



993SM - Laboratory of Computational Physics

lecture I - I part

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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

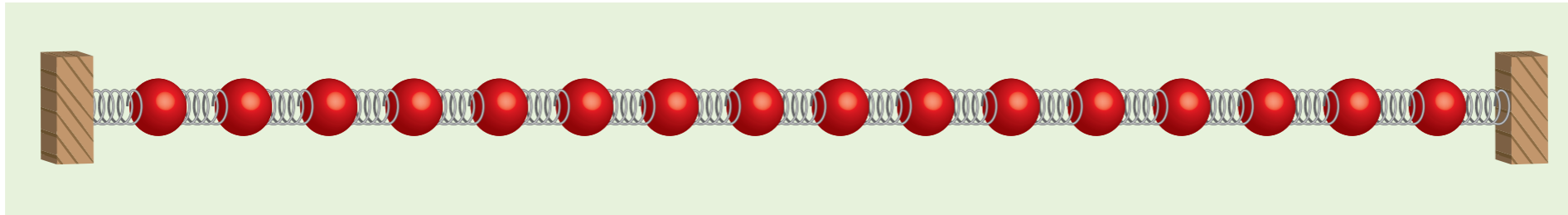
- control of instruments, data collection and analysis
- visualization
- symbolic manipulation
- . . .

.....

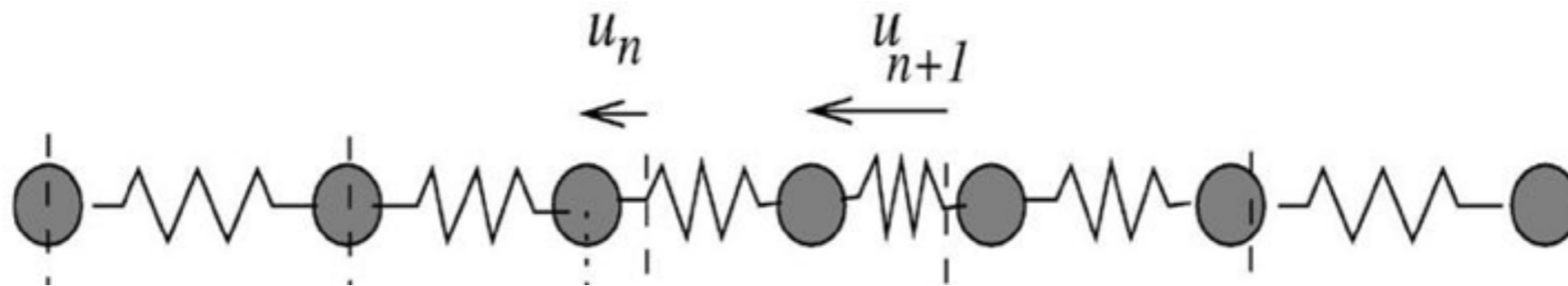
- **numerical analysis:** to solve equations which could not be tackled by analytical methods. This allows to measure theories, in a similar way as natural phenomena are measured by experiments, the ultimate goal of science being the insight and understanding gained from the comparison of these two kinds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

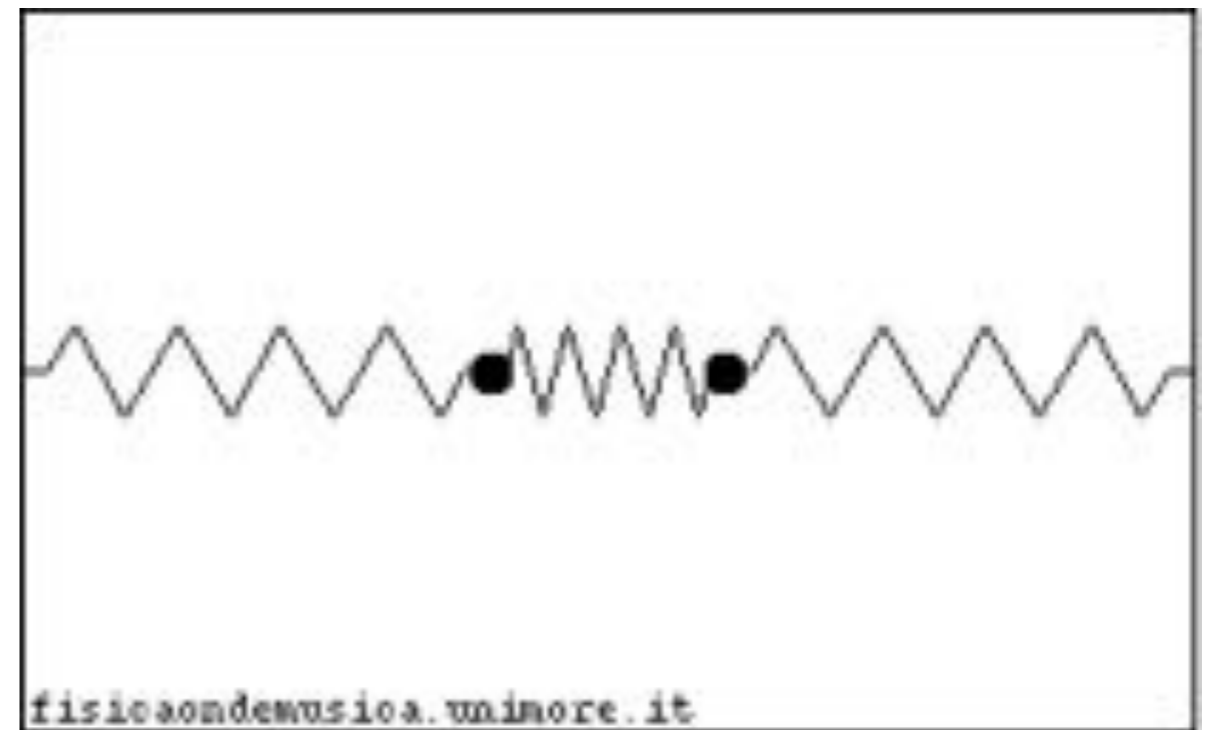
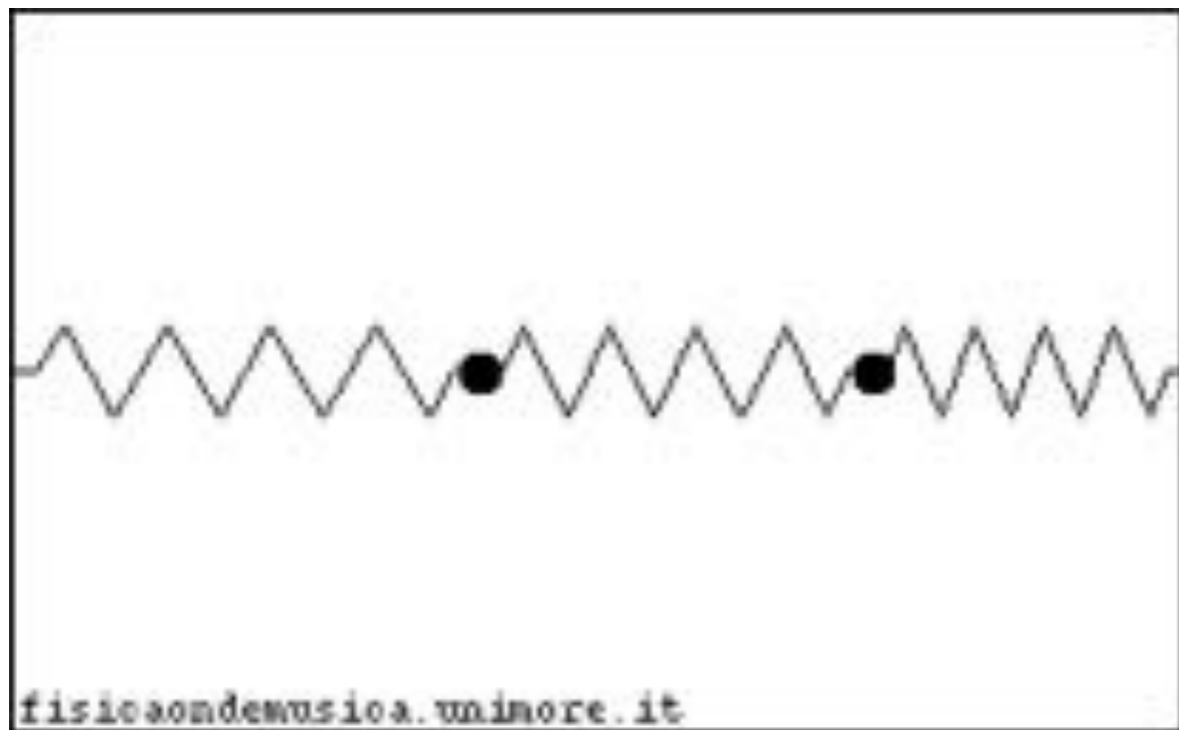


Linear interaction (Hooke's law):

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

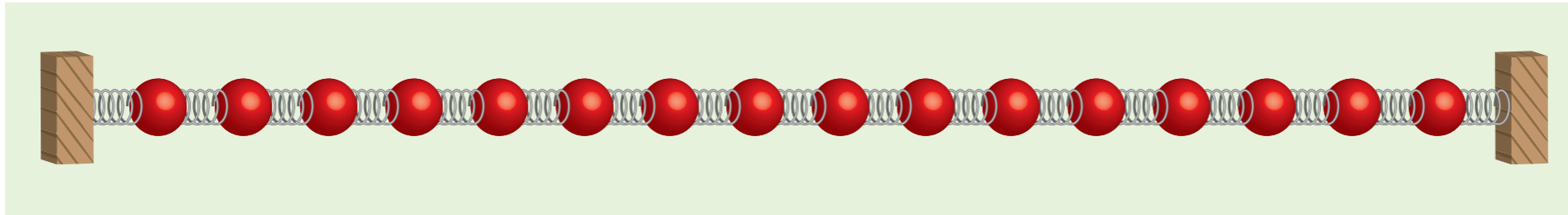


http://fisicaondemusica.unimore.it/Oscillatori_accoppiati.html

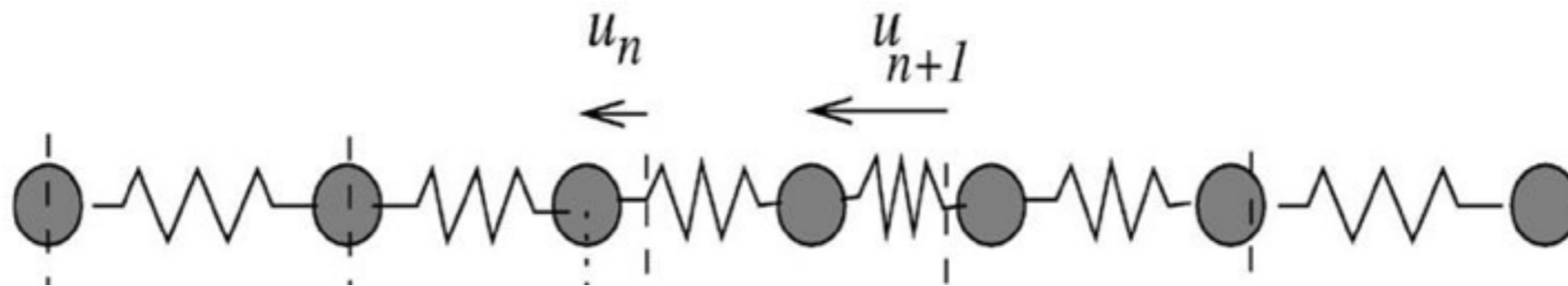
More in: http://fisicaondemusica.unimore.it/Catena_di_Fermi_Pasta_Ulam.html

The birth of computational physics

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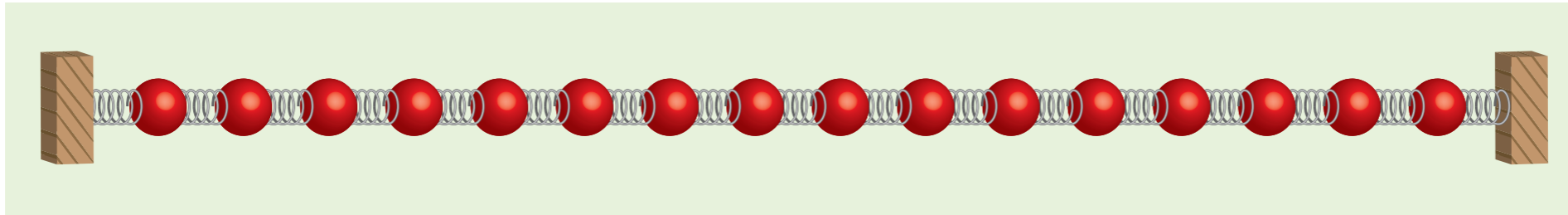


Linear interaction (Hooke's law):
analytical solution

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

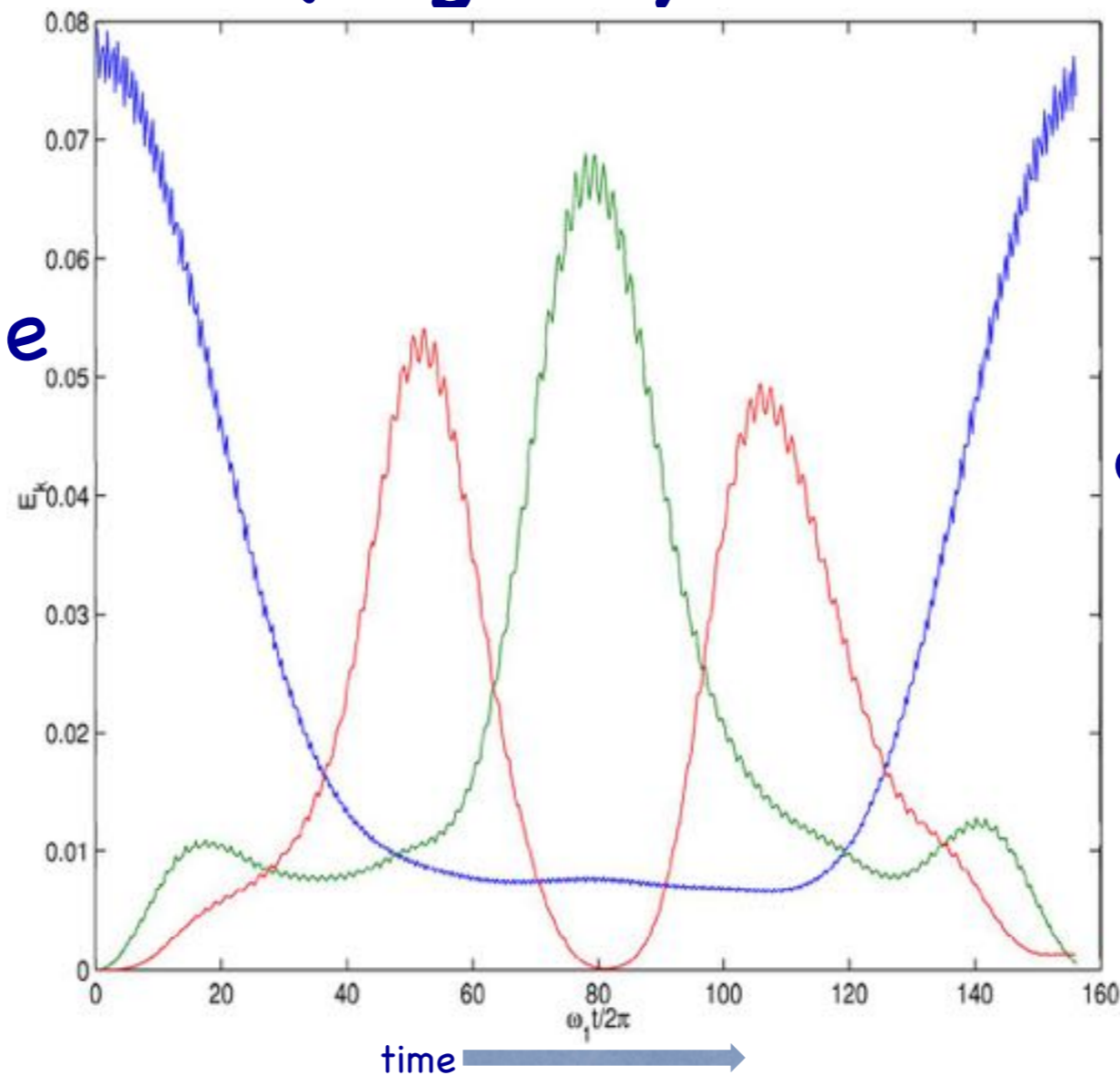
The birth of computational physics

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 !!!

Simulations as “virtual experiments”

A few similarities between experiments:

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

Simulations as “virtual experiments”

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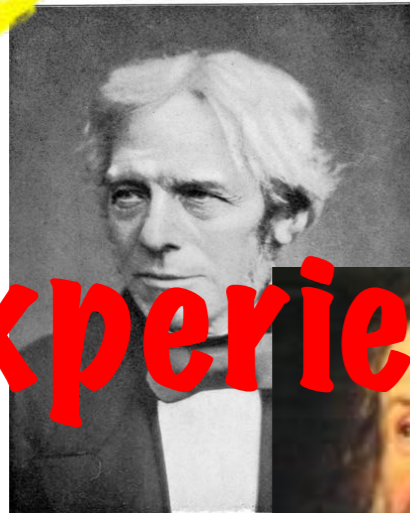
“real” (in lab)	“virtual” (computational)
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With errors!!!

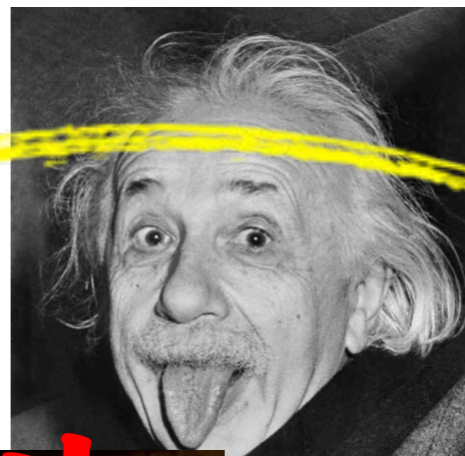


- Importance of simulations: “**what-if**” **experiments** (large flexibility in varying parameters; e.g. material properties can be studied also under conditions not accessible in real labs) ; **predictions**, not just description.
- Use of simulations: not “**final goal**”, but “**instruments**” to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

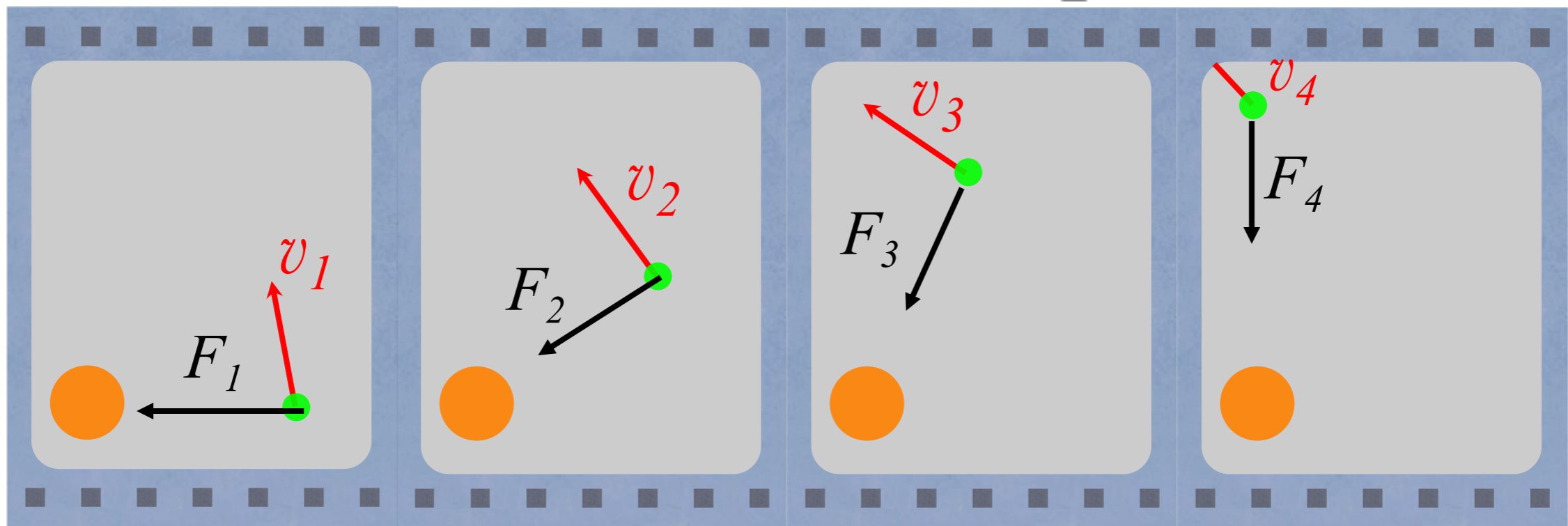
(the equation for the velocity is 1st order),
whether the force is dependent or not on the
velocity,
to which order...

Example (classical):

The deterministic approach

Discretization of the equation of motion and iteration:

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



$x(1)$ $v(1)$ $F(1)$

$x(2)$ $v(2)$ $F(2)$

$x(3)$ $v(3)$ $F(3)$

... ..

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

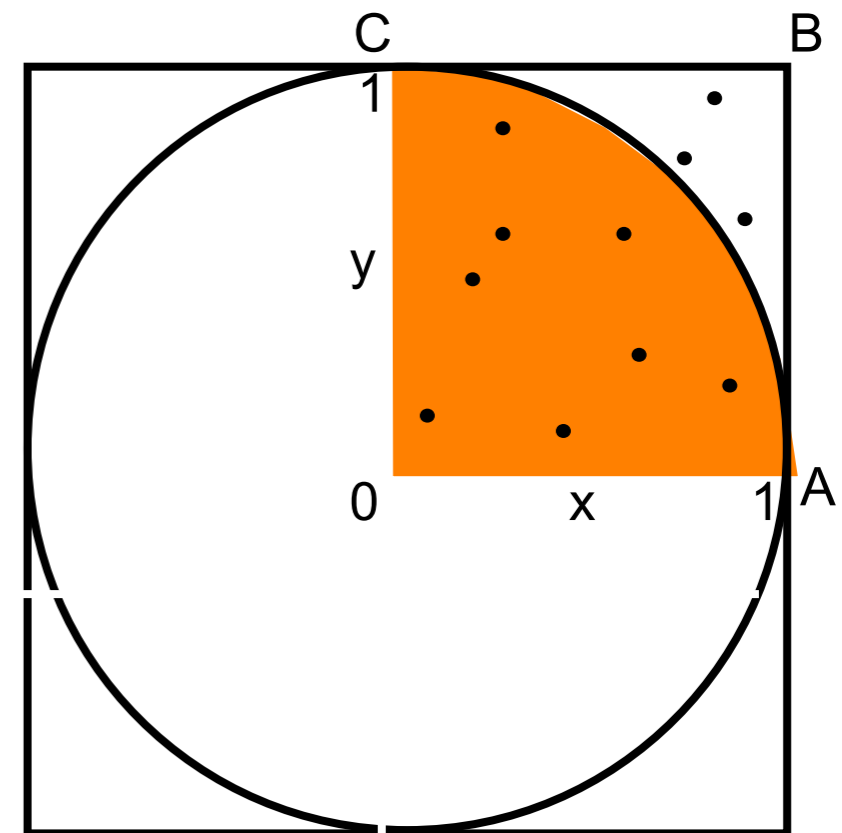
(*) a sequence of random numbers is a set of numbers which looks unpredictable but with well defined statistical properties

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



$$\begin{aligned}\pi &\approx \frac{4 \times \text{Area Under Curve CA}}{\text{Area of Square OABC}} \\ &= \frac{4\tau_{hit}}{\tau_{tot}}\end{aligned}$$

A few selected examples of applications

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

From "normal" scales...

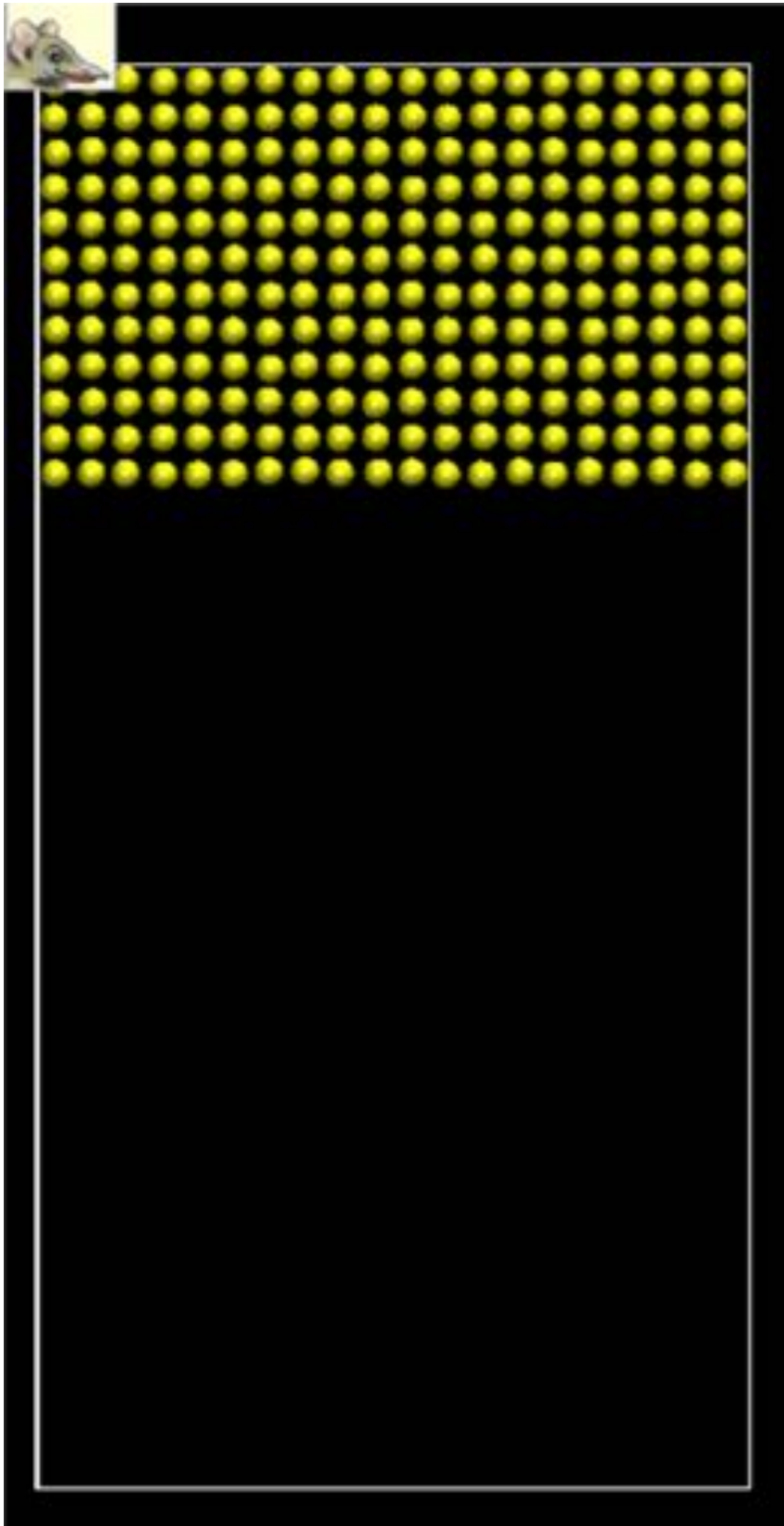
(classical)

SIMULATION
of the Brownian motion

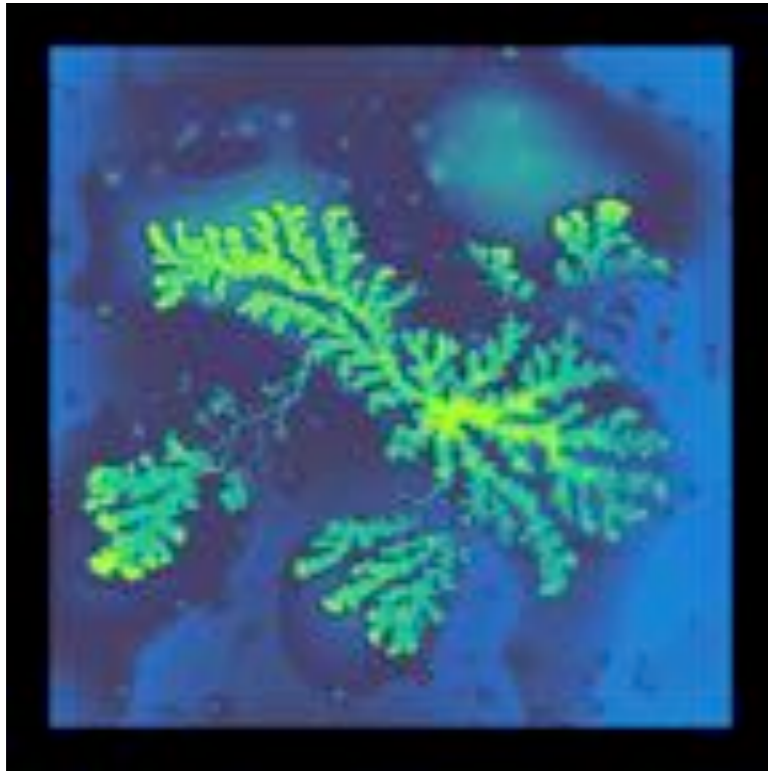
Sedimentation of hard spheres in a 2D
system with walls.

Included interactions with smaller
particles (not shown here) representing
the thermohydrodynamic solvent

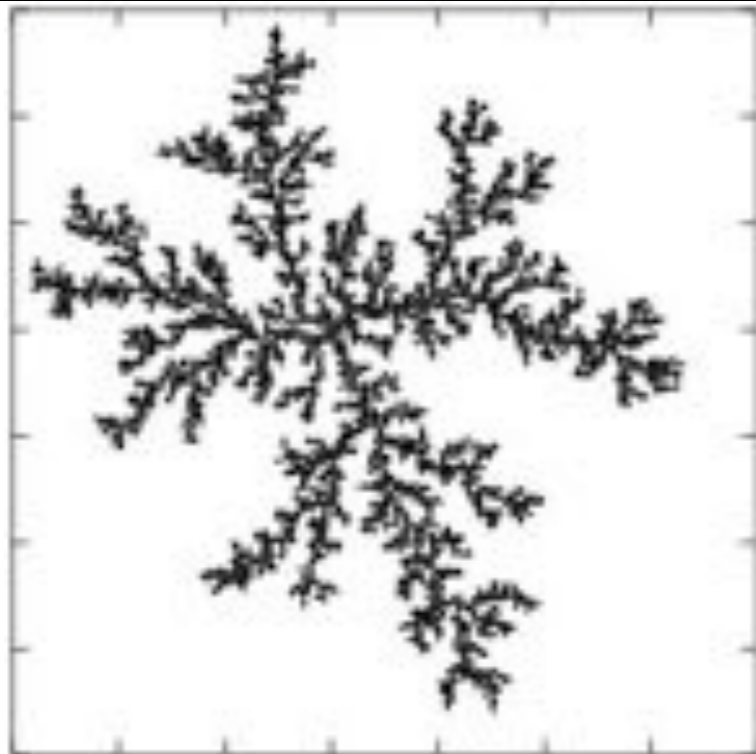
**(deterministic, classical
simulation)**



... 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)

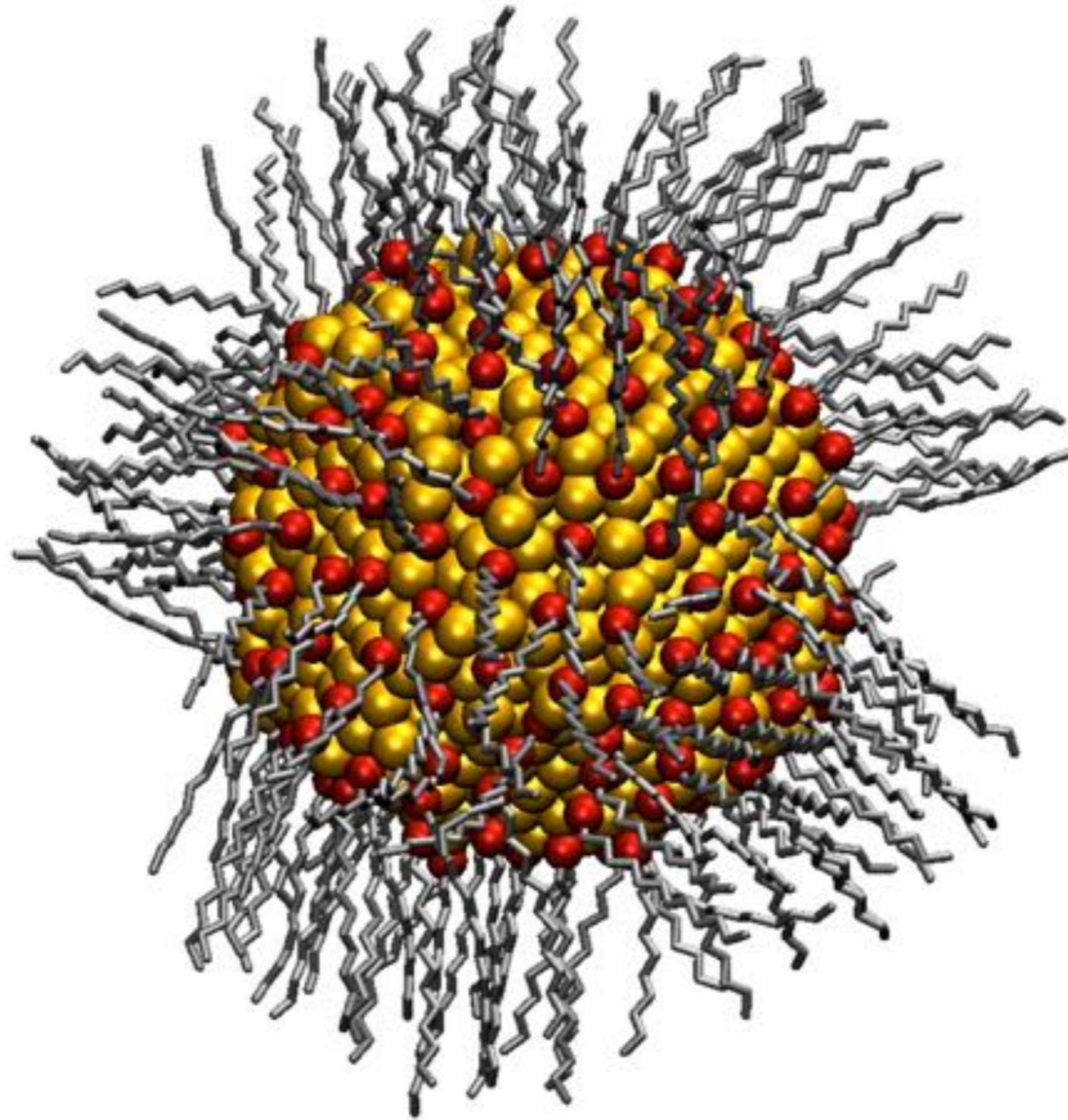
(stochastic, classical simulation)

... to the nanoscale: passivation of nanoparticles

with organic molecules
(thiols)

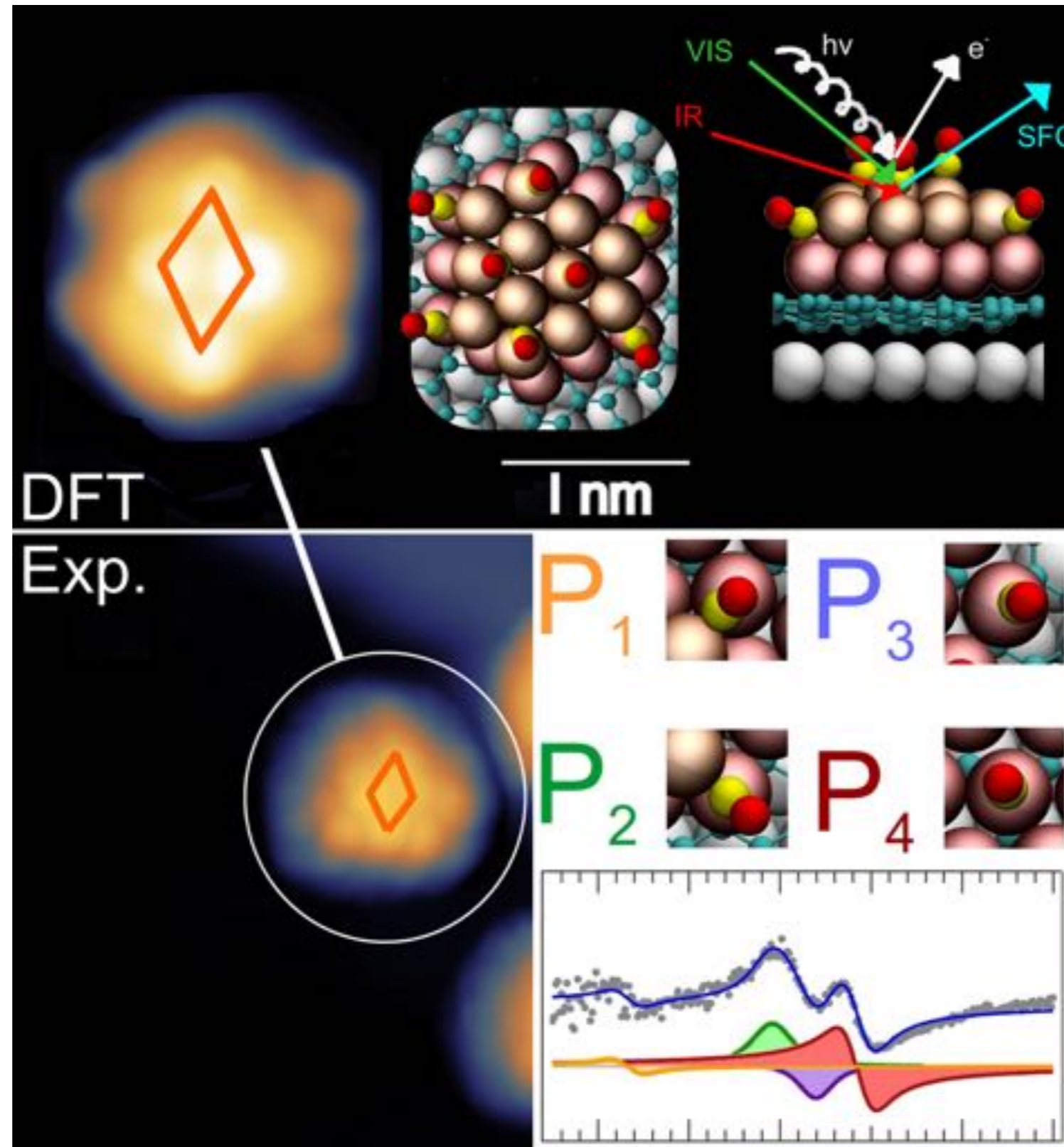
Au

S



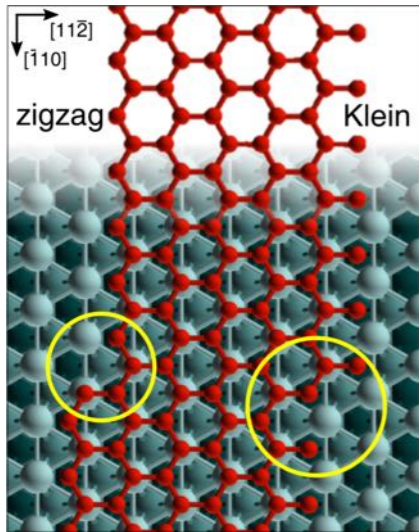
Credits: J. Olmos-Asar

... to the atomic scale



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

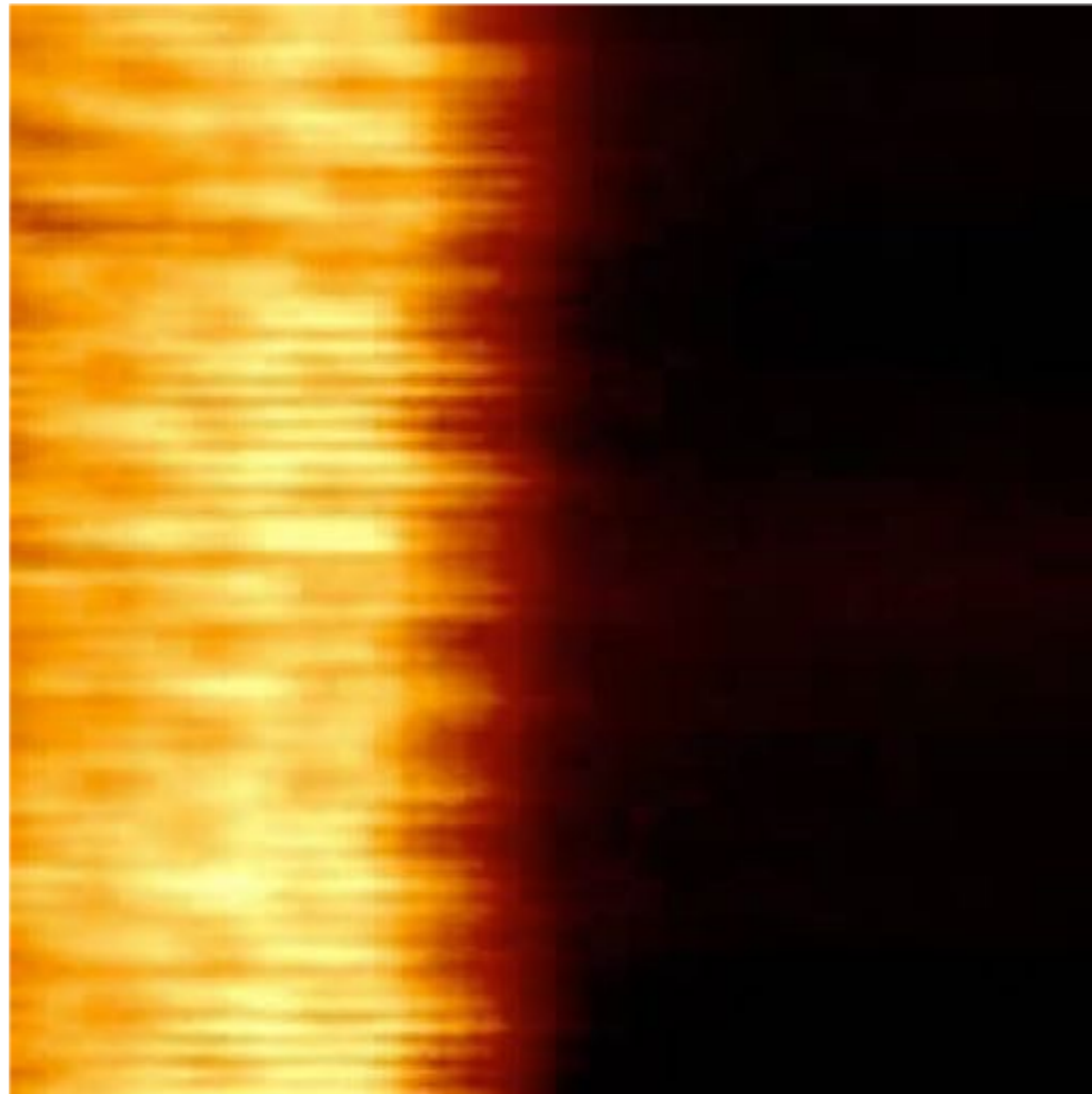
... another example



Grafene @Ni(111)

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

EXPERIMENTAL
FAST-STM
MOVIE

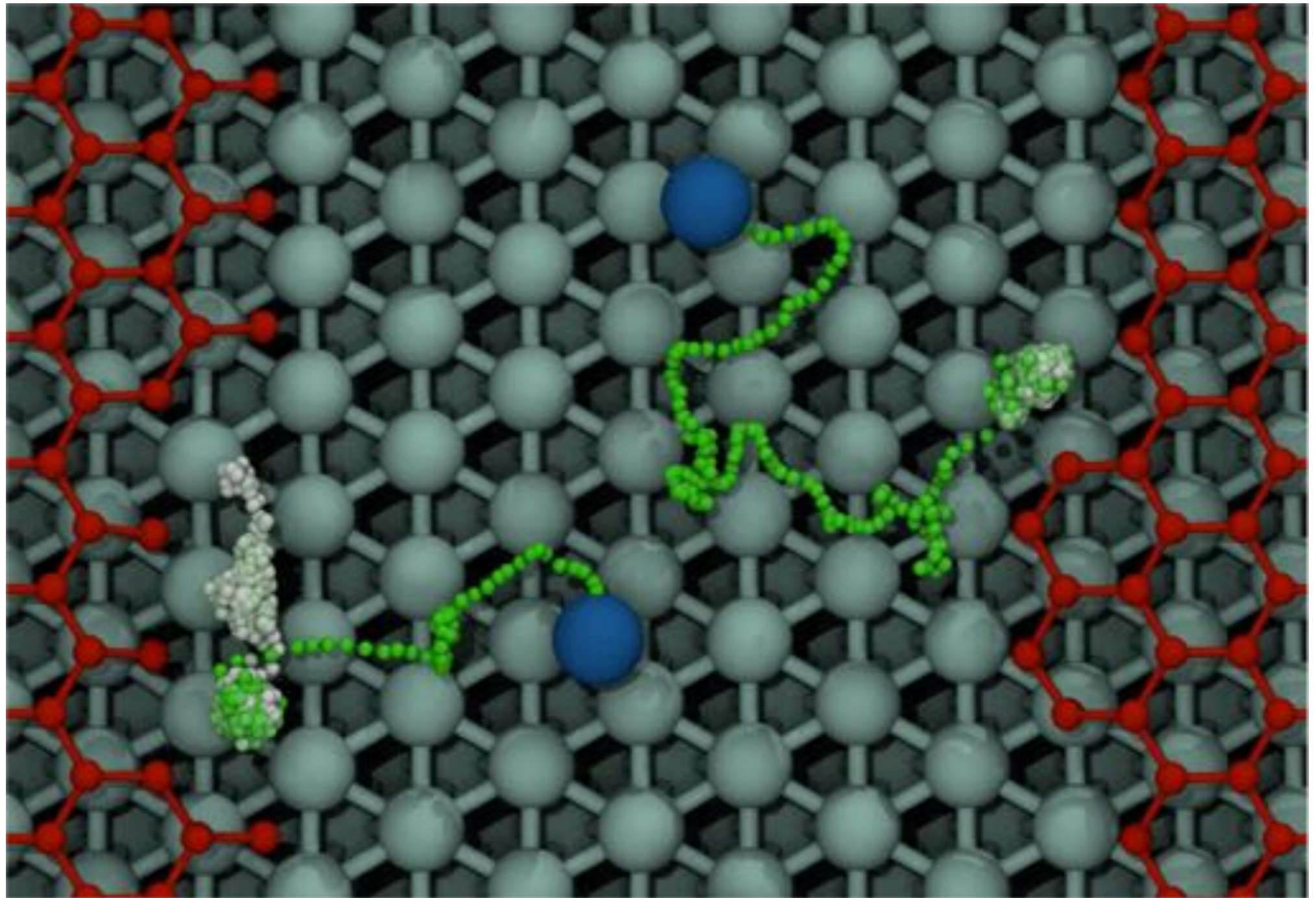


... another example

Grafene @Ni(111)

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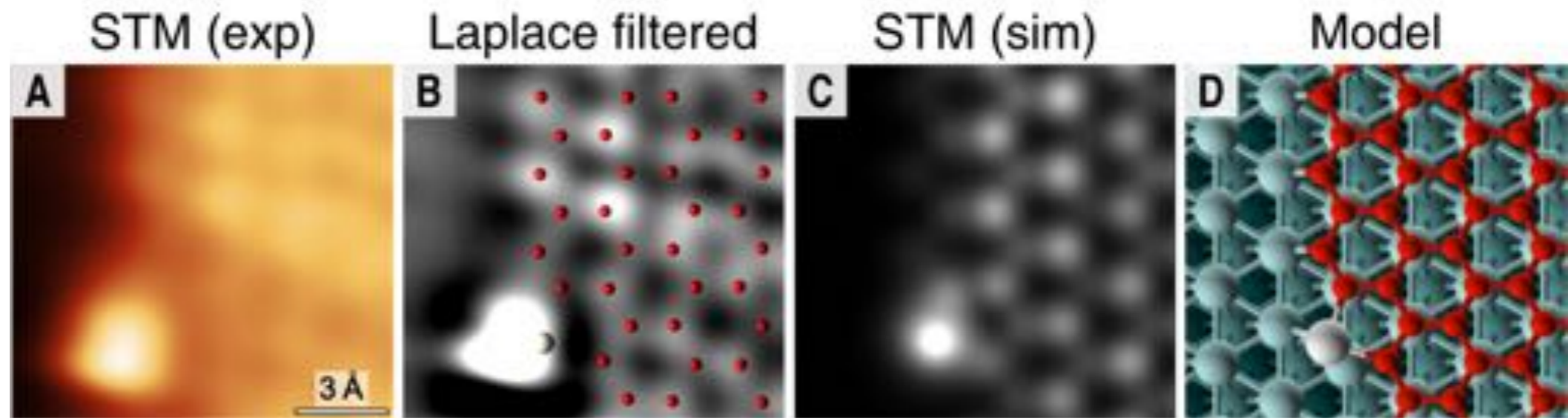
CLASSICAL
MOLECULAR
DYNAMICS
SIMULATION



... another example

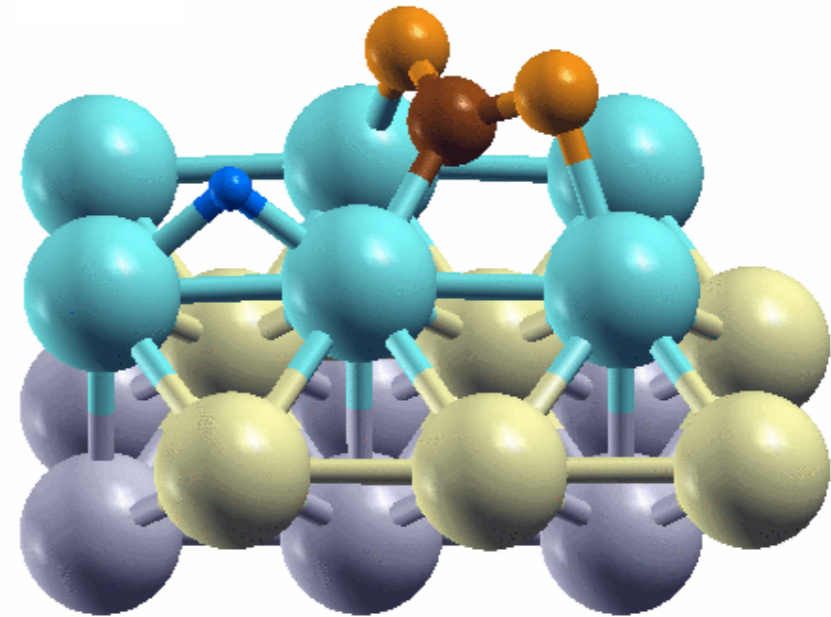
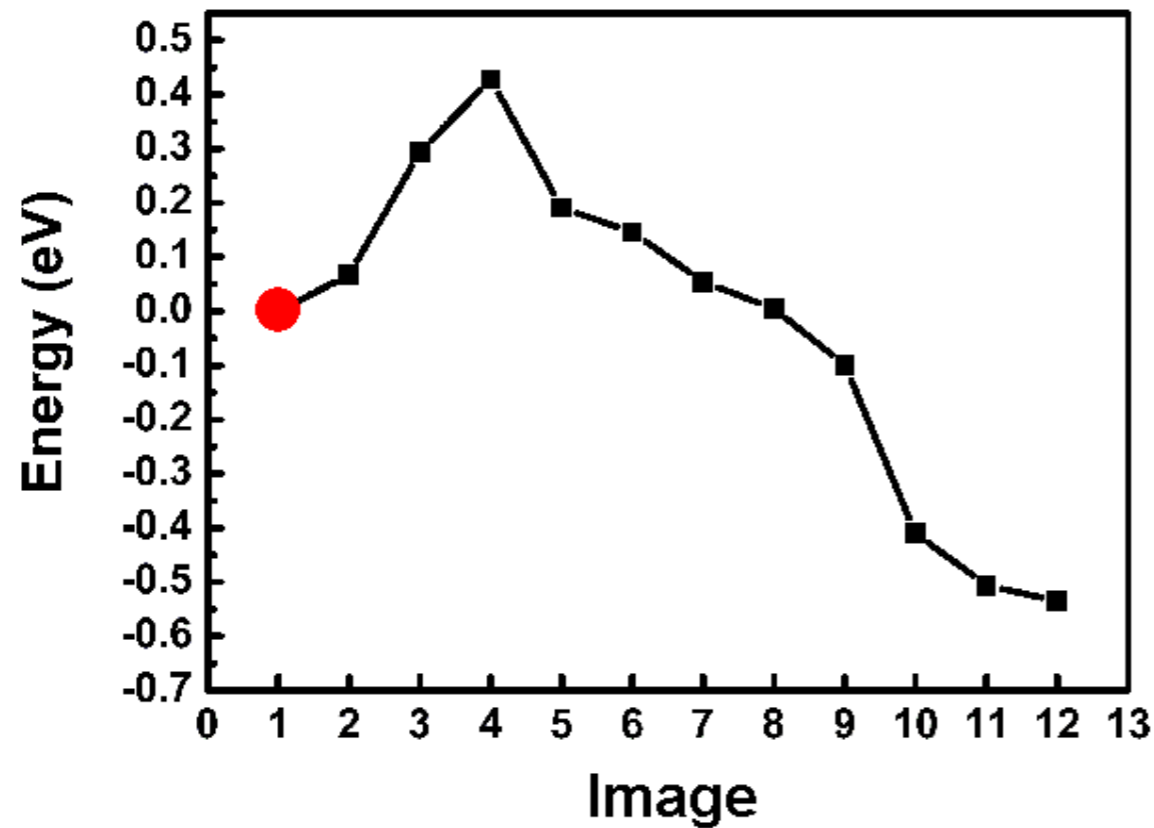
Grafene @Ni(111)

(M.P. in
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Science, 2018)



QUANTUM
MECHANICAL
SIMULATION

...including chemical reactions



(deterministic, quantum mechanical simulation)

even within the condensed matter:

- wide range of **length scales**: ≈ 12 orders of magnitude (nuclei/electrons/atoms/chemical bonds $\sim 10^{-12}$ m, fracture/macroscale mechanical phenomena ~ 100 m; nano / micro / meso / macroscale scales)
- wide range of **time scales**: ≈ 12 orders of magnitude (nuclei/electrons/atoms/chemical bonds $\sim 10^{-12}$ s, fracture/macroscale mechanical phenomena \sim 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 $\sim 10^3$ 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

<https://www.top500.org/lists/top500/2020/11/>

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
3	Sierra - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438

High performance computing

<https://www.top500.org/lists/top500/2020/11/>



➔

8	HPC5 - PowerEdge C4140, Xeon Gold 6252 24C 2.1GHz, NVIDIA Tesla V100, Mellanox HDR Infiniband, Dell EMC Eni S.p.A. Italy	669,760	35,450.0	51,720.8	2,252
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➔

11	Marconi-100 - IBM Power System AC922, IBM POWER9 16C 3GHz, Nvidia Volta V100, Dual-rail Mellanox EDR Infiniband, IBM CINECA Italy	347,776	21,640.0	29,354.0	1,476
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(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 stochastic algorithms;

Monte Carlo algorithms.

Error estimate and reduction of the variance methods.

Metropolis algorithm for arbitrary random number generation.

Metropolis method in the canonical ensemble.

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.

Chaos and determinism: classical billiards and chaotic billiards, logistic maps; Lyapunov exponents.

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

Course on moodle2

You can find the material lecture by lecture

- 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

SUBSCRIBE TO THE COURSE on moodle2 !

<https://moodle2.units.it>

Then select:

⇒ Dipartimento di Fisica

⇒ Laurea Magistrale

⇒ SM23 - FISICA

⇒ A.A. 2020-2021

Or point directly to:

<https://moodle2.units.it/course/view.php?id=7238>

Fortran compiler on the virtual Lab

- **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!

Other possible Fortran compilers

- 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)