Laboratory of Computational Physics

Maria Peressi

Universita' di Trieste - Dipartimento di Fisica

Sede di Miramare (Strada Costiera 11, Trieste)

e-mail: peressi@ts.infn.it

tel: +39 040 2240242

http://www-dft.ts.infn.it/~peressi/comp-phys.htm

Introduction

(1) Computational Physics

- Simulations and "what-if" experiments

- Deterministic and stochastic approaches

- A few examples

(2) This course

(3) Other Courses concerning computational Physics in our Physics training track

(1) Computational Physics

Computers in physics

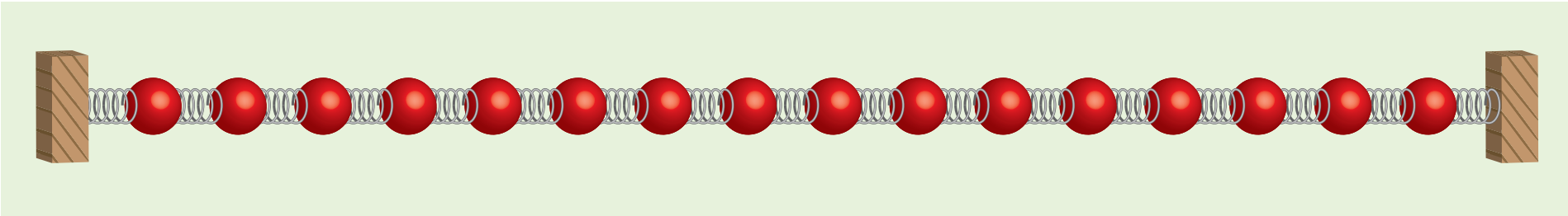
- control of instruments, data collection and analysis
- visualization
- symbolic manipulation
- . . .

- **numerical analysis**: to solve equations which could not be tackled by analytical methods. This allows to measure theories, in a similar way as natural phenomena are measured by experiments, the ultimate goal of science being the insight and understanding gained from the comparison of these two kinds of measures.

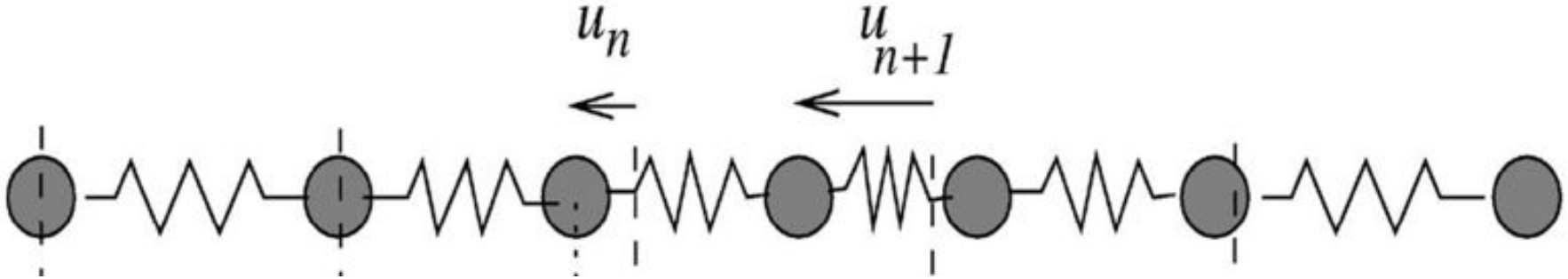
- **simulations**: to model and study physical phenomena with numerical techniques. This means doing virtual experiments in which our representation of the physical reality, though necessarily schematic and simplified, can be

computational physics

OBLEM: Fermi-Pasta-Ulam-Tsingou 1955



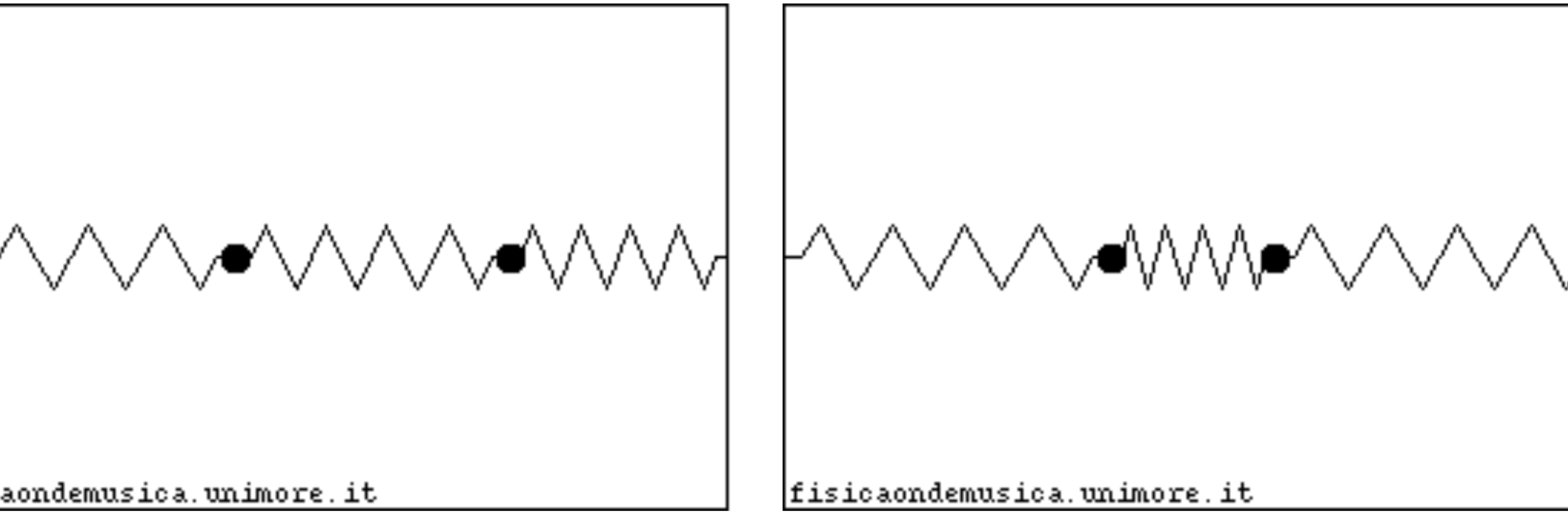
A chain of N particles linked by springs
(one-dimensional analogue of atoms in a crystal)



Linear interaction (Hooke's law):

there are N 'normal' modes

Example with 2 oscillators: 'normal' modes



http://fisicaondemusica.unimore.it/Oscillatori_accoppiati.html

More in: http://fisicaondemusica.unimore.it/Catena_di_Fermi_Pasta_Ulam.html

computational physics

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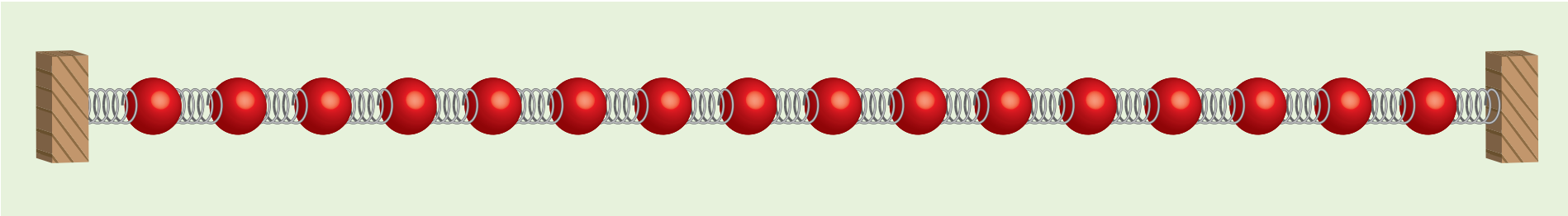

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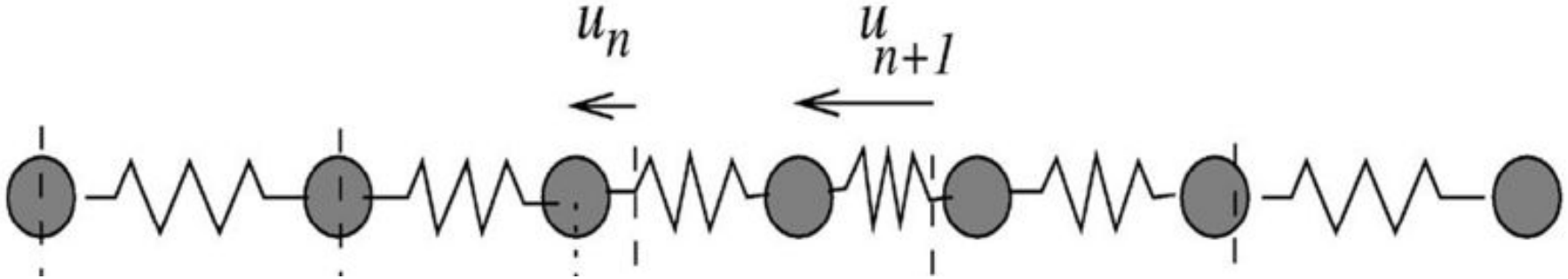
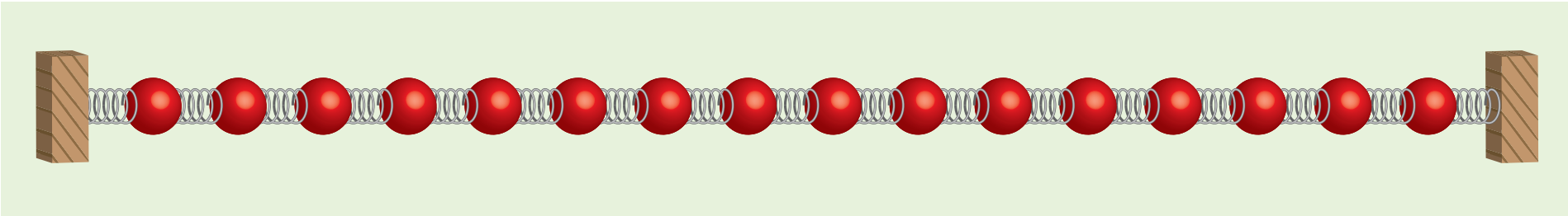


Linear interaction (Hooke's law):
analytical solution

computational physics

OBLEM: Fermi-Pasta-Ulam-Tsingou 1955



in presence of a weak non linear coupling

uadratic or cubic correction to the linear term

which modes will be excited after a long enough time?

Expected behavior based on *the equipartition theorem*: the energy will be equally distributed among all the degrees of freedom of the system.

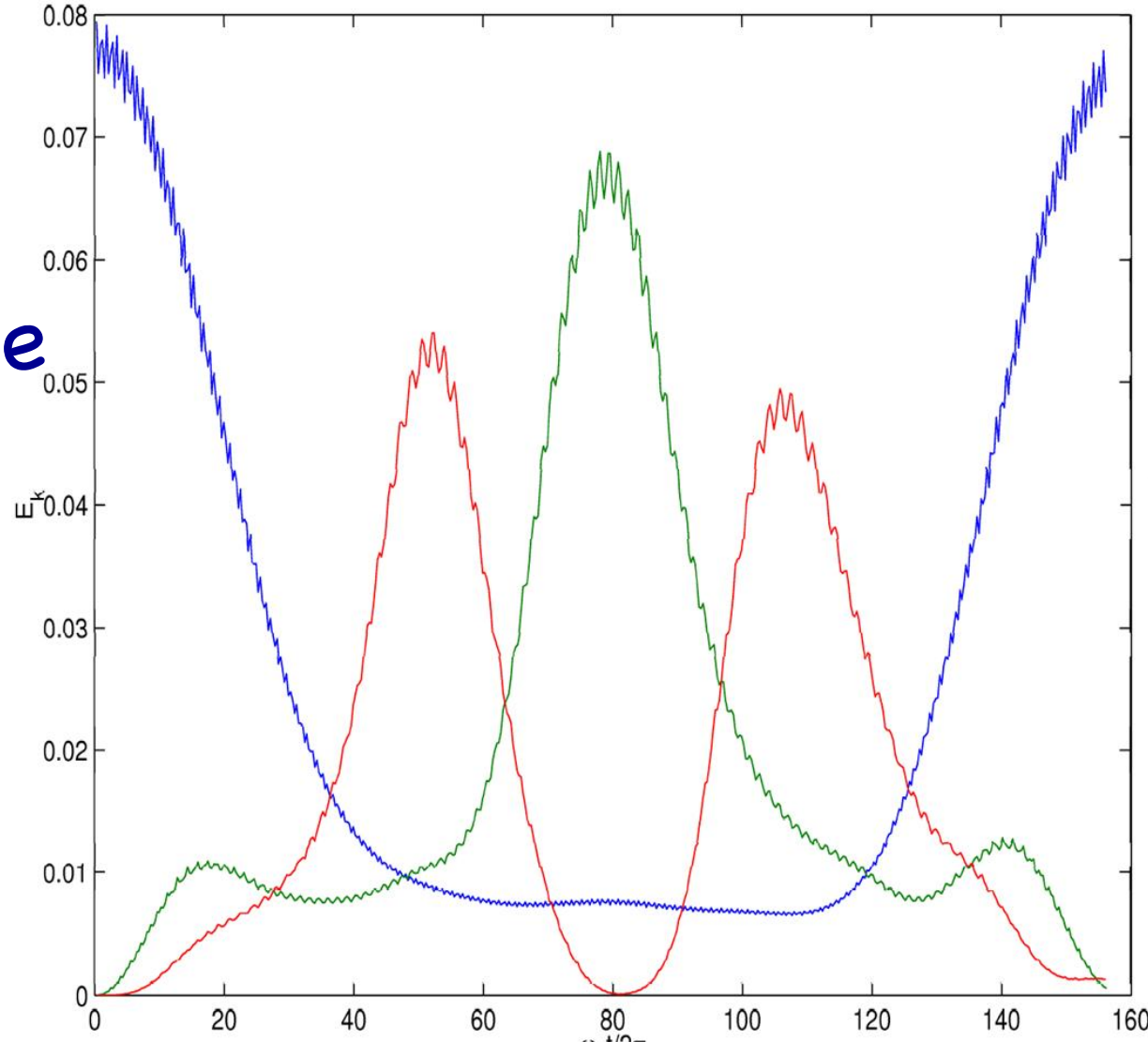
computational physics

OBLEM: Fermi-Pasta-Ulam-Tsingou 1955

umerical solution (originally: calculations for N=5)

ergy vs. time
or the first
hree modes:

1 2 3



After initial
excitation of t
mode k=1 an
157 periods,
almost all th
energy is bac
to this mode

Simulations as "virtual experiments"

A few similarities between experiments:

eal" (in lab)	"virtual" (computatio
nple	model and algorithms
ysical apparatus	code
ibration of instruments	test of the code
asurements	numerical results
a analysis	data analysis

Simulations as "virtual experiments"

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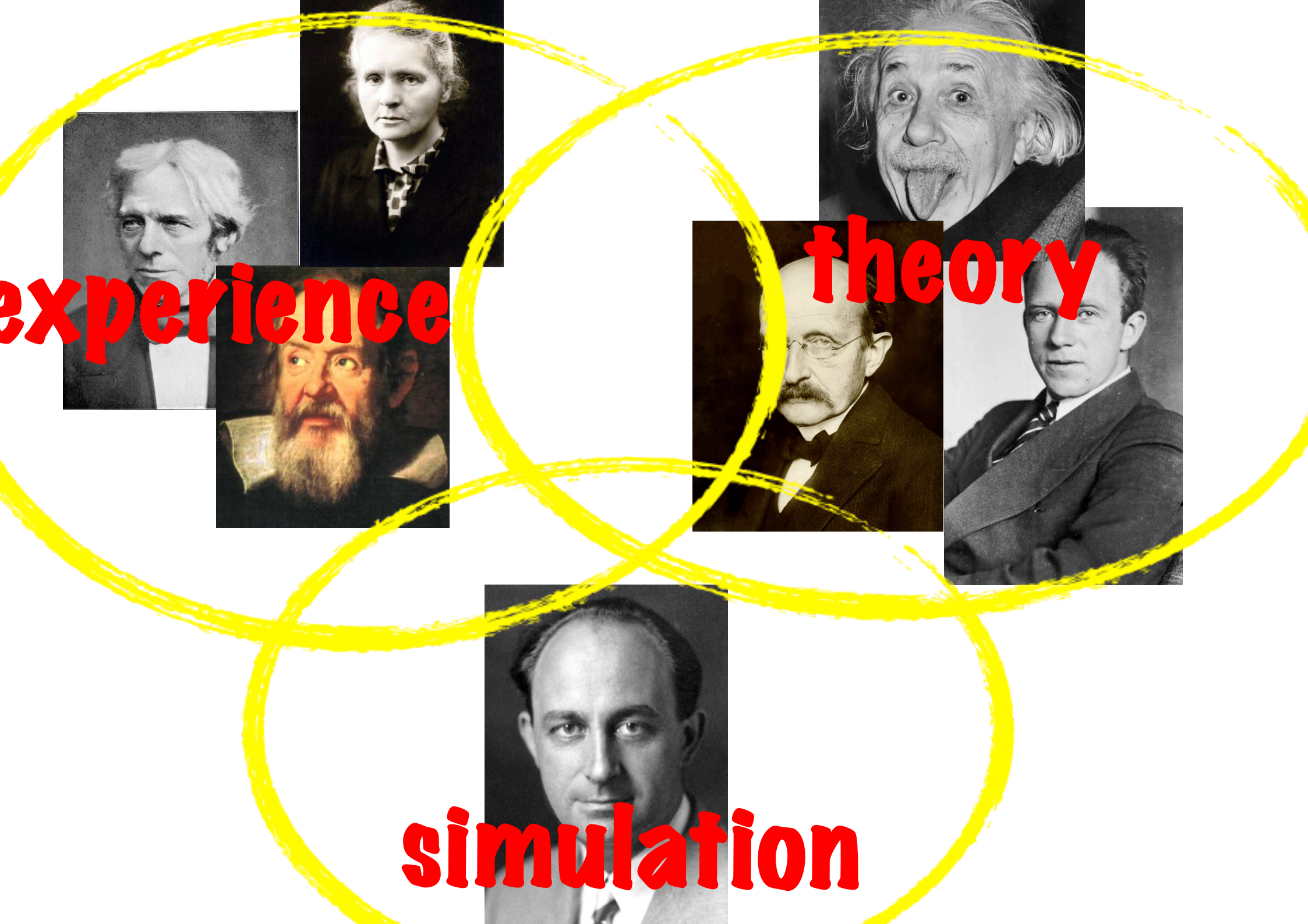
- **Importance of simulations**: **"what-if" experiments** (large flexibility in varying parameters; e.g. material properties can be studied also under conditions not accessible in real labs) ; **predictions**, not just description.

- **Use of simulations:** **not "final goal", but "instruments"** to study and shed light on complex phenomena and/or systems with many degrees of freedom or many variables and parameters

- in the last ~4 decades simulation has emerged as the third fundamental paradigm


experience
theory
simulation

The purposes of the scientific calculus

- "The computer is a tool for clear thinking" (Freeman J. Dyson)
- ". . . whose [of the calculations] purpose is insight, not numbers" (V. Hamming)

TWO different approaches for numerical simulations

- **deterministic**

Info can be obtained both on the equilibrium properties and on the dynamics of the system

- **stochastic** (Monte Carlo, MC)

Typically to simulate random processes, and/or sampling of most likely events

The deterministic approach

We can write the equations of motion
(Classical => Newton; Quantum => Schroedinger)

and we know the initial condition

the problem is related to the
numerical integration of differential equations
(or integral-differential in quantum problems)

(like the FPUT problem)

The deterministic approach

Numerical integration of the eqs. of motion: discretization and iteration

Different algorithms according whether
the equation is 1st , 2nd order...
(the equation for the velocity is 1st order),
whether the **force is dependent or not on the velocity,**
to which order...

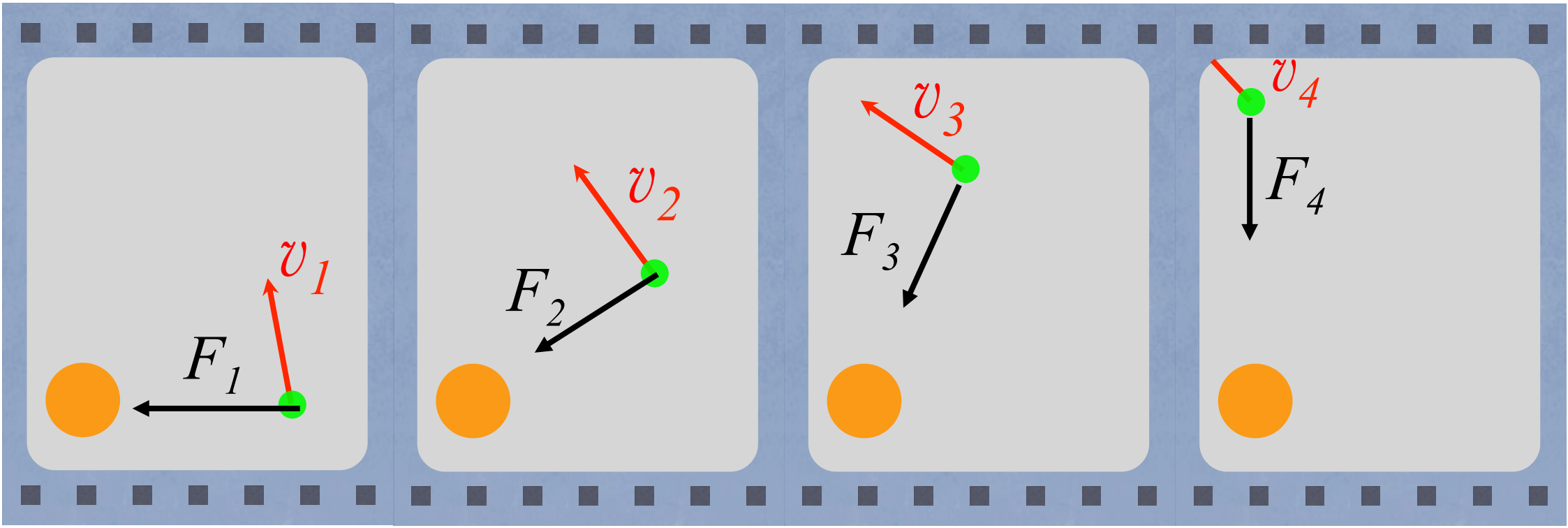
The deterministic approach

Discretization of the equation of motion and iteration:

$$a(t) = m\frac{d^2x(t)}{dt^2} = \frac{F(t)}{m}$$

$$x(t) = x(0) + v(0)t + \frac{1}{2}\frac{F}{m}t^2$$

$$x(t+\Delta t) = x(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2$$



The stochastic approach

seful to model:

Some physical processes which are herently probabilistic.

) Many large classical systems which ave so many variables, or degrees of reedom, that an exact treatment is tractable and not useful.

Probabilistic physical processes

e attempt to follow the `time dependenc
a model for which change, or growth, doe
t proceed in some rigorously predefined
shion (e.g. according to Newton's
uations of motion) but rather in a
ochastic manner which depends on a
quence of random numbers which is
nerated during the simulation.

g.: radioactive decay

with many degrees of freedom

g.: Thermodynamic properties of gases

possible and not useful to know the exact positions a
ocities of all molecules.

eful properties are statistical averages: average ener
particles (temperature), average momentum change
m collisions with walls of container (pressure), etc.

e error in the averages decreases as the number of
rticles increases. Macroscopic volume of gas has
0^23) molecules. Thus a statistical approach works ve

Monte Carlo

Monte Carlo refers to any procedure which makes use of random numbers (*)

Monte Carlo is used in:

- Numerical analysis
- Statistical Mechanics Simulation

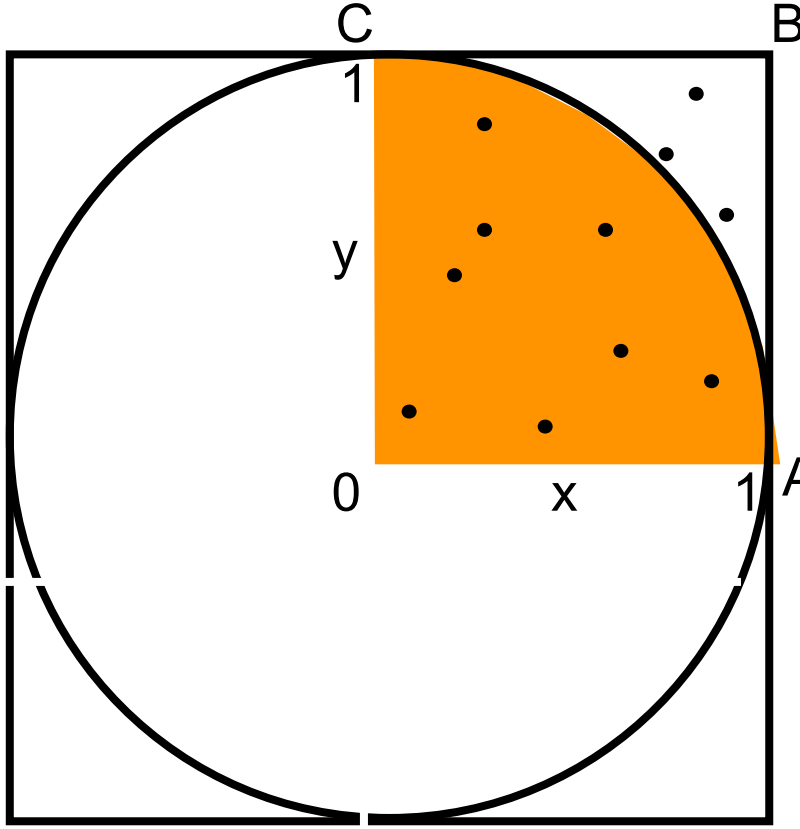
(*) a sequence of random numbers is a set of numbers which looks unpredictable but with well defined statistical properties

Monte Carlo Methods: to calculate integrals

"Hit or Miss" Method: How much is π ?

lgorithm:

- Generate uniform, random x and y between 0 and 1
- Calculate the distance from the origin: $d=(x^2+y^2)^{1/2}$
- If $d \le 1$, $\tau_{hit} = \tau_{hit} + 1$



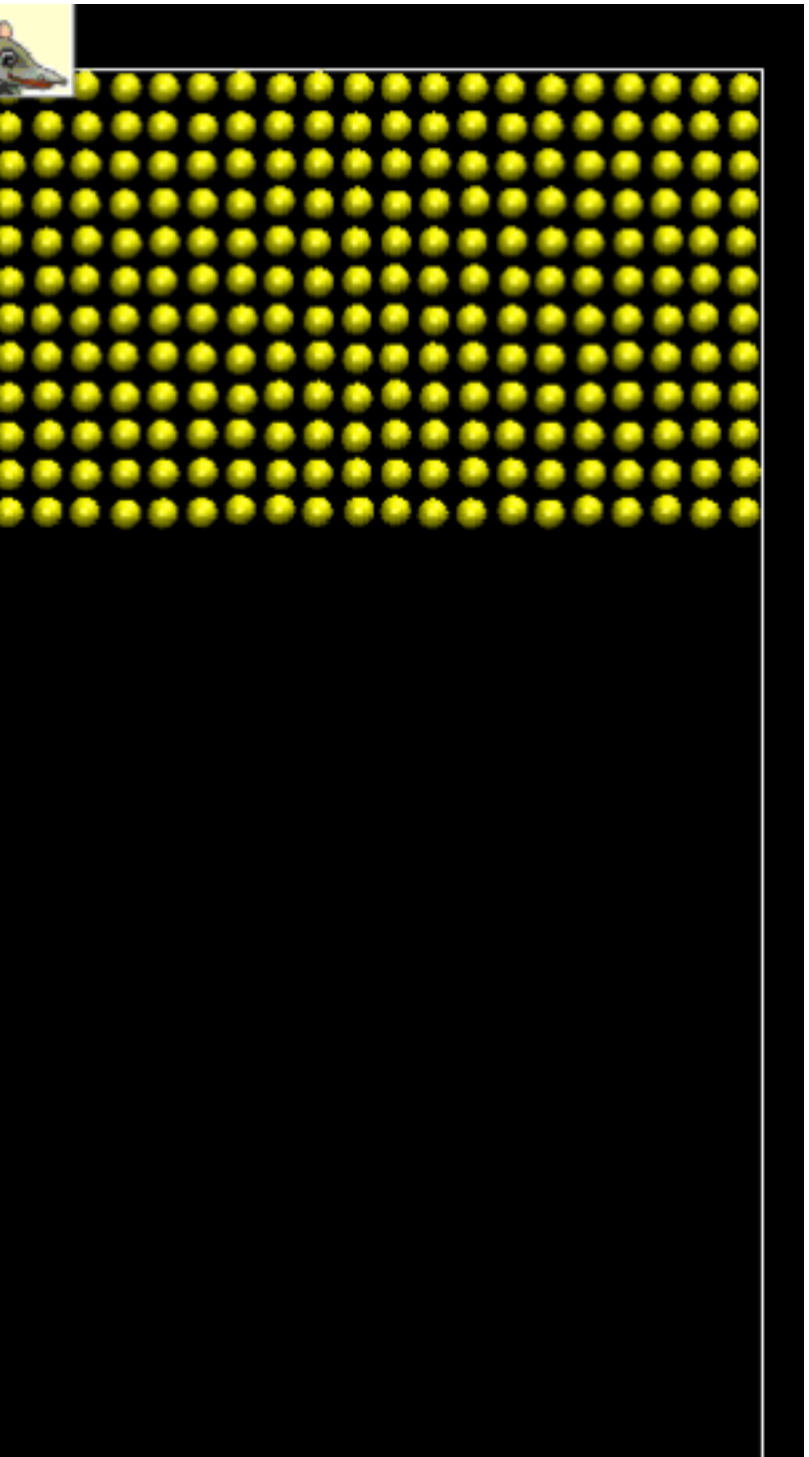
$$\pi \approx \frac{4 \times \text{Area Under Curve CA}}{\text{Area of Square OABC}}$$

$$= \frac{4\tau_{hit}}{}$$

A few selected examples of applications

(here: atomistic simulations
in condensed matter...)

From "normal" scales...



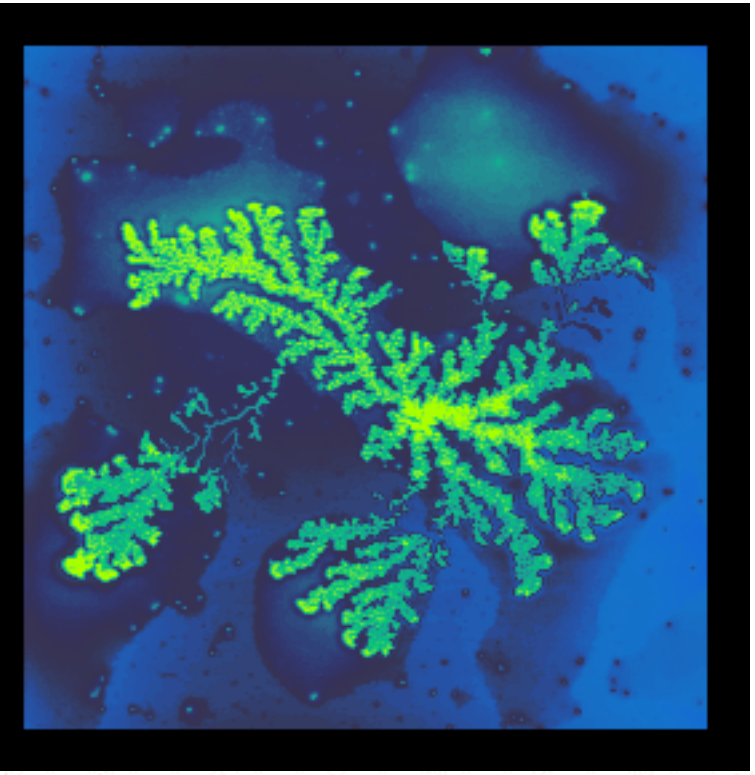
(classical)

SIMULATION
of the Brownian motion

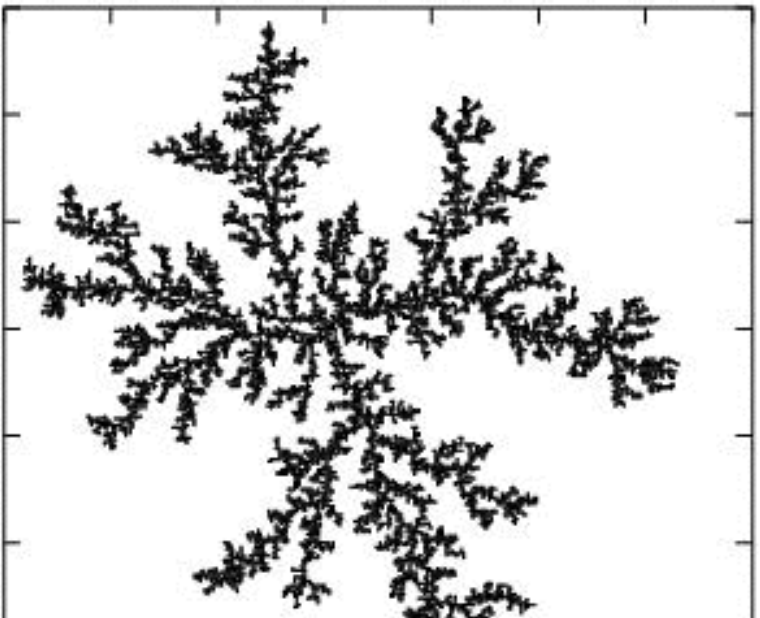
Sedimentation of hard spheres in a 2D system with walls.
Included interactions with smaller particles (not shown here) representing the thermohydrodynamic solvent

(deterministic, classical

substrate...



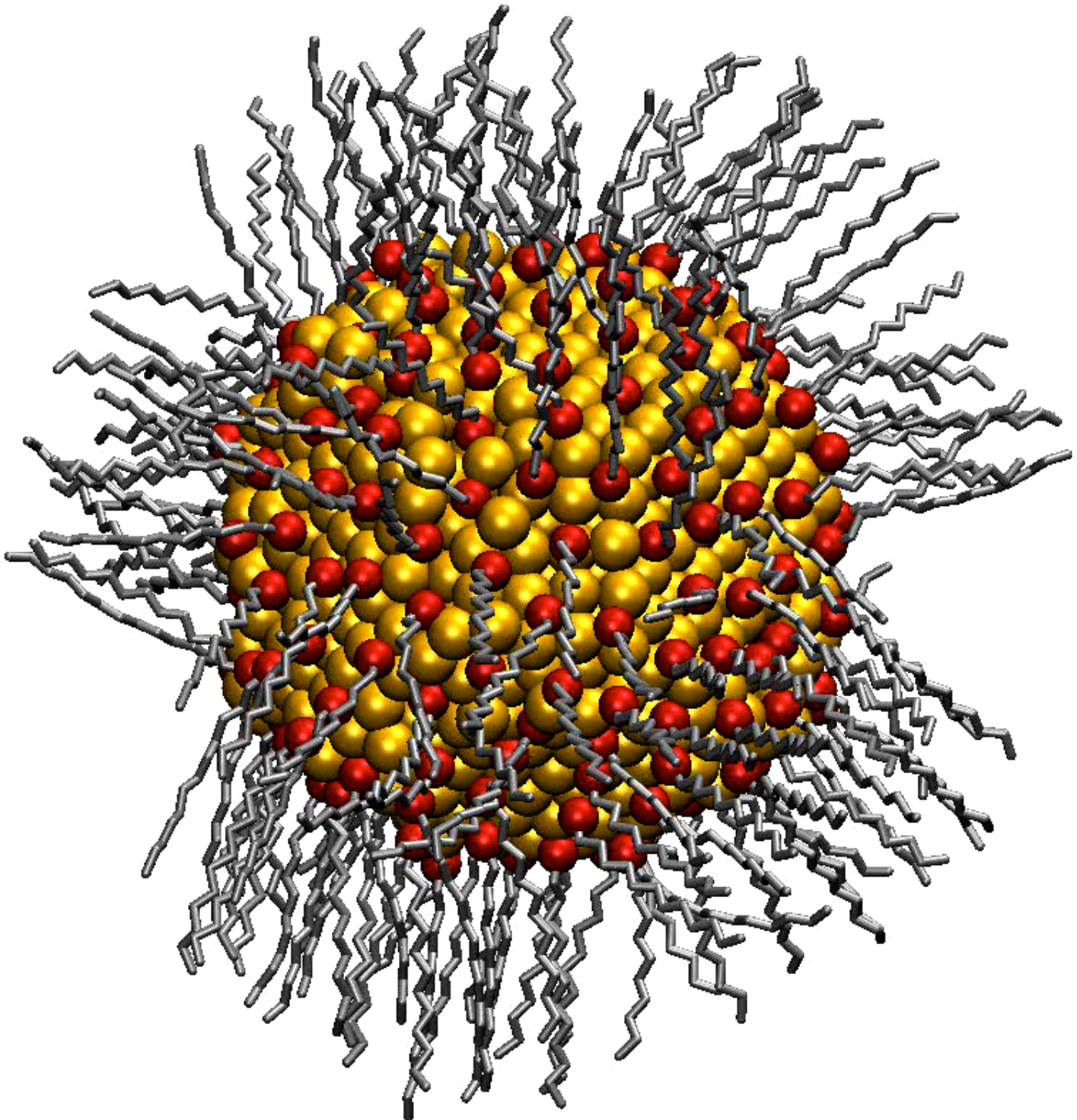
REAL IMAGE (by Atomic Field Microscopy) of a gold colloid of about 15 nm on a mica substrate



SIMULATION of a diffusion-limited auto-aggregation model (fractal)

passivation of nanoparticles

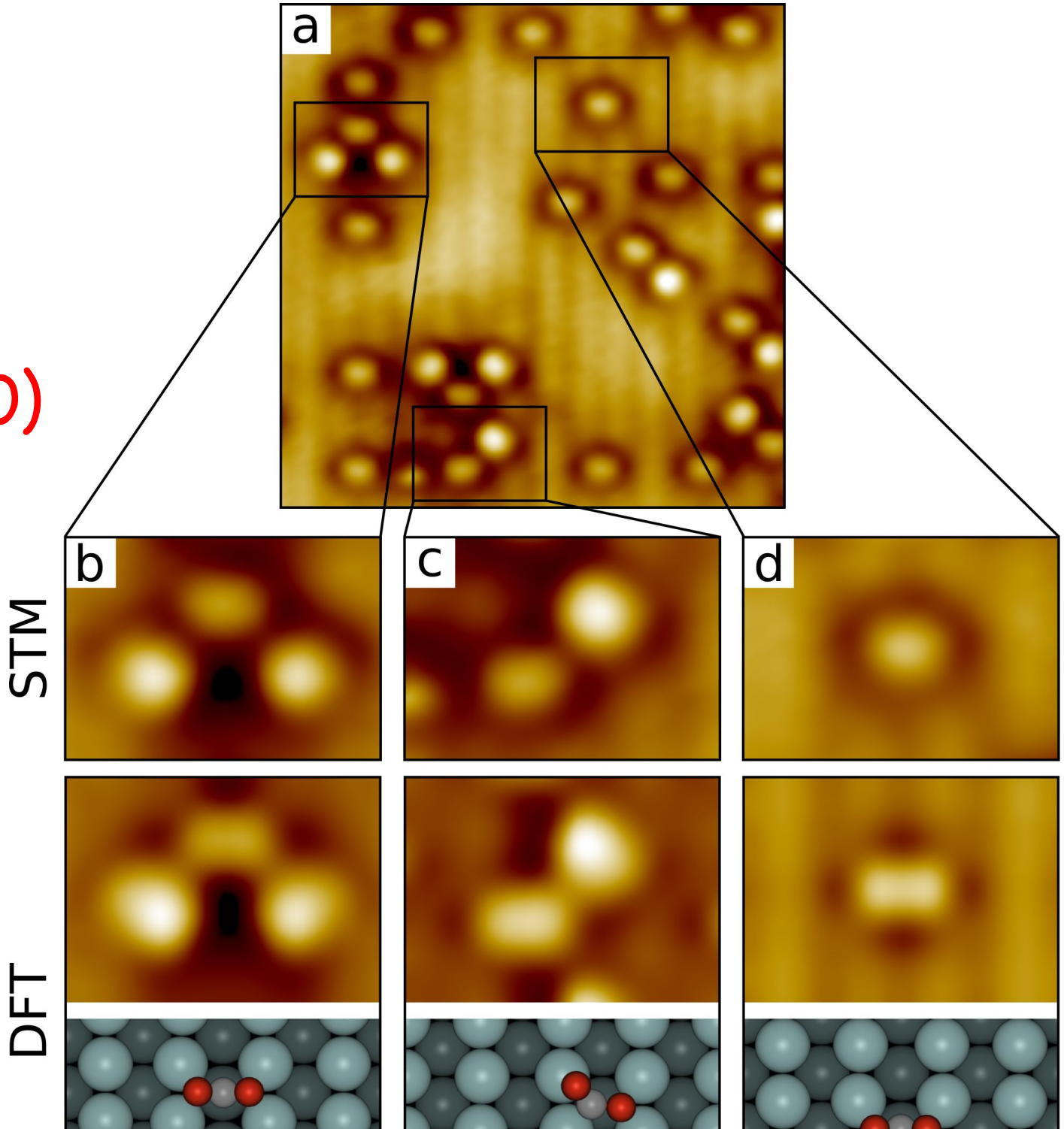
rganic molecules
)



... to the atomic scale

O_2@Ni(110)

ollaboration
h Surf Sci
tivity Group
of TASC)



Exp Low
STM ima

Simulat
STM ima

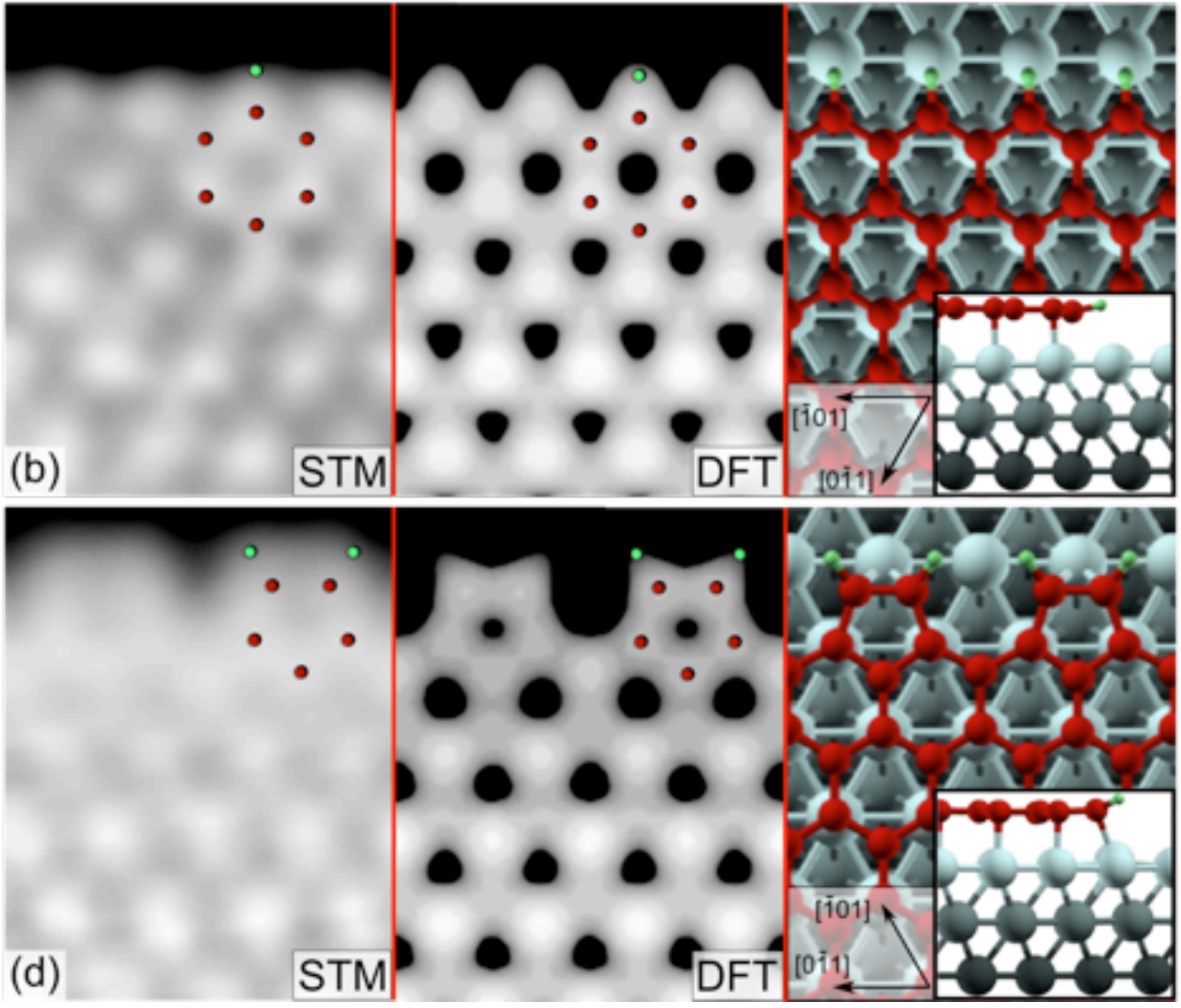
... another example

afene
Ni(111)

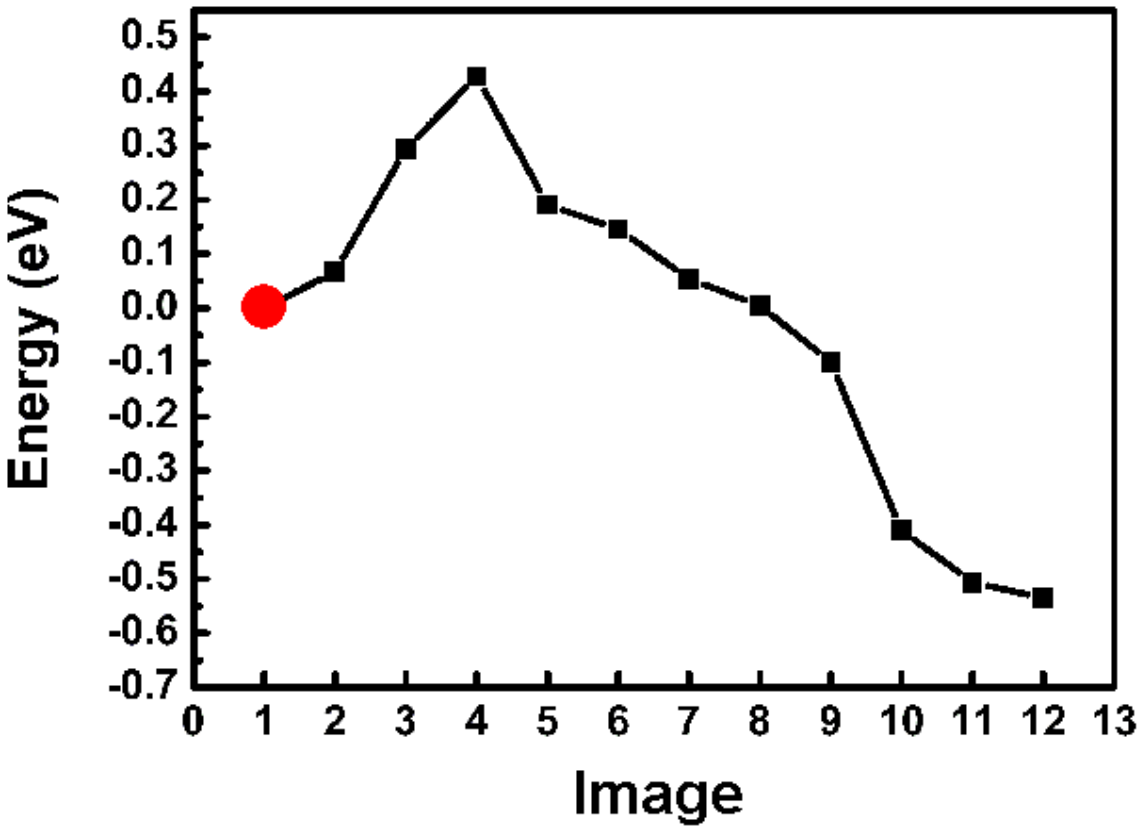
ollaboration
ith TASC)

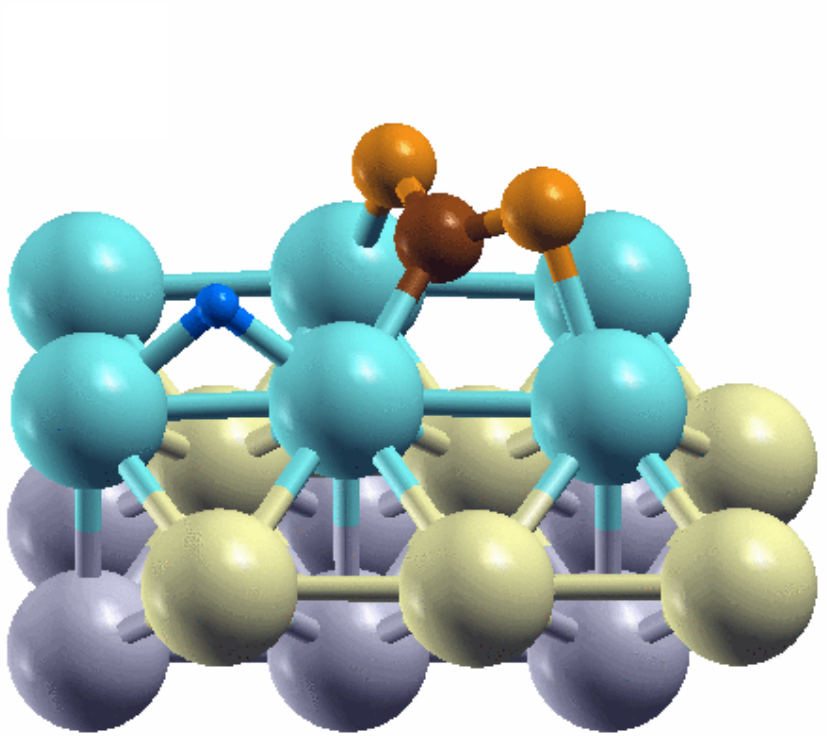
RT

(H-terminated edges)



...including chemical reactions





CO_2 + H -> HCOO @ Ni(110)

- wide range of **length scales**: ≈12 orders of magnitude (nuclei/electrons/atoms/chemical bonds ~ 10—12 m, fracture/macroscopic mechanical phenomena ~ 100 m nano / micro / meso / macroscopic scales)

- wide range of **time scales**: ≈12 orders of magnitude (nuclei/electrons/atoms/chemical bonds ~ 10—12 s, fracture/macroscopic mechanical phenomena ~ year)

- wide range of chemical-physical **properties**: structural, elastic, vibrational, electronic, dielectric, magnetic, optical, thermal . . .

- wide range of **materials**: different phases, traditional materials (crystalline / amorphous , metals/ semiconductors / insulators . . .), new materials. . .

different kind of interactions

- Classic
- Quantum

different approaches

- Deterministic
- Stochastic

...and also different specific techniques

corresponding to different size/time scales:

- **continuous models** (for macroscopic systems)
- **atomistic simulations**

- ab - initio techniques (or "first-principles"): up ~10^3 atoms, 10 ps

- Semiempirical techniques: up to 10~7 atoms, 1 m

- models at different levels

...and different computational workload

Some techniques and systems are
not computationally very demanding
our experiments will be quite small and simple

others, they are...

High performance computing

PERCOMPUTER SITES

: November 2015

Tianhe-2 (MilkyWay-2) NUDT

tional Super Computer Center in Guangzhou)

000 nodes, with 3,120,000 cores with CPU+GPU

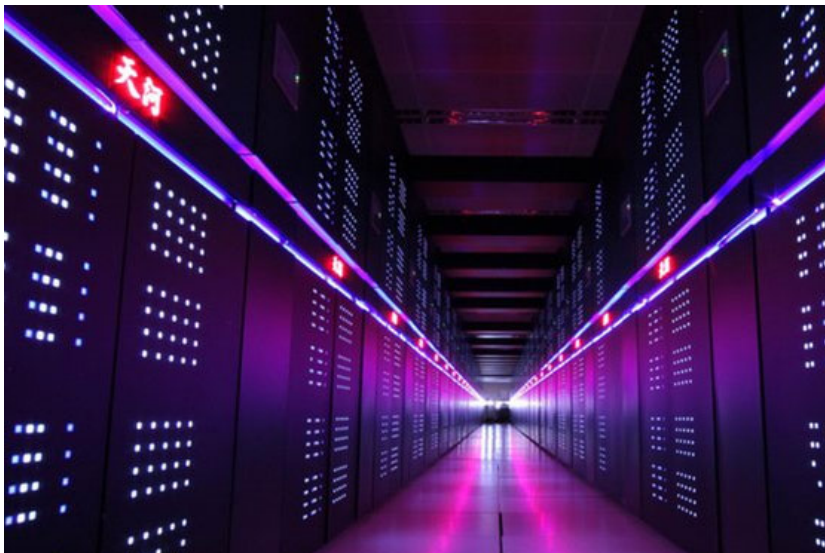
ch node: different Intel Xeon types of processors

d GPU, like those for videogames!!!)

ak performances: up to 34 PFlop

ta = 10^{15})

op = "floating-point" operation / second)

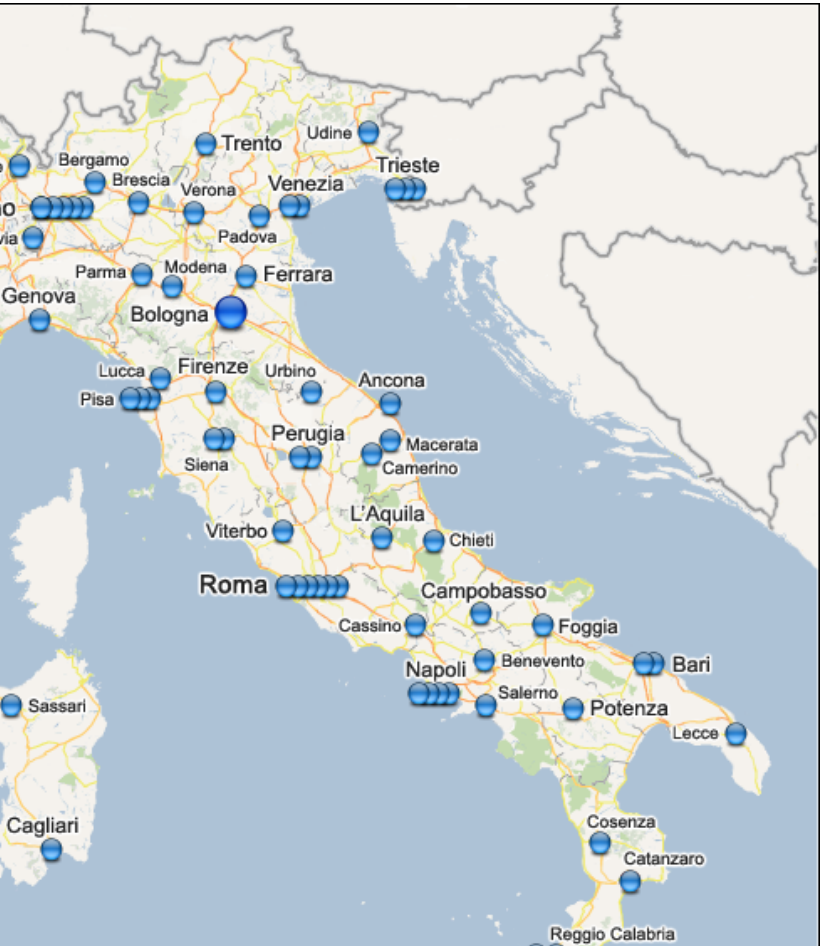


PERCOMPUTER SITES

: November 2015

FERMI - BlueGene/Q IBM, CPU+GPU

e with grants; agreement also with UniTS)



163.840 computing cores ar
peak performace of 2,1 PFl

(2) This course

This course

- IS NOT a course on Information Technology, Computer Science, Programming languages…
- BUT a **PHYSICS LAB.**
- **focusing on modeling, problem solving and algorithms**
- Not exhaustive, of course…

This course

- **Stochastic approach, classical interactions (mainly)**

- + basic ingredients of the **deterministic approach** (Molecular Dynamics) and **quantum mechanics** (Variational Monte Carlo)
  (1 week each topic)

Web page of the course

http://www-dft.ts.infn.it/~peressi/comp-phys.ht

With:

- important announcements
- detailed contents of each lecture
- lectures notes
- exercises
- info about textbooks
- links, tutorials (for surviving with Linux/Unix, Fortran90, gnuplot...)
- info about exams

Use it!

e Carlo simulation of Random Walks.

rical integration in 1 dimension: deterministic and stocastic algorithms;·

e Carlo algorithms.·

estimate and reduction of the variance methods.·

opolis algorithm for arbitrary random number generation.·

opolis method in the canonical ensamble.·

model and Metropolis-Monte Carlo simulation.·

cal fluids: Monte Carlo and Molecular Dynamics simulation of hard spheres and ennard-Jones fluids.·

states and macrostates: efficient algorithm for the numerical calculation of ent

tional Monte Carlo in quantum mechanics (basics).·

ce gas: vacancy diffusion in a solid.·

and determinism: classical billiards and caotic billiards, logistic maps; Lyapunov kponents.·

als: diffusion and aggregation models for surface growth simulation. Percolation

Available computational resources: INFIS

p://df2.units.it/?q=it/modulistica

p://df2.units.it/?q=it/node/2919/

DATTICA => SERVIZI AGLI STUDENTI

Remote connection:

$ssh username@w01.infis.units.it

Your address at INFIS:

username@infis.univ.trieste.it

You can copy **the source codes lecture by lecture** (wait
updates!!! Do not copy everything today!!!) from:

tp://www.infis.units.it/~peressi/ **(PUBLIC ACCE**

on INFIS, you find the **source codes** in the directory (you
need to have an account on INFIS):

home/peressi/comp-phys

d subdirectories (I-basic, etc. etc....)

om your directory, do:

cp /home/peressi/comp-phys/I-basics/* .

Fortran compilers on INFIS

- **g95 or gfortran (free):** ([] for optional)

  $ g95 [-o test.o] test.f90 or

  $ gfortran [-std=f95] [-o test.o] test.f90

- OTHERS (NOT SUPPORTED ON INFIS):

  ifort (Fortran Intel compiler, NOT free)

  F (free; useful options: -ieee=full for floating point exception manipulation)

- executables (e.g. test.o or a.out by default):

  $ ./a.out (or $bash a.out)

A few useful UNIX (Linux, MacOSx,...) commands:

Check your space!

$ quota

or "du" (displays disk usage statistics):

$ du ~ | more

(if "-k" flag is specified, the number of 1024-byte blocks used by the file is displayed):

$ du -k ~ | more (Last line shows the total)

5) Other courses concerning computational Physics in our Physics training track

- complementary to **"Classical simulations of many body systems"** (E. Smargiassi, I semester I year) (deterministic, classical
- complementary to **"Numerical Methods of Quantum Mechanics"** (P. Giannozzi, I semester I year) (deterministic, quantum