CSIC

CIN2 CENTRE D'INVESTIGACIÓ EN NANOCIÈNCIA I NANOTECNOLOGIA

ICN2 Institut Català de Nanotecnologia

Computing Needs for Materials Science

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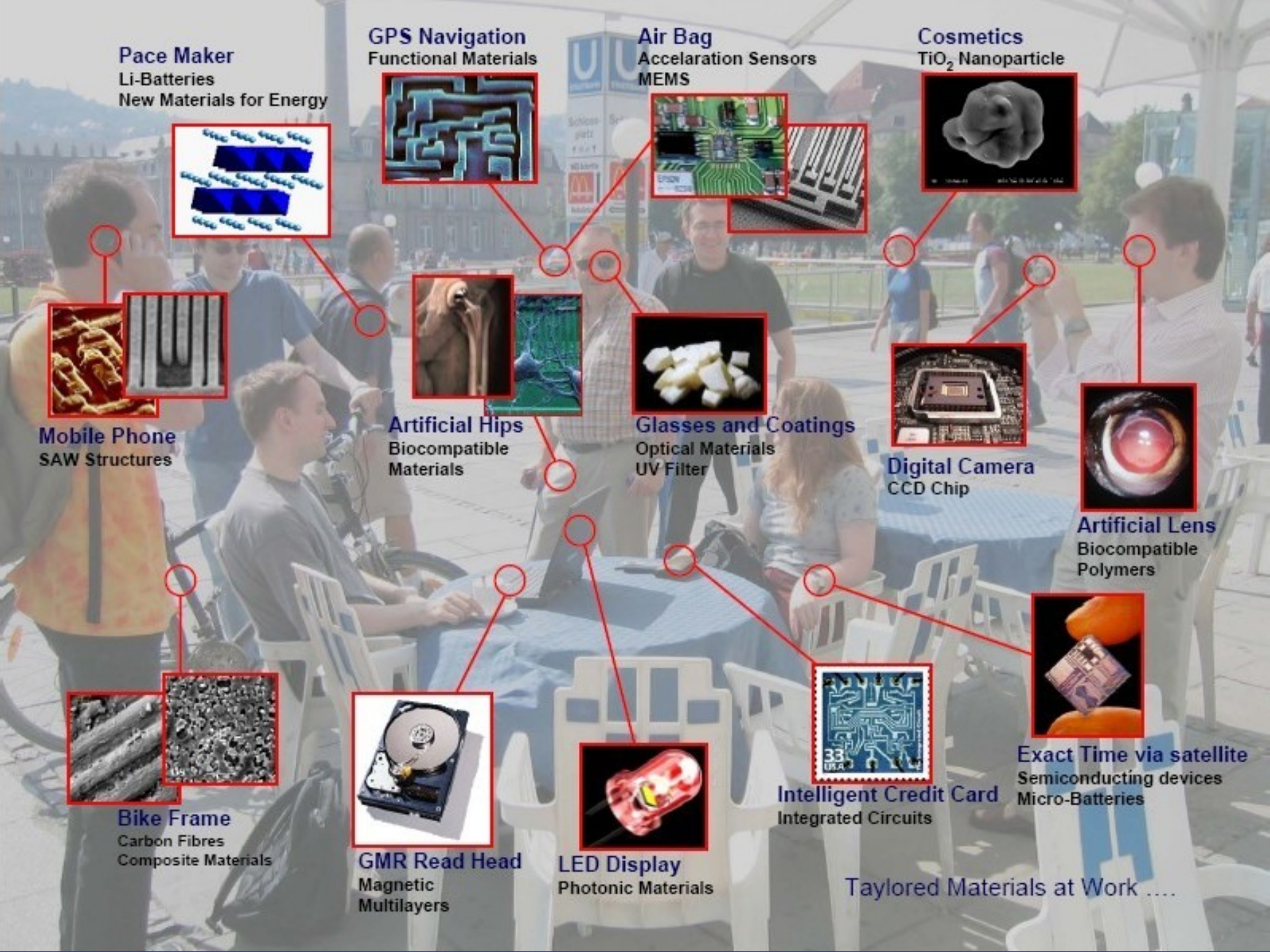
CIN2 – CSIC/ICN (Barcelona)


On a typical day in Stuttgart .....
Courtesy of Prof. Helmut Dosch
Max Planck Institute for Metal Research
Stuttgart (Germany)


Pace Maker
Li-Batteries
New Materials for Energy
GPS Navigation
Functional Materials
Air Bag
Accelaration Sensors
MEMS
Cosmetics
TiO_2 Nanoparticle
Mobile Phone
SAW Structures
Artificial Hips
Biocompatible
Materials
Glasses and Coatings
Optical Materials
UV Filter
Digital Camera
CCD Chip
Artificial Lens
Biocompatible
Polymers
Bike Frame
Carbon Fibres
Composite Materials
GMR Read Head
Magnetic
Multilayers
LED Display
Photonic Materials
Intelligent Credit Card
Integrated Circuits
Exact Time via satellite
Semiconducting devices
Micro-Batteries
Taylored Materials at Work ....

Materials Simulations: The "Virtual Lab"

- Basic understanding
- Aid in interpretation of experiments
- Systems and conditions not feasible in experiment
- Focus on specific details
- Specify external conditions
- Prediction and design! → **Materials with predefined properties**

Materials Simulations

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…).

Ingredients:

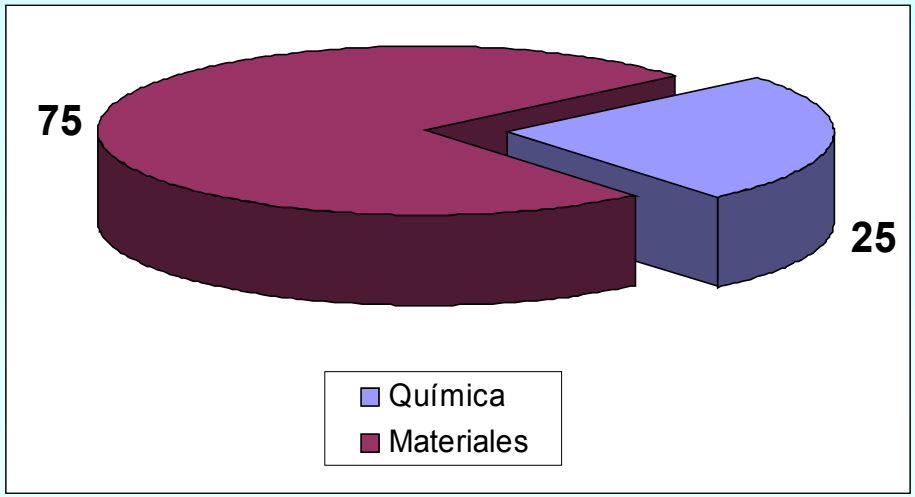
1. A **model of the interactions** between the "blocks" that build the material.

   Here: atomistic models.

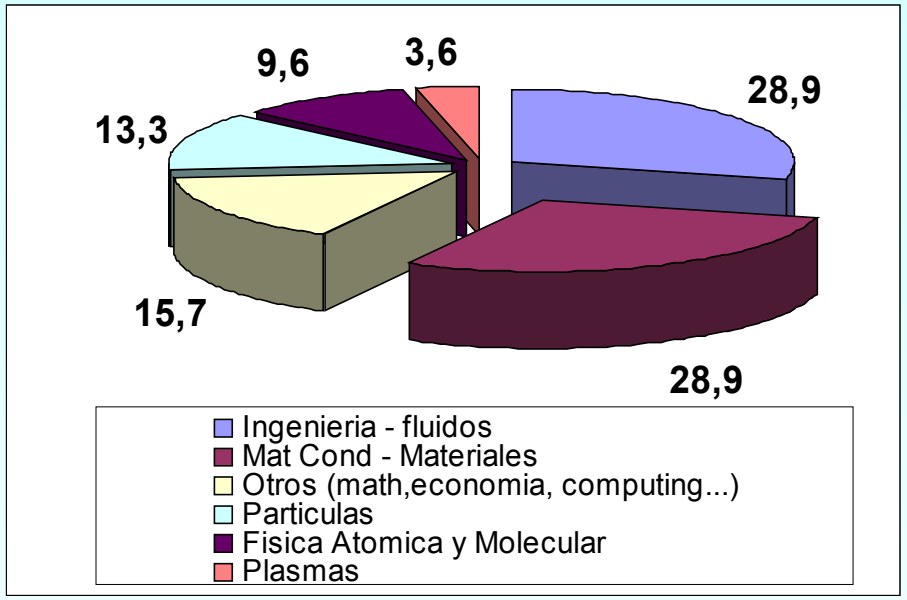
2. A **simulation algorithm**: the numerical solution to the equations that describe the model.

3. A set of **tools for the analysis** of the results of the simulation.

Química y Materiales (25%)



Física e Ingeniería (25%)



Simulaciones en Materiales: **Aprox 26% de la CPU de la RES**

15.6 Millones de Horas / año

Challenges in Materials Simulations

Multiple scales

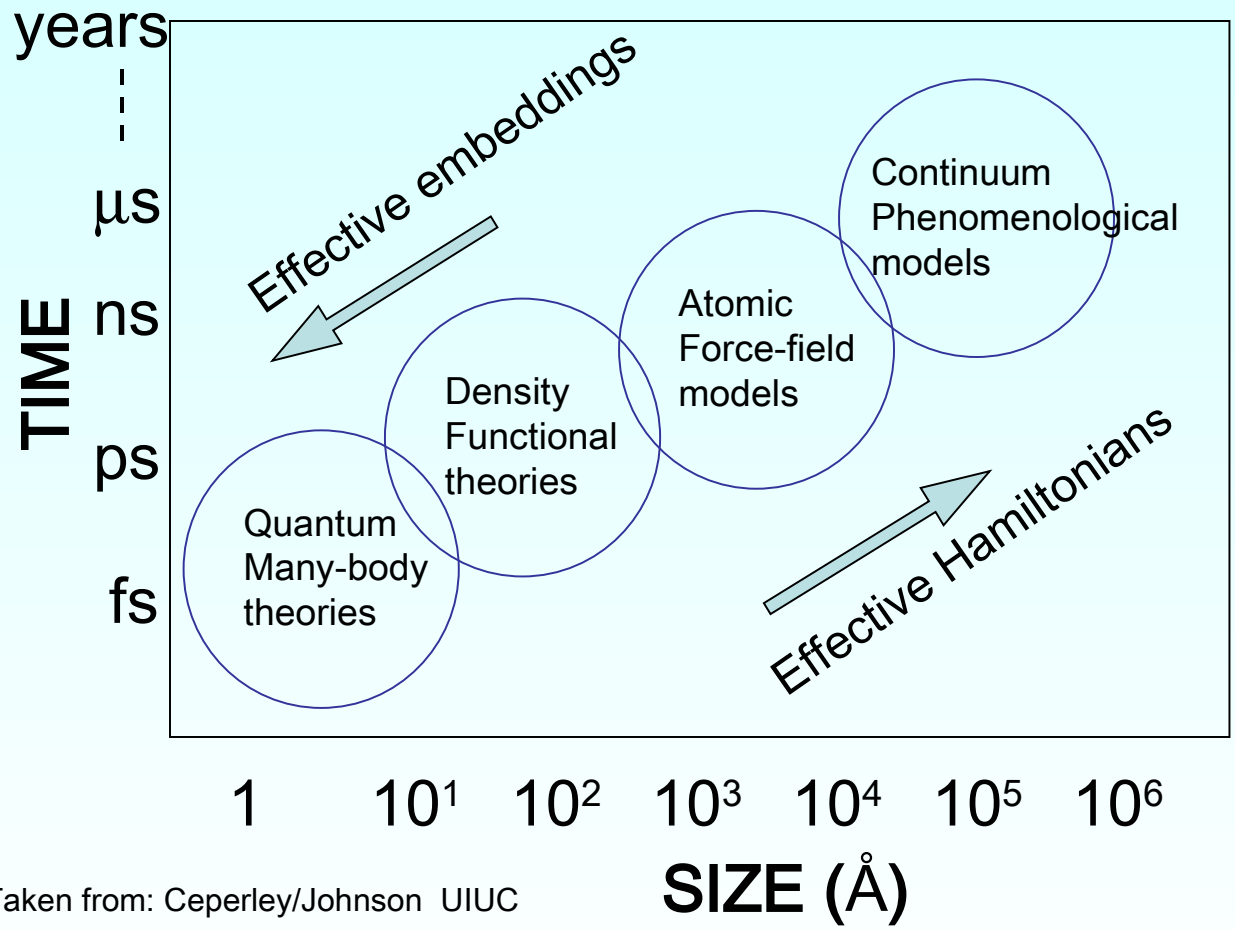
cm — Å (10^{-10} m)

years — fs (10^{-15} s)

Macro – and *mesoscopic* phenomena; Thermodynamics

Atomic structure and dynamics

Electronic states Chemical bonds and reactions, excitations …



Taken from: Ceperley/Johnson UIUC

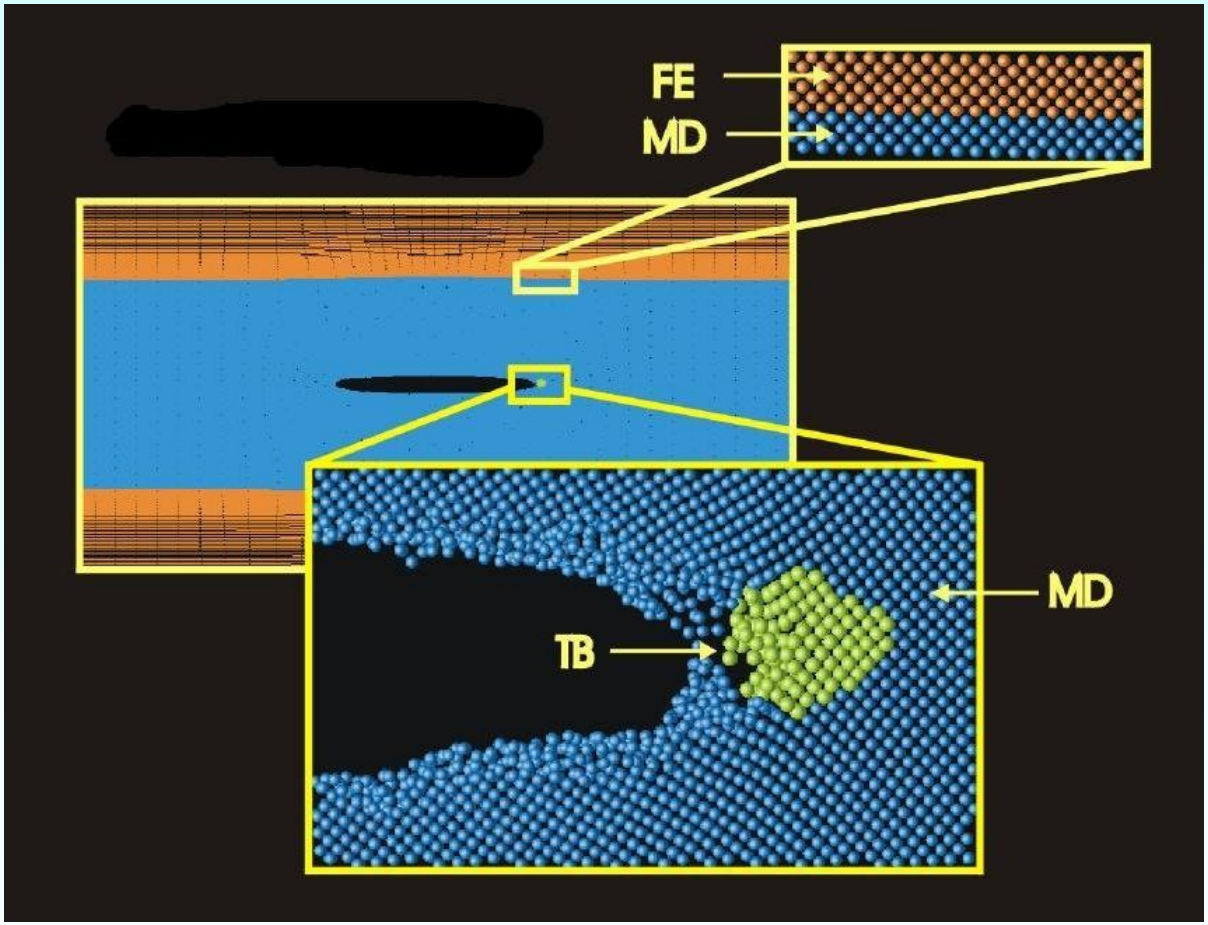
Challenges in Materials Simulations

Multi-scale methods

FE: Finite Elements
(continuum models)

MD: Classical dynamics with Interatomic Potentials

TB: Tight Binding
(Quantum mech.)

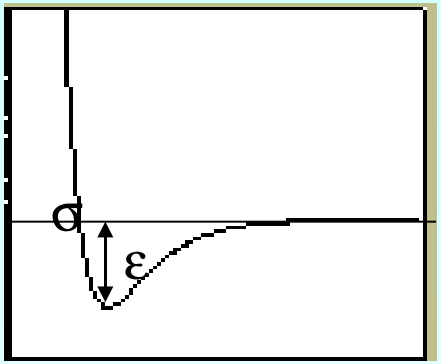


Crack propagation in Silicon (Prof. E. Kaxiras, Harvard)

Interatomic Potentials

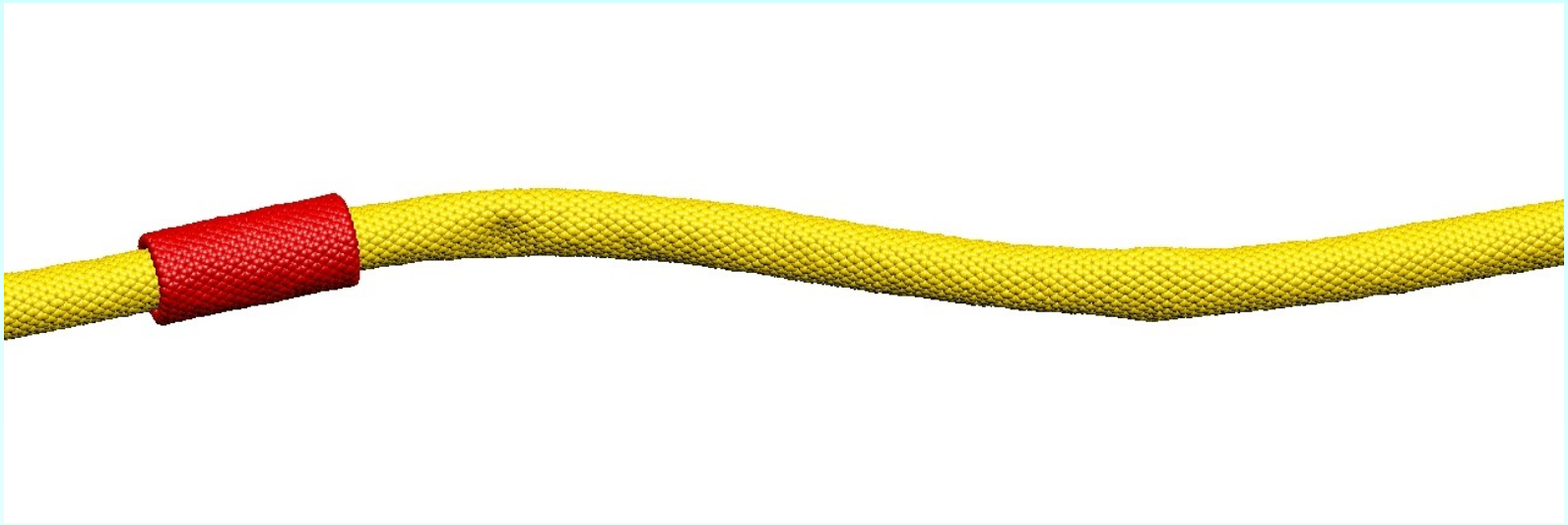
- Only atoms are considered (e.g. Lennard-Jones)

$$v(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^{6}]$$



- Parameters determined from experimental information or from *ab-initio* calculations
- Easy/fast to compute. Allow calculations in very large systems (100,000+ atoms, nanoseconds - microseconds)
- CPU and Memory typically scale as O(N) with the size of the system
- Very easy to parallelize efficiently: excellent scaling with thousands of processors

Interatomic Potentials



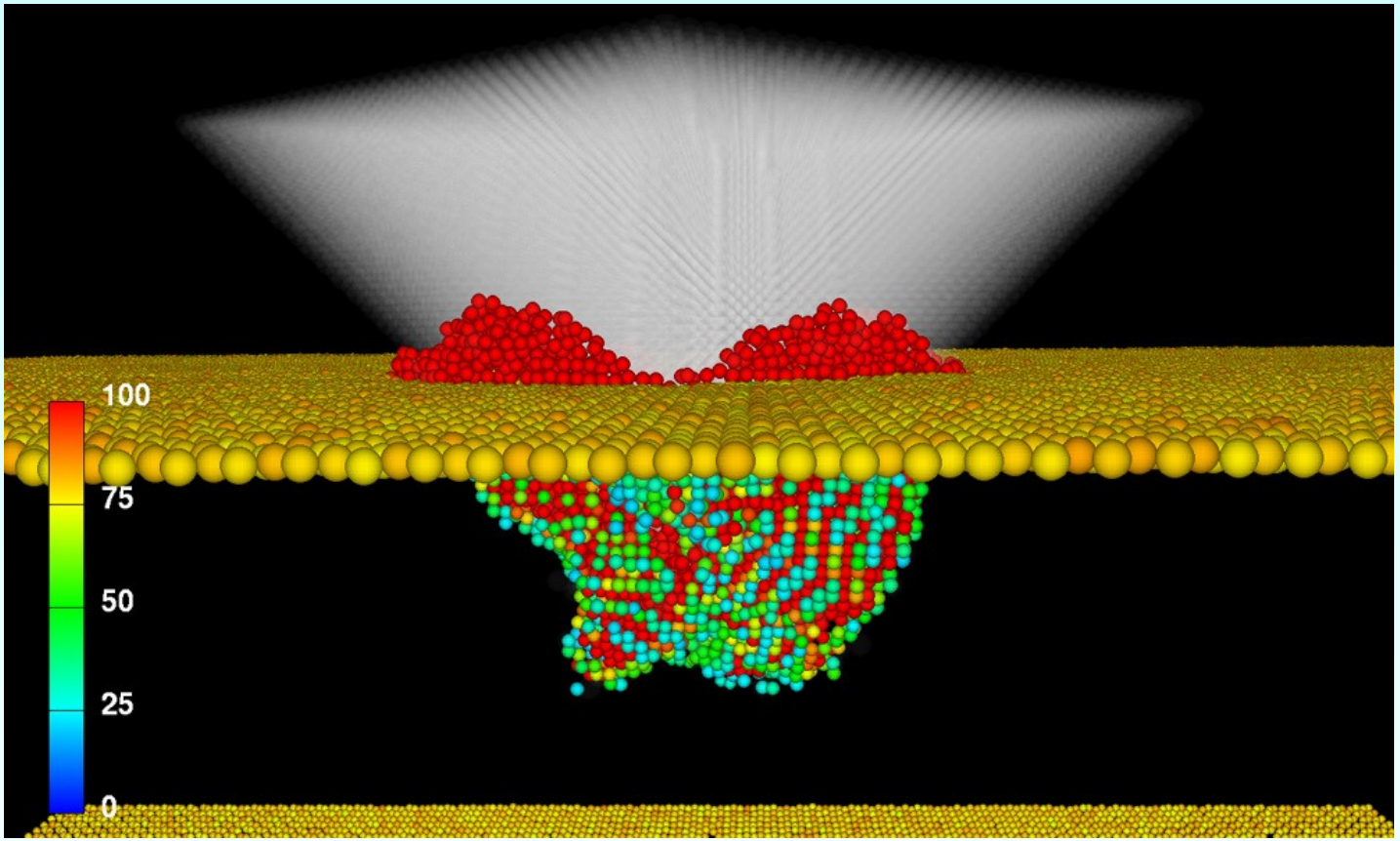
Mass transport driven by thermal gradients

A. Barreiro, R. Rurali, E. Hernandez et al., Science **320**, 775 (2008)

20.000 C atoms 200 ps = 0.2 ns

1-2 days of CPU in a single Pentium-4 processor

Interatomic Potentials



Nanoindentation - Priya Vashishta et al. (U. Southern California)

Multimillion atom simulation - Hundreds of nodes

Quantum-Mechanical Simulations

- Explicit fundamental interactions between electrons and nuclei
- No parameters to fit!: Ab-initio
- Computationally expensive, possible for only relatively small systems (100+ atoms)
- Necessary to describe chemical reactions, breaking/forming of bonds.
- Typical scaling is $O(N^3)$ with the number of atoms (linear scaling methods are starting to become available: **SIESTA**)
- Very difficult to parallelize!!. Efficient scaling up to tens or hundreds of processors, at most.

Quantum-Mechanical Simulations

Matter at high pressure and temperature

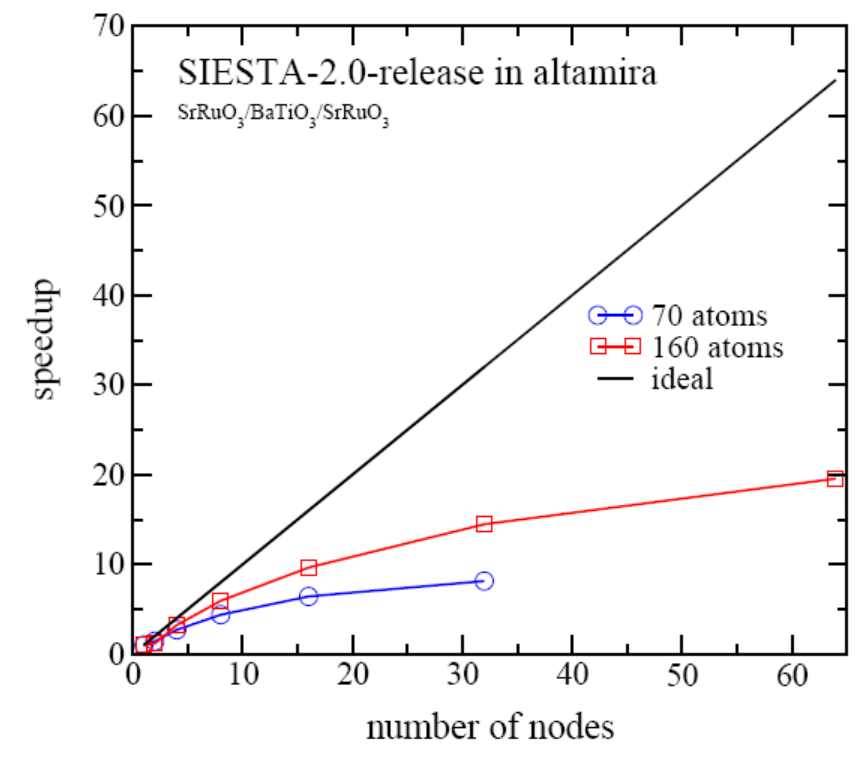
Liquids at Neptune and Uranus
H_2O, CH_4, NH_3

Simulation: 376 atoms
20 GPa - 750^{o}C - 1 ps

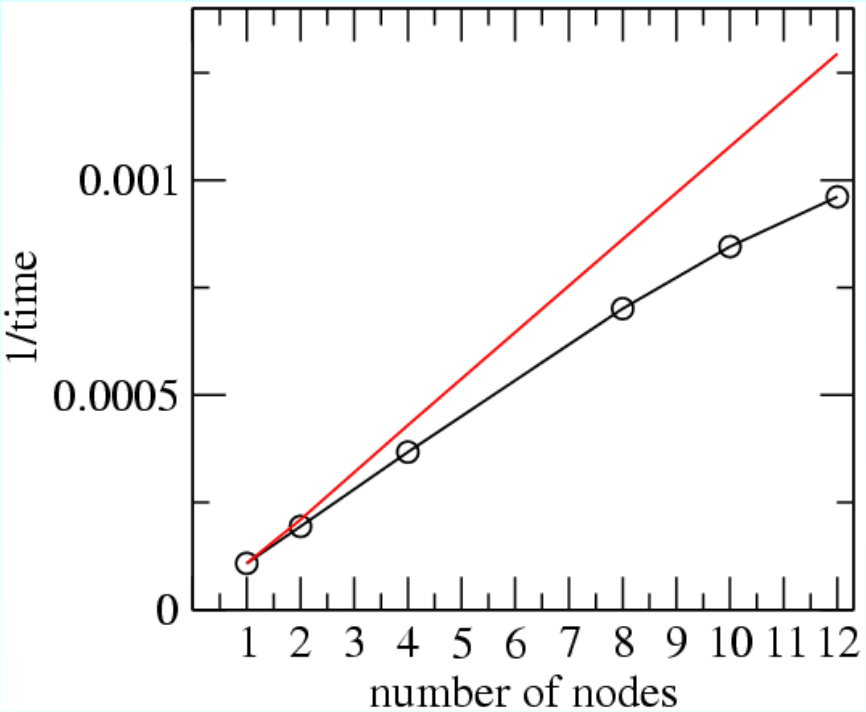
3-4 days of CPU in 32 Processors (MN)

Quantum-Mechanical Simulations

Parallel scaling



SIESTA



VASP

Computing Needs for Mat. Simul.

- Methodological Advances
- Graphical I/O: GUI's
- Visualization/analysis tools
- GRID infrastructures
- Better parallel codes for existing hardware
- Future hardware: Multicore processors?

Computing Needs for Mat. Simul.

- Methodological Advances
  - Time scale problem: 'complexity'
  - Rare events
  - True, robust multi-scaling methods

- Graphical I/O: GUI's
- Visualization/analysis tools
- GRID infrastructures
- Better parallel codes for existing hardware
- Future hardware: Multicore processors?

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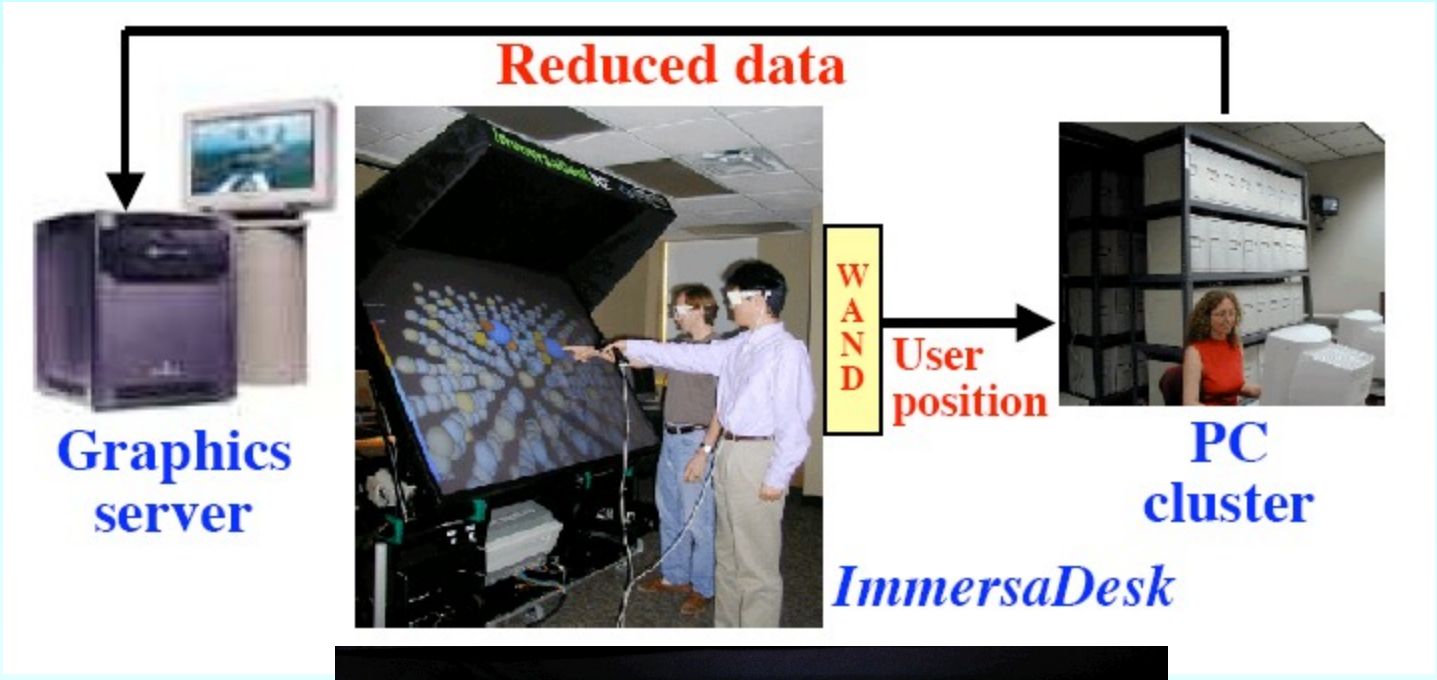
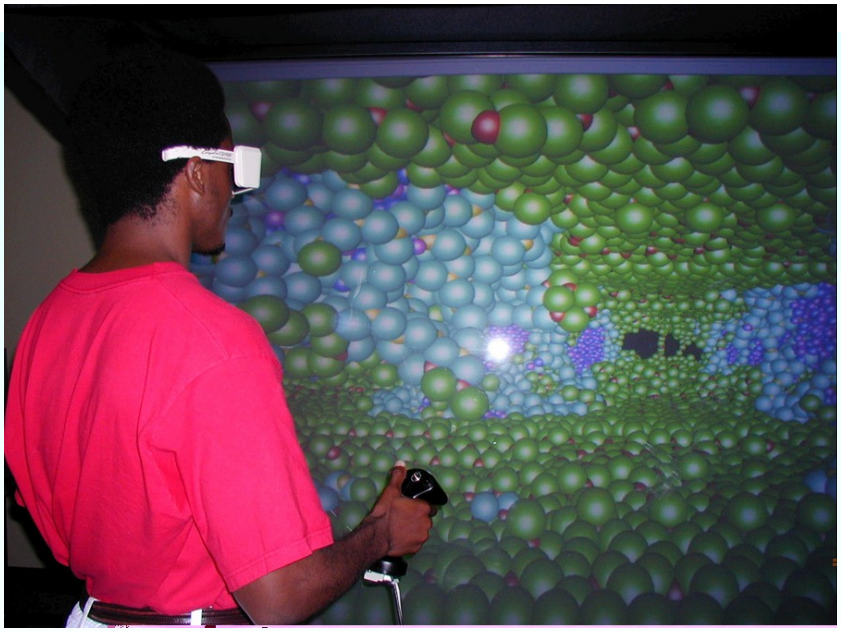
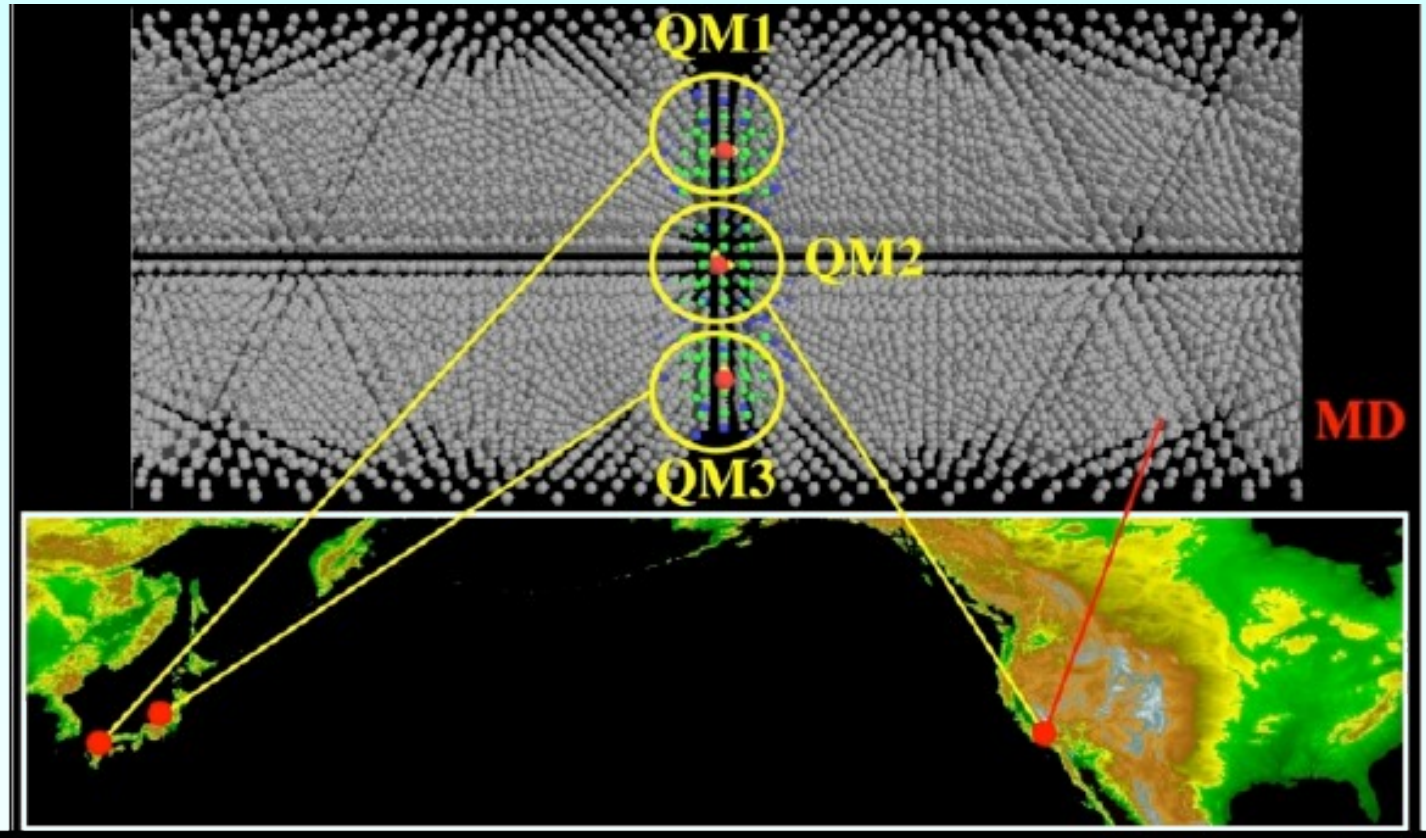

Reduced data
Graphics server
WAND
User position
PC cluster
ImmersaDesk



Computing Needs for Mat. Simul.

- Methodological Advances
- Graphical I/O: GUI's
- Visualization/analysis tools
- GRID infrastructures
  - Monte Carlo, Mol. Dyn. of independent events
  - Parameter Optimization
  - "Divide and Conquer" strategies
- Better parallel codes for existing hardware
- Future hardware: Multicore processors?

Divide and Conquer



GRID Computing between USA and Japan

P. Vashishta, USC.

Computing Needs for Mat. Simul.

- Methodological Advances
- Graphical I/O: GUI's
- Visualization/analysis tools
- GRID infrastructures
- Better parallel codes for existing hardware
  - Distributed Memory
  - Shared Memory
- Future hardware: Multicore processors?

Computing Needs for Mat. Simul.

- Methodological Advances
- Graphical I/O: GUI's
- Visualization/analysis tools
- GRID infrastructures
- Better parallel codes for existing hardware
- Future hardware: Multicore processors? (CELL and others)
  - Enhanced power but huge coding difficulty
  - High-level programming and parallelization languages/tools
  - Compilers

Concluding Remarks

- Simulations in Materials: an important area of research, with increasing demands.
- The methods and supercomputing needs depend on the specific problem.
- Need for faster, more powerful machines, but also for:
  - Programming support/toos (specially for the future multicore processors generation)
  - Graphic interfaces (input/output/analysis)
  - GRID Infrastructures and Tools
  - **Professional support for all this!!!**