UNIVERSITÀ DEGLI STUDI DI TRIESTE

Dipartimento di Fisica
Dipartimento d'Eccellenza 2023-2027

Laboratorio di Fisica Computazionale FI020004-4

Maria Peressi
Università degli Studi di Trieste - Dipartimento di Fisica
Sede di Miramare (Strada Costiera 11, Trieste)
e-mail: peressi@units.it

Computer in FISICA: qual è la vostra esperienza?

- Visualizzazione
- Raccolta e Analisi dati
- Controllo strumenti
- Manipolazione simbolica
- ...
- ...
- ...
- ...
- Analisi numerica?
- Simulazioni numeriche?

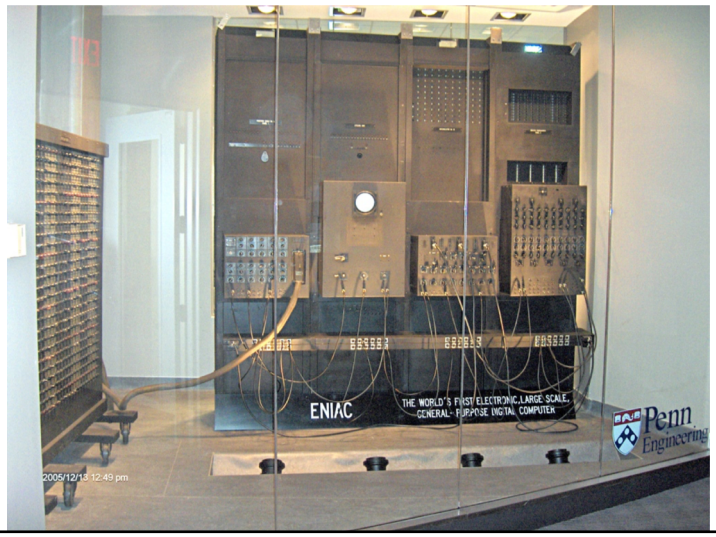
- analisi numerica: risolvere equazioni che non possono essere affrontate con metodi analitici
- simulazioni: modellare e studiare fenomeni fisici con tecniche numeriche. Ciò significa fare esperimenti virtuali in cui la nostra rappresentazione della realtà fisica, sebbene necessariamente schematica e semplificata, possa essere modificata e variata a piacimento.

Introduzione

- La nascita della fisica computazionale
- Simulazioni ed esperimenti "what-if"
- Approcci deterministici e stocastici
- Alcuni esempi

Qual è il primo computer «general purpose»?

Electronic Numerical Integrator And Computer



Perché ci è utile un computer per fare fisica?

moltissime operazioni in pochissimo tempo!

Ieri (1946): ENIAC poteva eseguire 357 moltiplicazioni o 38 divisioni al secondo. Alla presentazione ufficiale, eseguì 5.000 volte la moltiplicazione di 97.367 per se stesso in meno di un secondo.

Qual è la potenza di calcolo disponibile oggi?

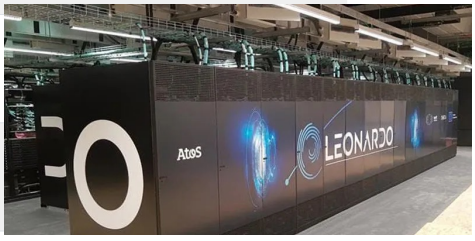
Oggi... (aggiornamento giugno 2023)

https://www.top500.org/

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				
3	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland				
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

Flop/s: numero di operazioni in virgola mobile eseguite in un secondo

TERA(T) / PETA(P) / EXA(E) : prefissi che indicano 10^{12}, 10^{15}, 10^{18}

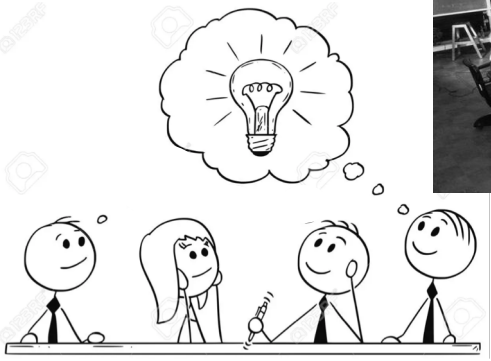


X

La nascita della fisica computazionale

Un PROBLEMA per il computer MANIAC (Los Alamos, 1955)

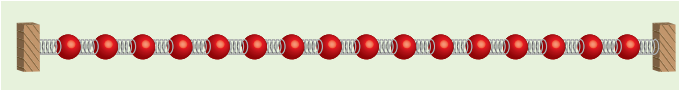
termalizzazione!



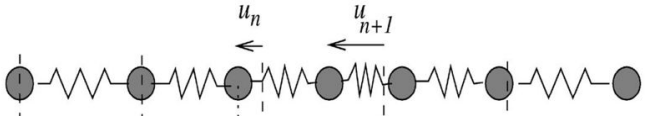
https://discover.lanl.gov/publications/national-security-science/2020-winter/we-thank-miss-mary-tsingou/

La nascita della fisica computazionale

PROBLEMA: Fermi-Pasta-Ulam-Tsingou 1955



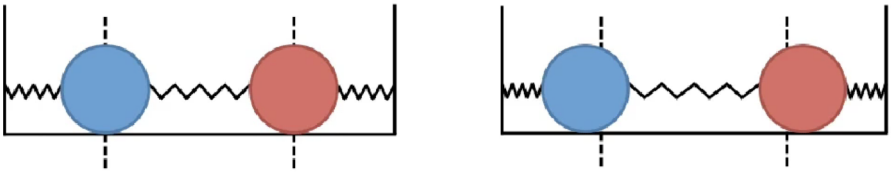
Una catena di N particelle legate da molle (analogo unidimensionale degli atomi in un cristallo)



Interazione lineare (legge di Hooke)

ci sono N «modi normali» (cioè schemi di movimento in cui tutte le parti del sistema oscillano con la stessa frequenza e con una relazione di fase fissa)

Esempio con 2 oscillatori: Modi normali

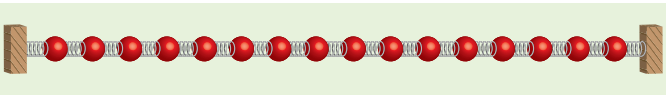


http://fisicaondemusica.unimore.it/Oscillatori_accoppiati.html

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

La nascita della fisica computazionale

PROBLEMA: Fermi-Pasta-Ulam-Tsingou 1955



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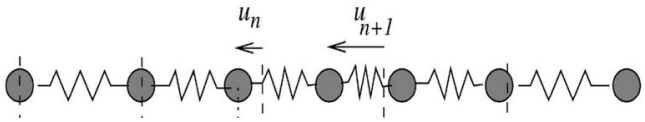
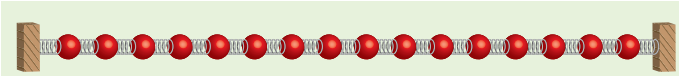


Interazione lineare (legge di Hooke)
soluzione analitica:
L'energia fornita a un singolo «modo normale» rimane sempre in quel modo

La nascita della fisica computazionale

PROBLEMA: Fermi-Pasta-Ulam-Tsingou 1955



in presenza di un **debole accoppiamento non lineare** (correzione quadratica o cubica al termine lineare), quali modi verranno eccitati dopo un tempo sufficientemente lungo?

Comportamento atteso in base al teorema di equipartizione: l'energia sarà equamente distribuita tra tutti i gradi di libertà del sistema. Tuttavia: **soluzione analitica impossibile**

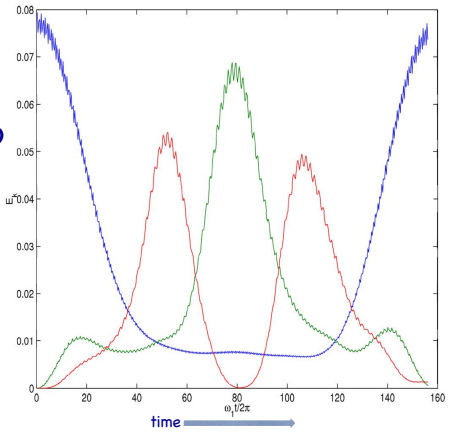
La nascita della fisica computazionale

PROBLEMA: Fermi-Pasta-Ulam-Tsingou 1955

Soluzione numerica con MANIAC (originalmente: calcolo per N=5)

Energia verso tempo per 3 modi normali:

K= 1 2 3



qui: N=32; dopo l'eccitazione iniziale del modo k=1 e 157 periodi, quasi tutta l'energia ritorna in questo modo!!!

Immagini da: 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 e altri siti web

Simulazioni come "esperimenti virtuali"

Alcune similitudini:

Esperimento reale (in laboratorio tradizionale)	Esperimento virtuale (computazionale)
campione	modelli e algoritmi
apparato fisico	codice
calibrazione degli strumenti	test del codice
misure	risultati numerici
analisi dati	analisi dati

Con errori!!!

- **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

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…

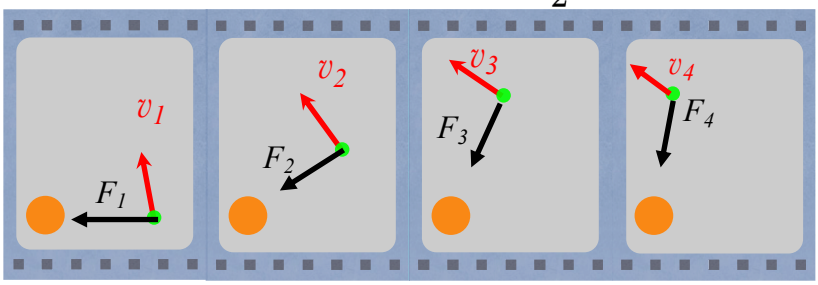
Examples =>

The deterministic approach

1) Classical Discretization of the equation of motion and **iteration**:

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

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



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 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

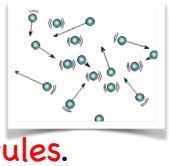
We attempt to follow the `time dependence' of a model where change, or growth, does not proceed in some rigorously predefined fashion (e.g. according to Newton's equations of motion) but rather in a stochastic manner which depends on a sequence of random numbers which is generated during the simulation.

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.

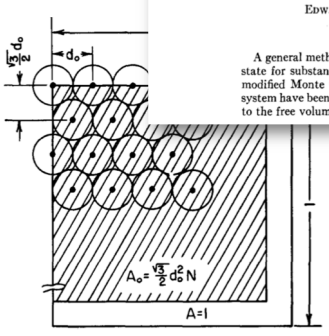


FIG. 3. The close-packed arrangement for determining A_0.

(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

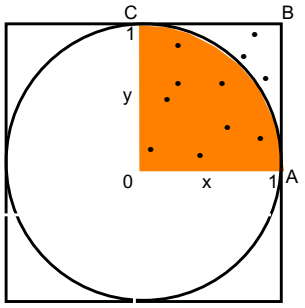
(*) a sequence of random numbers is a set of numbers which looks unpredictable but with well defined statistical properties

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

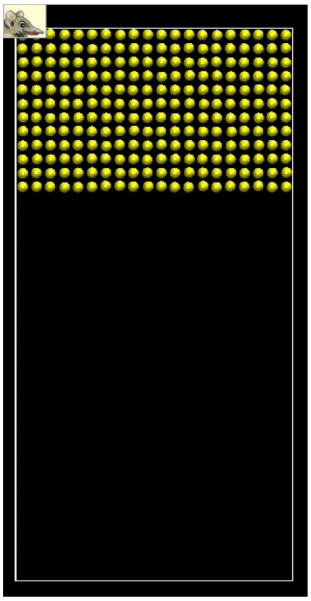


$$\pi \approx \frac{4 \times \text{Area Under Curve CA}}{\text{Area of Square OABC}} = \frac{4\tau_{hit}}{\tau_{tot}}$$

A few selected examples of applications

(here: limited to condensed matter field !!!)

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

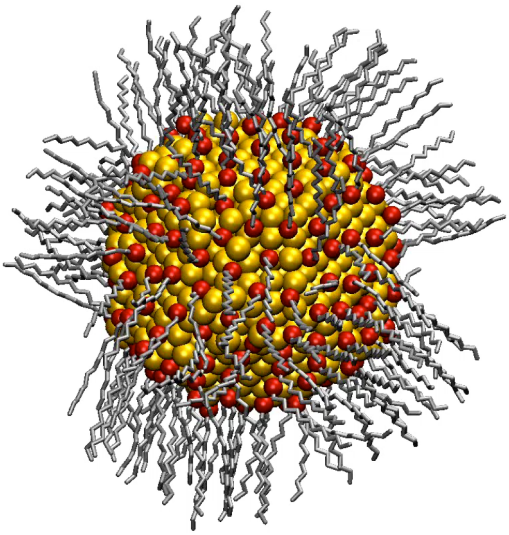
(deterministic, classical simulation)

… to the nanoscale: passivation of nanoparticles

with organic molecules (thiols)

Au

S



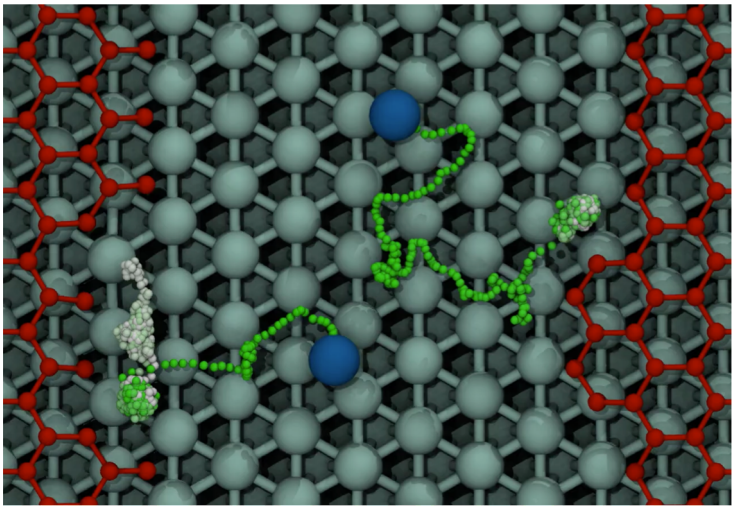
Credits: J. Olmos-Asar

… to the atomic scale

Grafene @Ni(111)

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

CLASSICAL MOLECULAR DYNAMICS 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

This minicourse

- 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…

A few possible examples

- **deterministic approach**
  - gas diffusion & thermodynamics
  - gravitational problems
  - Chaos and determinism: classical billiards and chaotic billiards, logistic maps
- **stochastic approach**
  - Monte Carlo approach for measuring areas
  - Random walks

Which tools?

- (Do-it-yourself?) Codes in different languages (Fortran90, C++, Java, Python, …) + visualization tools
- Excel (electronic sheets)
- Many nice applets available on the web
- …

Consider several factors to reach a goal….

- expertise & interests
- time
- resources
- …

Course material on Moodle

FI020004-4 - LABORATORIO DI FISICA COMPUTAZIONALE 2023

Iscrizione spontanea con chiave d'accesso:
FI020004-4