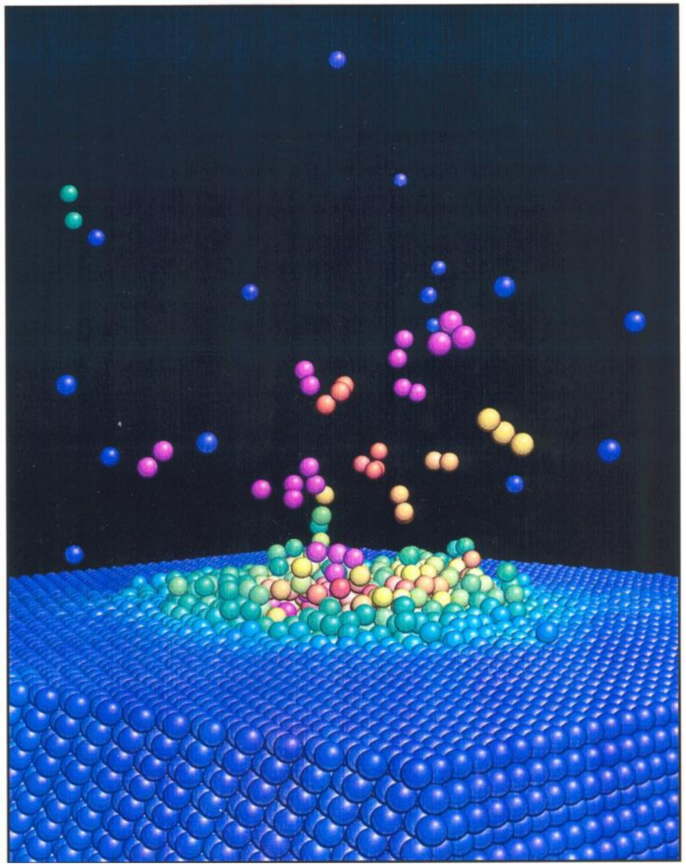
Computational Materials Science
- overview -

Herbert M Urbassek



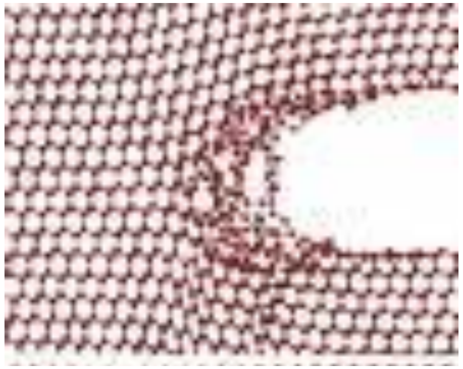
ion impact

fracture

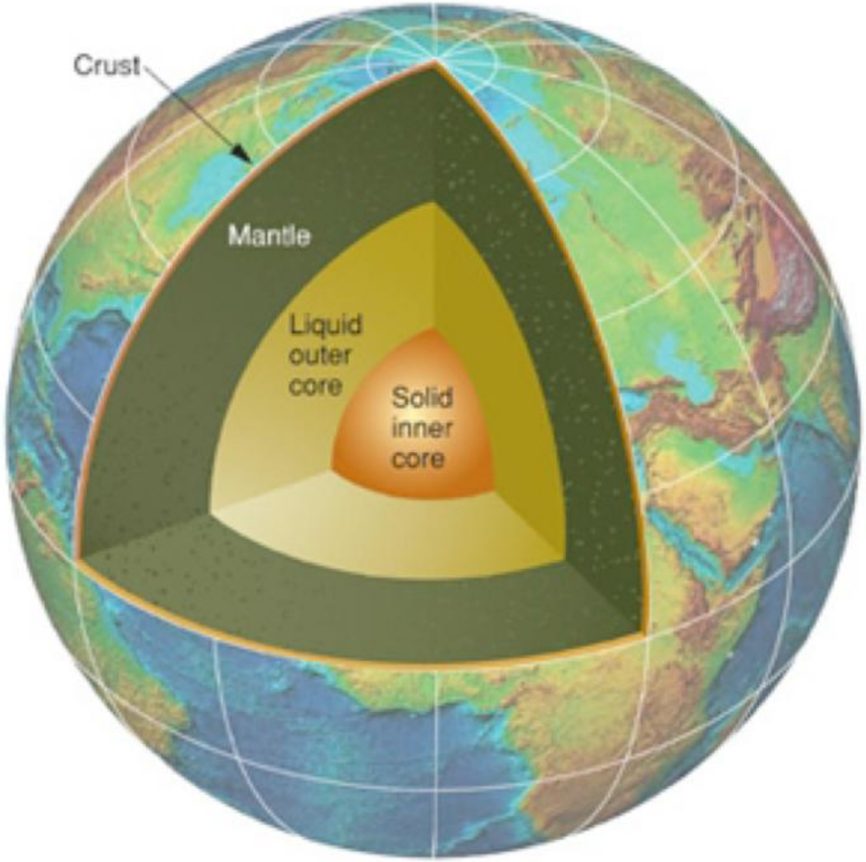
Objective:

understand properties of materials
using modelling
in particular computation

here: atomistic methods



Why modelling?



Fe at temperature 5000 K pressure 300 GPa

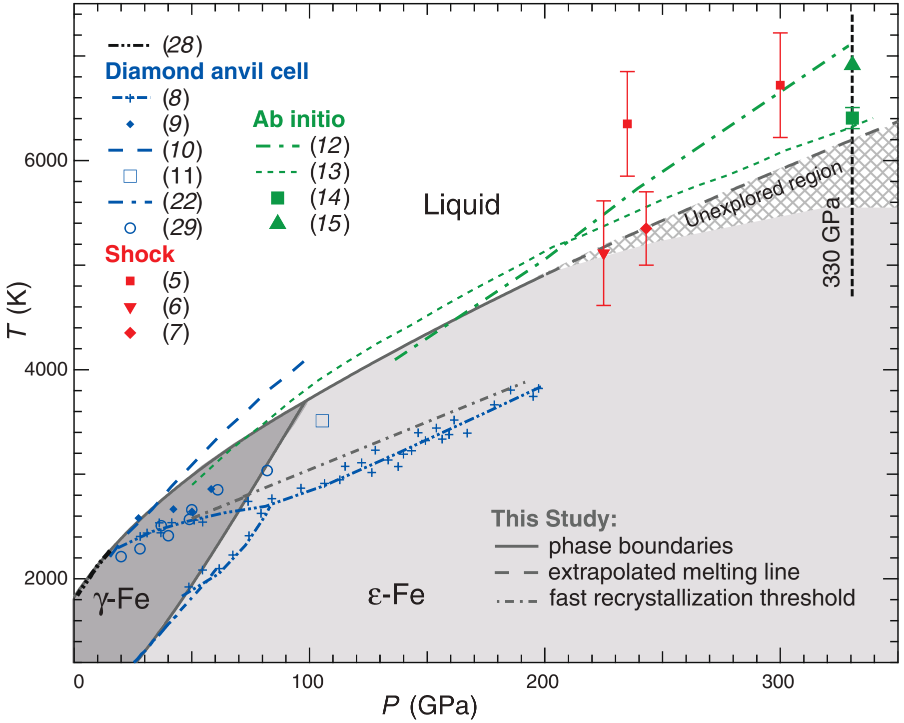


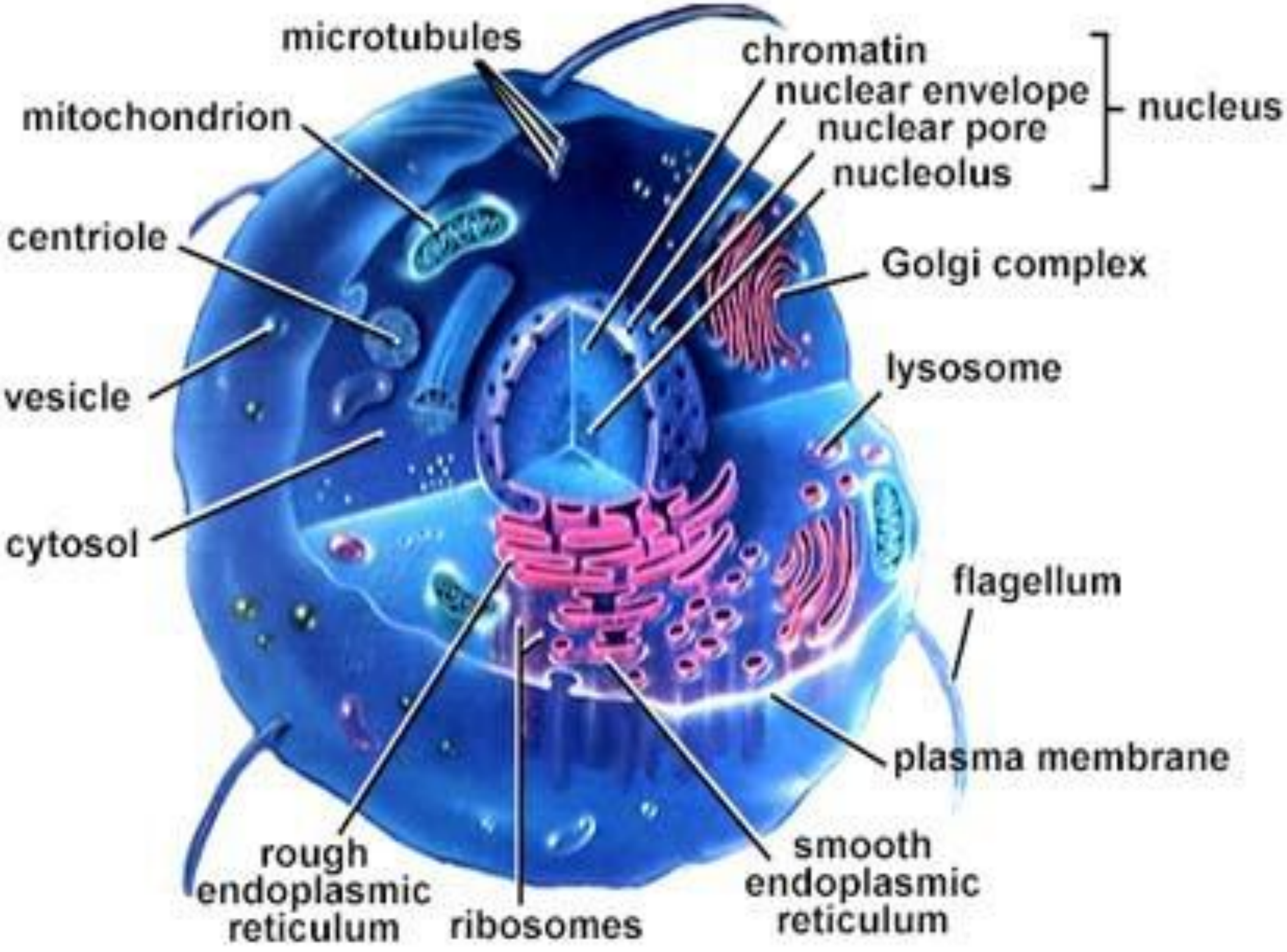
Fig. 3. Phase stability domains for Fe obtained in the literature and in this study. The stability field for ε-Fe is based on the current study data and data from (*19*).

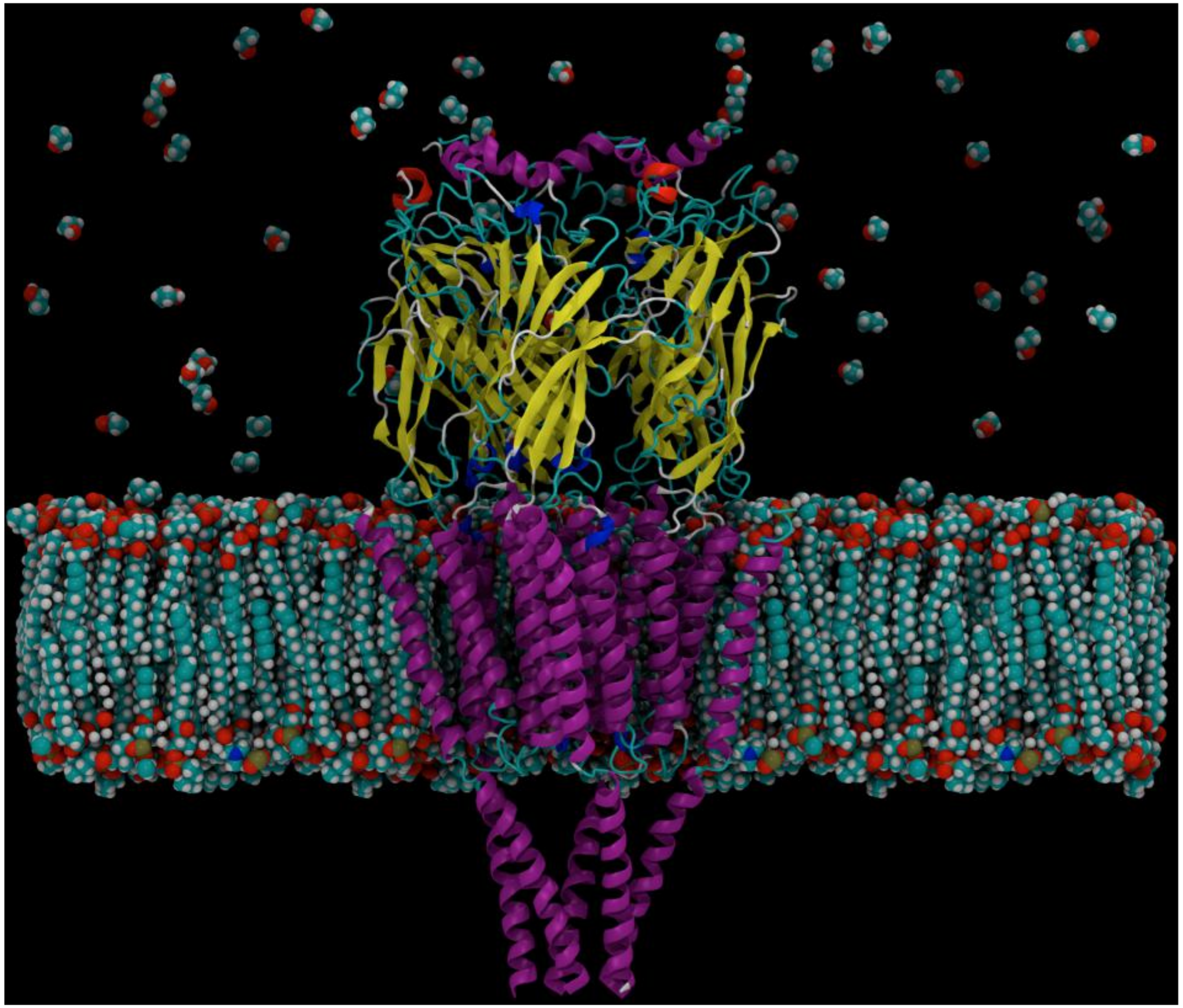
When does iron melt?

Ab initio simulations can help

Anzellini et al., Science 340 (2013) 464

In a cell


microtubules
mitochondrion
centriole
vesicle
cytosol
chromatin
nuclear envelope
nuclear pore
nucleolus
nucleus
Golgi complex
lysosome
flagellum
plasma membrane
rough endoplasmic reticulum
ribosomes
smooth endoplasmic reticulum



passage of ethanol through acetylcholine receptor

Outline

Introduction:
- Why simulation?

Simulation techniques
- Length and time scales
- Multiscale Modelling

Outlook:
- The future of modelling
- Computation and education

Why modeling?

Experiment

observation
measurement

Theory

analytical models
differential equations
mathematical models

Why modeling?

Experiment

observation
measurement

Theory

analytical models
differential equations
mathematical models

Computational Science

numerical methods
large-scale simulation
optimization
big data
virtual reality

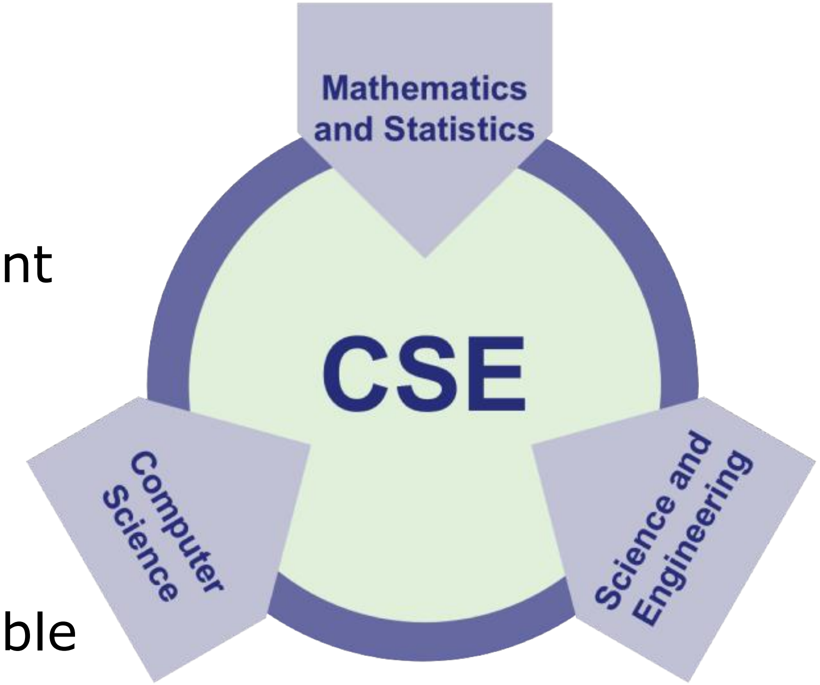
Computational Science and Engineering

Predictive power of computing
marks a new era in science

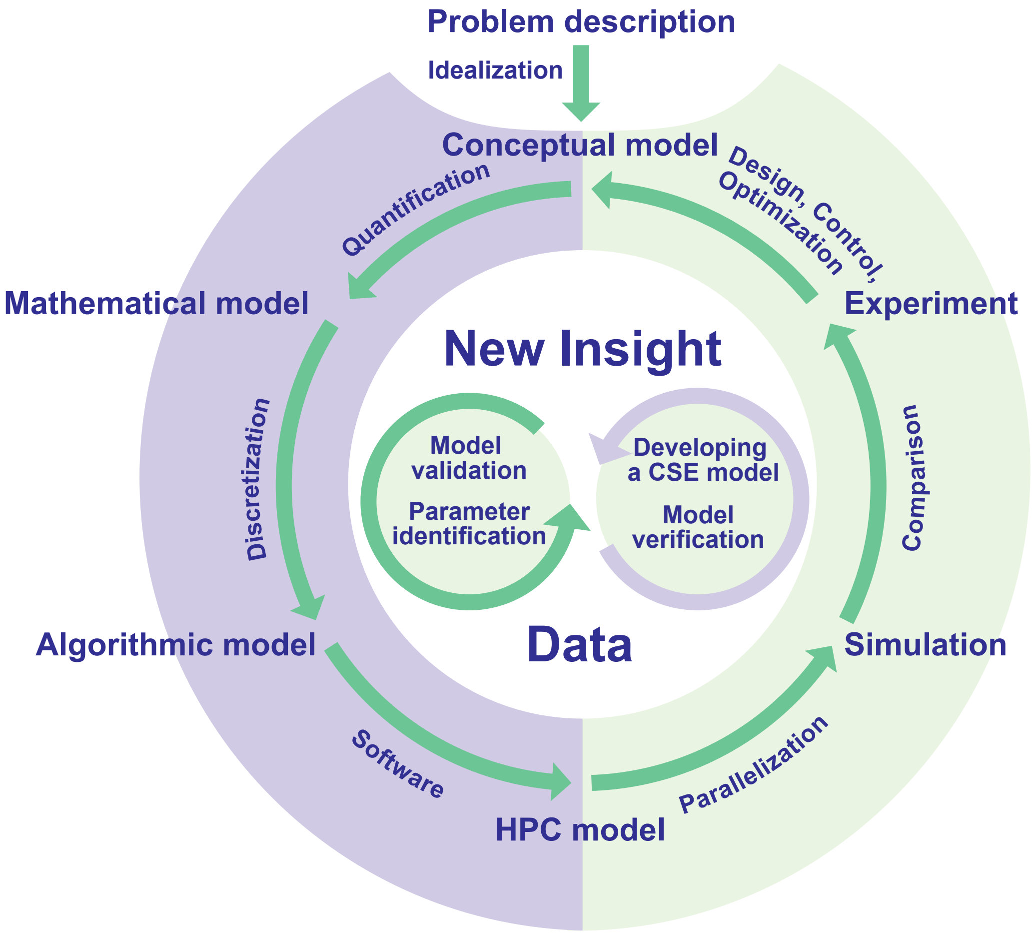
closes the gap
between theory and experiment
of complex models

can get rid of approximations

for some theories
only numerical solutions possible



Rüde et al 2016: Research and Education in Computational Science and Engineering

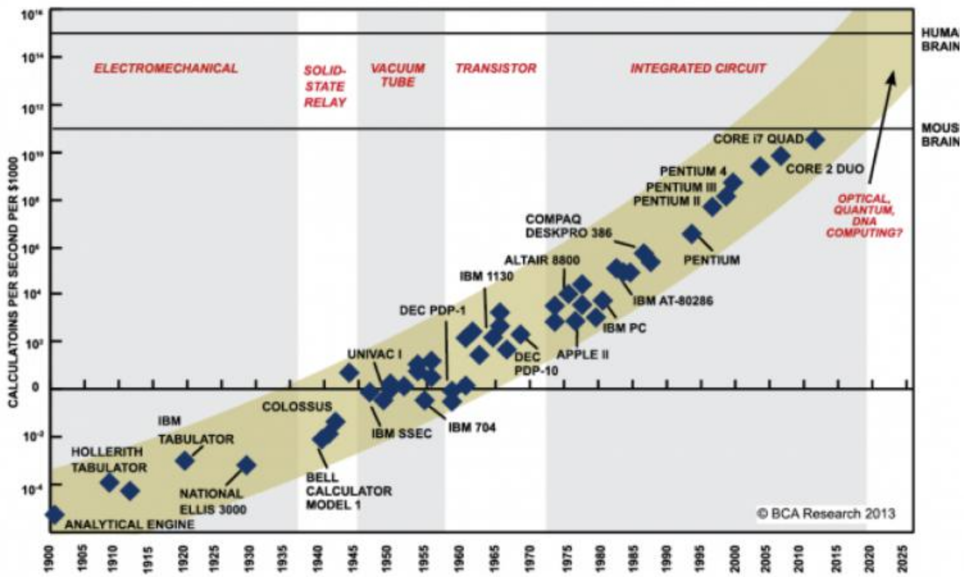


Problem description
Idealization
Conceptual model
Quantification
Mathematical model
Discretization
Algorithmic model
Software
HPC model
Parallelization
Simulation
Comparison
Experiment
Design, Control, Optimization
New Insight
Model validation
Parameter identification
Developing a CSE model
Model verification
Data

A loop: requires multiple passes and feedbacks

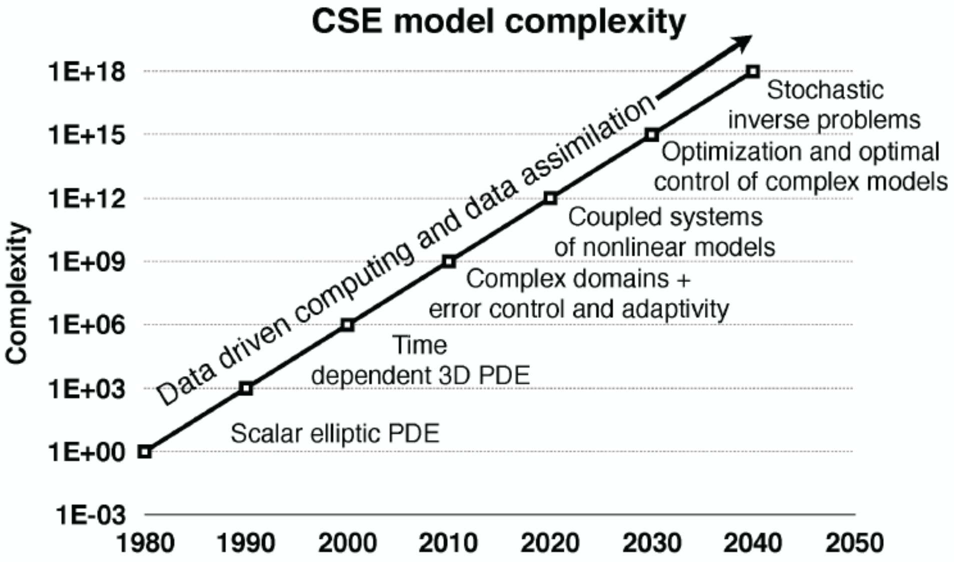
HPC: High Performance
Computing

Moore’s law

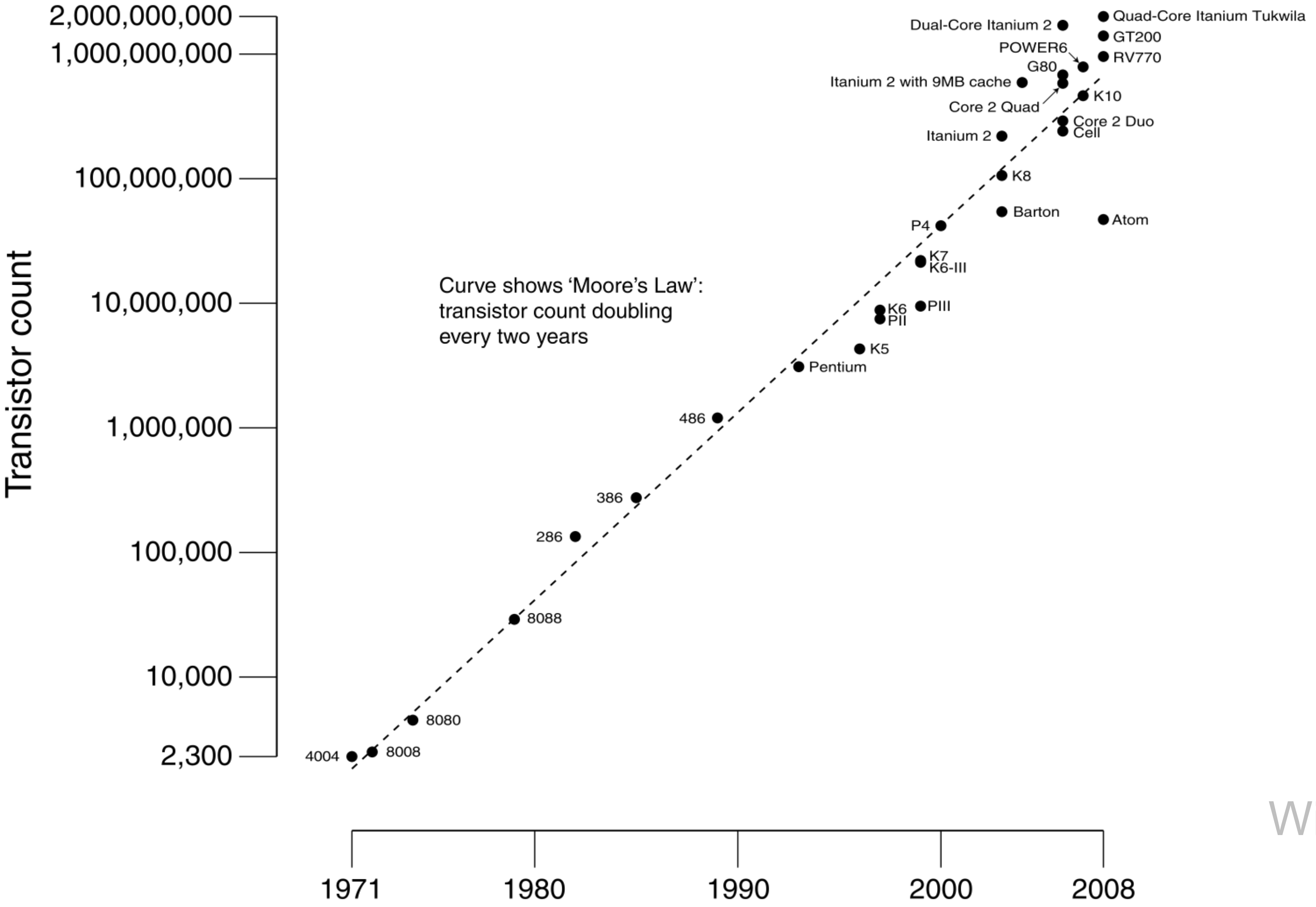


SOURCE: RAY KURZWEIL, "THE SINGULARITY IS NEAR: WHEN HUMANS TRANSCEND BIOLOGY", P.67, THE VIKING PRESS, 2006. DATAPOINTS BETWEEN 2000 AND 2012 REPRESENT BCA ESTIMATES.

calculations per second
per 1000 $

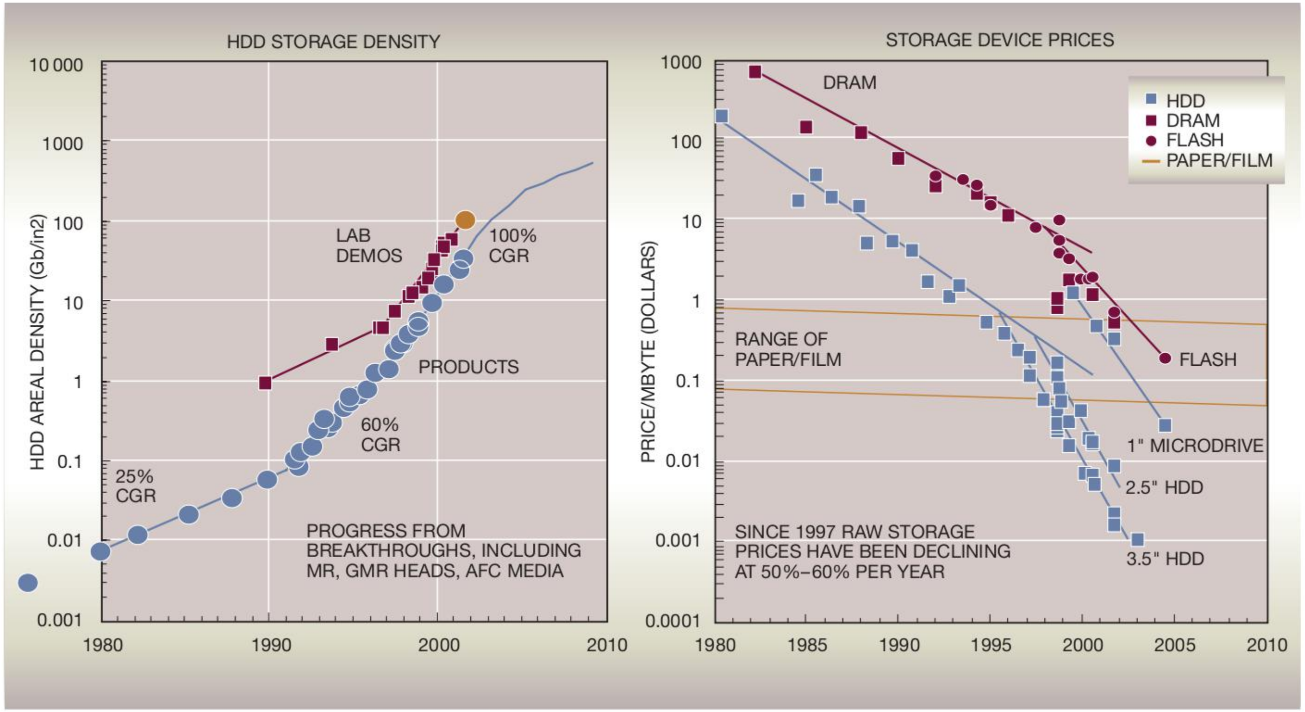


complexity for the example of
3-dimensional Poisson equation


Transistor count
2,000,000,000
1,000,000,000
100,000,000
10,000,000
1,000,000
100,000
10,000
2,300
Curve shows 'Moore's Law': transistor count doubling every two years
Quad-Core Itanium Tukwila
Dual-Core Itanium 2
GT200
POWER6
RV770
G80
Itanium 2 with 9MB cache
Core 2 Quad
K10
Core 2 Duo
Cell
Itanium 2
K8
Barton
Atom
P4
K7
K6-III
K6
PII
PIII
K5
Pentium
486
386
286
8088
8080
8008
4004
1971
1980
1990
2000
2008

Wikipedia

Development of storage



IBM SYSTEMS JOURNAL (2003)42:205

Supercomputer

AHRP **Kaiserslautern**

- Elwetritsch II
  - Dell
  - 144 nodes
  - 2122 Cores

- Mogon II
  - Megware
  - 824 nodes
  - 16.280 cores
  - TOP 500: #265

JUQUEEN

- Blue Gene/Q architecture
- 458,752 PowerPC A2 cores
- 16 cores (1.6 GHz) per node
- 16 GiB RAM per node
- 5D torus interconnect
- 5.8 PFlops Peak
- TOP 500: #19

Sunway TaihuLight

- SW26010 processor
- 10,649,600 cores
- 260 cores (1.45 GHz) per node
- 32 GiB RAM per node
- 125 PFlops Peak
- Power consumption: 15.37 MW
- TOP 500: #1

“Extreme scale” simulations

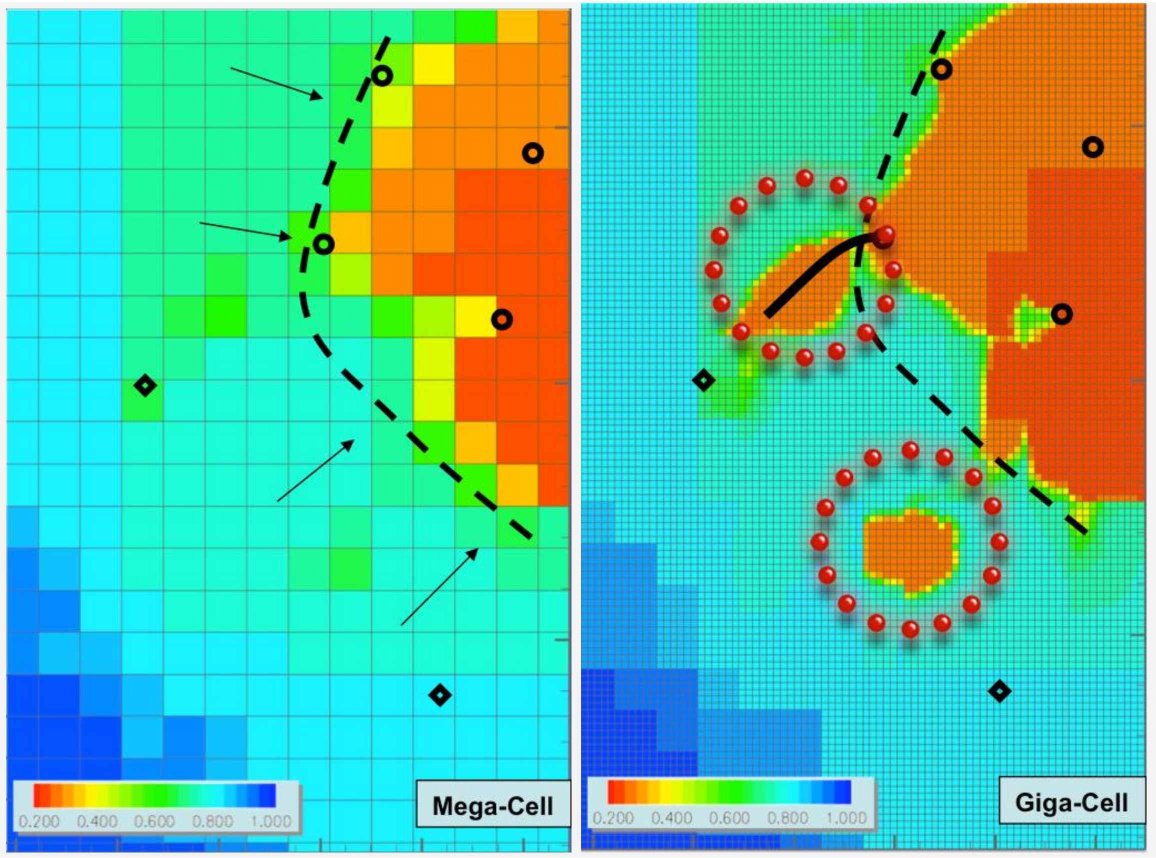
On Juqueen vectors with 10^{13} elements can be stored

10^{12} - these are BIG problems

Energy				
computer generation	gigascale: 10^9 FLOPS	terascale 10^{12} FLOPS	petascale 10^{15} FLOPS	exascale 10^{18} FLOPS
desired problem size DoF=N	10^6	10^9	10^{12}	10^{15}
energy estimate (kWh) 1 NJoule × N^2 all-to-all communication	**0.278 Wh** 10 min of LED light	**278 kWh** 2 weeks blow drying hair	**278 GWh** 1 month electricity for Berlin	**278 PWh** 100 years world electricity production
TerraNeo prototype (kWh)	**0.13 Wh**	**0.03 kWh**	**27 kWh**	**?**

Example:
Petroleum industry

“Correctly predicting a pocket of oil left behind can justify an entire corporate simulation department.”



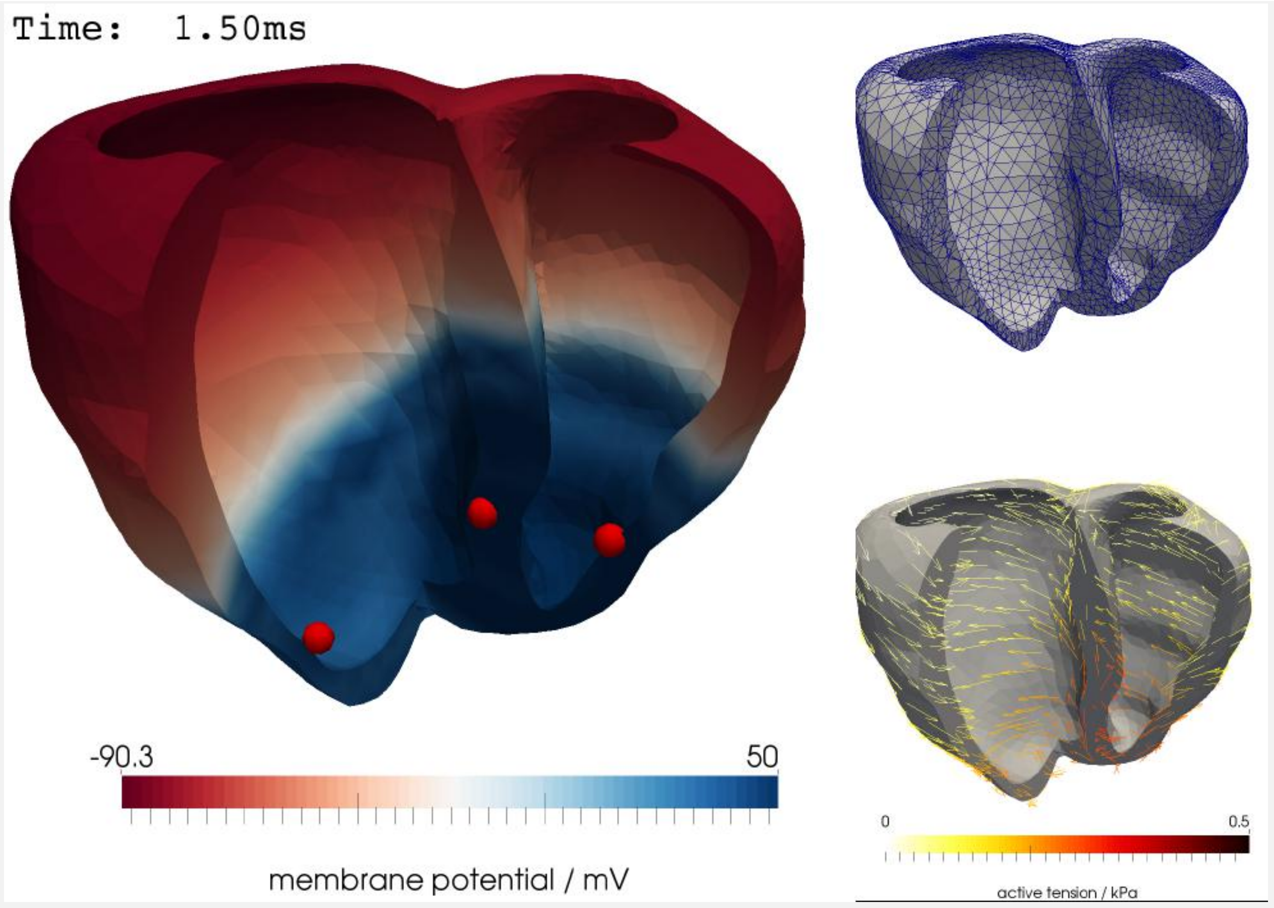
Grid refinement identifies two reservoirs

Rüde et al 2016

Example:
Computational Medicine

Electromechanical activity
in heart:
  - detect scars
  - study diseases
  - place electrodes

"The virtual design and testing of new drugs and therapies accelerate medical progress and reduce cost for development and treatment."

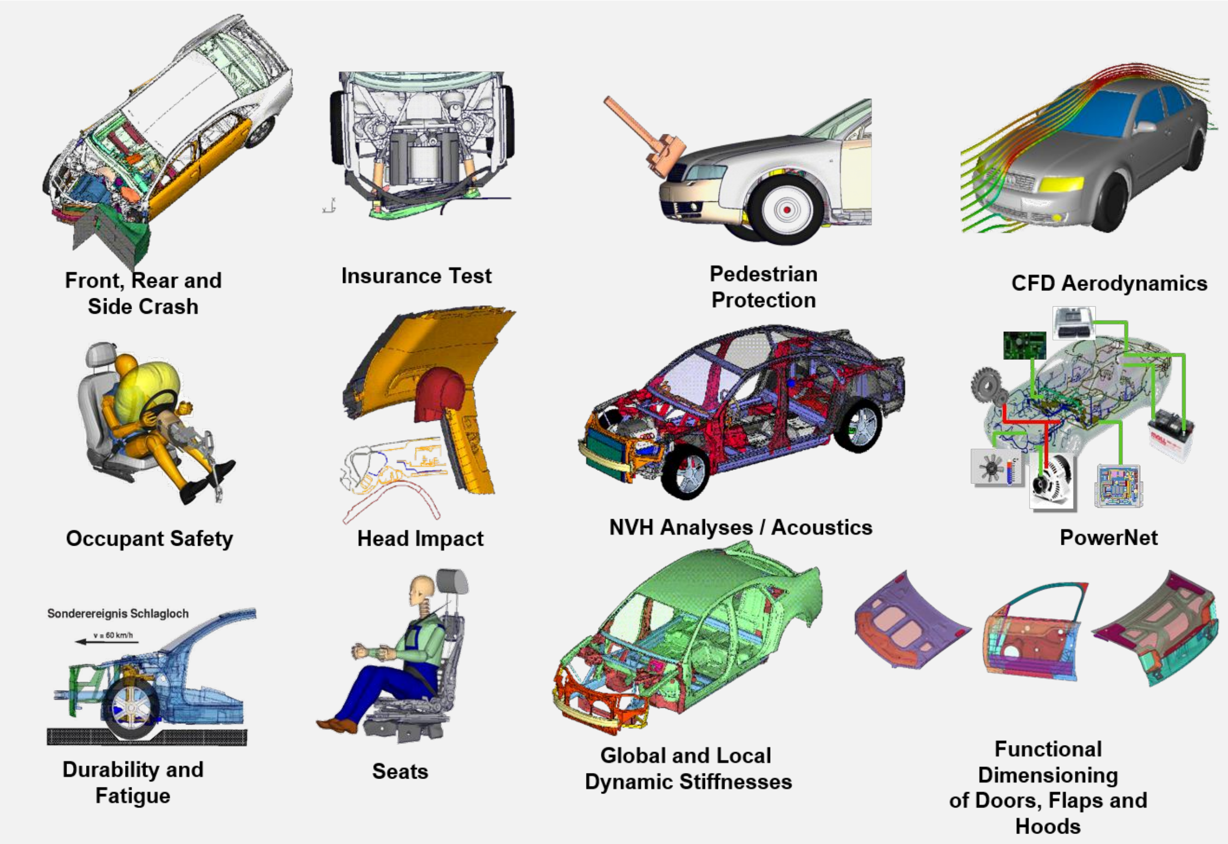


T. Dickopf, T. Krause, R. Kraus, and M. Potse,
SIAM J Sci Comput 36(2), C163- C189, 2014.

Example: Computer-Aided Engineering

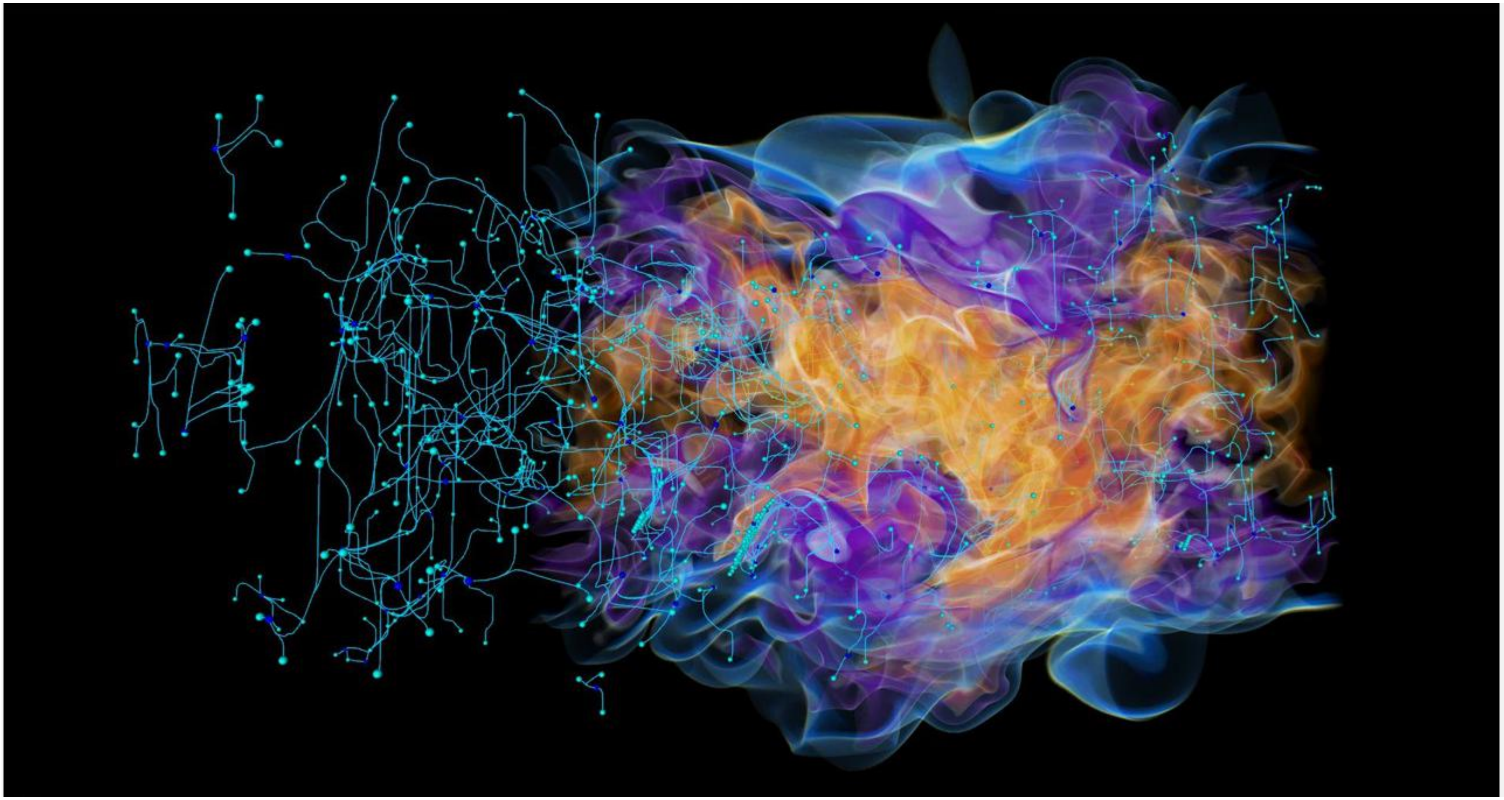
Assess the functional behavior of products early in the design cycle when physical prototypes are not yet available.

„The many advantages of virtual testing compared with physical testing, include flexibility, speed, and cost.“



Rüde et al 2016

Example:
Visual analytics brings insight to TByte of data



Topological analysis (ignition and extinction events) and volume rendering of a combustion simulation.

Rüde et al 2016

Outline

Introduction:
- Why simulation?

Simulation techniques in Materials Science
- Length and time scales
- Multiscale Modelling

Outlook:
- The future of modelling
- Computation and education

Length and time scales

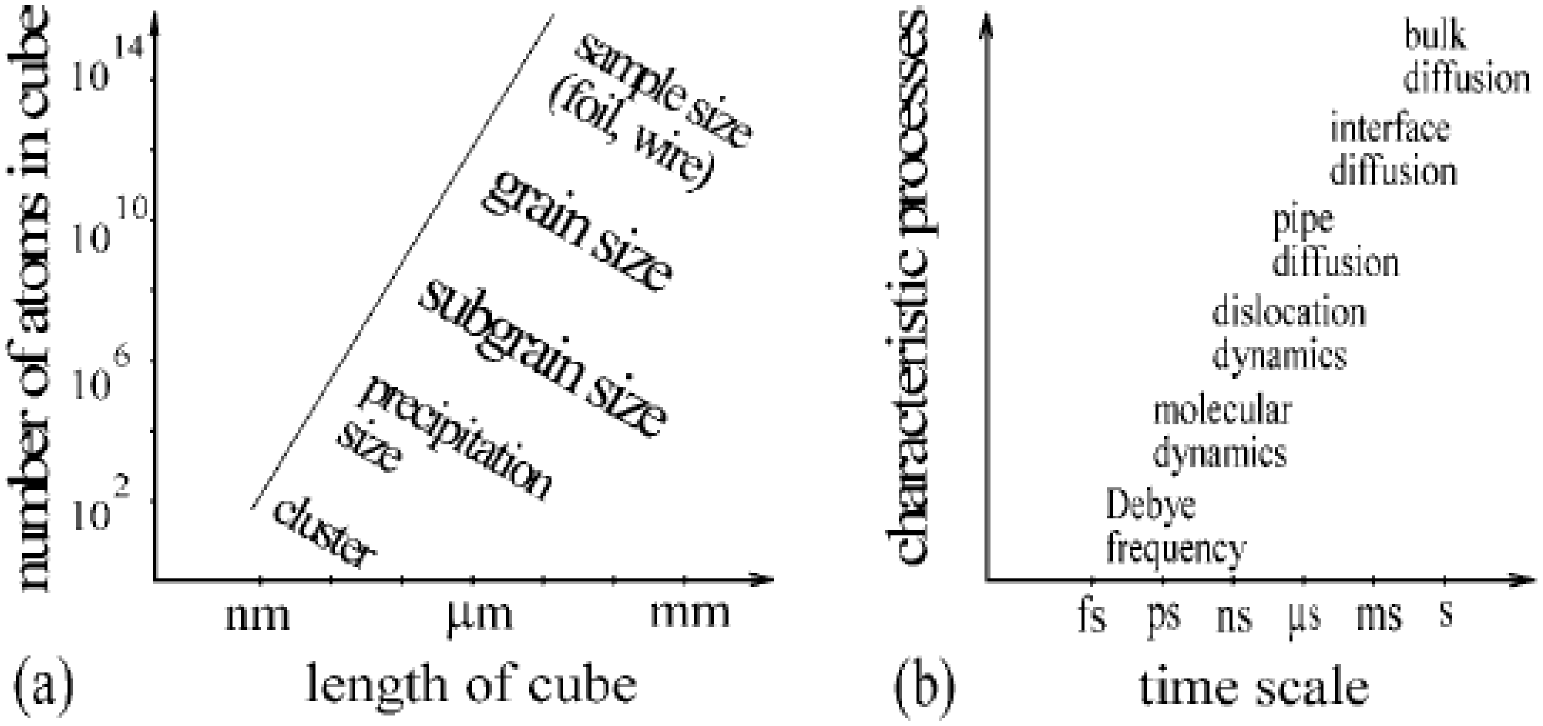
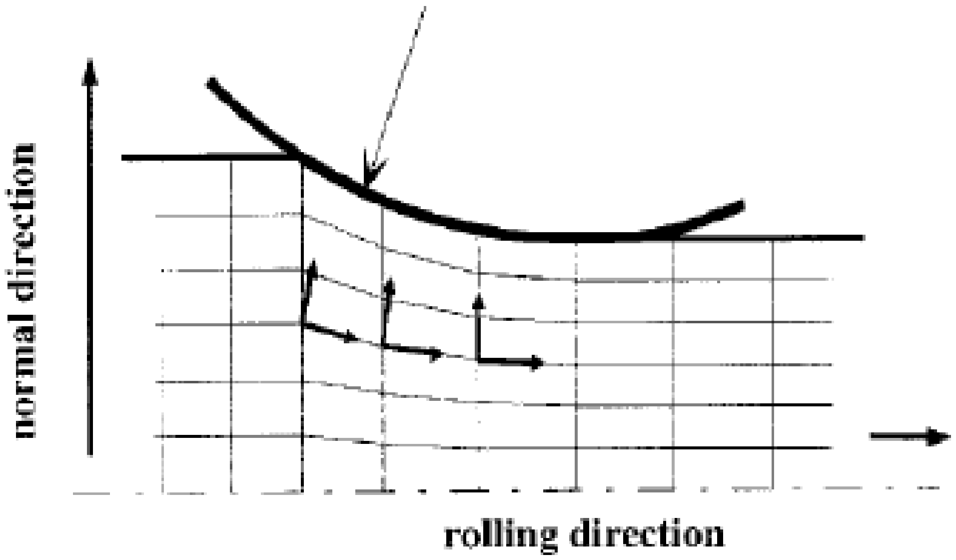


Figure 1.1: Some characteristic space and time scales, (a) number of atoms in a cube, (b) characteristic times of typical simulation problems.

Raabe 98

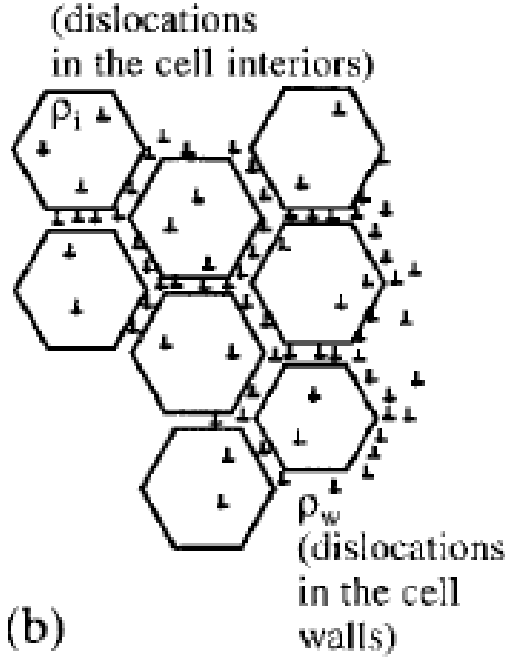
Example:

Plasticity at various scales:

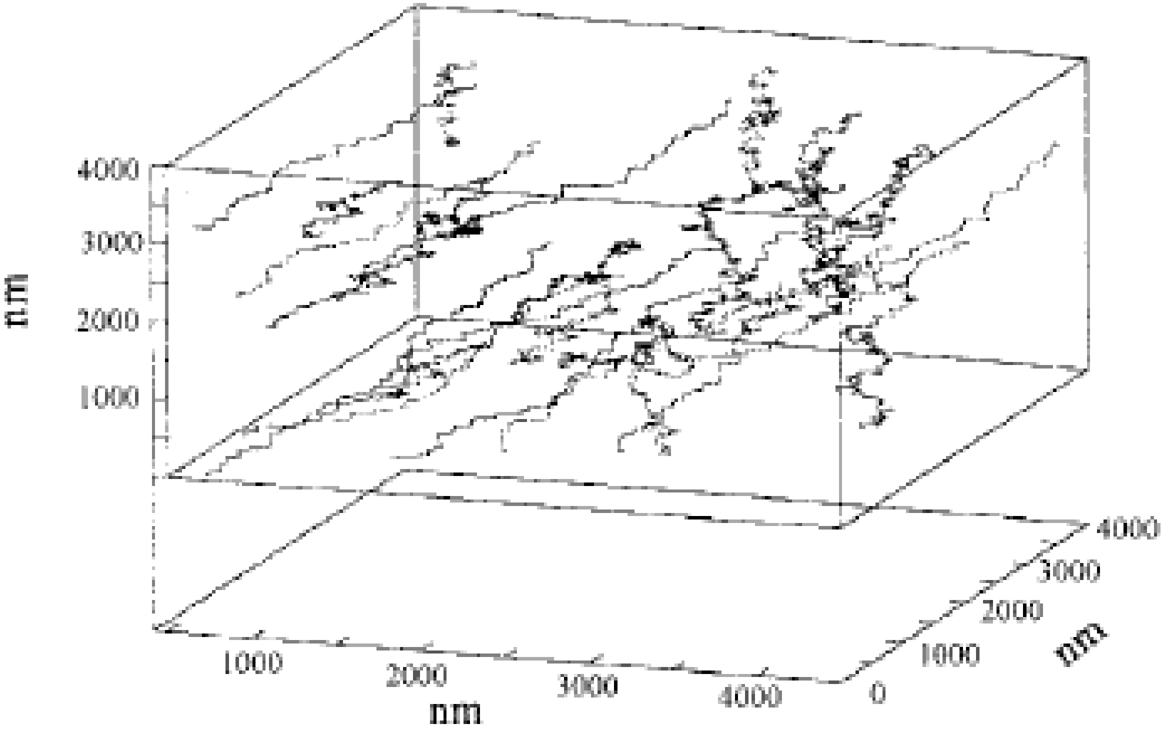


2-dimensional finite-element simulation

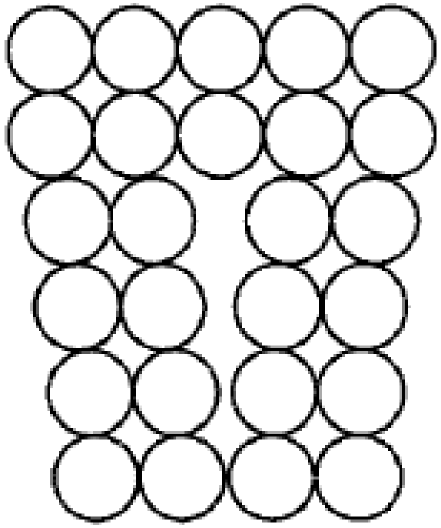
statistical simulations based on parameterized constitutive laws



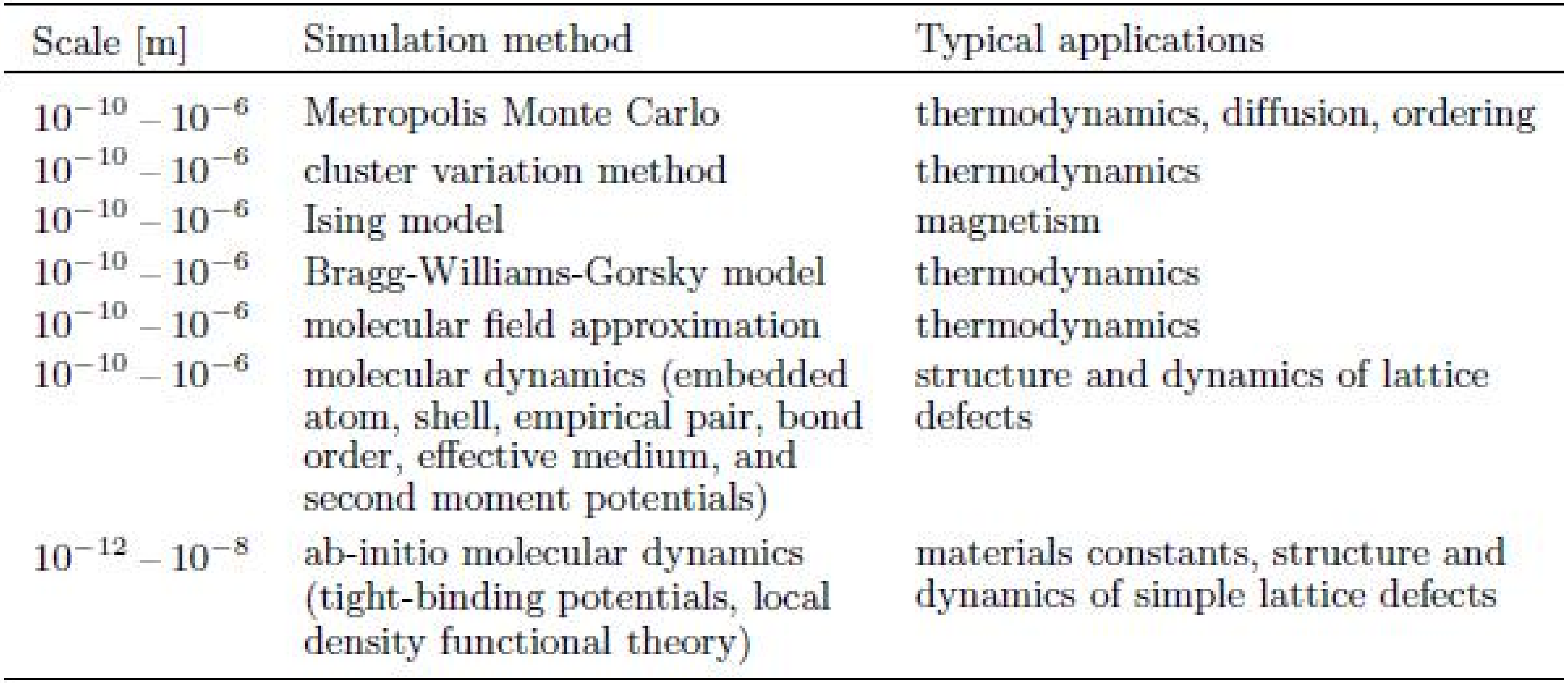
dislocation dynamics



molecular dynamics

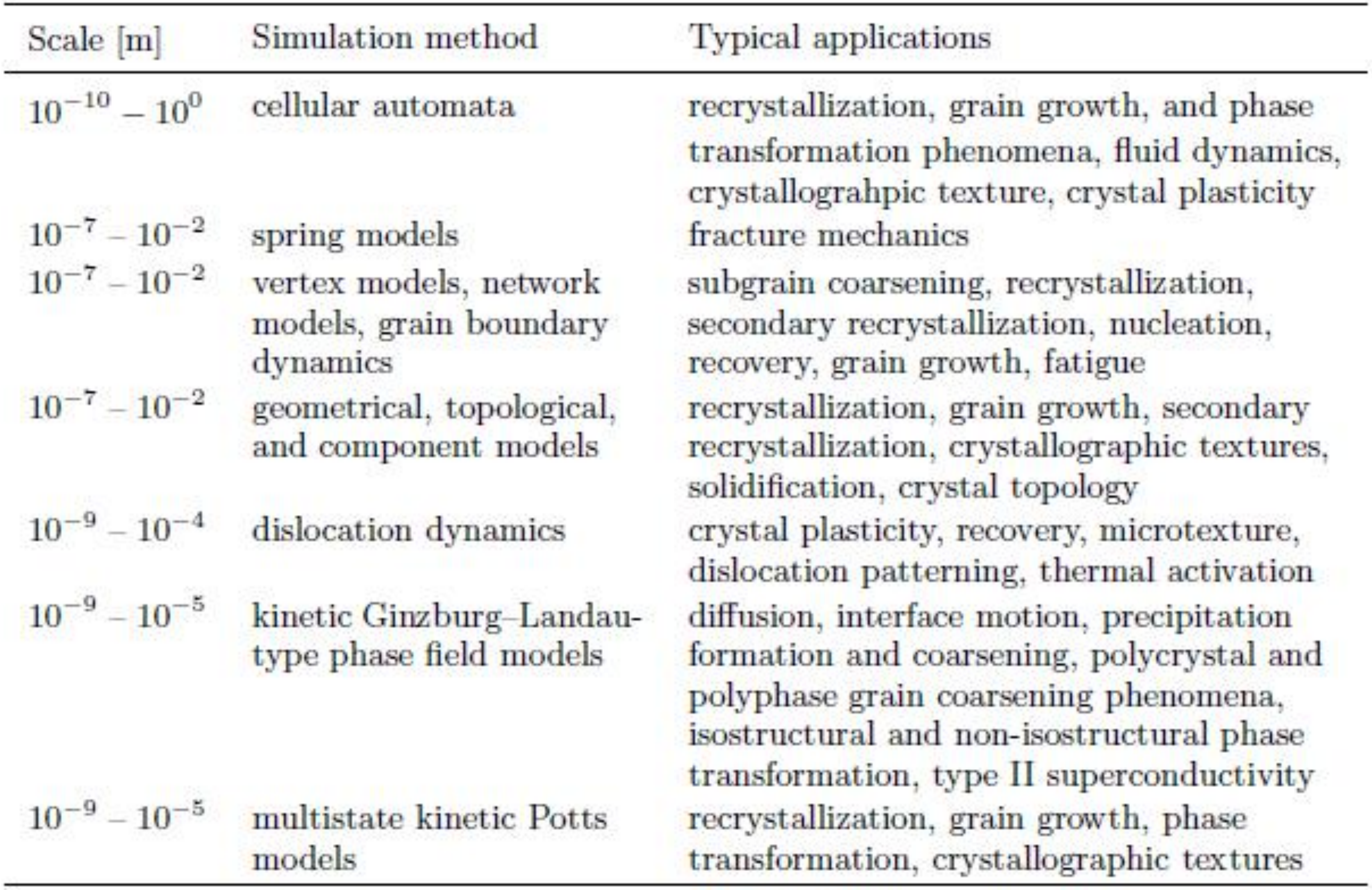


Methods
at the nano-micro level



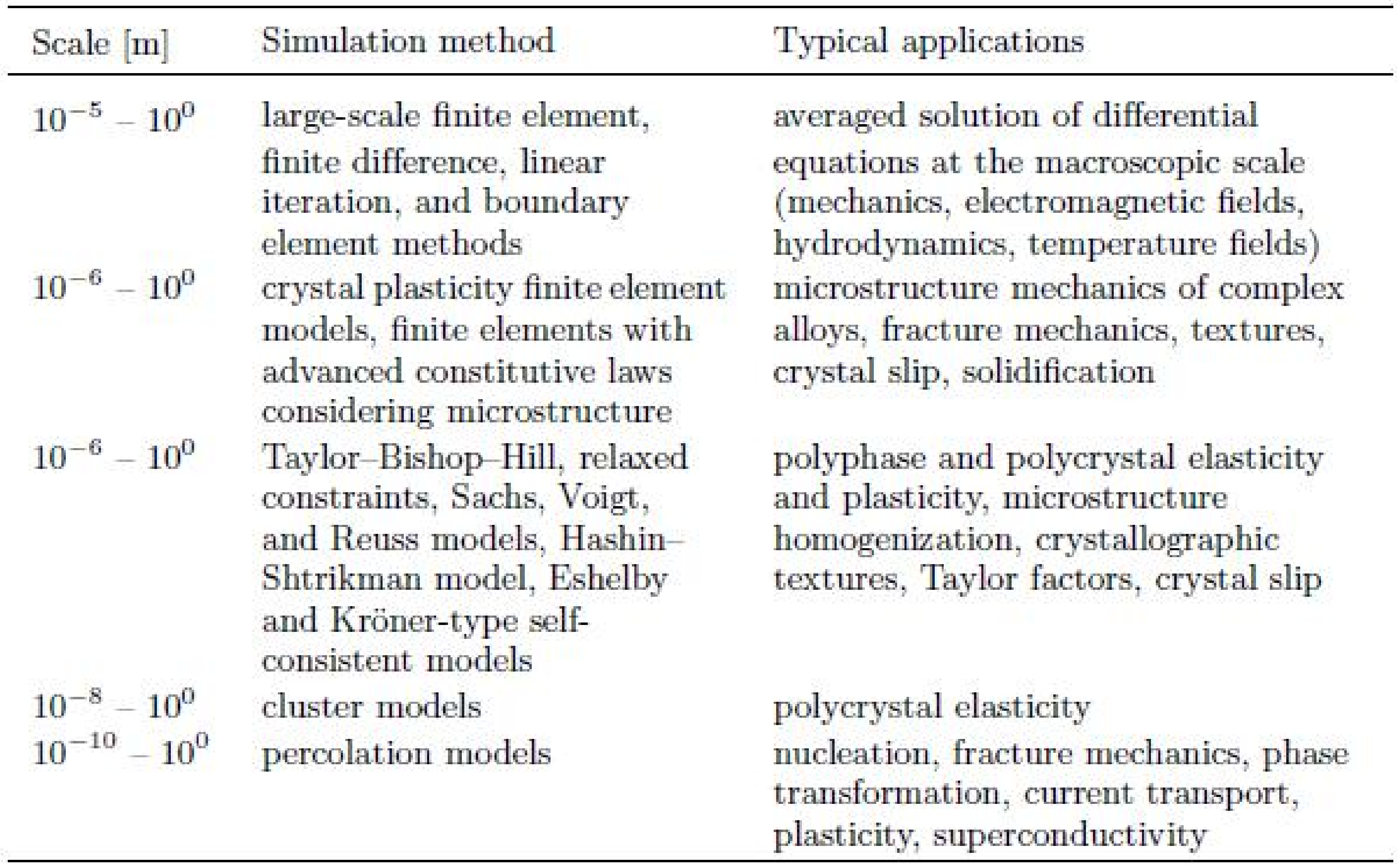
Scale [m]	Simulation method	Typical applications
$10^{-10} - 10^{-6}$	Metropolis Monte Carlo	thermodynamics, diffusion, ordering
$10^{-10} - 10^{-6}$	cluster variation method	thermodynamics
$10^{-10} - 10^{-6}$	Ising model	magnetism
$10^{-10} - 10^{-6}$	Bragg-Williams-Gorsky model	thermodynamics
$10^{-10} - 10^{-6}$	molecular field approximation	thermodynamics
$10^{-10} - 10^{-6}$	molecular dynamics (embedded atom, shell, empirical pair, bond order, effective medium, and second moment potentials)	structure and dynamics of lattice defects
$10^{-12} - 10^{-8}$	ab-initio molecular dynamics (tight-binding potentials, local density functional theory)	materials constants, structure and dynamics of simple lattice defects

Methods at the micro-meso level



Scale [m]	Simulation method	Typical applications
$10^{-10} - 10^{0}$	cellular automata	recrystallization, grain growth, and phase transformation phenomena, fluid dynamics, crystallograhpic texture, crystal plasticity
$10^{-7} - 10^{-2}$	spring models	fracture mechanics
$10^{-7} - 10^{-2}$	vertex models, network models, grain boundary dynamics	subgrain coarsening, recrystallization, secondary recrystallization, nucleation, recovery, grain growth, fatigue
$10^{-7} - 10^{-2}$	geometrical, topological, and component models	recrystallization, grain growth, secondary recrystallization, crystallographic textures, solidification, crystal topology
$10^{-9} - 10^{-4}$	dislocation dynamics	crystal plasticity, recovery, microtexture, dislocation patterning, thermal activation
$10^{-9} - 10^{-5}$	kinetic Ginzburg–Landau-type phase field models	diffusion, interface motion, precipitation formation and coarsening, polycrystal and polyphase grain coarsening phenomena, isostructural and non-isostructural phase transformation, type II superconductivity
$10^{-9} - 10^{-5}$	multistate kinetic Potts models	recrystallization, grain growth, phase transformation, crystallographic textures

Methods
at the meso-macro level

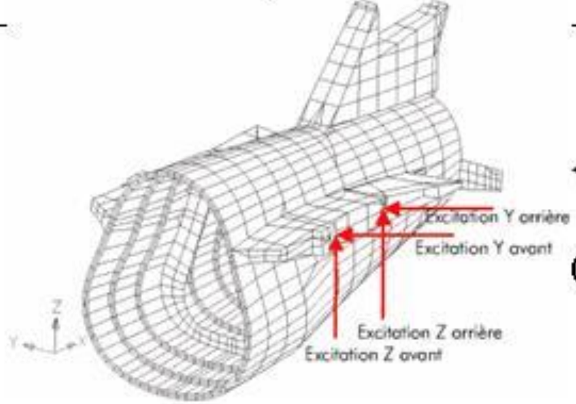


Scale [m]	Simulation method	Typical applications
10^{-5} – 10^{0}	large-scale finite element, finite difference, linear iteration, and boundary element methods	averaged solution of differential equations at the macroscopic scale (mechanics, electromagnetic fields, hydrodynamics, temperature fields)
10^{-6} – 10^{0}	crystal plasticity finite element models, finite elements with advanced constitutive laws considering microstructure	microstructure mechanics of complex alloys, fracture mechanics, textures, crystal slip, solidification
10^{-6} – 10^{0}	Taylor–Bishop–Hill, relaxed constraints, Sachs, Voigt, and Reuss models, Hashin–Shtrikman model, Eshelby and Kröner-type self-consistent models	polyphase and polycrystal elasticity and plasticity, microstructure homogenization, crystallographic textures, Taylor factors, crystal slip
10^{-8} – 10^{0}	cluster models	polycrystal elasticity
10^{-10} – 10^{0}	percolation models	nucleation, fracture mechanics, phase transformation, current transport, plasticity, superconductivity

Multiscale modelling

Pertinent scales

Macroscopic scale



1m

Finite Element Method

Constitutive law

Scale of the grains

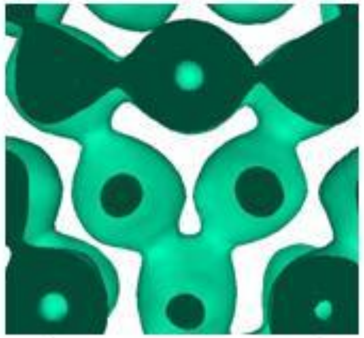
1mm

Homogenization

Constitutive law,
Elastic limit
Hardening coef.

Multiscale modeling:
Transfer information from the finer to the higher scales

Scale of the electrons

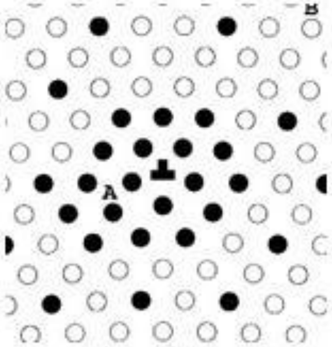


1 Å

Ab Initio Methods

Energies

Scale of the atoms

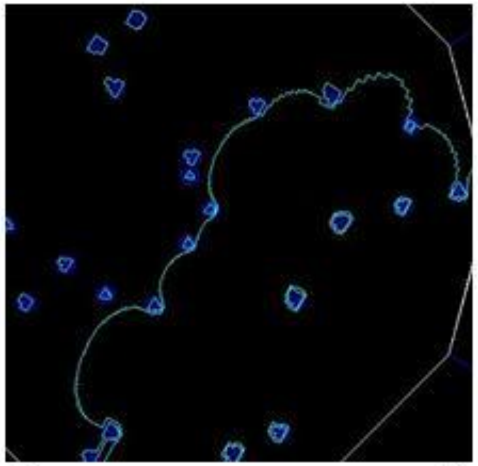


1 nm

Molecular Dynamics
Monte Carlo

Dislo mobility
Annihilation dist.
Precipitate shape

Scale of the defects



1 µm

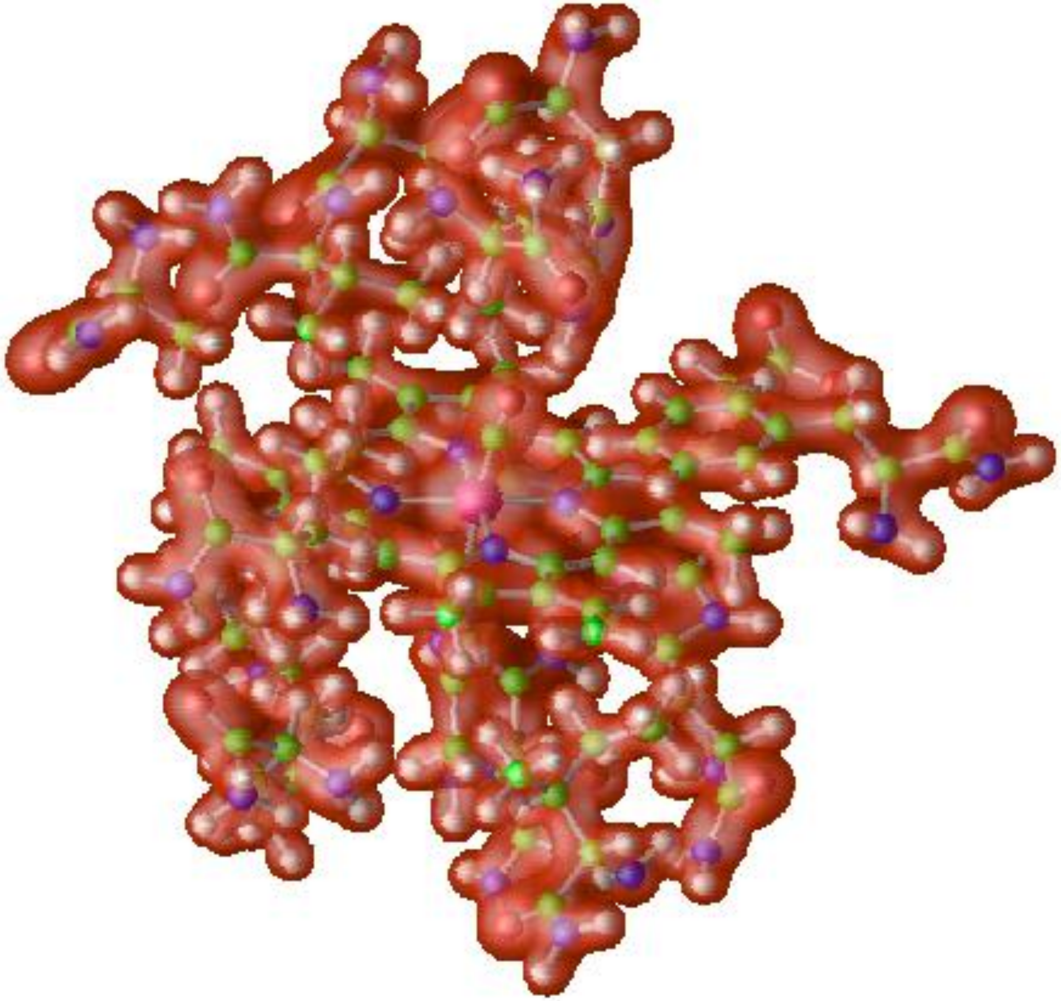
Dislocation Dynamics
Phase field

Simulation techniques:
Outline

- ab initio techniques: electron structure
- atomistic techniques: molecular dynamics
- statistical techniques: kinetic Monte Carlo
- mesoscopic technique: granular mechanics

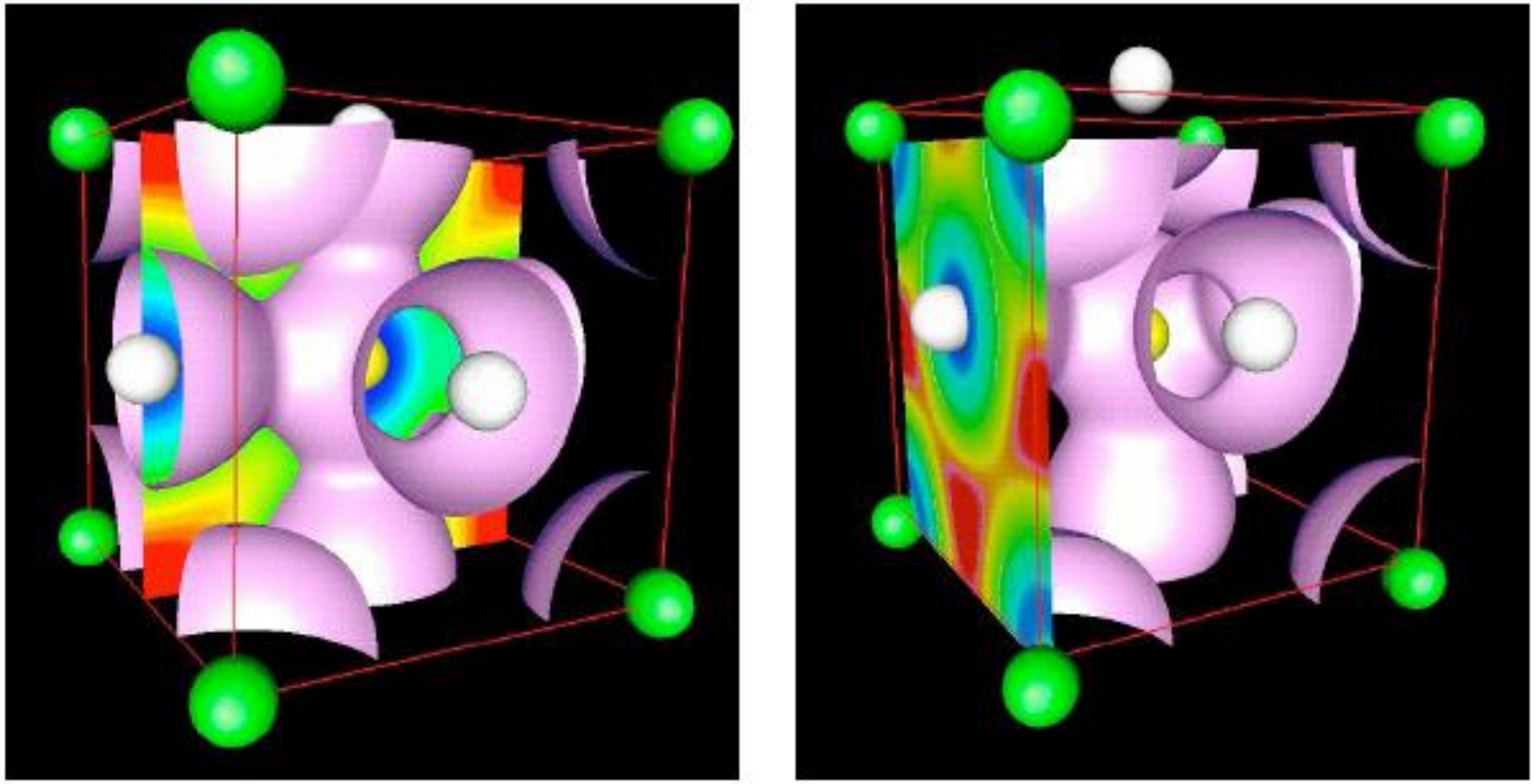
Ab initio modelling

IT'S A QUANTUM WORLD !



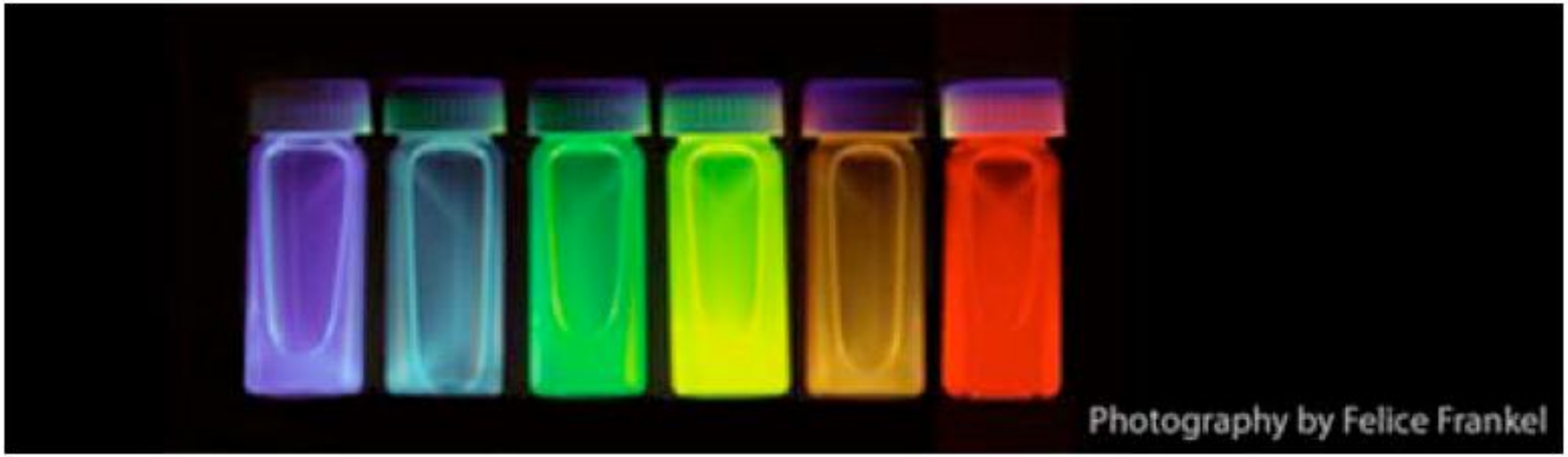
Why do we need quantum mechanics ?

1) Bonding and Structure



Paraelectric (cubic) and ferroelectric (tetragonal) phases of $PbTiO_3$

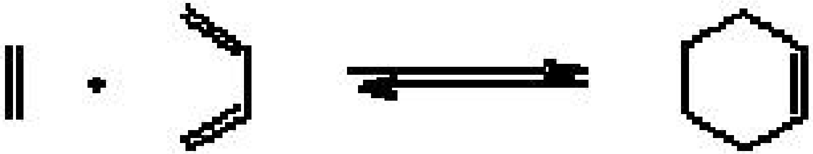
2) Electronic, optical, magnetic properties


Photography by Felice Frankel

3) Dynamics, chemistry

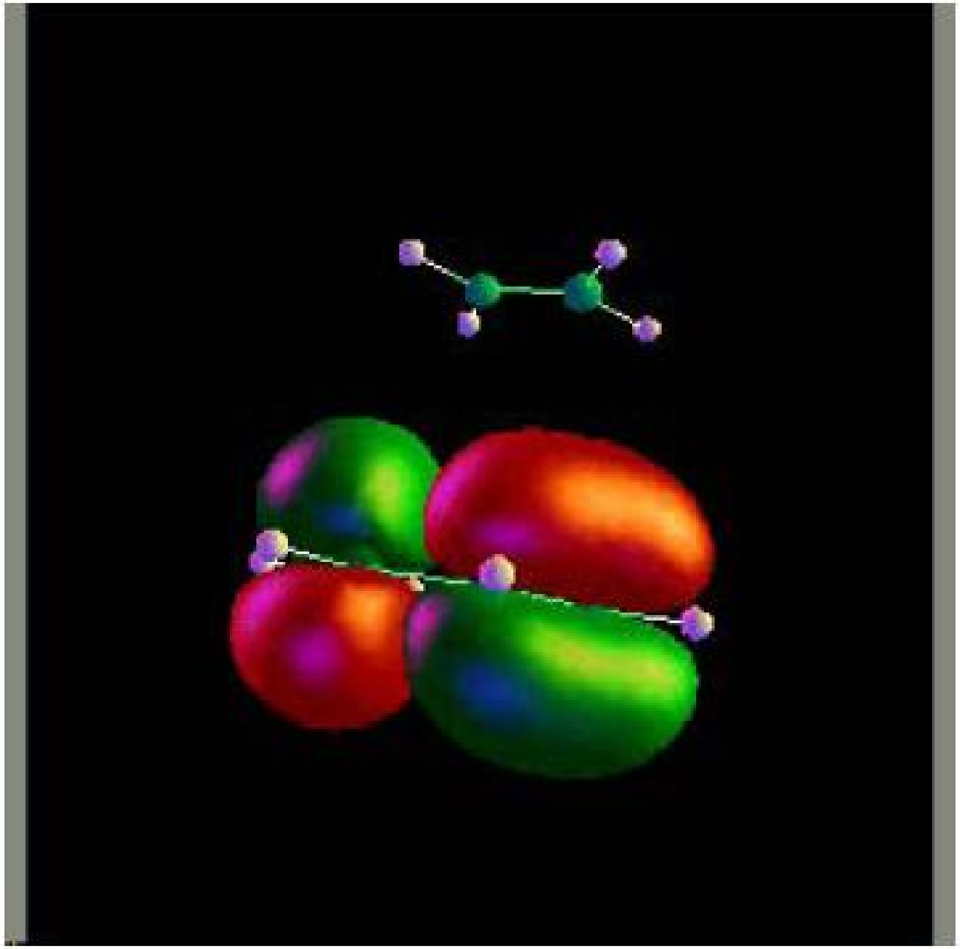
Diels-Alder Reaction:

1,3-butadiene + ethylene → cyclohexene

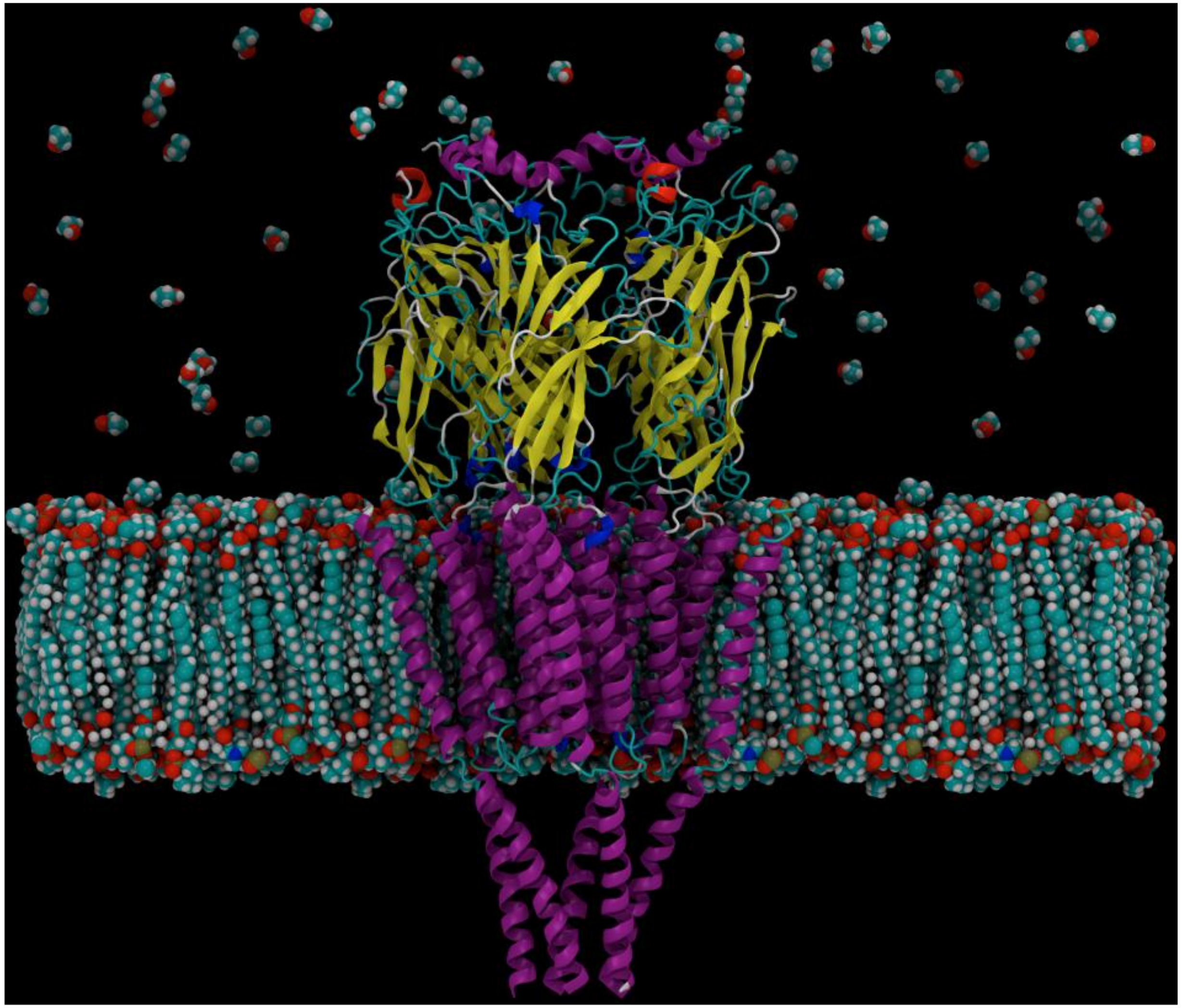


http://www.wag.caltech.edu/home-pages/jim/

Courtesy of James Kendall. Used with permission.



Molecular dynamics



Outline

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Simulation techniques

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computational cluster

The future of modeling

What does more computing buy you ?

Doubling every two years

40 years -> 10^6 increase in performance

But, … scaling

Molecular Dynamics with potentials	**O(N)**
DFT (LDA, GGA)	**O(N^3 or N^2log(n))**
Hartree Fock	**O(N^4)**

Method	Today (atoms)	+40 years
MD (potentials)	10^8 atoms	10^{14} atoms
LDA (N^3)	1000	100,000
LDA(N)	1000	10^9
HF +CI(N^6)	10	100

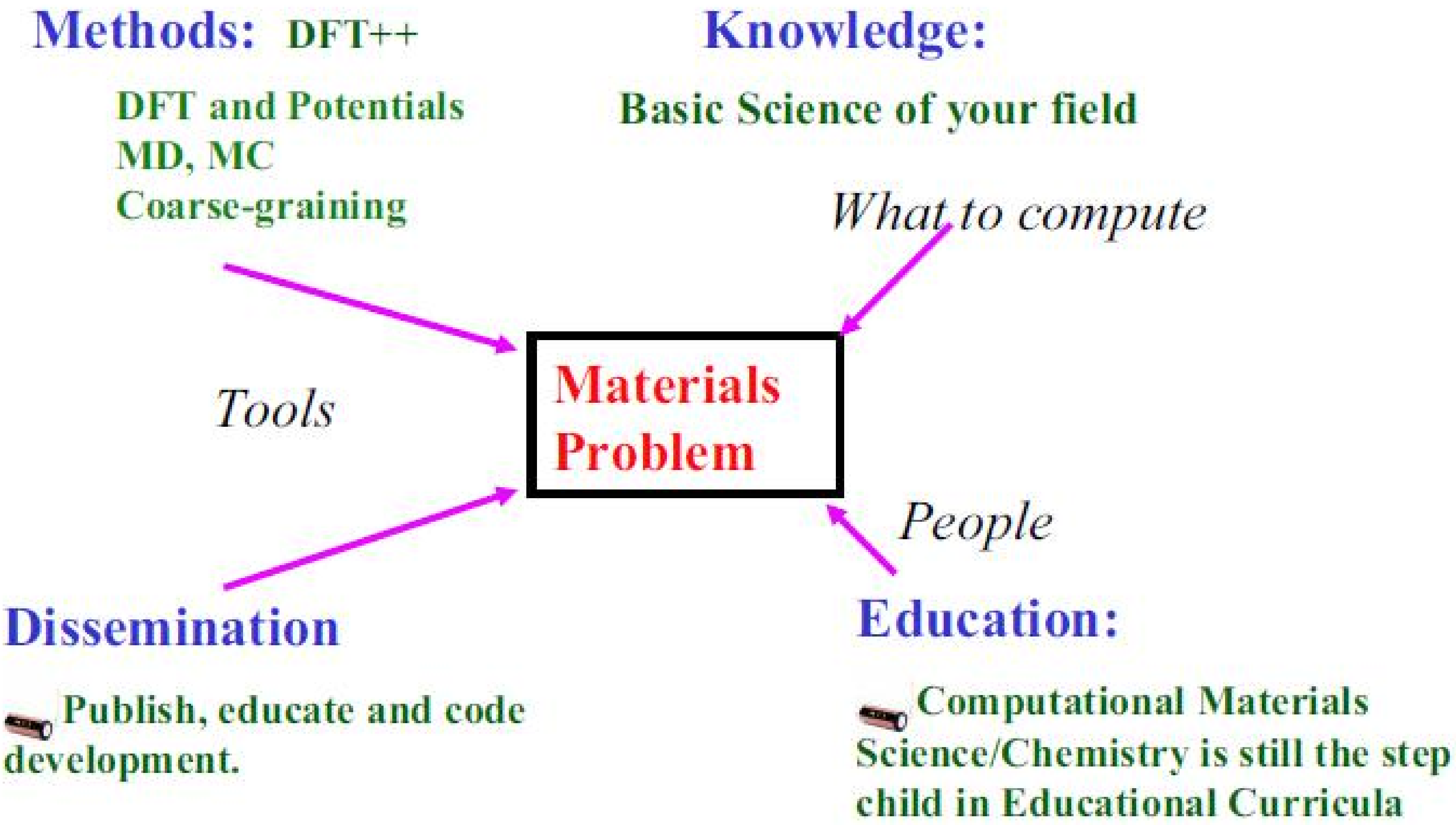
Scaling for length

$N = L^3$

Towards Predictive Science

Computation and education

Issues: How to make impact ?



Methods: **DFT++**

DFT and Potentials
MD, MC
Coarse-graining

Tools

Knowledge:

Basic Science of your field

What to compute

Materials Problem

Dissemination

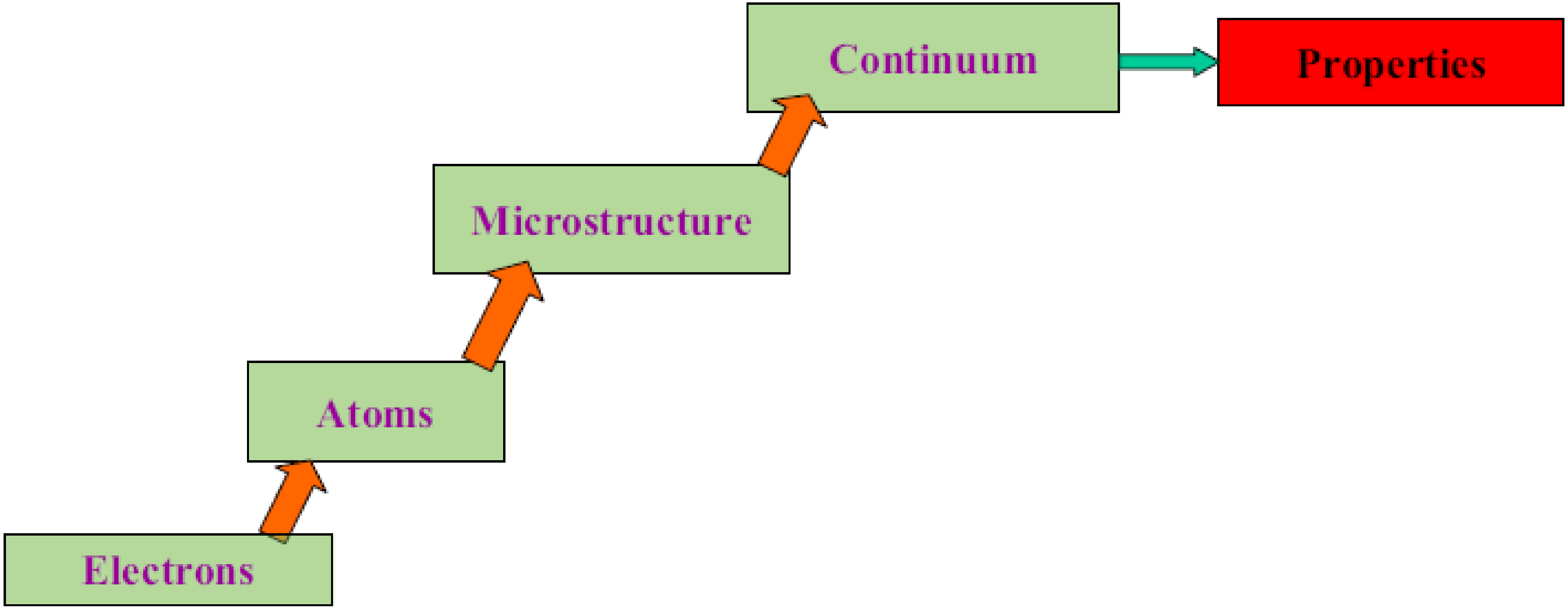
Publish, educate and code development.

People

Education:

Computational Materials Science/Chemistry is still the step child in Educational Curricula

Theory of Properties: The Multi-Scale Materials View



Electrons

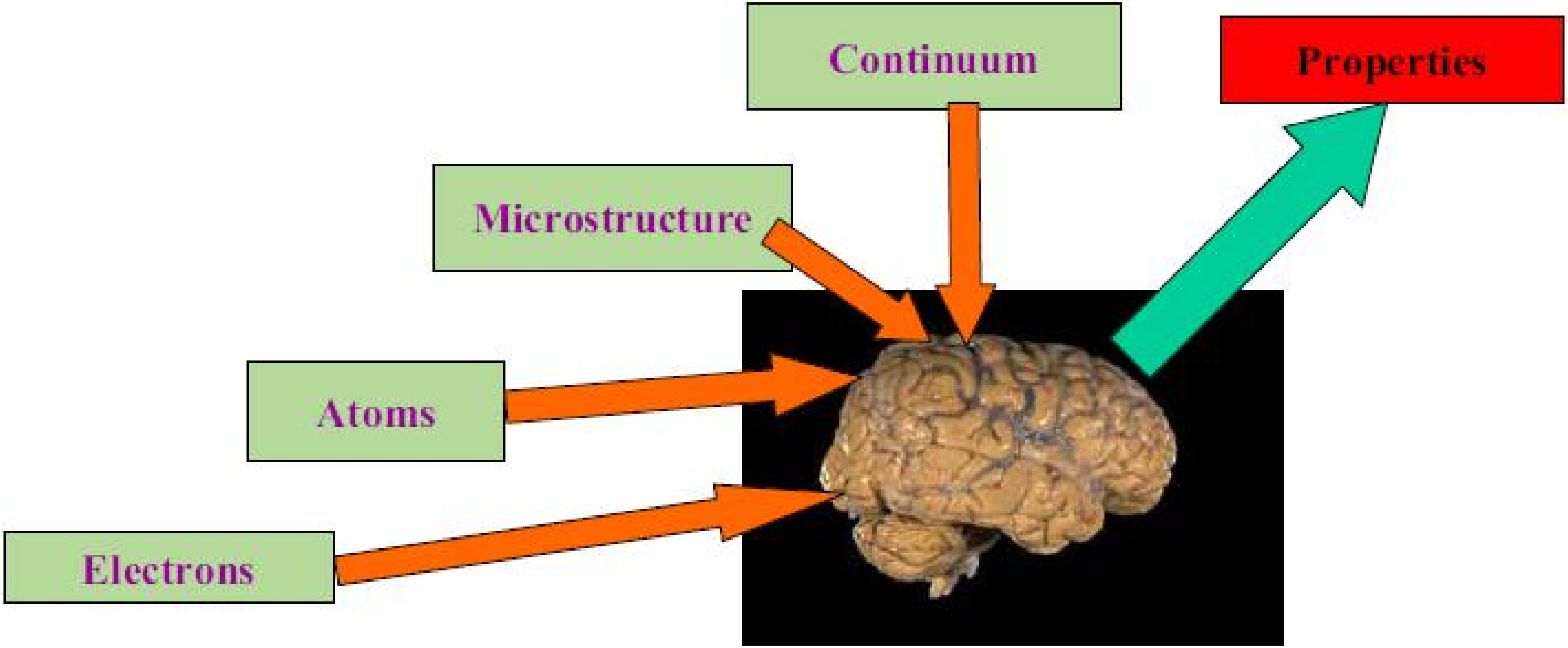
Atoms

Microstructure

Continuum

Properties

Theory of Properties: A More Realistic View



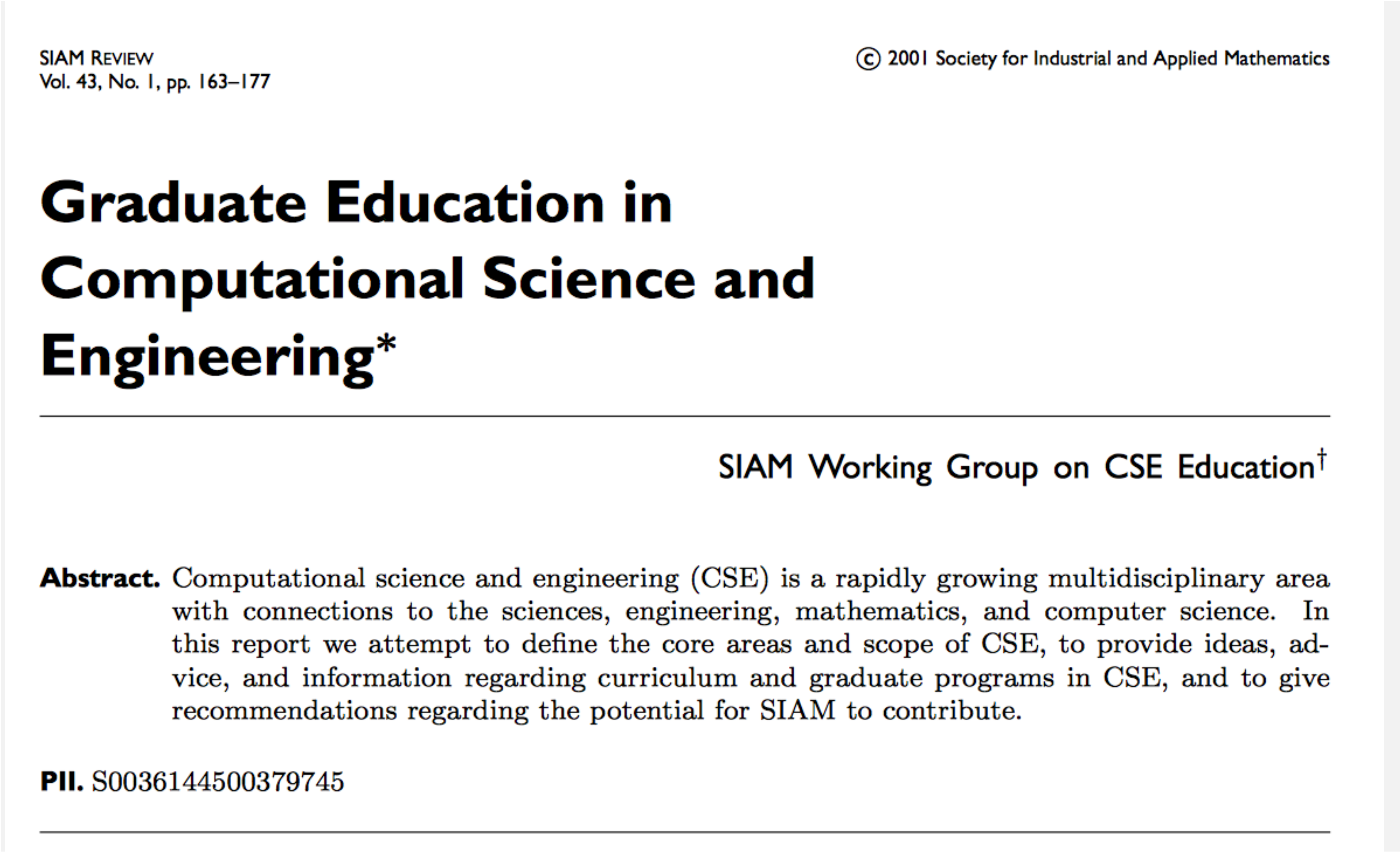
Continuum

Properties

Microstructure

Atoms

Electrons



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Vol. 43, No. 1, pp. 163–177

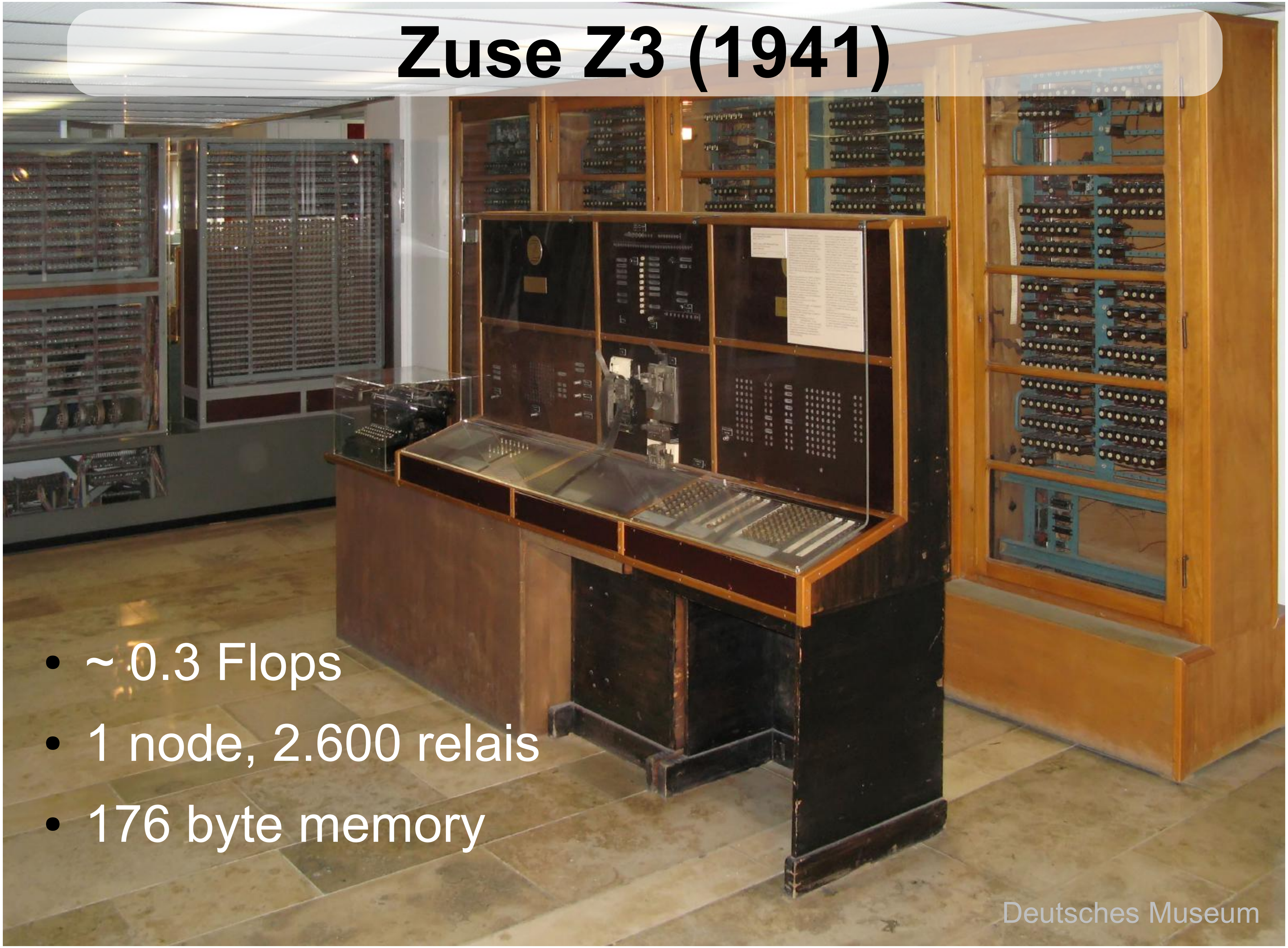
Graduate Education in Computational Science and Engineering*

SIAM Working Group on CSE Education†

Abstract. Computational science and engineering (CSE) is a rapidly growing multidisciplinary area with connections to the sciences, engineering, mathematics, and computer science. In this report we attempt to define the core areas and scope of CSE, to provide ideas, advice, and information regarding curriculum and graduate programs in CSE, and to give recommendations regarding the potential for SIAM to contribute.

PII. S0036144500379745

Rüde et al 2016



Zuse Z3 (1941)

- ~ 0.3 Flops
- 1 node, 2.600 relais
- 176 byte memory

Deutsches Museum