Introduction to atomistic simulation methods in condensed matter

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Outline of the talk:

What is an atomistic simulation

How to compute material properties from first-principles.

Overview of approximations

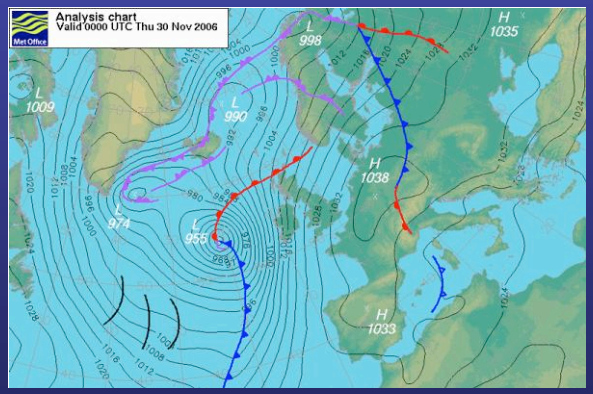
Examples of realistic simulations

What is a Computer Simulation?

By “computer simulation” we understand the use of a computer to “solve” numerically the equations that govern a certain process.

Simulations are present in every branch of science, and even increasingly in every day life

Weather forecast



Flight simulations

Finances

What is a Computer Simulation?

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Simulations are present in every branch of science, and even increasingly in every day life

Simulations in materials: study the way in which the blocks that build the material interact with one another and with the environment, and determine the internal structure, the dynamic processes and the response to external factors (pressure, temperature, radiation, etc.)

Why are simulations interesting?

Simulations are the only general method to solve models describing many particles interacting among themselves.

Experiments are sometimes limited (control of conditions, data acquisition, interpretation,…) and generally expensive

Simulations scale up with the increase of computer power
(that roughly doubles every year!!)

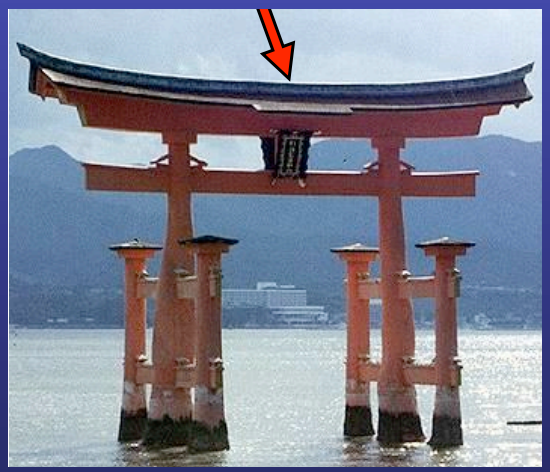
Why are simulations interesting?

Alternative to approximate solutions for models (traditional theory)

Complement and alternative to experimental research

First-principles simulations

The Torii metaphore
(Prof. H. Nakamura)



Theory Experiment

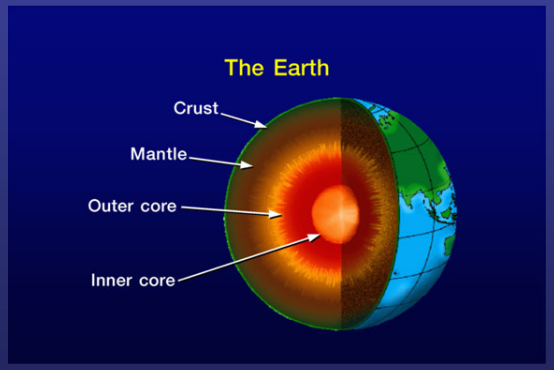
Why are simulations interesting?

Alternative to approximate solutions for models (traditional theory)

Complement and alternative to experimental research

Increasing scope and power with improving computers and codes

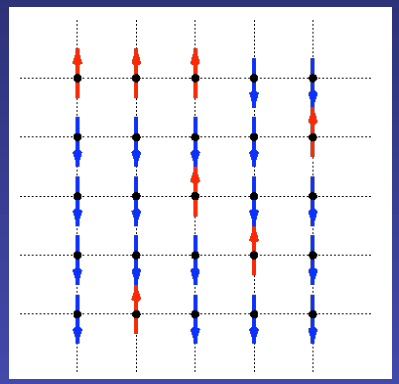
Level of accuracy ⟹ "Computer experiments"

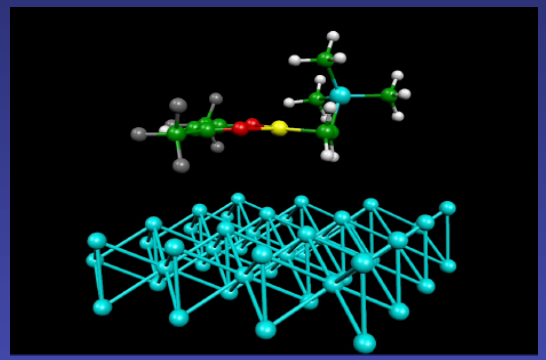


Model of materials under circumstances far away from the conditions achievable in a lab., under extreme conditions

Components of a simulation

1. A model of the interactions between the blocks that build the material





Ising model:

A mathematical model of ferromagnetism in statistical physics.

Spins are treated as discrete variables that can be in one of two states.

Spins are arranged in a lattice or graph, and each spin interacts at most with its nearest neighbors.

$$\hat{H}(\sigma) = -\sum_{i \neq j} \sigma_i \sigma_j - \sum_j h_j \sigma_j$$

Atomistic models
Wave function methods
DFT

Components of a simulation

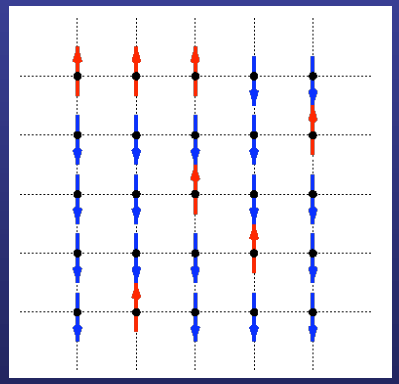
1. A model of the interactions between the blocks that build the material

2. A simulation algorithm: the numerical solution to the equations that describe the model.

For the same model, there might be many different implementations, many availables codes

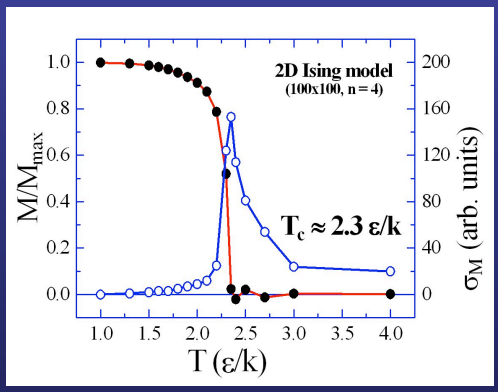
3. A set of tools for the analysis of the results of the simulations

Ising model + Monte Carlo simulations ⟹ phase transitions



Results:
Emergent properties not evident just looking at the equations

Use of computer essential for the exploration of the model



Challenge of simulation of materials

Physical and mathematical foundations

What approximations come in?

The simulation is only as good as the model being solved

Systems with many particles and long-time scales are problematic

Computed time is limited: relatively small number of atoms for relatively short times

Space-time is 4D $\quad 2 \times L_i \rightarrow \mathrm{CPU} \times 16$

How we do estimate errors? (Statistical and systematic)

How do we manage ever more complex codes?

Challenge of simulation of materials

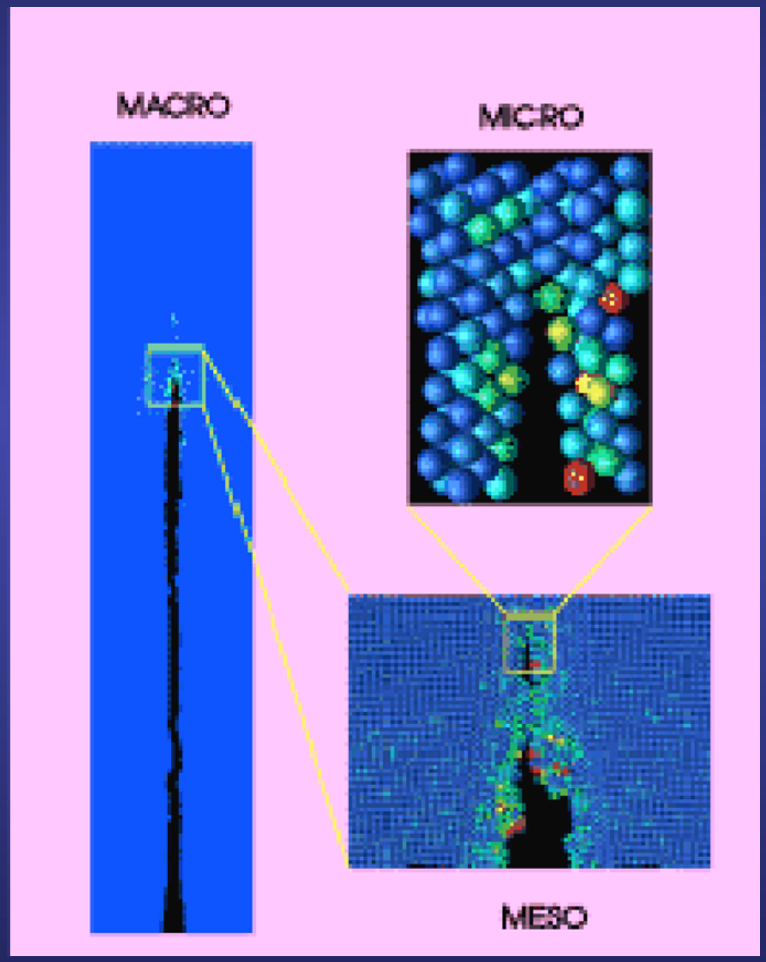
Multiple scales

Length scales:

1 cm – 1 Å (10^{-10} m)

Time scales:

1 year – 1 fs(10^{-15}s)



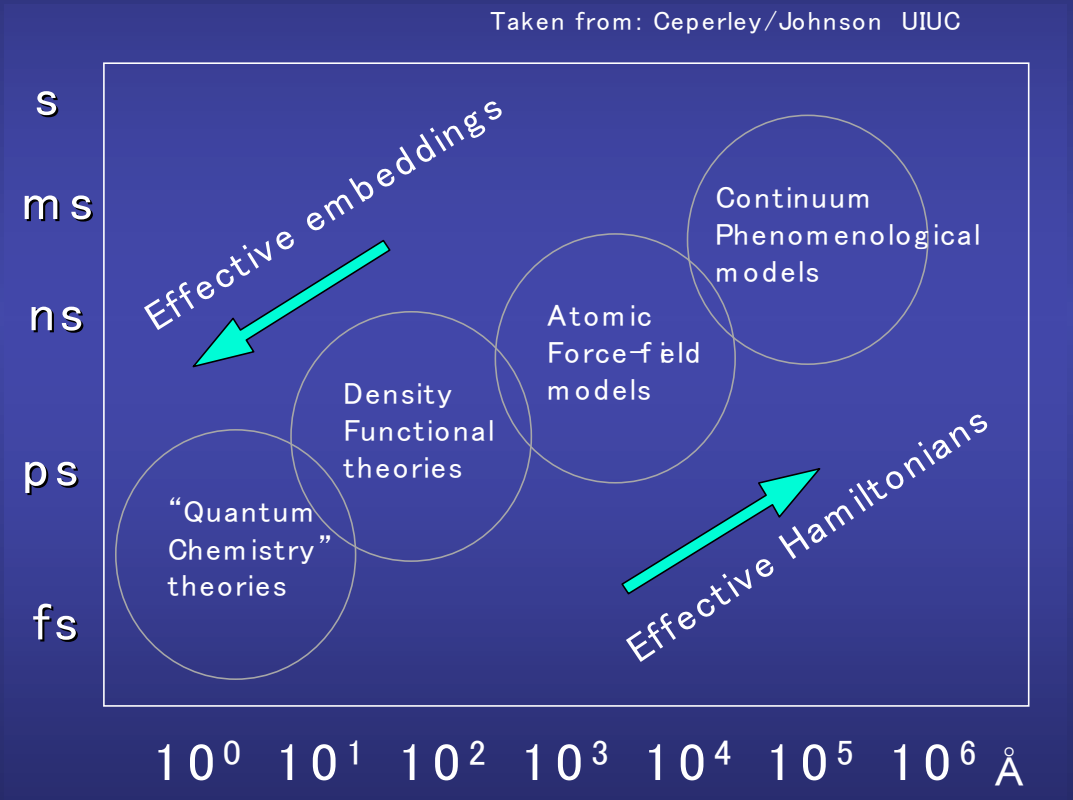
Challenge of simulation of materials

Multiple scales

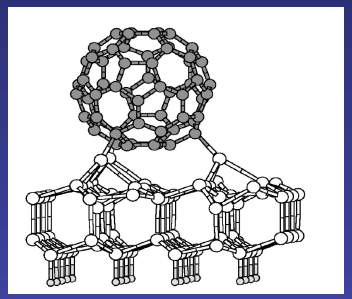
Macro and mesoscopic thermodynamic properties

Atomic structure and dynamics

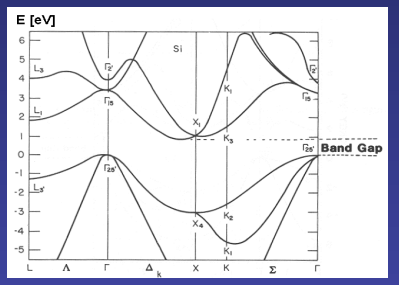
Electronic states chemical bonds and reactions, excitations…



Goal: Describe properties of matter from theoretical methods firmly rooted in fundamental equations



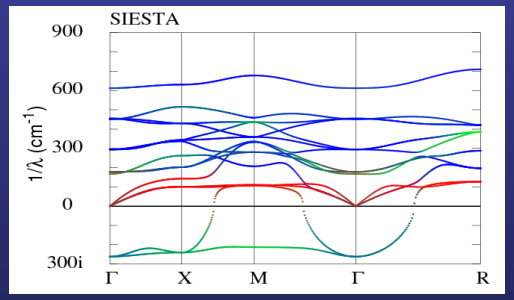
structural



electronic

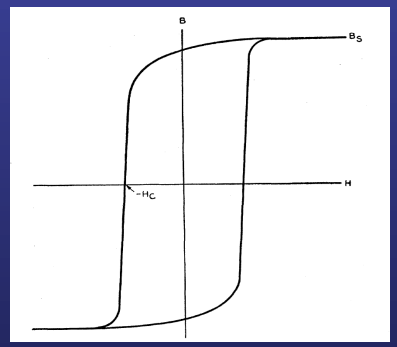
PROPERTIES

vibrational

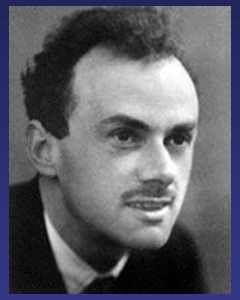


optical

magnetic



Modern atomic simulations follow Dirac's intructions (1929)



"The general theory of quantum mechanics is now almost complete. 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."

Goal of modern atomic simulations: implement that dream

The most important point: analysis and modelization of the results

In a first-principles simulations, what we have is the ultimate modeling of materials, whose solution requires the use of computers

"A simple model can shed more light on Nature's workings than a series of "ab-initio" calculations of individual cases, which,even if correct, are so-detailed that they hide reality instead of revealing it… A perfect computation simply reproduces Nature, it does not explain it."

Philip W. Anderson