buy a pile of mass market commodity hardware for node computers
2. Connect all nodes via a private cluster network (the fastest you can afford)
3. Run the free Linux operating system and packages to support distributed parallel computing: PVM, MPI, PBS
4. Run your code in parallel on hundreds, thousands, or millions of CPUs

⇒ supercomputer power for a fraction of the price
In the latest list (June 2022):

- 452 of the 500 fastest computers in the world are clusters (90.4%)
- Top cluster system in the list (rank 4): Summit, Oak Ridge National Laboratory, 2,414,592 CPUs

Frontera (Texas Advanced Computing Center)
**Pegasus cluster and the Foundry**

**Pegasus cluster:**
- used by Vojta research group
- 192 diskless compute nodes (total 832 CPU cores)
- parallel computing via Message Passing Interface (MPI)

**The Foundry:**
- campus cluster
- CPU and GPU nodes, more than 11,000 CPU cores
- funded by $2 million NSF award in 2019
Monte Carlo simulations

Monte Carlo method:
class of computational algorithms for simulating various physical and mathematical systems; they are ... stochastic, usually by using random numbers.

Example: Monte Carlo calculation of Pi

- fire random data points at a circle inscribed within a square
- ratio of the areas of circle and square is $\pi/4$
- ratio can be estimated as the number of hits in the circle and the total number of points in the square
Computational Physics Projects:

- some **programming experience** in required
- projects involve:
  developing Monte Carlo programs,
  running large-scale parallel simulations,
  analyzing and visualizing numerical data