

Simulazioni al computer: la terza via

Congressino di Dipartimento, 23/04/2015



www.phdcomics.com

Andrea Giuntoli,
Scuola di Dottorato,
Università di Pisa

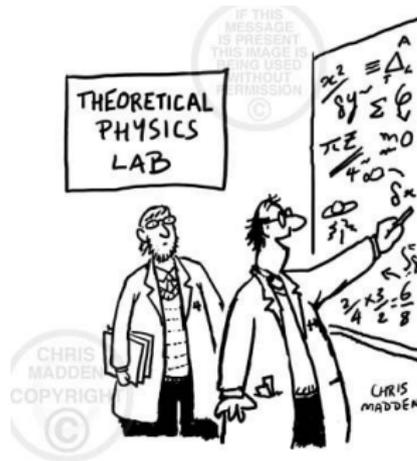
andrea.giuntoli@for.unipi.it

L'eterna domanda: sperimentale o teorico?



"LET 'ER RIP! SAYS HERE WE'VE GOT TO GET IT TO 77 K!"

©1985 Tom Swanson



"Soon I will be able to answer one of the fundamental questions about the structure of the universe: just how long is a piece of string?"

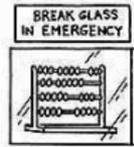
"...the craft of experimental physics is the sublime quality of patience - patience in accumulating data - patience with recalcitrant equipment..."
-Abdus Salam

*"(1) write down the problem
(2) think very hard
(3) write down the answer"*
-Richard Feynman

La terza via

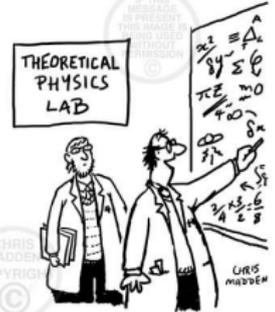


©1988 Tom Swenson



search ID: sea0478

©Original Artist
Reproduction rights obtainable from
www.CartoonStock.com

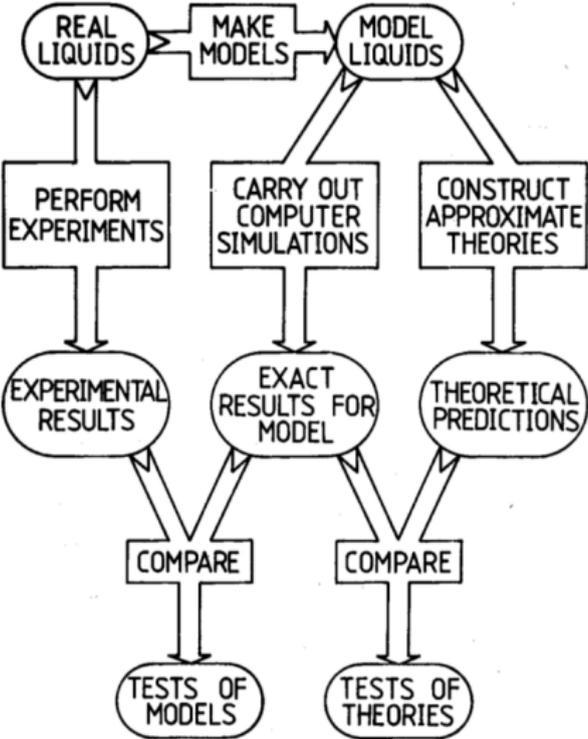


"Soon I will be able to answer one of the fundamental questions about the structure of the universe:
just how long is a piece of string?"

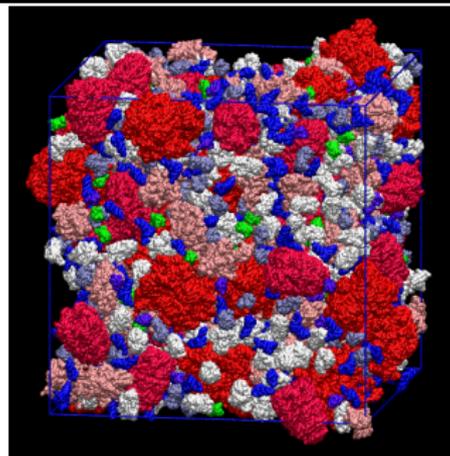
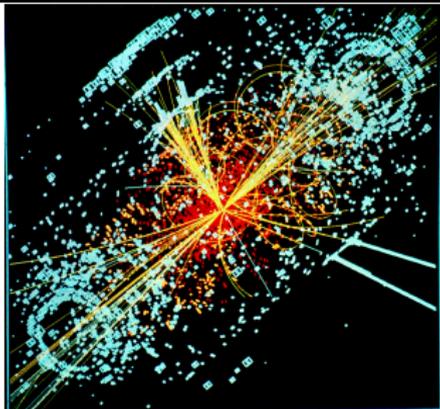
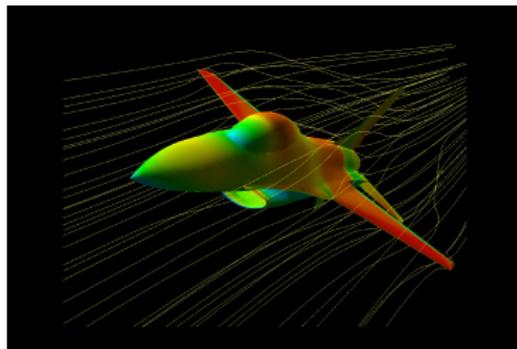
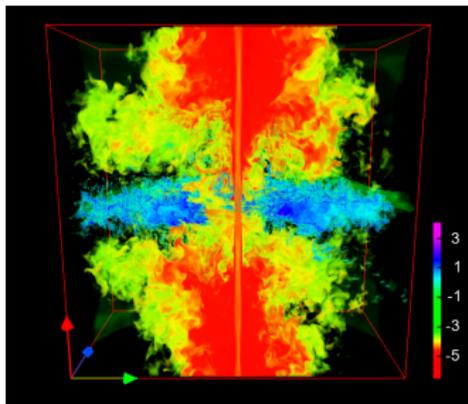
"Traditional scientific knowledge has generally taken the form of either theory or experimental data. However, where theory and experiment stumble, simulations may offer a third way."

-Simulation, Johannes Lenhard et al.

Un ponte tra teoria ed esperimento



Simulazioni: dove e perchè



Pro e contro della simulazione

Grandi vantaggi rispetto all'esperimento:

- Controllo dei parametri
- Ampio range di spazio e tempo
- Semplicità di esecuzione
- Isolamento delle proprietà di interesse

E allora perchè andiamo ancora in laboratorio??

Non tutto è oro quel che luccica, vari problemi delle simulazioni:

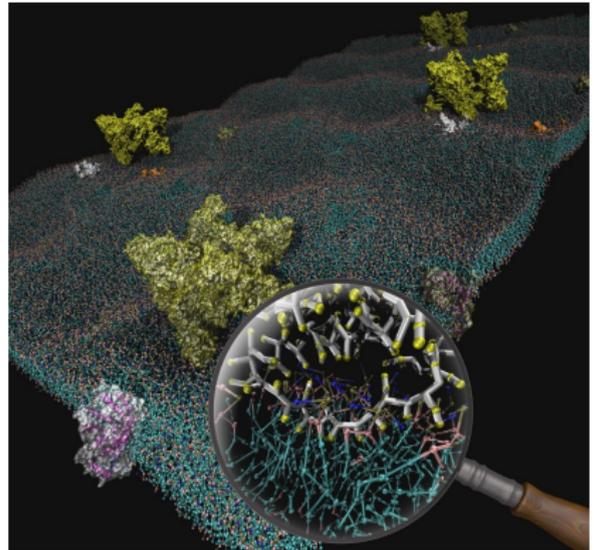
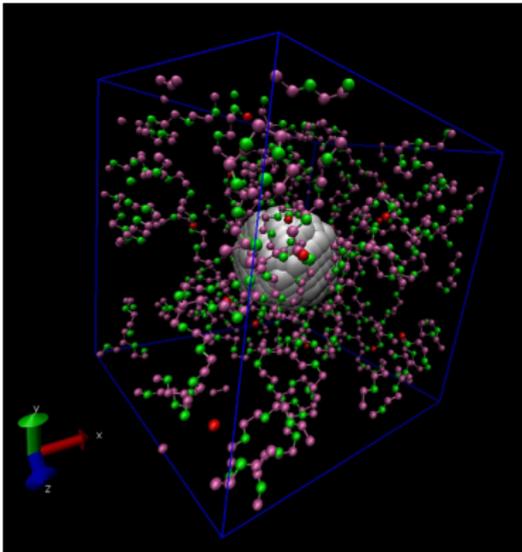
- Errori numerici
- Limiti di potenza di calcolo
- Un modello, niente di più

"All models are wrong, but some are useful"

- G. Box

Dinamica Molecolare

"... I took a number of rubber balls and stuck them together with rods of a selection of different lengths ranging from 2.75 to 4 inches. I tried to do this in the first place as casually as possible, working in my own office, being interrupted every five minutes or so and not remembering what I had done before the interruption" - J.D. Bernal, 1962



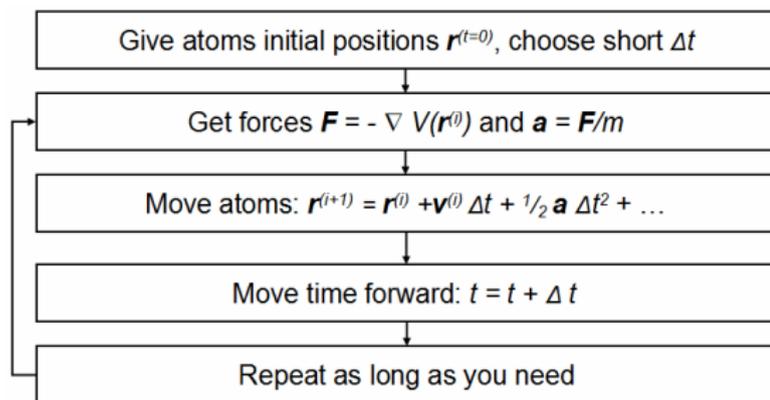
Dinamica molecolare

L'ingrediente principale: come interagiscono due elementi del sistema?

Le proprietà di ogni elemento e l'interazione di coppia definiscono completamente il modello.

Se diventano tanti, però...
(10^{24} atomi in una mole!)

Un problema algoritmico



Così semplice che anche un computer è in grado di farlo!

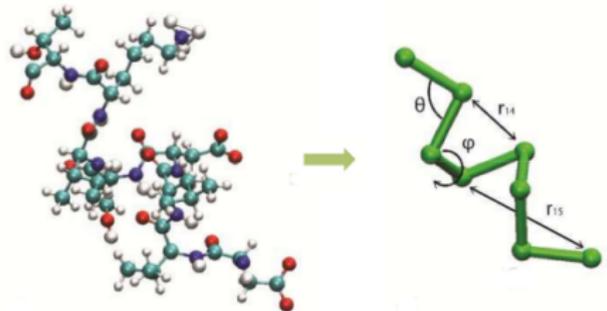
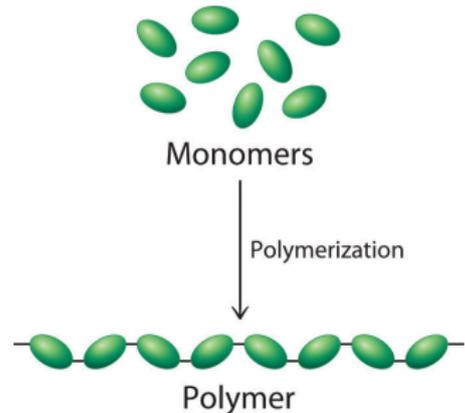
Cos'è un polimero?

Polimero: una lunga catena di elementi ripetuti (i monomeri)

Grande varietà, sia naturali che artificiali:

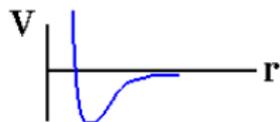
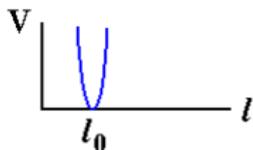
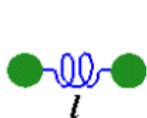
- proteine
- DNA
- plastiche

Si possono simulare a varie risoluzioni, in base al fenomeno fisico di interesse



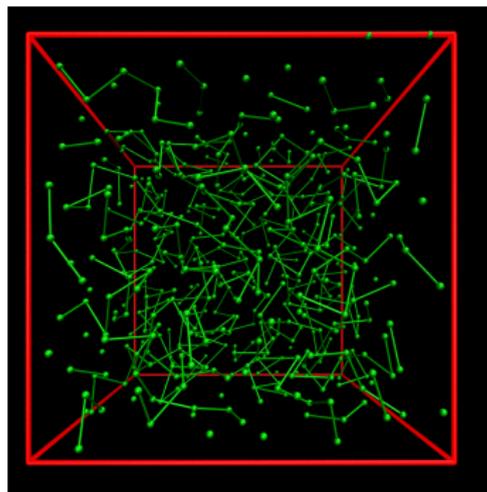
Liquidi polimerici

Studio delle proprietà collettive, in un modello semplificato:



Simulazione caratterizzata da numero e lunghezza delle catene, volume, temperatura, pressione...

Si ottengono informazioni sulle proprietà macroscopiche e di singolo monomero



La transizione vetrosa

Repentino raffreddamento: aumento del tempo di rilassamento strutturale a $T = T_g$

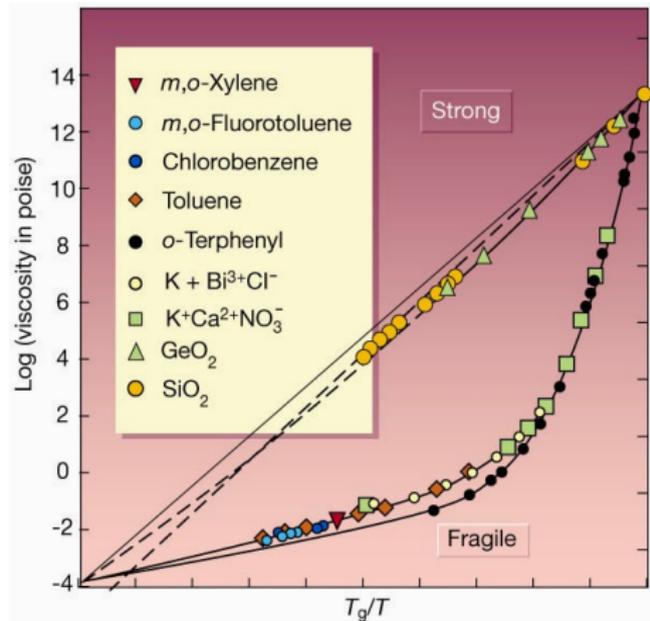
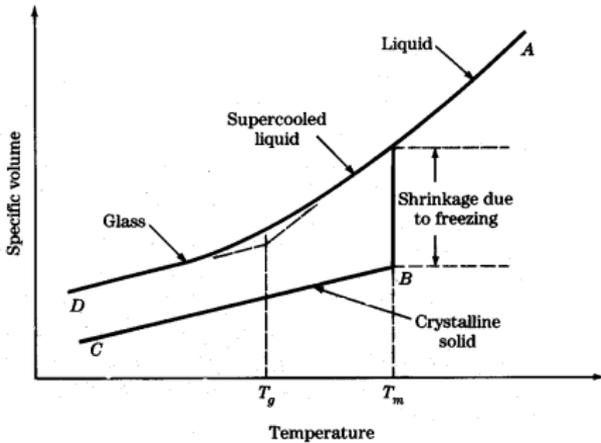


Figure da:

- www.phdcomics.com
- blogs.scienceforums.net/swansont
- www.cartoonstock.com
- www.chrismadden.co.uk
- M.P. Allen, D.J. Tildesley *"Computer Simulation of Liquids"*
- www.ita.uni-heidelberg.de
- www.psc.edu/science/Farhat
- home.web.cern.ch
- T. Ando, J. Skolnick, doi: 10.1073/pnas.1011354107
- www.uh.edu/engines/epi2838.htm
- Karo J, Peterson P, Vendelin M, PMID: 22241474
- catalog.flatworldknowledge.com/bookhub
- Giulia Spampinato, Tesi di Laurea
- condensedconcepts.blogspot.it
- www.benbest.com/cryonics