993SM - Laboratory of Computational Physics

lecture I - I part

Sept. 25, 2023

Maria Peressi - Antimo Marrazzo

Università degli Studi di Trieste - Dipartimento di Fisica

Sede di Miramare (Strada Costiera 11, Trieste)

e-mail: peressi@units.it , antimo.marrazzo@units.it

And you?

https://www.menti.com/al7fyr7o428e
or
https://www.menti.com
ond enter the code
3152 8582

Computers in Physics: what is your experience?

https://www.menti.com/aljohokzeb8h

or

https://www.menti.com

ond enter the code

8521 0628

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.

- **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.

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

(4) Local resources

(1) Computational Physics

The birth of computational physics

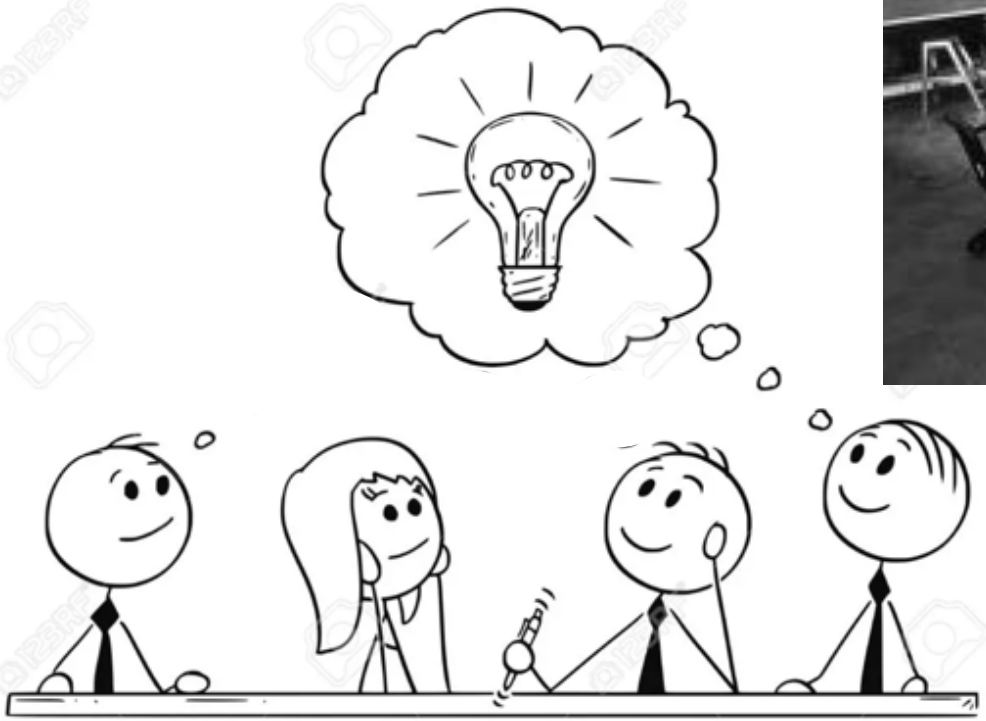
A PROBLEM for the MANIAC computer (Los Alamos, 1955)

Fermi-Pasta-Ulam-Tsingou

The birth of computational physics

A PROBLEM for the MANIAC computer (Los Alamos, 1955)

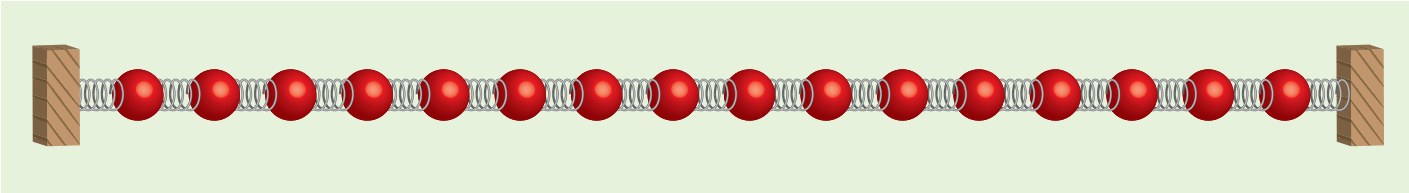
thermalization!



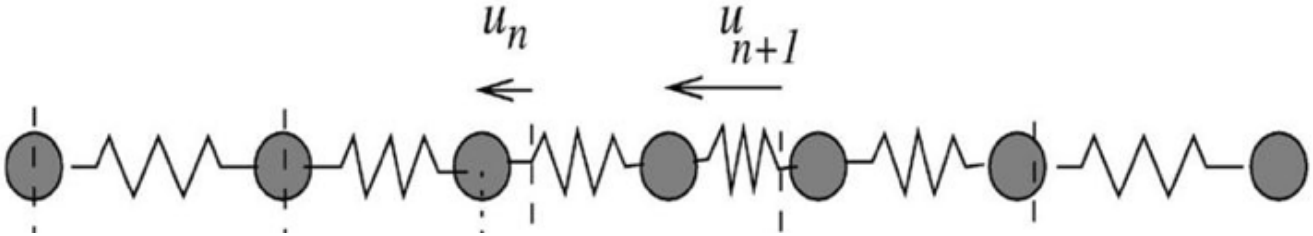
https://discover.lanl.gov/publications/national-security-science/2020-winter/we-thank-miss-mary-tsingou/

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)

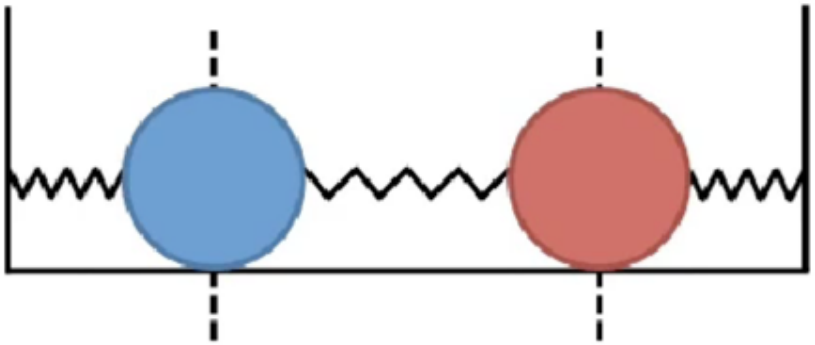


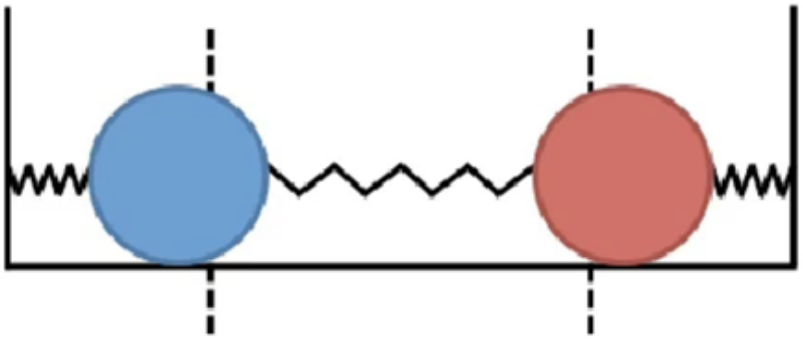
Linear interaction (Hooke's law):

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



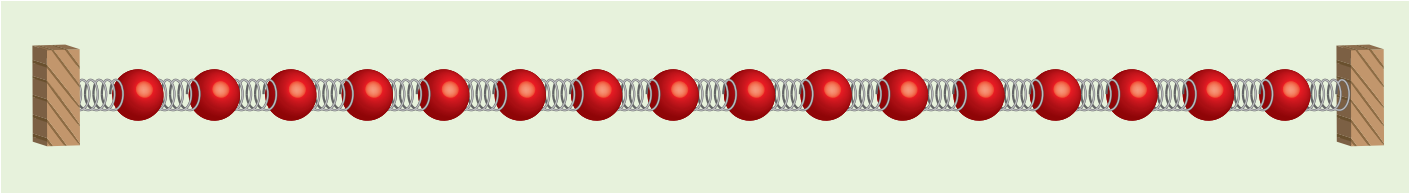


http://fisicaondemusica.unimore.it/Oscillatori_accoppiati.html

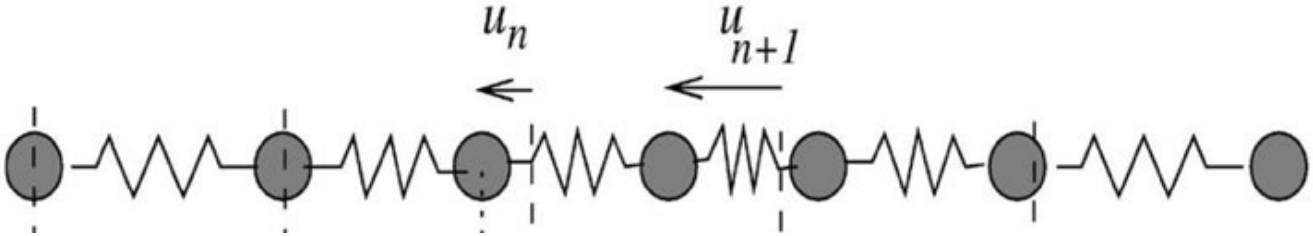
More on: https://fisicaondemusica.unimore.it/Catena_di_Fermi-Pasta-Ulam.html

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)

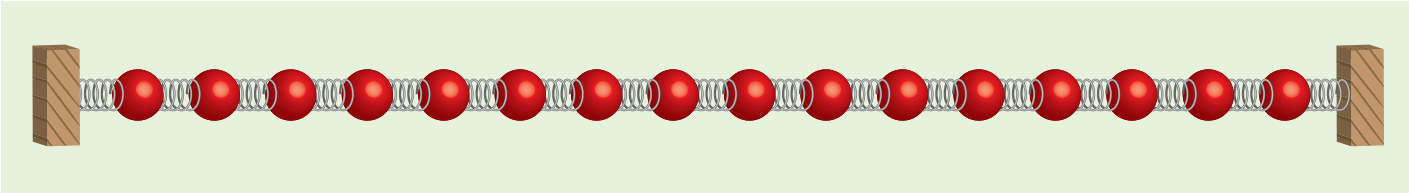


Linear interaction (Hooke's law):
analytical solution

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

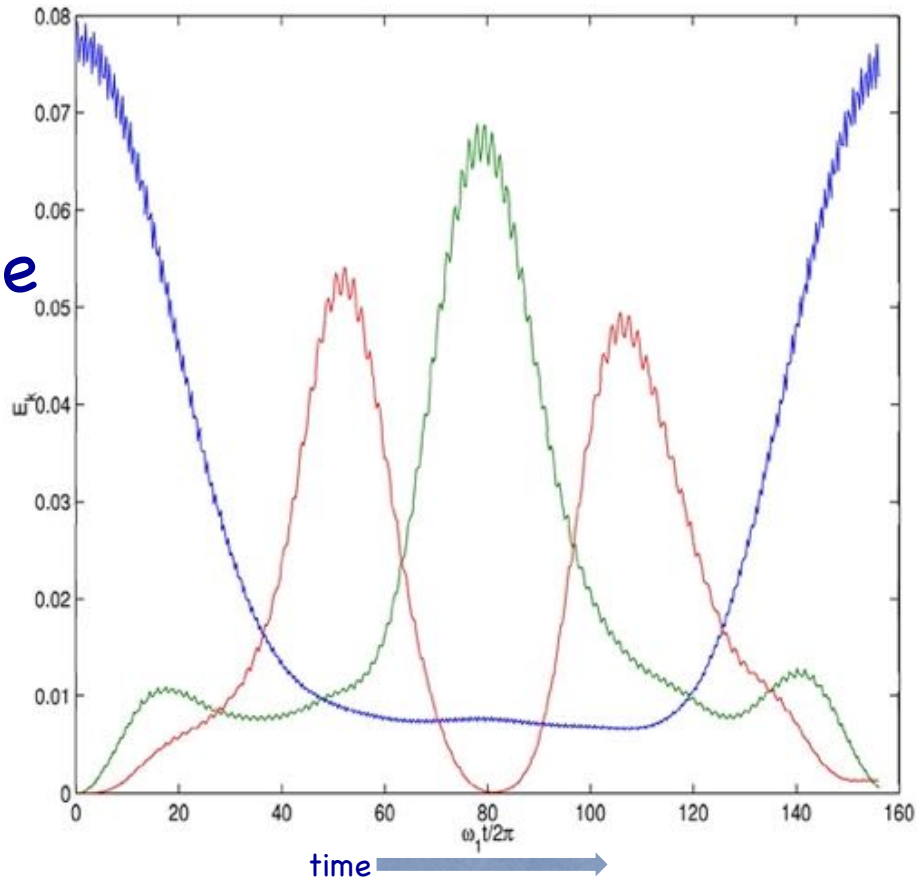
The birth of computational physics

PROBLEM: Fermi-Pasta-Ulam-Tsingou 1955

Numerical solution with MANIAC (originally: calculations for N=5)

Energy vs. time for the first three modes:

K= 1 2 3



here: N=32; 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 decades, the numerical 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...

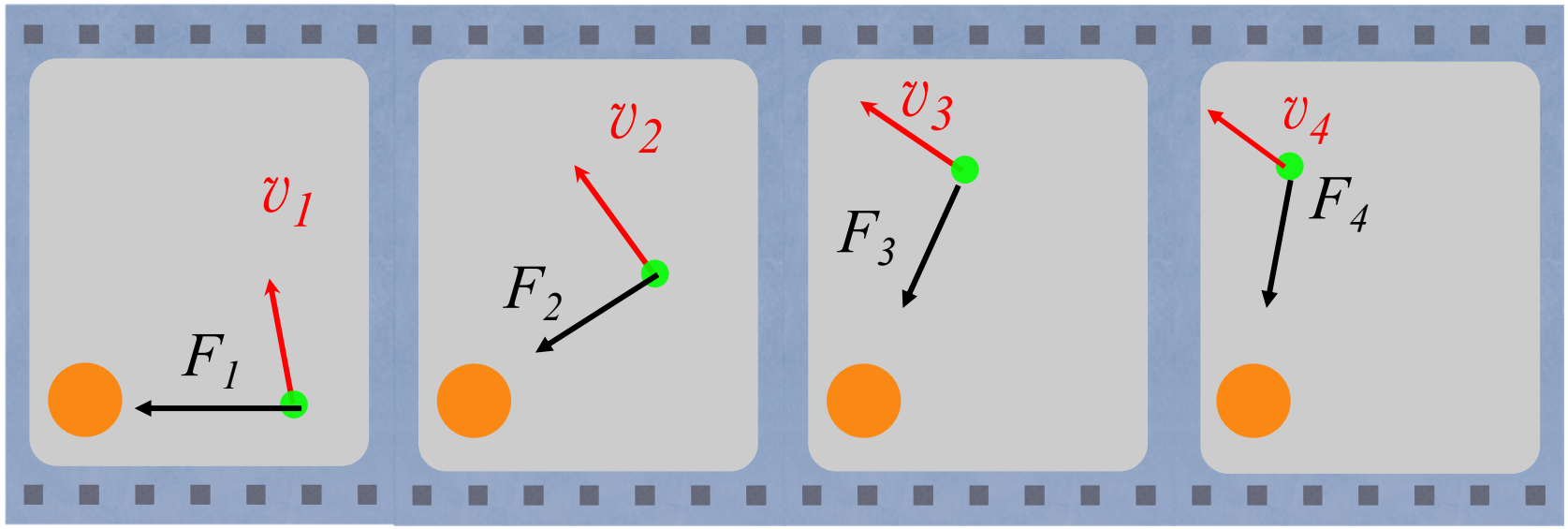
Examples =>

The deterministic approach

1) Classical 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 deterministic approach

2) Quantum

Discretization of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$$

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.

The stochastic approach

1) Probabilistic physical processes

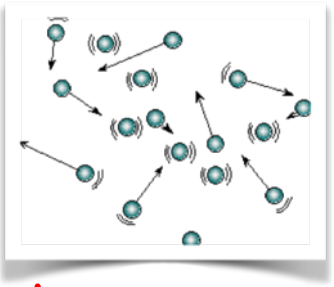
We attempt to follow the `time dependence' of a model where change, or growth, does not proceed in some rigorously predefined fashion (e.g. according to Newton's equations of motion) but rather in a stochastic manner which depends on a sequence of random numbers which is generated during the simulation.

E.g.: radioactive decay

The stochastic approach

2) 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!

The stochastic approach

2) Systems with many degrees of freedom

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

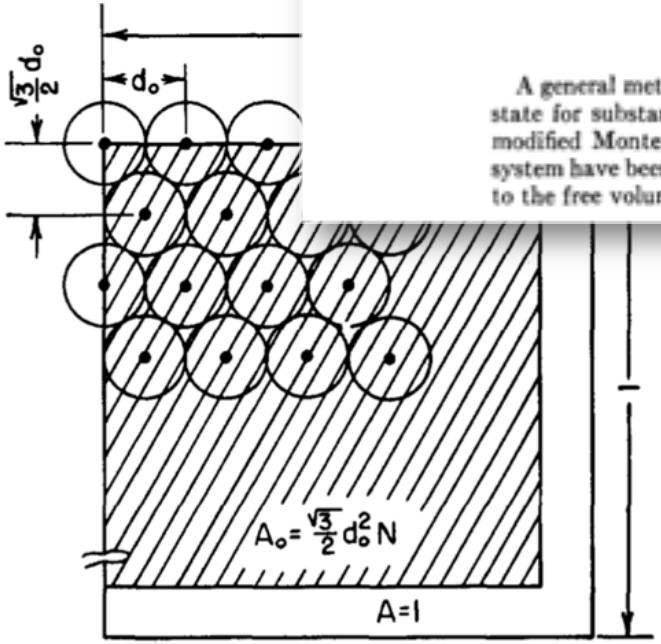


FIG. 3. The close-packed arrangement for determining A_0.

(problem faced with MANIAC computer)

Monte Carlo

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

Monte Carlo is used in:
-Numerical analysis
-Stochastic Simulations

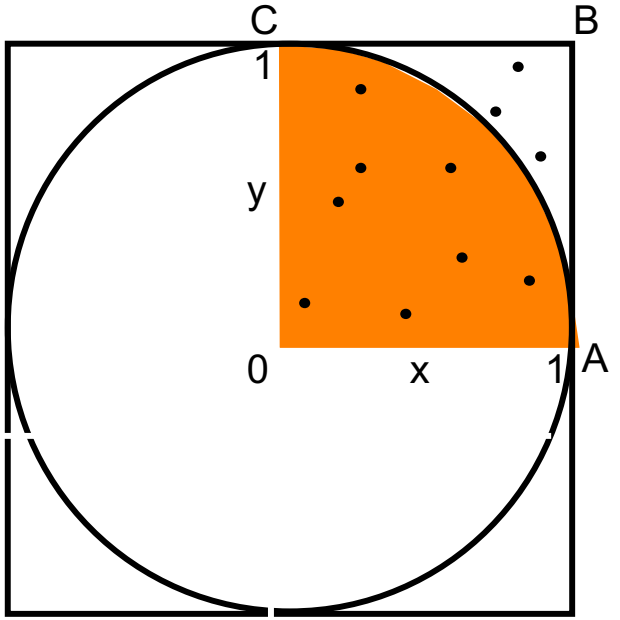
(*) a sequence of random numbers is a set of numbers which looks unpredictable but with well defined statistical properties

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

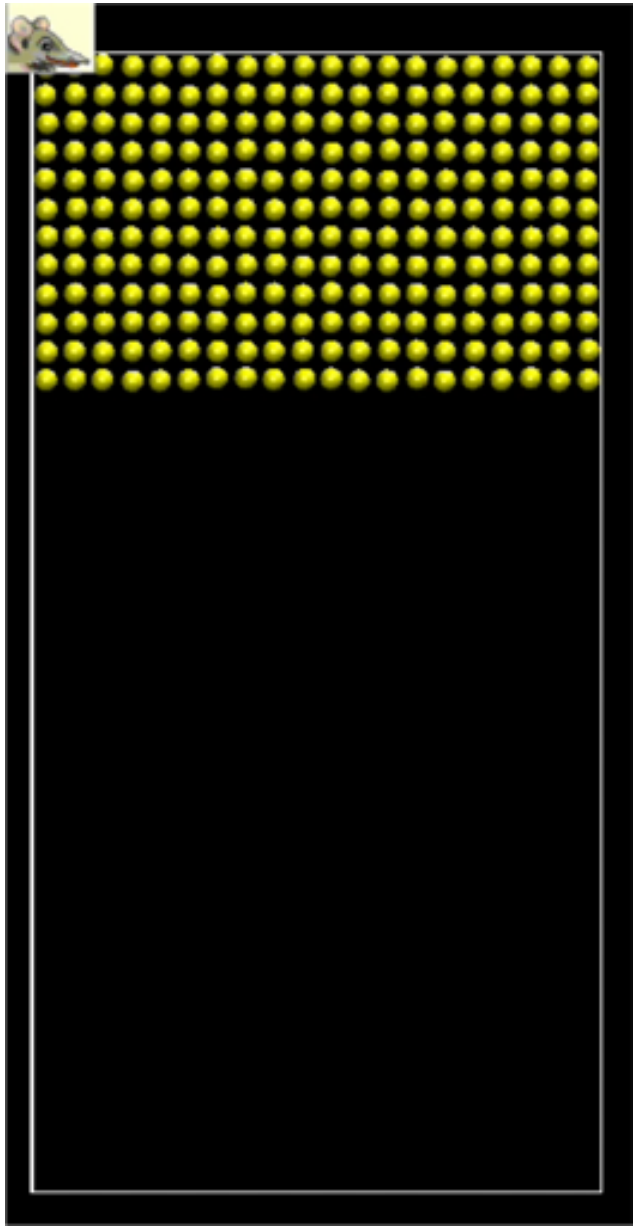


$$\pi \approx \frac{4 \text{ x Area Under Curve CA}}{\text{Area of Square OABC}} = \frac{4\tau_{hit}}{\tau_{tot}}$$

A few selected examples of applications

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

From "normal" scales...



(classical)

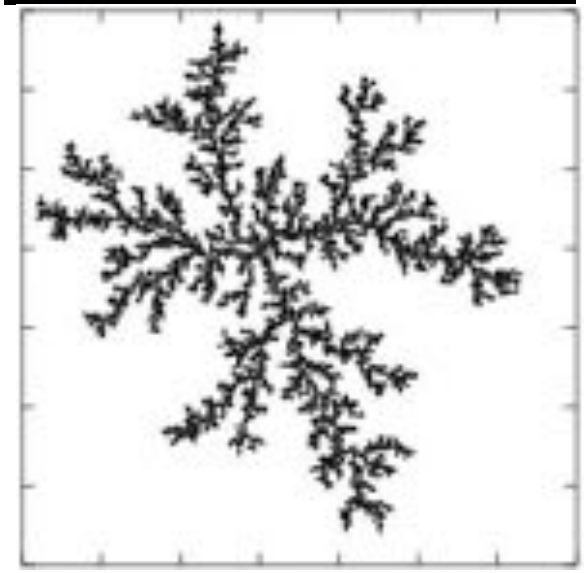
SIMULATION
of the Brownian motion

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

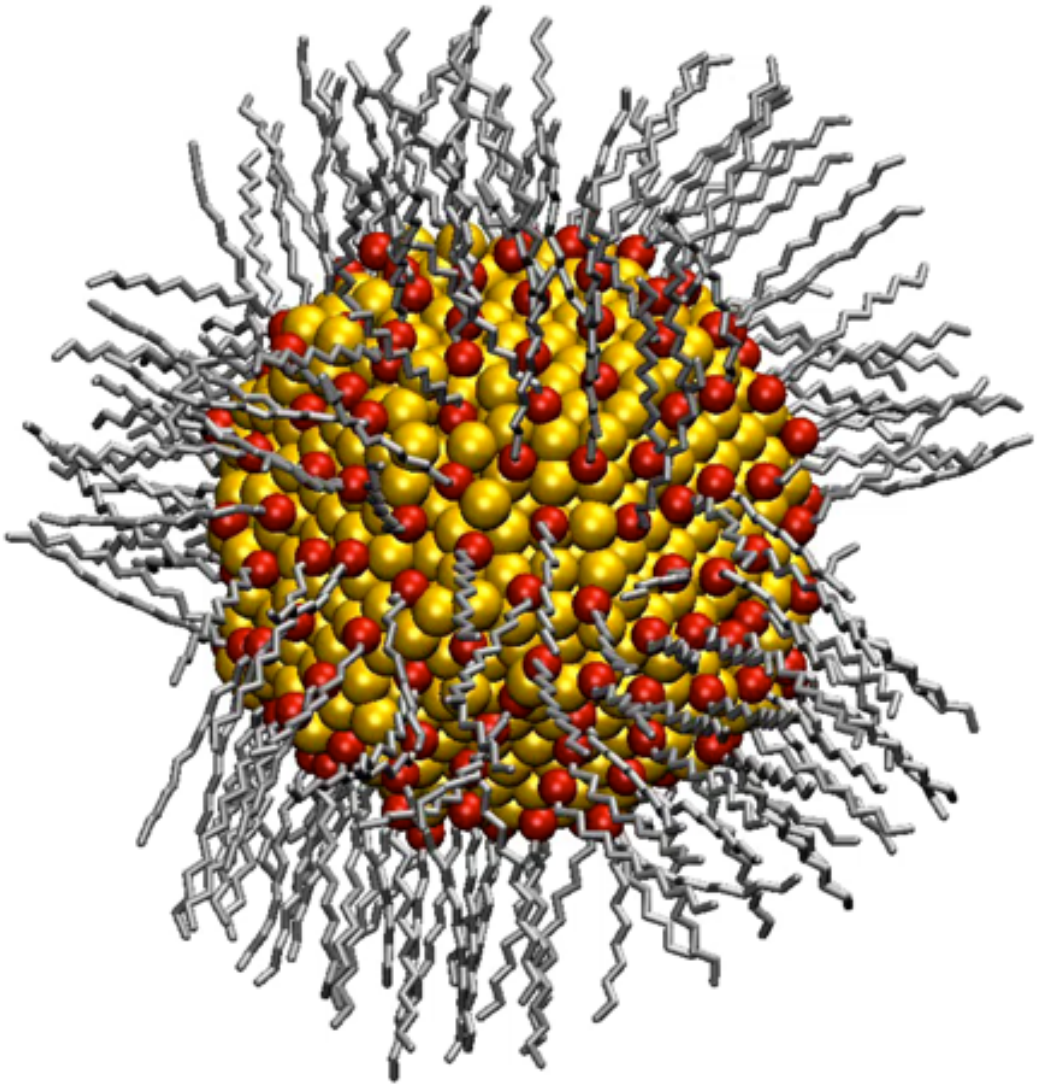


SIMULATION of a diffusion-limited auto-aggregation model (fractal)

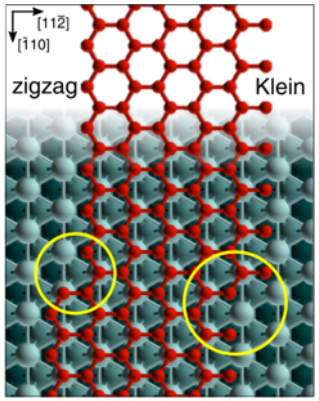
(stochastic, classical simulation)

... to the nanoscale: passivation of nanoparticles

with organic molecules
(thiols)
Au
S



Credits: J. Olmos-Asar

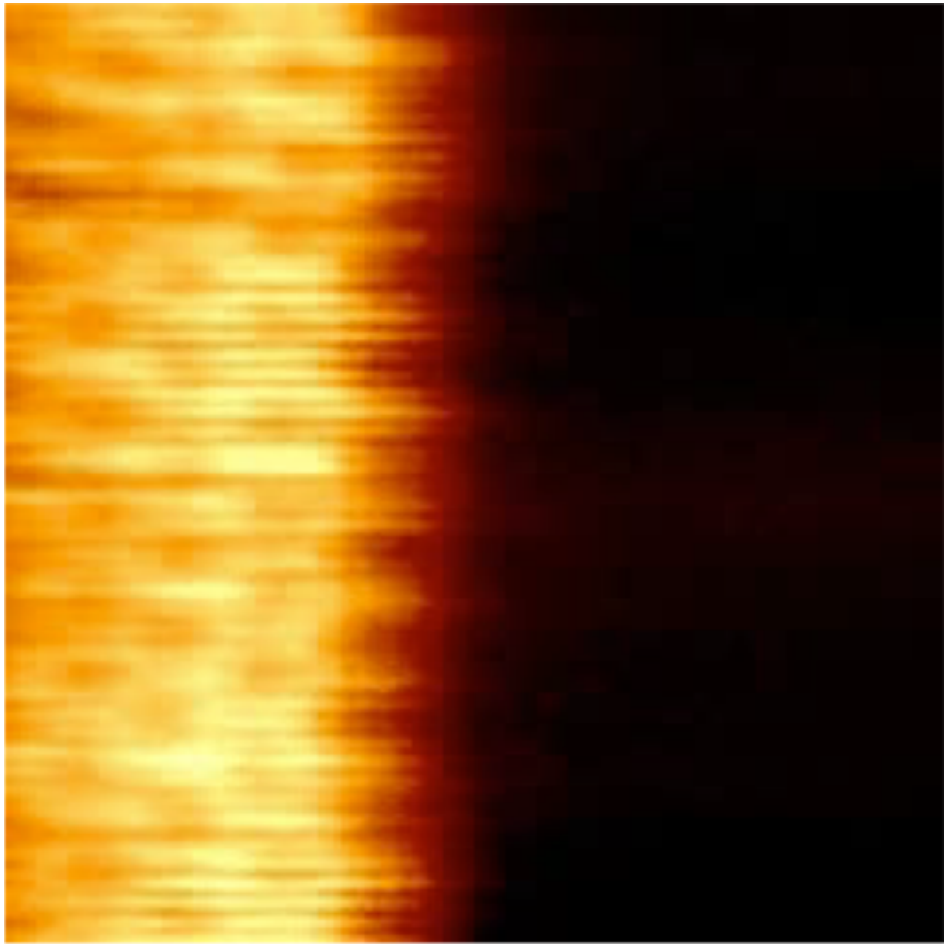


… to the atomic scale

Grafene @Ni(111)

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

EXPERIMENTAL FAST-STM MOVIE

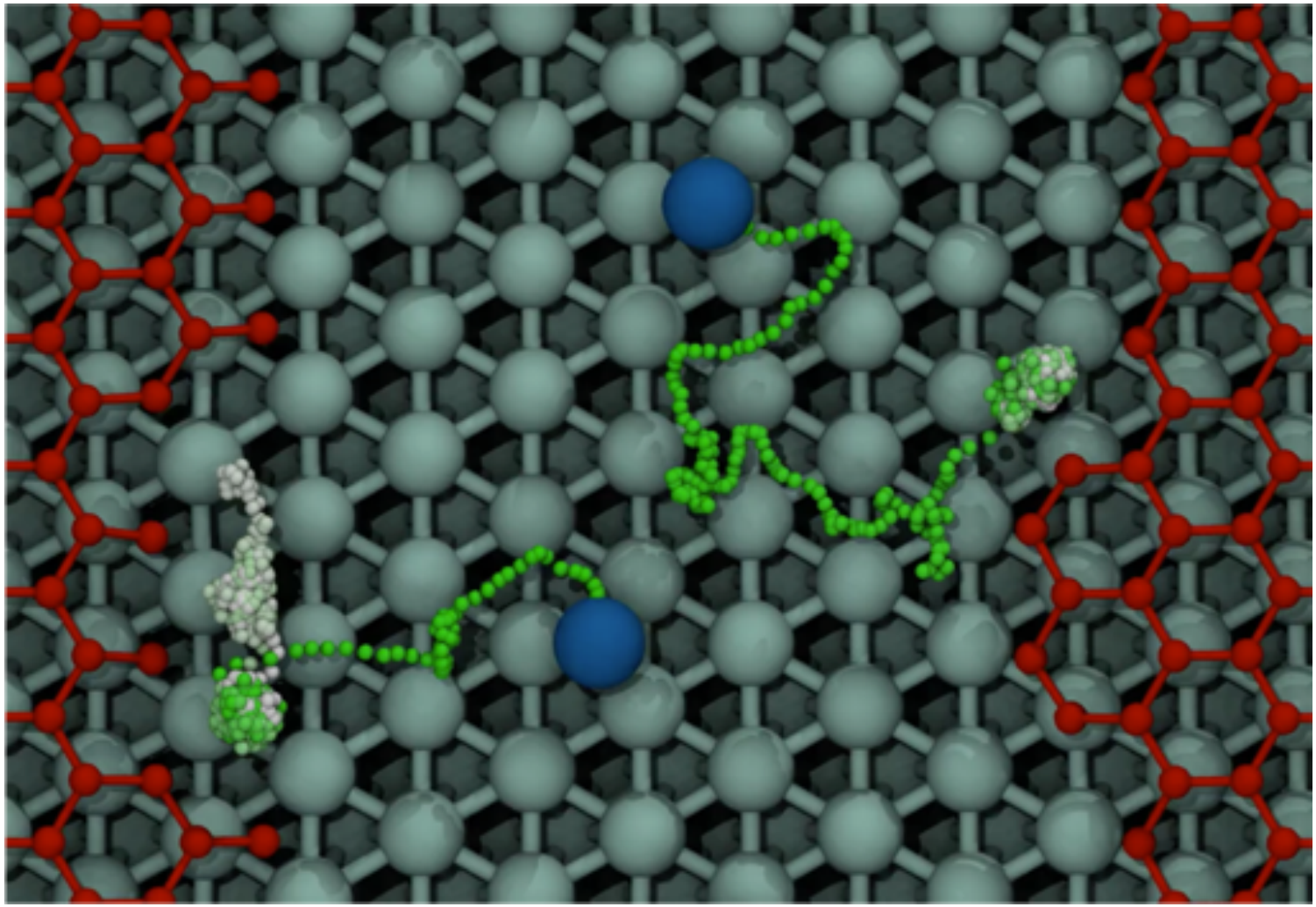


… to the atomic scale

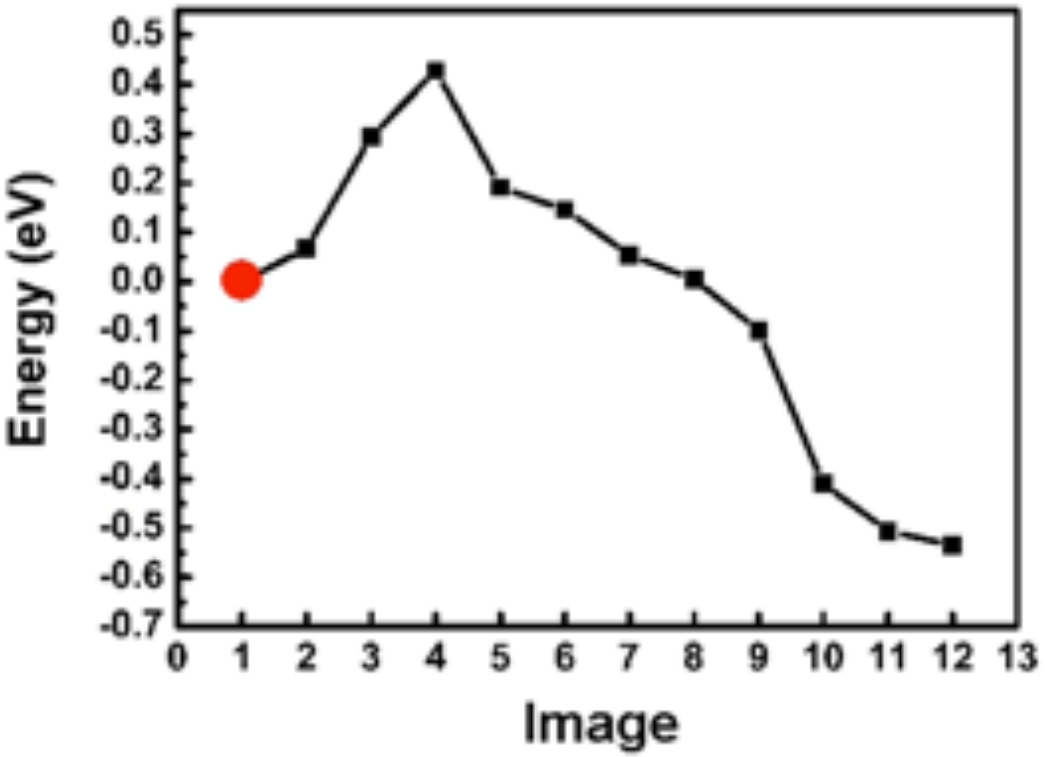
Grafene
@Ni(111)

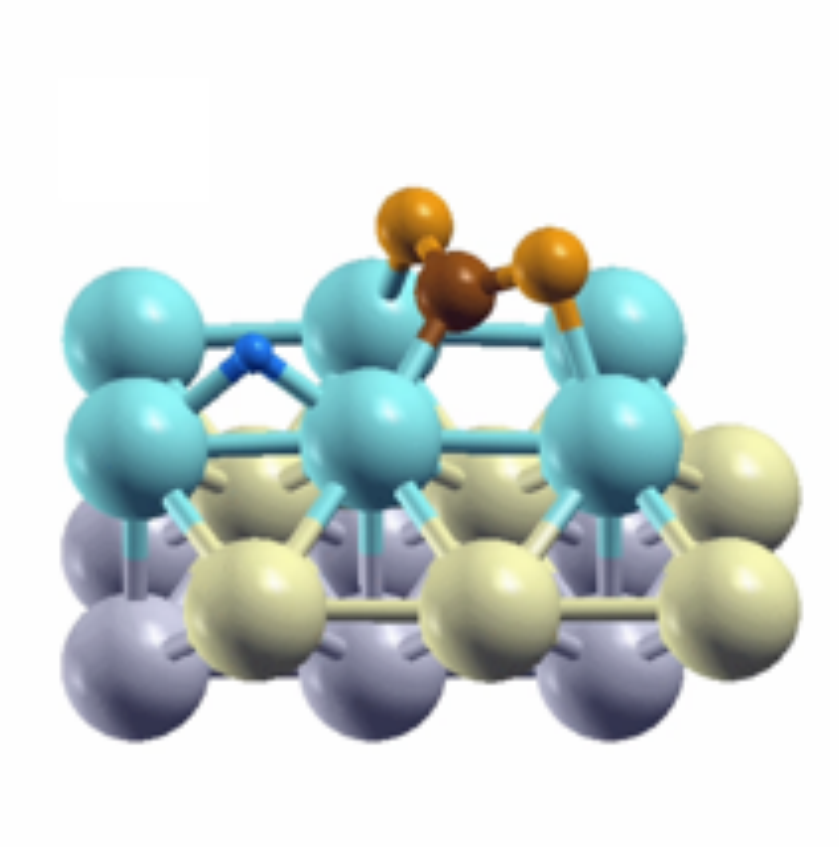
(M.P. in collaboration with TASC; Science, 2018)

CLASSICAL MOLECULAR DYNAMICS SIMULATION



...including chemical reactions





CO_2 + H -> HCOO @ Ni(110)

(deterministic, quantum mechanical simulation)

A wide scenario...
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!!!)

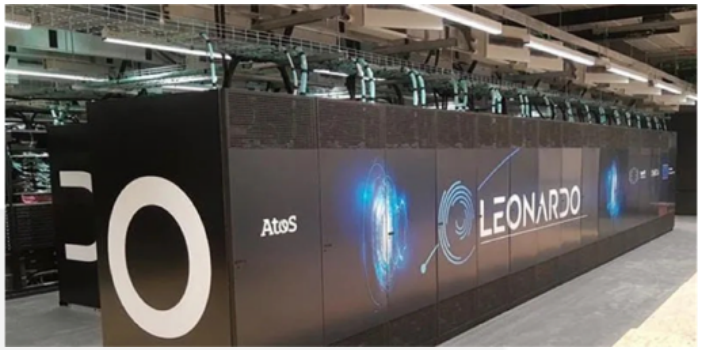
others are very hard and need

High Performance Computing resources

High performance computing

https://www.top500.org/ - updated June 2023

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, **HPE** DOE/SC/Oak Ridge National Laboratory **United States**	8,699,904	1,194.00	1,679.82	22,703
2	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, **Fujitsu** RIKEN Center for Computational Science **Japan**	7,630,848			
3	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, **HPE** EuroHPC/CSC **Finland**	2,220,288			
4	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, **Atos** EuroHPC/CINECA **Italy**	1,824,768	238.70	304.47	7,404



High performance computing

Possible access to CINECA HPC resources for research but also for thesis
(direct calls or through UniTS-CINECA agreement)

And...

a cluster @DF!

(2.1) This course -contents-

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

- basic ingredients of the **deterministic approach**

  (only **quantum**)

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

TENTATIVE LIST OF ARGUMENTS

Discretization of differential equation: Numerov algorithm.

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.

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.

(Genetic algorithms. Population dynamics and epidemic models.)

Course material on:
MS Teams & moodle2

On MS Teams: registration of lectures (42nd2c3)

On moodle: everything else https://moodle2.units.it

Then select:

⇒Dipartimento di Fisica

⇒Laurea Magistrale

⇒SM23 - FISICA

⇒A.A. 2023-24

Or point directly to:

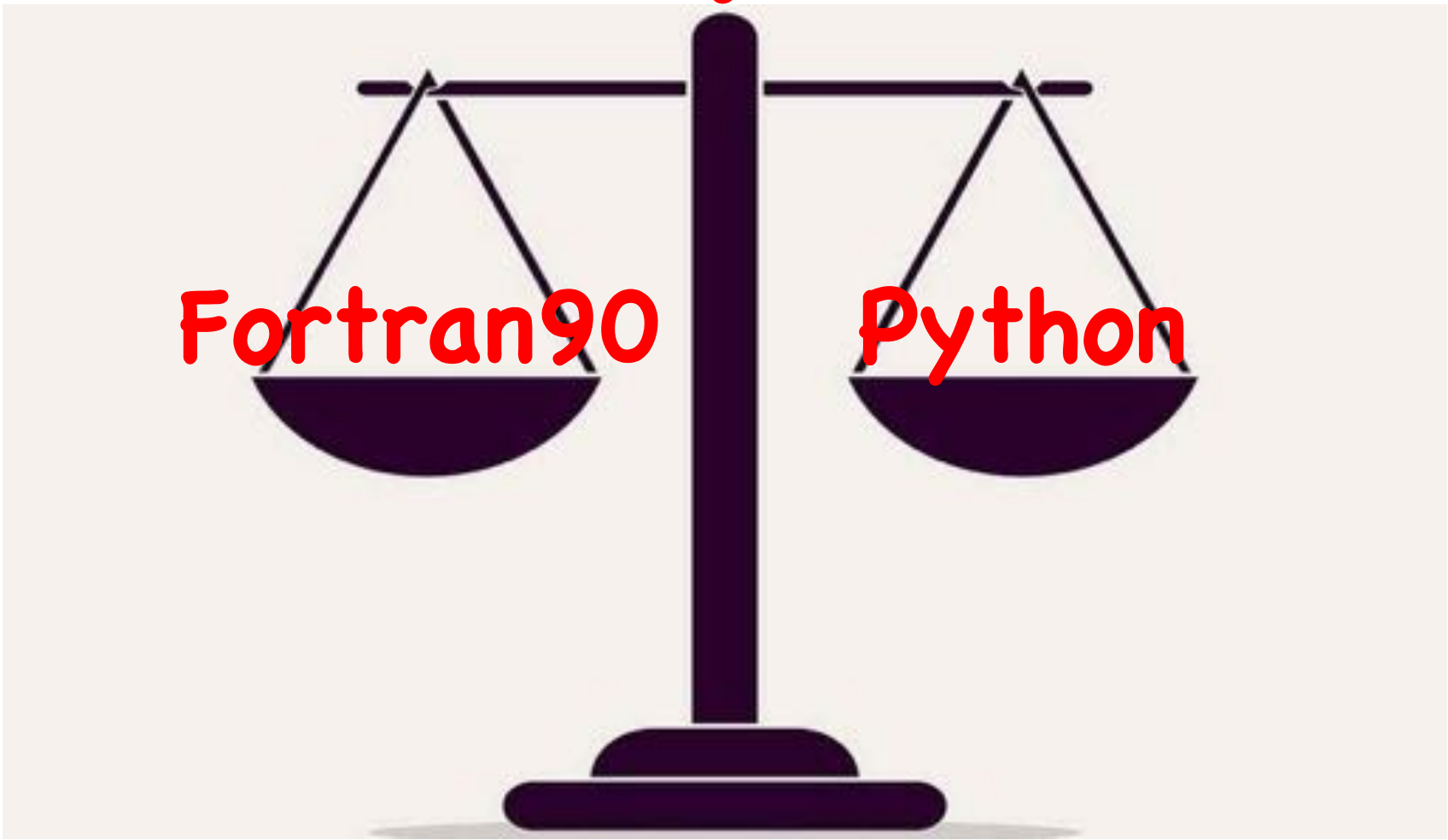
https://moodle2.units.it/course/view.php?id=11402

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, Python, gnuplot...)
-Info about exams

SUBSCRIBE TO THE COURSE to:
-register your attendance lecture by lecture
-be able to upload homeworks

Languages ?



Fortran compilers

- **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)

Python:
Wednesday

(2.2) This course

- lectures schedule
- rules for attendance
- exams

Schedule:

1 topic / week: 3 h lectures + 3 h lab

	Monday 25/09	Tuesday 26/09	Wednesday 27/09
14:00	LABORATORIO DI FISICA COMPUTAZIONALE - Lezione PERESSI MARIA, MARRAZZO ANTIMO Aula B [Edificio F] 14:00 - 16:00 Lezione	LABORATORIO DI FISICA COMPUTAZIONALE - Lezione PERESSI MARIA, MARRAZZO ANTIMO Aula N [Edificio A - corpo centrale] 14:00 - 15:00 Lezione	LABORATORIO DI FISICA COMPUTAZIONALE - Laboratorio PERESSI MARIA, MARRAZZO ANTIMO Lab. informatico Poropat [Edificio F] 14:00 - 17:00 Lezione
14:30			
15:00		with Python (A. Marrazzo)	
15:30			Hands-on session
16:00	Introduce the topic + sketch solutions in Fortran90		
16:30	+ give exercises (M. Peressi)		

Start do-it-yourself!

Attendance, homeworks, exams:

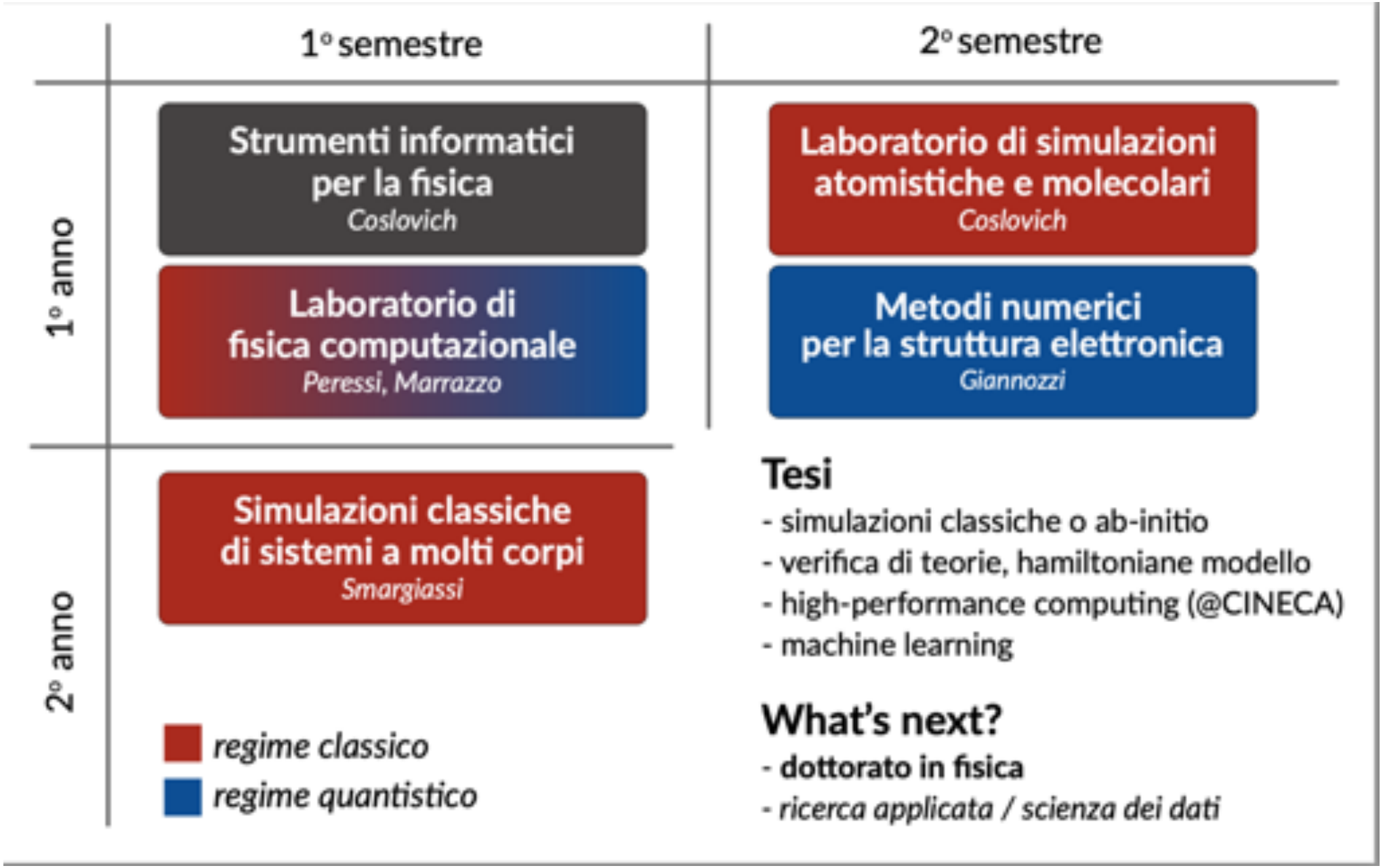
- attendance: 75% compulsory (this is a lab course!)
- Exercises during the course (for some of them, a short report will be requested as homework within ~1 week from the lecture)
- Exam: homework reports (if not uploaded during the course, they must be given at the end with some additional request) + a final project

(3) Activity/Courses in Computational Physics

in the Condensed Matter training track

others

- **"Information Technology Tools for Physics"** (D. Coslovich, I semester)
- **"Numerical Methods for Electronic Structure"** (P. Giannozzi, II semester) (deterministic, quantum)
- **"Classical simulations of many body systems"** (E. Smargiassi, I semester) (deterministic, classical)
- **"Laboratory of Atomistic and Molecular Simulations"** (D. Coslovich, II semester) (also mesoscale, solid & soft matter, machine learning approaches)


1° semestre
2° semestre
1° anno
2° anno
Strumenti informatici per la fisica
Coslovich
Laboratorio di fisica computazionale
Peressi, Marrazzo
Laboratorio di simulazioni atomistiche e molecolari
Coslovich
Metodi numerici per la struttura elettronica
Giannozzi
Simulazioni classiche di sistemi a molti corpi
Smargiassi
regime classico
regime quantistico
Tesi
- simulazioni classiche o ab-initio
- verifica di teorie, hamiltoniane modello
- high-performance computing (@CINECA)
- machine learning
What's next?
- dottorato in fisica
- ricerca applicata / scienza dei dati

(4) Local resources

virtual Lab of Physics Dept.

Access:
on VPN UNITS (Forticlient)
through Vmware Horizon client
using your own UniTS credentials
⇒AULA-CORSI-FISICA
⇒It's a temporary space! Save your work!
⇒Do LOGOUT at the end

```
=> Select properly the keyboard language
=> You may increase font size:
gsettings set org.gnome.desktop.interface scaling-factor 2
```

993SM - Laboratory of Computational Physics

lecture I - II part

September 25, 2023

Maria Peressi - Antimo Marrazzo

Università degli Studi di Trieste - Dipartimento di Fisica

Sede di Miramare (Strada Costiera 11, Trieste)

e-mail: peressi@units.it , antimo.marrazzo@units.it