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

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
- . . .

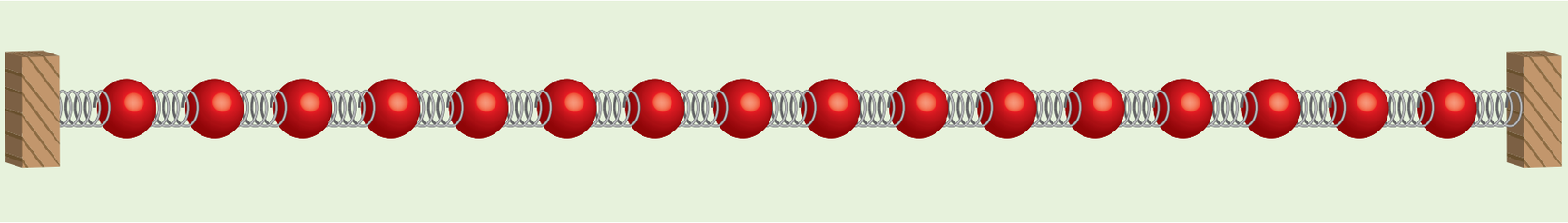
……

- **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.

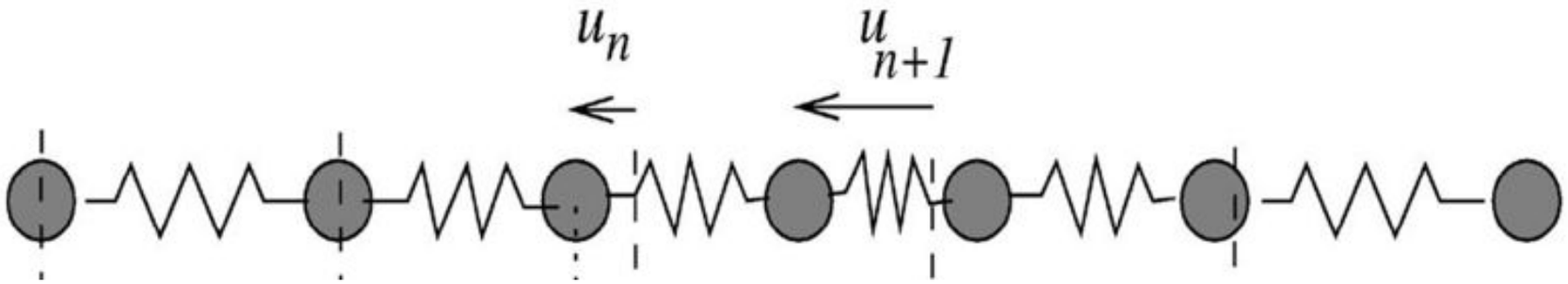
- **simulations**: to model and study physical phenomena with numerical techniques. This means doing virtual experiments in which our representation of the physical reality, though necessarily schematic and simplified, can be tuned and varied at will.

The birth of computational physics

PROBLEM: Fermi-Pasta-Ulam-Tsingou 1955



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

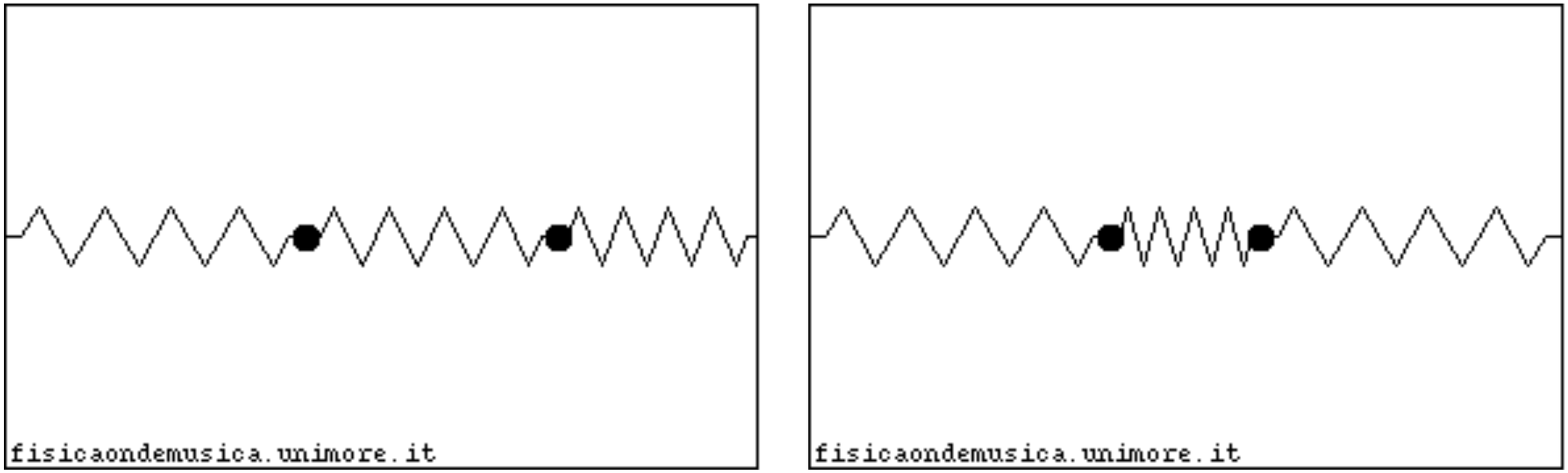


Linear interaction (Hooke's law):

there are N 'normal' modes

(i.e., patterns of motion in which all parts of the system oscillate with the same frequency and with a fixed phase relation)

Example with 2 oscillators: 'normal' modes

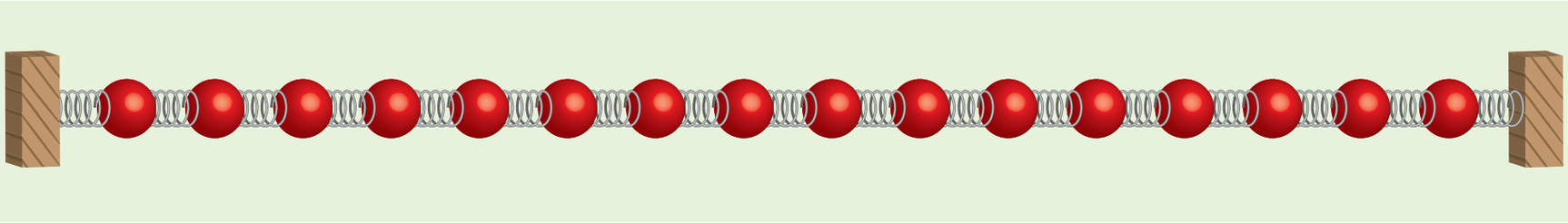


http://fisicaondemusica.unimore.it/Oscillatori_accoppiati.html

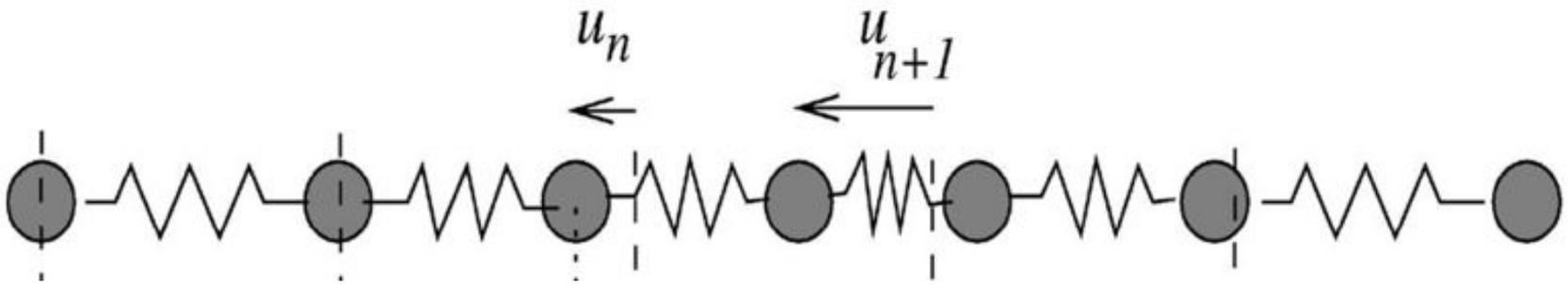
More in: http://fisicaondemusica.unimore.it/Catena_di_Fermi_Pasta_Ulam.html

The birth of computational physics

PROBLEM: Fermi-Pasta-Ulam-Tsingou 1955



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

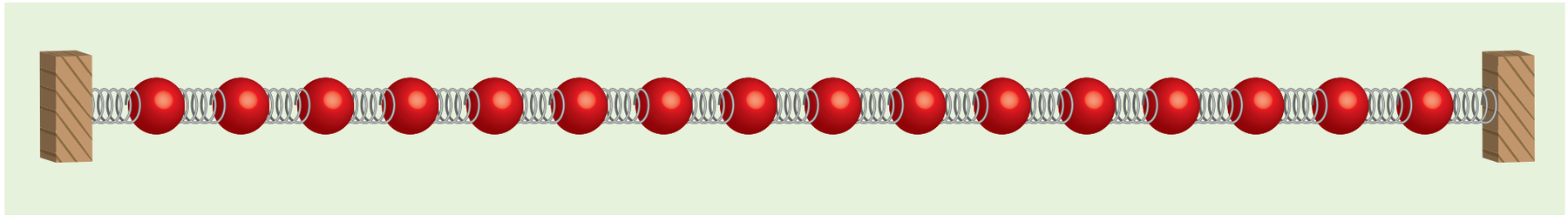


Linear interaction (Hooke's law):
analytical solution

The energy given to a single 'normal' mode
always remains in that mode.

The birth of computational physics

PROBLEM: Fermi-Pasta-Ulam-Tsingou 1955



in presence of a weak non linear coupling (quadratic 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.

However: analytical solution impossible

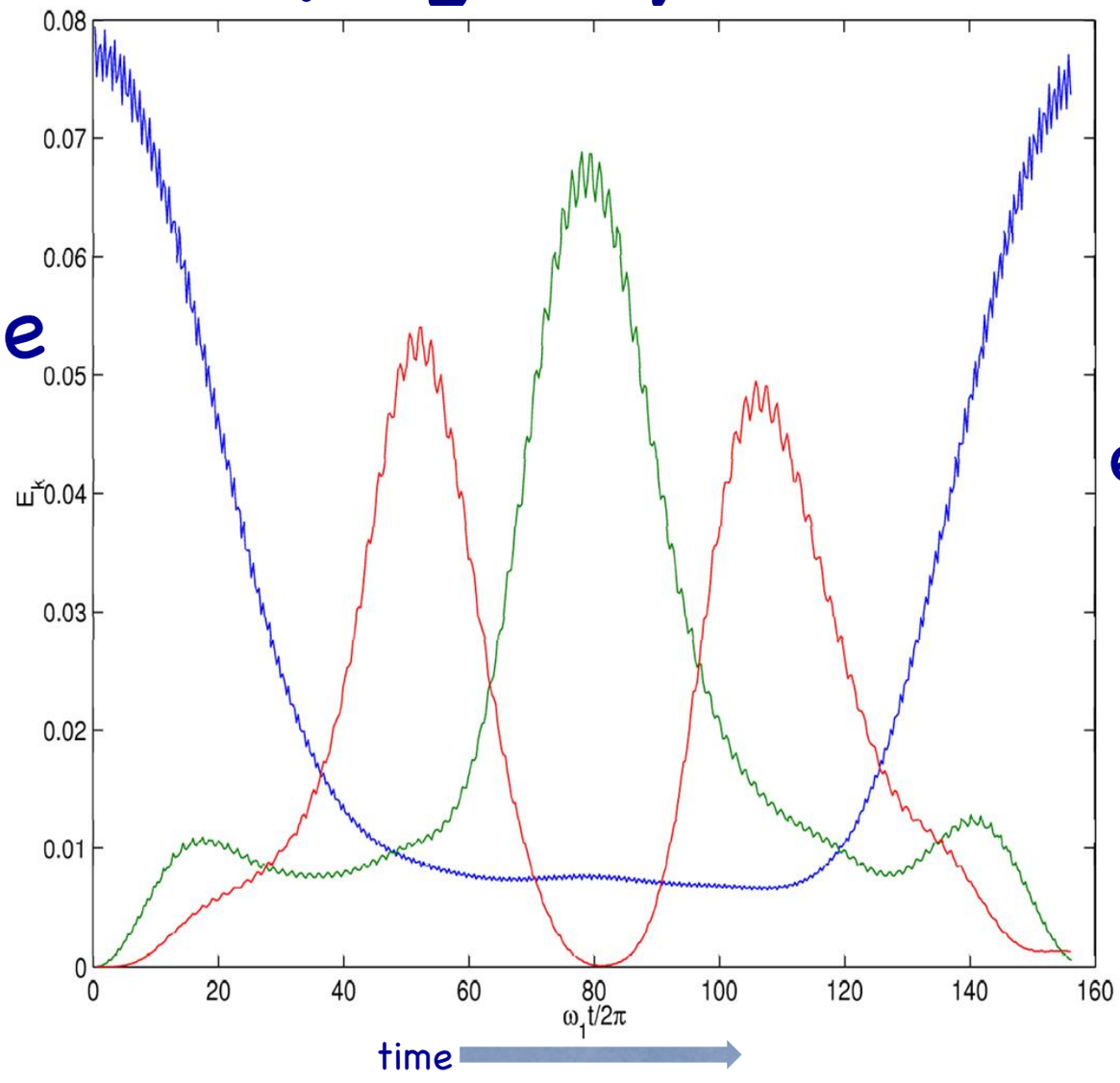
The birth of computational physics

PROBLEM: Fermi-Pasta-Ulam-Tsingou 1955

Numerical solution (originally: calculations for N=5)

Energy vs. time for the first three modes:

K= 1 2 3



After initial excitation of the mode k=1 and 157 periods, almost all the energy is back to this mode !!!

Pictures from: Thierry Dauxois and Stefano Ruffo (2008), Scholarpedia, 3(8):5538. doi:10.4249/scholarpedia.5538 http://www.scholarpedia.org/article/Fermi-Pasta-Ulam_nonlinear_lattice_oscillations and other web sites

Simulations as "virtual experiments"

A few similarities between experiments:

"real" (in lab)	"virtual" (computational)
sample	model and algorithms
physical apparatus	code
calibration of instruments	test of the code
measurements	numerical results
data analysis	data analysis

Simulations as "virtual experiments"

A few similarities between experiments:

"real" (in lab)	"virtual" (computational)
sample	model and algorithms
physical apparatus	code
calibration of instruments	test of the code
measurements	numerical results
data analysis	data analysis

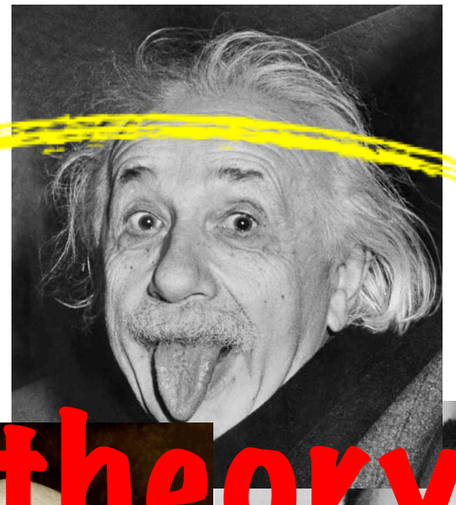
With errors!!!

- **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.

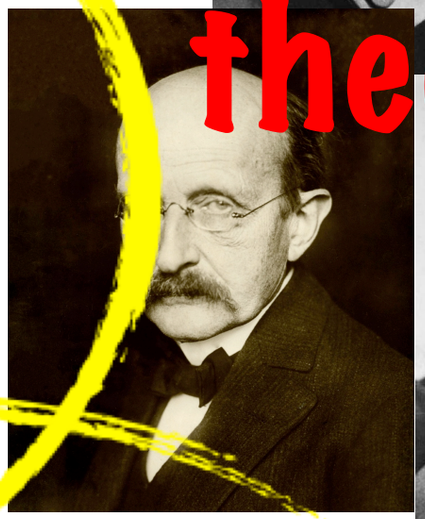
- **Use of simulations:** **not "final goal", but "instruments"** to study and shed light on complex phenomena and/or systems with many degrees of freedom or many variables and parameters

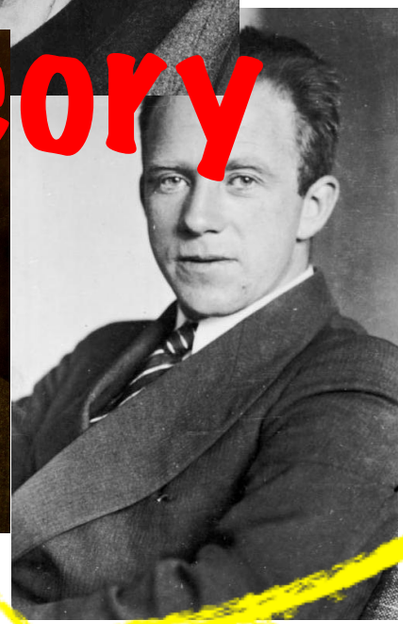
- in the last ~4 decades simulation has emerged as the third fundamental paradigm of science, beside theory and experiment

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" (Richard W. 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...

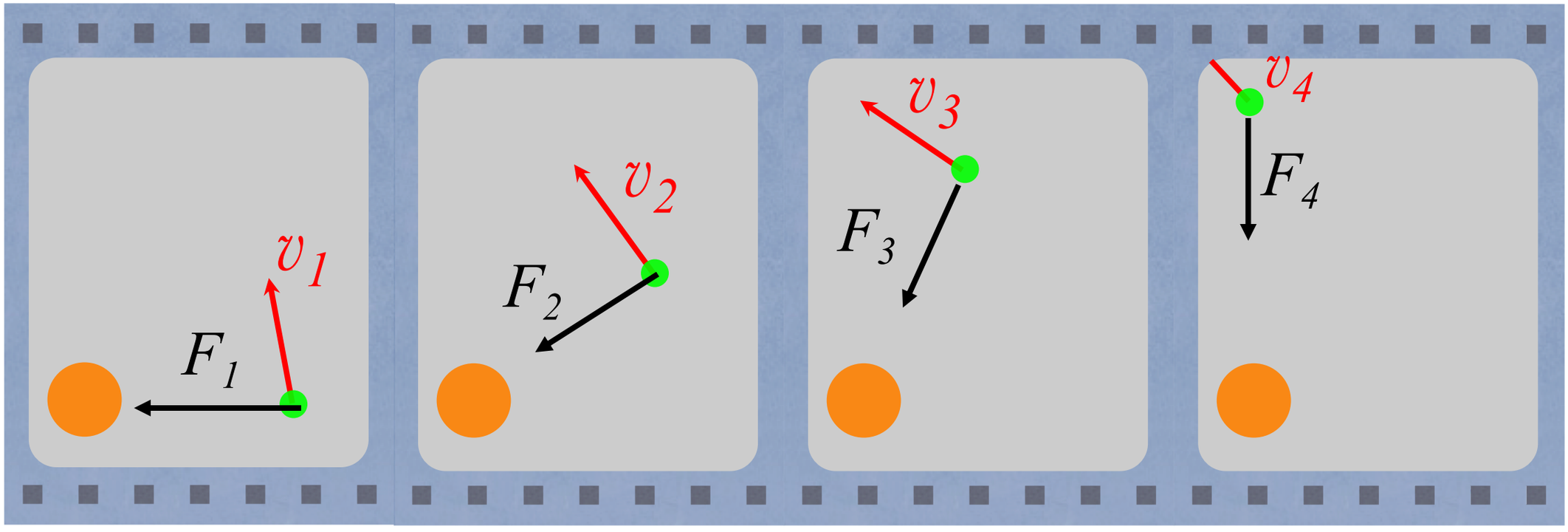
Example (classical):

The deterministic approach

Discretization of the equation of motion and iteration:

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

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



x(1) v(1) F(1) x(2) v(2) F(2) x(3) v(3) F(3) ... ...

The stochastic approach

Useful to model:

1) Some physical processes which are inherently probabilistic.

2) Many large classical systems which have so many variables, or degrees of freedom, that an exact treatment is intractable and not useful.

Probabilistic physical processes

We attempt to follow the `time dependence' of a model for which change, or growth, does not proceed in some rigorously predefined fashion (e.g. according to Newton's equations of motion) but rather in a stochastic manner which depends on a sequence of random numbers which is generated during the simulation.

E.g.: radioactive decay

Systems with many degrees of freedom

E.g.: Thermodynamic properties of gases

Impossible and not useful to know the exact positions and velocities of all molecules.

Useful properties are statistical averages: average energy of particles (temperature), average momentum change from collisions with walls of container (pressure), etc.

The error in the averages decreases as the number of particles increases. Macroscopic volume of gas has O(10^23) molecules. Thus a statistical approach works very well!

Monte Carlo

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

Monte Carlo is used in:

-Numerical analysis
-Statistical Mechanics Simulation

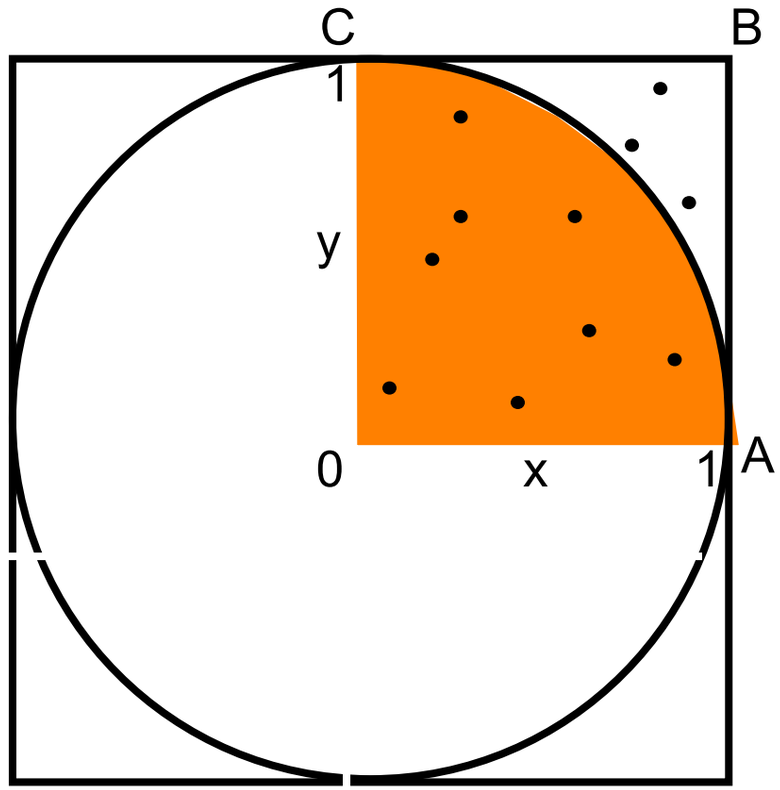
(*) a sequence of random numbers is a set of numbers which looks unpredictable but with well defined statistical properties

Monte Carlo Methods: to calculate integrals

"Hit or Miss" Method: How much is π?

Algorithm:

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

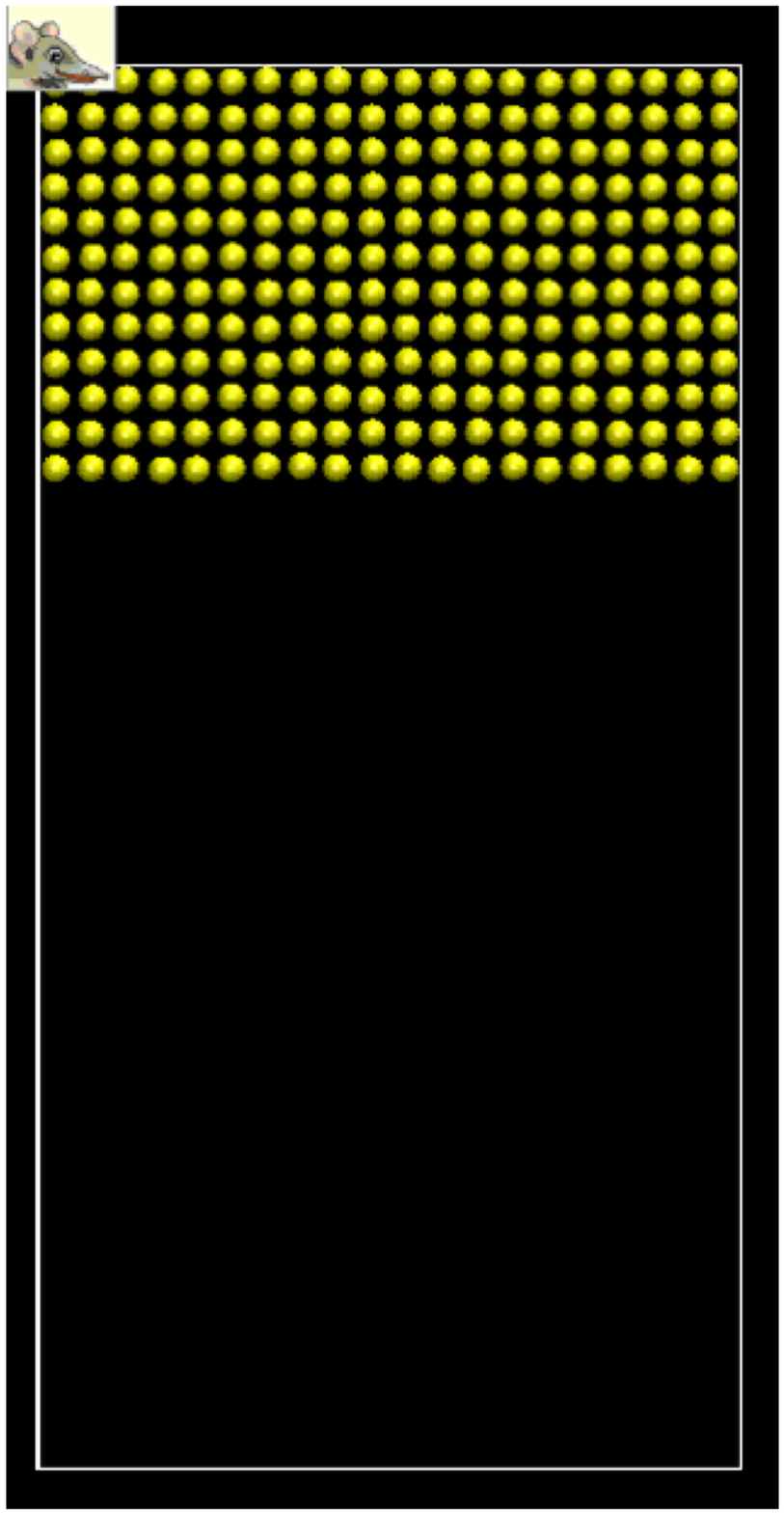


$$\pi \approx \frac{4 \text{ x Area Under Curve CA}}{\text{Area of Square OABC}} = \frac{4\tau_{hit}}{\tau_{tot}}$$

A few selected examples of applications

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

From "normal" scales…



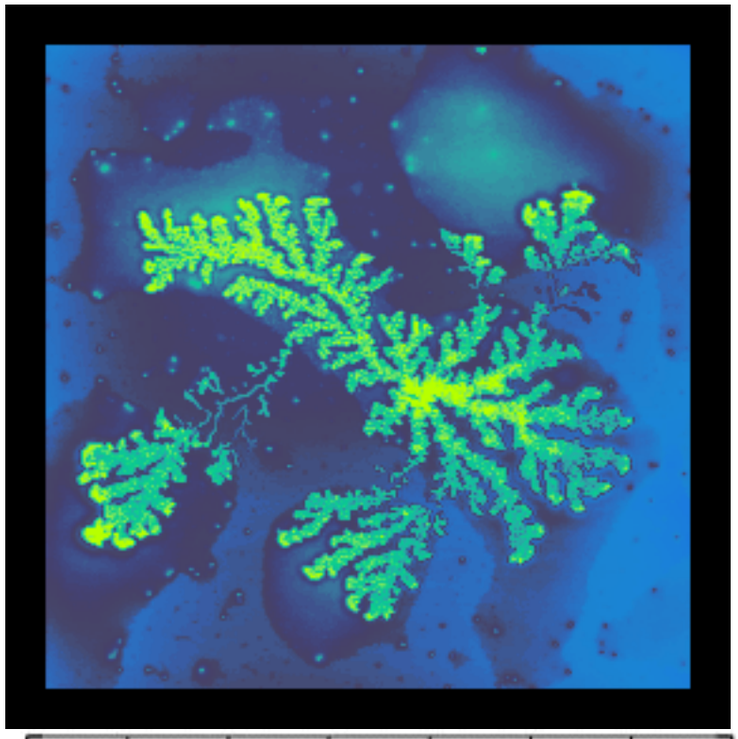
(classical)

SIMULATION
of the Brownian motion

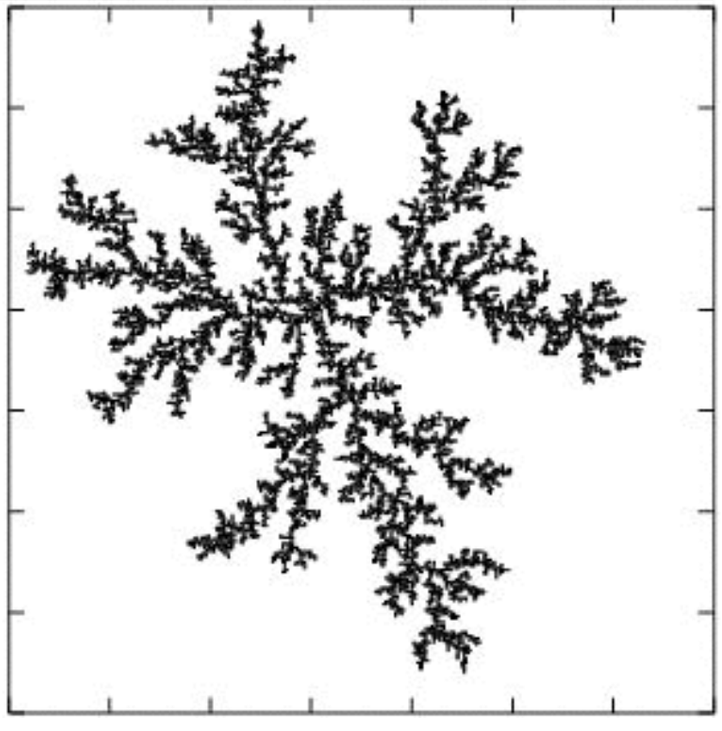
Sedimentation of hard spheres in a 2D system with walls.
Included interactions with smaller particles (not shown here) representing the thermohydrodynamic solvent

(deterministic, classical simulation)

... colloidal systems growth on a substrate...



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

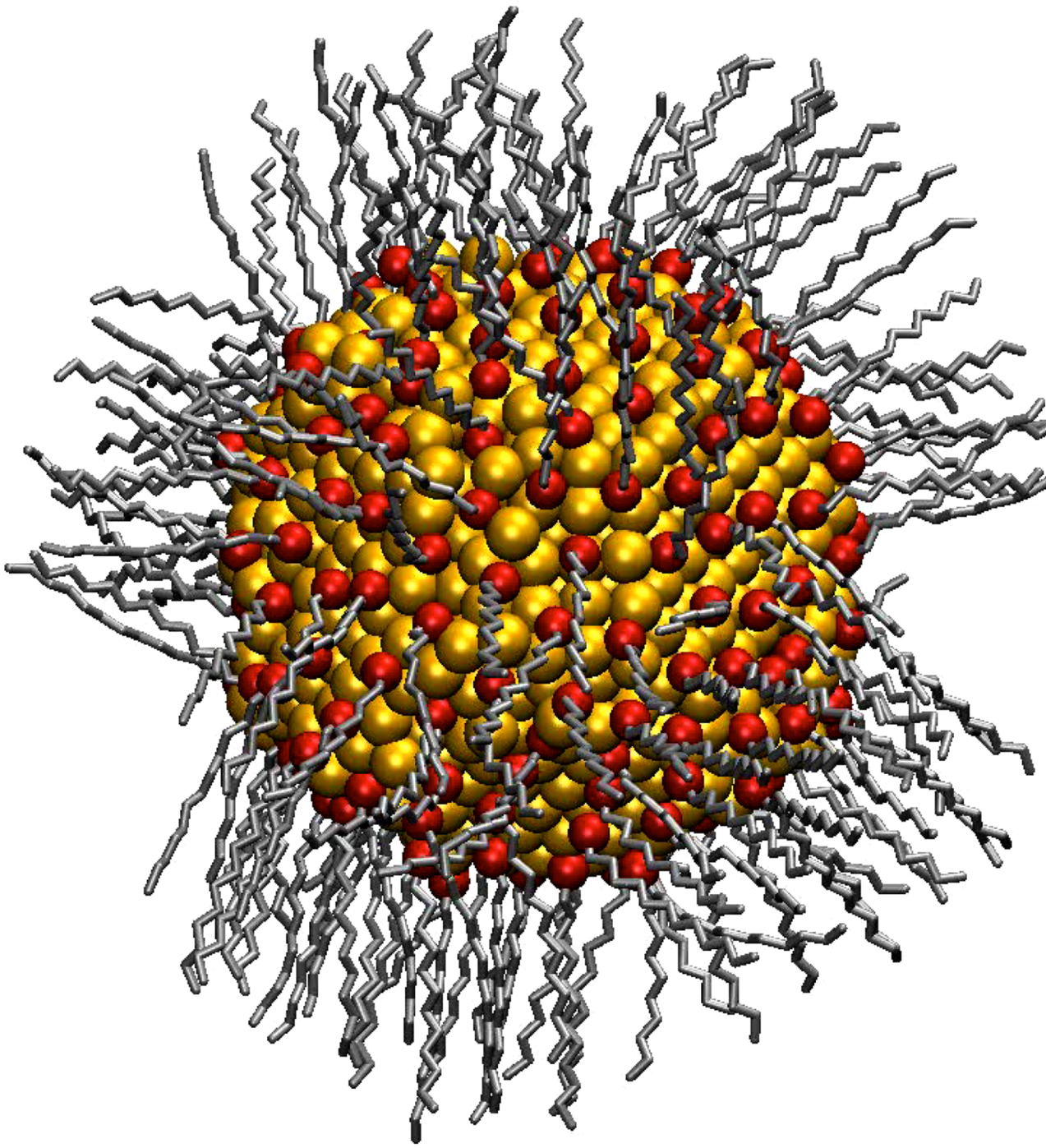


SIMULATION
of a diffusion-limited auto-aggregation model (fractal)

(stochastic, classical simulation)

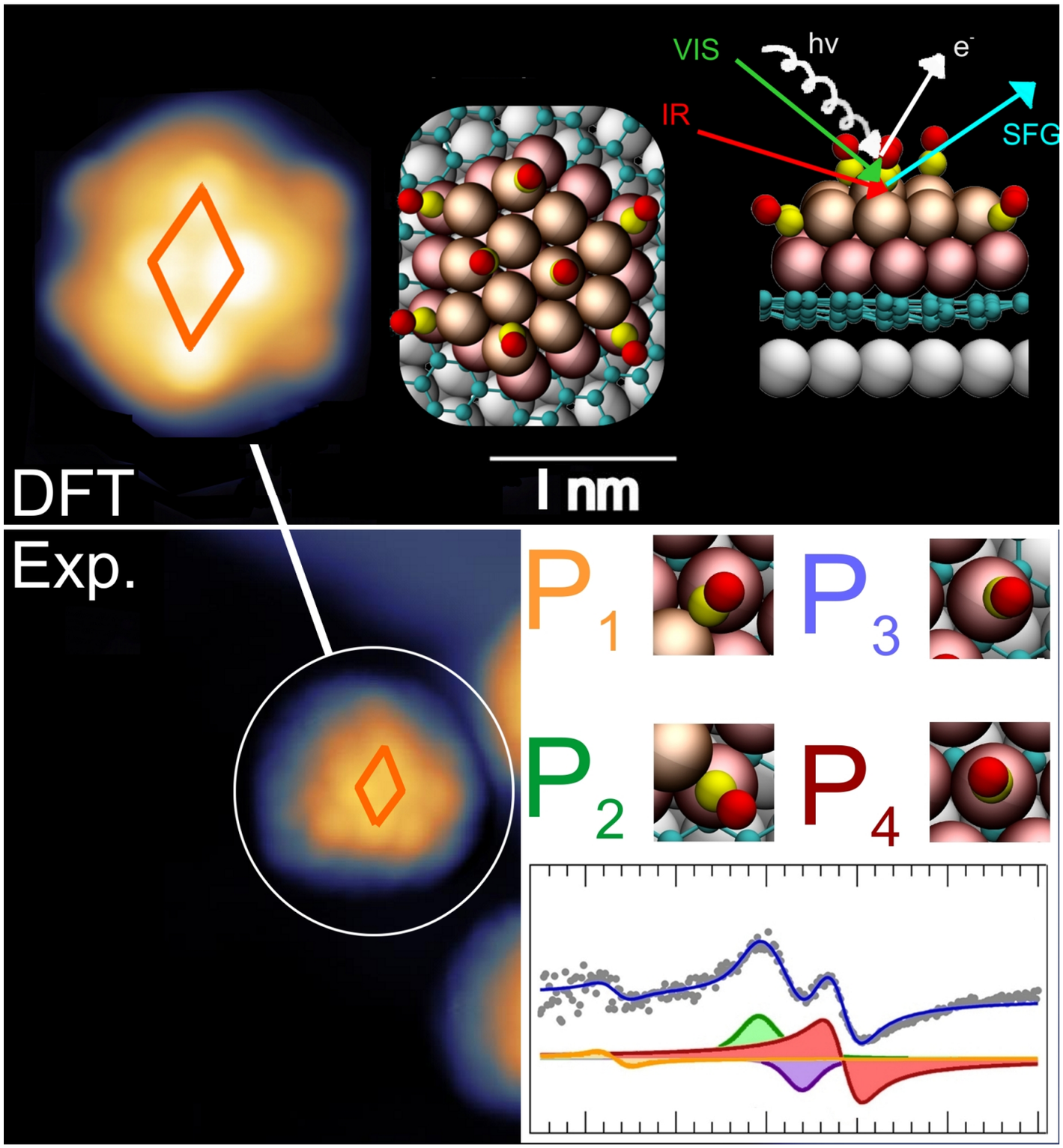
... to the nanoscale: passivation of nanoparticles

with organic molecules
(thiols)
Au
S



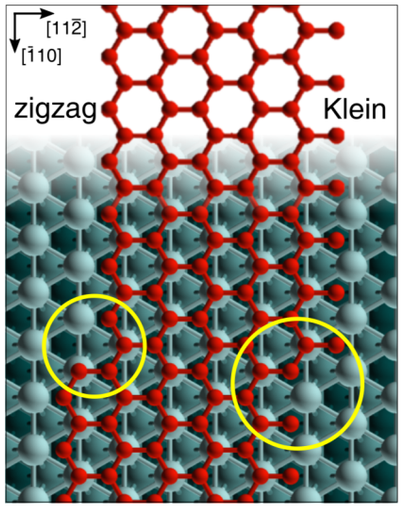
Credits: J. Olmos-Asar

… to the atomic scale



(M.P. in collaboration
with E. Vesselli
and G. Comelli)

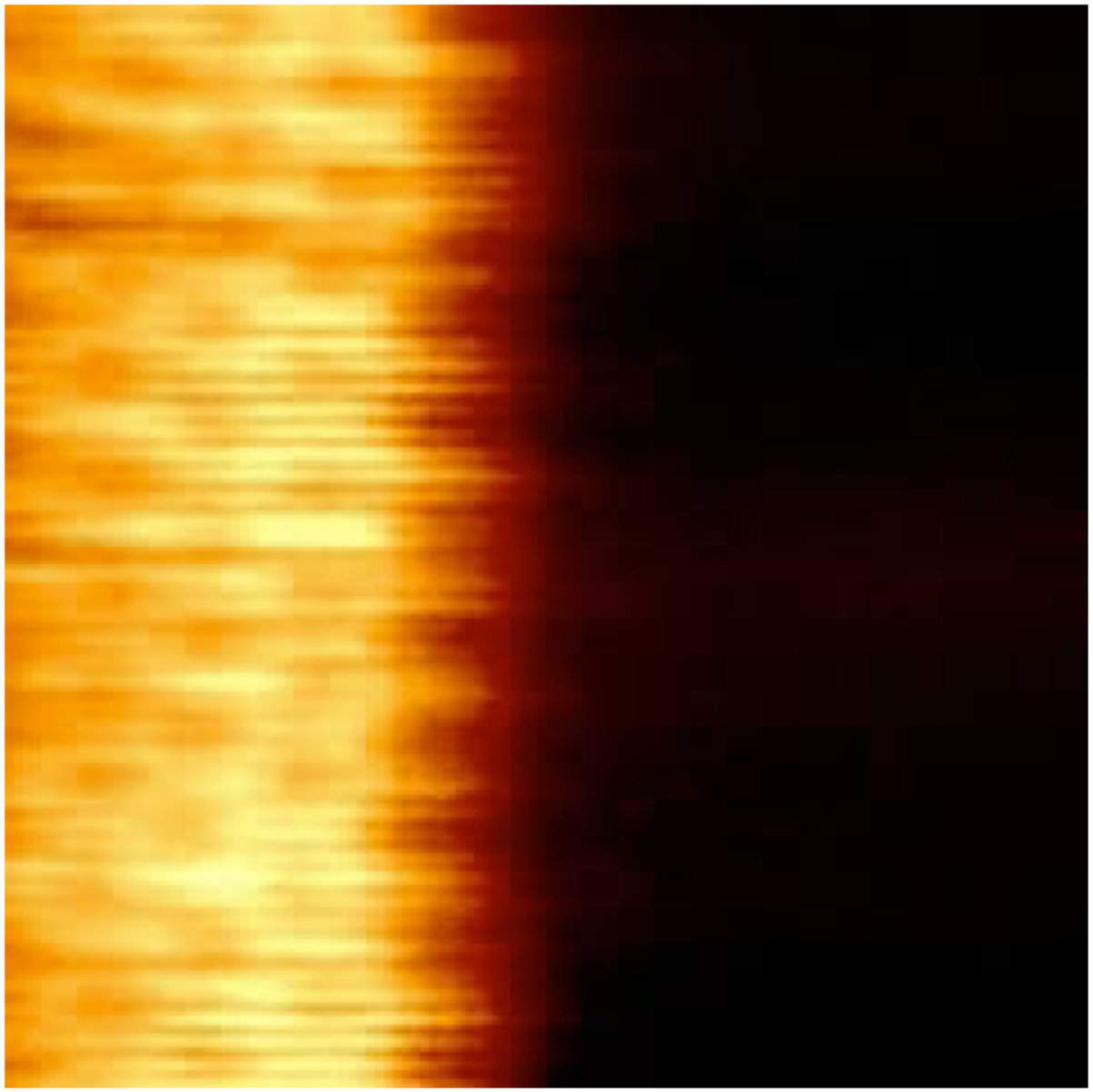
… another example



Grafene @Ni(111)

(M.P. in collaboration with TASC; Science, 2018)

EXPERIMENTAL FAST-STM MOVIE

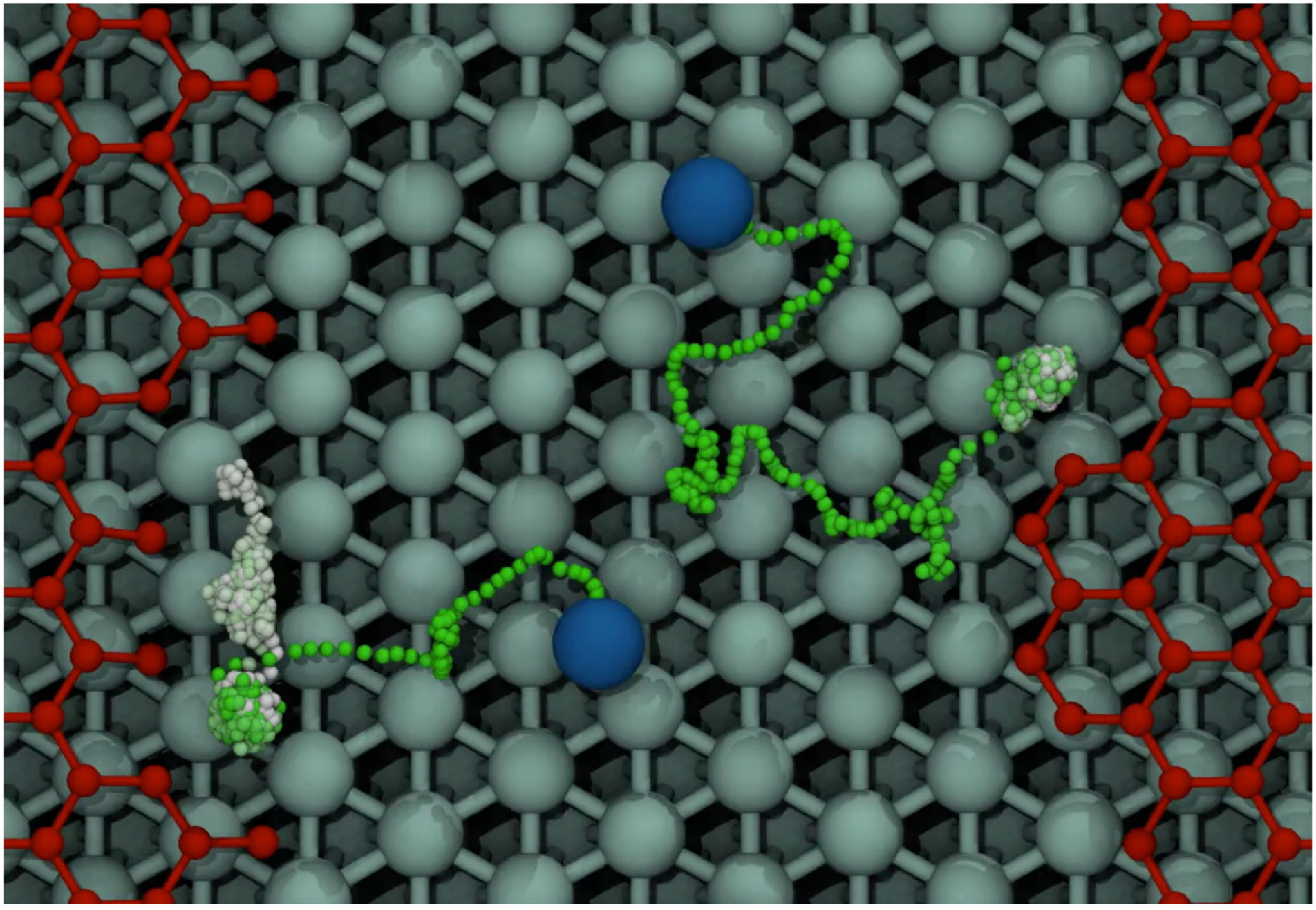


… another example

Grafene @Ni(111)

(M.P. in collaboration with TASC; Science, 2018)

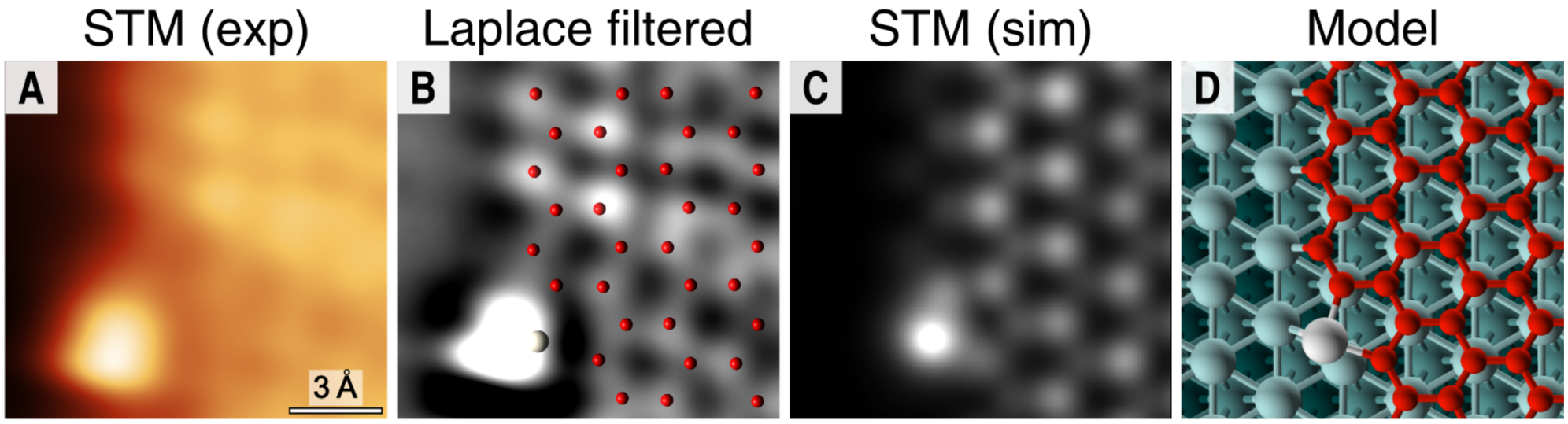
CLASSICAL MOLECULAR DYNAMICS SIMULATION



… another example

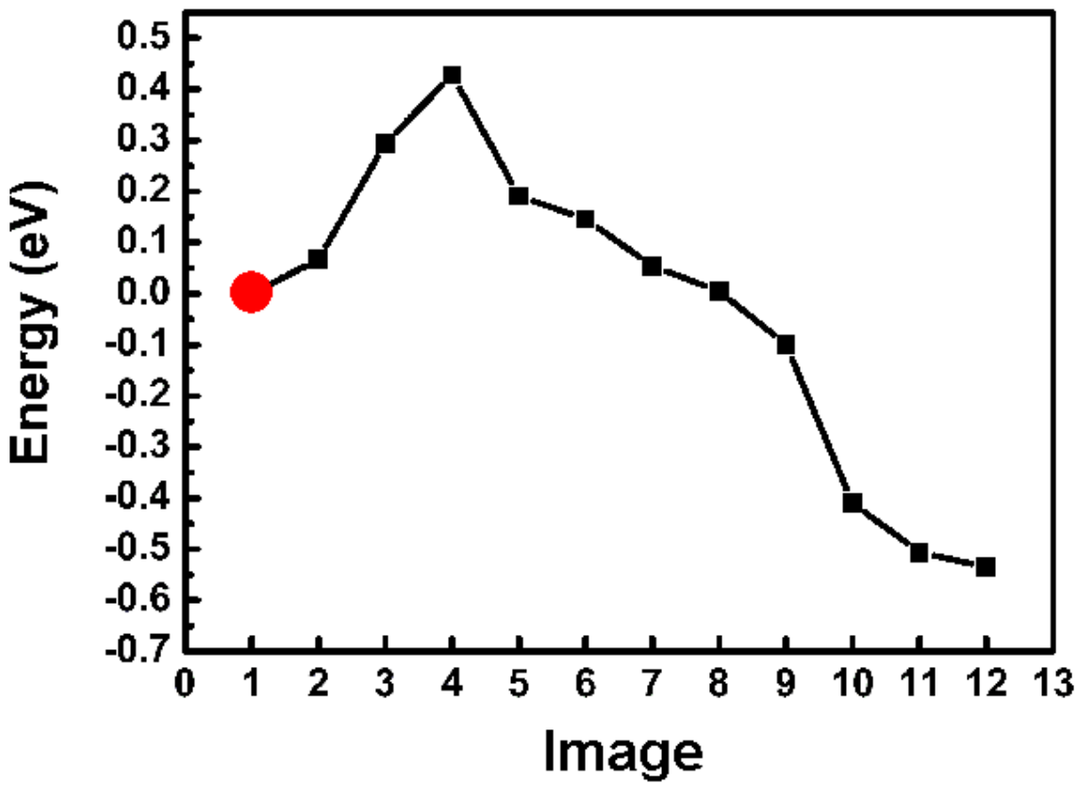
Grafene @Ni(111)

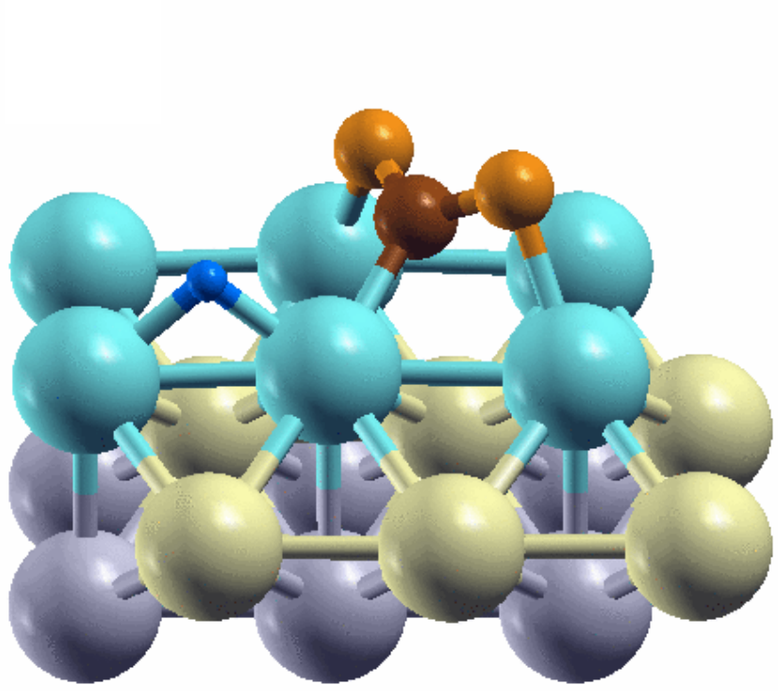
(M.P. in collaboration with TASC; Science, 2018)



QUANTUM MECHANICAL SIMULATION

...including chemical reactions





CO_2 + H -> HCOO @ Ni(110)

(deterministic, quantum mechanical simulation)

even within the condensed matter:

- 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:

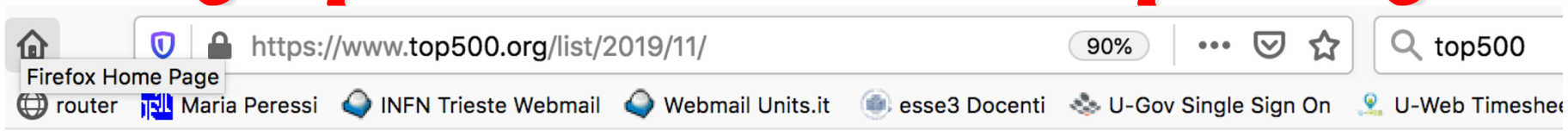
- **continuous models** (for macroscopic systems)
- **atomistic simulations**
  - ab - initio techniques (or "first-principles"): up to ~10^3 atoms, 10 ps
  - Semiempirical techniques: up to 10~7 atoms, 1 ms
  - models at different levels

...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



TOP500 List - November 2019

R_{max} and **R_{peak}** values are in TFlops. For more details about other fields, check the TOP500 description.

R_{peak} values are calculated using the advertised clock rate of the CPU. For the efficiency of the systems you should take into account the Turbo CPU clock rate where it applies.

previous | 1 | 2 | 3 | 4 | 5 | next

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	DOE/SC/Oak Ridge National Laboratory United States	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband IBM	2,414,592	148,600.0	200,794.9	10,096
2	DOE/NNSA/LLNL United States	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband IBM / NVIDIA / Mellanox	1,572,480	94,640.0	125,712.0	7,438
3	National Supercomputing Center in Wuxi China	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
4	National Super Computer Center in Guangzhou China	**Tianhe-2A** - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000	4,981,760	61,444.5	100,678.7	18,482

High performance computing

16	Eni S.p.A. Italy	**HPC4** - Proliant DL380 Gen10, Xeon Platinum 8160 24C 2.1GHz, Mellanox InfiniBand EDR, NVIDIA Tesla P100 HPE	253,600	12,210.0	18,621.1	1,320
17	Commissariat a l'Energie Atomique (CEA) France	**Tera-1000-2** - Bull Sequana X1000, Intel Xeon Phi 7250 68C 1.4GHz, Bull BXI 1.2 Atos	561,408	11,965.5	23,396.4	3,178
18	Texas Advanced Computing Center/Univ. of Texas United States	**Stampede2** - PowerEdge C6320P/C6420, Intel Xeon Phi 7250 68C 1.4GHz/Platinum 8160, Intel Omni-Path Dell EMC	367,024	10,680.7	18,309.2	
19	CINECA Italy	**Marconi Intel Xeon Phi** - CINECA Cluster, Lenovo SD530/S720AP, Intel Xeon Phi 7250 68C 1.4GHz/Platinum 8160, Intel Omni-Path Lenovo	348,000	10,384.9	18,816.0	

(usage with grants; agreement also with UniTS)

(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)

TENTATIVE LIST OF ARGUMENTS

Properties and generation of Random Numbers with different distributions.

Monte Carlo simulation of Random Walks.

Numerical integration in 1 dimension: deterministic and stocastic algorithms;

Monte Carlo algorithms.

Error estimate and reduction of the variance methods.

Metropolis algorithm for arbitrary random number generation.

Metropolis method in the canonical ensamble.

Ising model and Metropolis-Monte Carlo simulation.

Classical fluids: Monte Carlo and Molecular Dynamics simulation of hard spheres and Lennard-Jones fluids.

Microstates and macrostates: efficient algorithm for the numerical calculation of entropy.

Variational Monte Carlo in quantum mechanics (basics).

Lattice gas: vacancy diffusion in a solid.

Caos and determinism: classical billiards and caotic billiards, logistic maps; Lyapunov exponents.

Fractals: diffusion and aggregation, models for surface growth simulation. Percolation.

Course on moodle2

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

https://moodle2.units.it

Then select:

⇒Dipartimento di Fisica

⇒Laurea Magistrale

⇒SM23 - FISICA

⇒A.A. 2019-2020

Or point directly to:

https://moodle2.units.it/course/view.php?id=4367&lang=it

First steps to attend the Course:

1) Go on moodle2 and
REGISTER ON THE COURSE!

2) If you don't have, ask for an account on INFIS

3) "corso sicurezza studenti": you should have the certificate

Available computational resources: INFIS

If you don't have an account on INFIS, compile the form and ask for it (Modulo richiesta di account):

http://df.units.it/it/servizi-strumenti/node/798

Remote connection:
$ssh username@w01.infis.units.it

Your address at INFIS:
username@infis.units.it
nome.cognome@infis.units.it

Where are the examples

- You can find the material lecture by lecture from :

https://moodle2.units.it or

http://www.infis.units.it/~peressi/

(you can find, read and copy the source codes from there if you have an INFIS account)

$/home/peressi/comp-phys

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

From your directory, do:

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

(this last "." means: here, with the same name)

fortran compiler on INFIS

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

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

The option -std=f95 allows to obtain, after compilation, supplementary info about the commands you wrote in your code (the syntax, whether it is standard fortran or not...)

OPTIONS ARE IMPORTANT AND USEFUL!

fortran compilers on INFIS

- OTHERS (NOT SUPPORTED ON INFIS):

  g95 (free)

  ifort (Fortran Intel compiler, NOT free)

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

  ....

- To run the 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)

$ find . -size +20000 -print (to identify big files)

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

- complementary to **"Classical simulations of many body systems"** (E. Smargiassi, I semester) (deterministic, classical)

- complementary to **"Numerical Methods of Quantum Mechanics"** (P. Giannozzi, II semester) (deterministic, quantum)