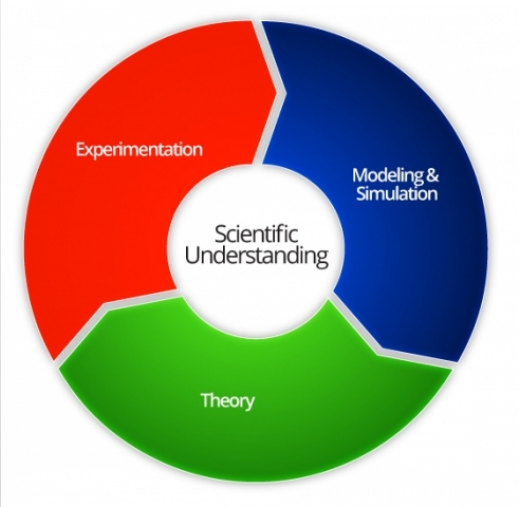
AC274: Computational Physics

The third route to scientific investigation



Sauro Succi,

IAC Rome and IACS Harvard

What is Computational Physics?

Interrogate Nature using computers

The **art** of filling the huge gap between the degrees of available to Nature and those affordable by our computers …

(A. Avogadro, 1776-1856)

Why an art?

The Avogadro syndrome:

- **10^23** molecules in a cc of water vs ~ **10^16** bits in the largest computers
- About **10^6 atoms/bit**
- Our best e-computers can simulate a few billions "molecules" over milliseconds: 1 computational molecule ~ sqrt(Avogadro) molecules.

YET IT WORKS!

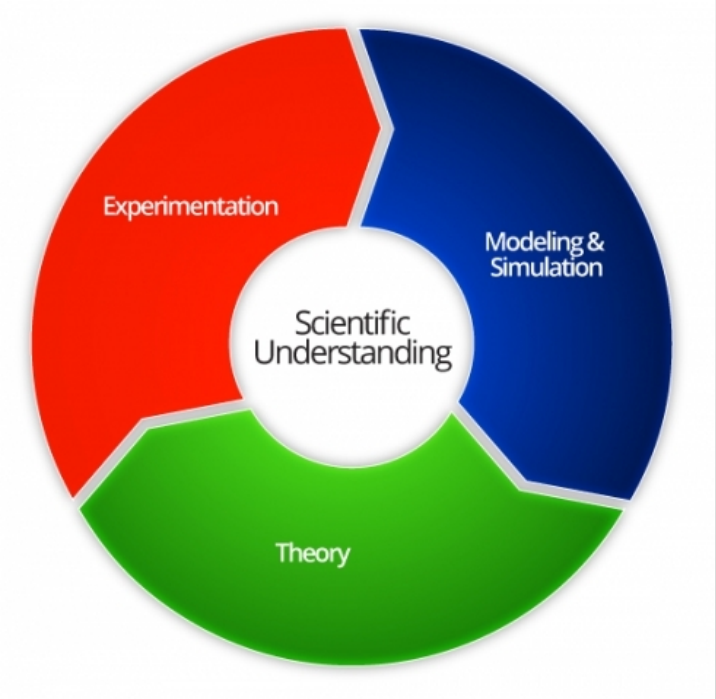
WHY? Because Nature is ***Hierarchical*** and (sometimes) ***Universale (detail insensitive)***
Hence: broad scope for clever proxies:

Mathematical Models&Algorithms

Why Computational Physics?

Experiment, problems with:

1. ***Access (extreme conditions)***
2. ***Costs***
3. ***Safety***
4. ***1+2+3…***



Theory: major barriers

1. **Non-linearity**
2. **Non-Locality**
3. **Large dimensions**
4. **Complex geometry**

The Pillars of Computational Physics

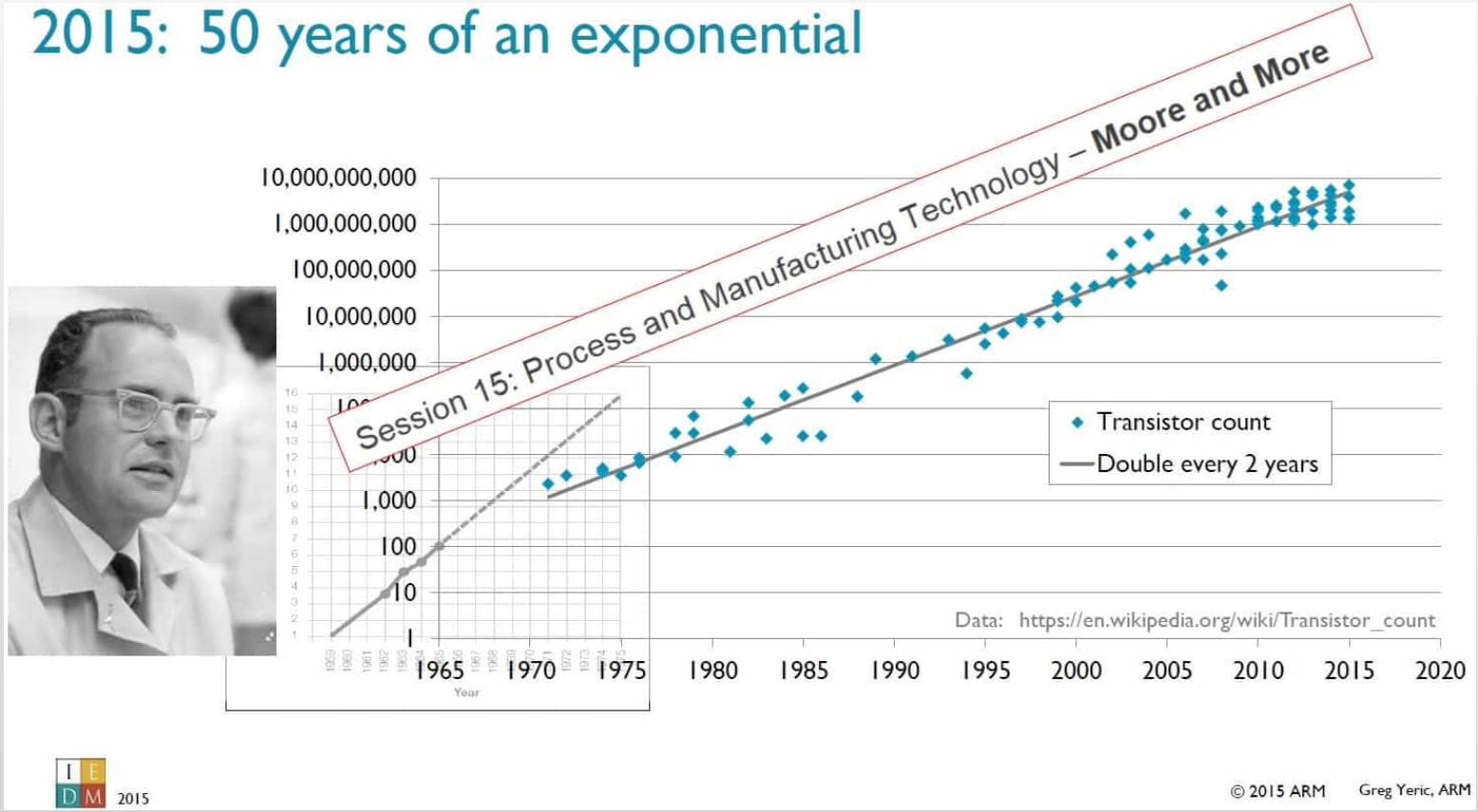
The two pillars of computational physics: **hardware** and **software**

HW SW

HW: Spectacular progress over the last 50 yrs: the compute power has **doubled every 1.5 yrs** (Moore's law): over a million in five decades!

SW: No less spectacular, proceeds by Revolution, see next slides...

Moore's law



With the same trend in automotive, today we would drive faster than light!

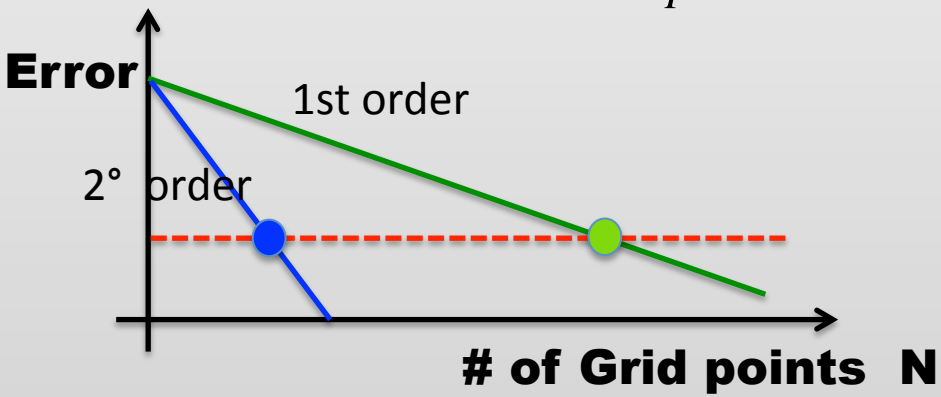
Top current machine: Yian-He2, China: how many Flops?

Methods&Algorithms

Algorithmic advances no less spectacular

SW: Computational methods proceed by **REVOLUTION.**
For instance, going from first to second order accuracy saves **decades** of Moore's time!!!

Error with p-th order method: $e_p \approx 1/N^p$



$$N_p = N_1^{1/p}$$

From first to second order accuracy means 10^3 grid points instead of 100^3 saves *at least* a factor 1000=**10 Moore years!!!**

The top 10 algorithms …

Monte Carlo: hyperdimensional quadratures

Molecular Dynamics: condmat,biology

Comp. Fluid Dynamics: fluids

Fast Fourier Transform: signals

The **Fortran** compiler: all equations

QR Decomposition: matrix algebra

Lanczos/Krylov iteration: iteration methods

Fast Multipole: long-range interactions

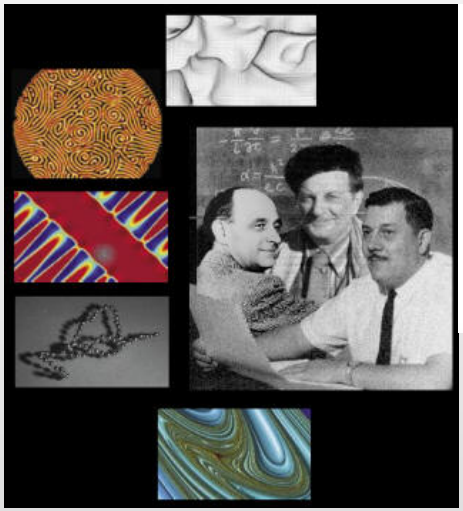
Simplex method: linear programming

Quicksort: search

(AC274 will cover several but not all (-:)

The birth of Computational Physics

Fermi-Pasta-Ulam-Tsingou (Los Alamos, 1955)



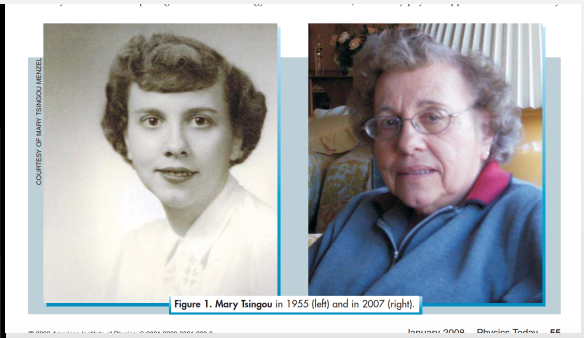


Figure 1. Mary Tsingou in 1955 (left) and in 2007 (right).

CP at its zenith: not just "number crunching"

NEW *model equations from THEORY!*

New paradigms beyond the original problem

$$\partial_t u + u\partial_x u = \lambda \partial_{xxx} u$$

From heat propagation in solids to Tsunamis!

Computational State of Mind

A beautiful description of CP at its highest:

*The growing computational capacity **will change the nature of the questions we ask**, the answers we seek and the investigations we pursue. Last but not least, it will change the nature of the investigator..*

Concepts and equations that computers can run will be powerfully leveraged, concepts and equations that cannot be turned into algorithms will be regarded as deficient.

That does NOT mean that mindless number crunching will replace imaginative insight, on the contrary ….

(F. Wilczek, Phys Today April 2016)

Now to AC274

Four main parts:

1. Grid methods for classical and quantum fields

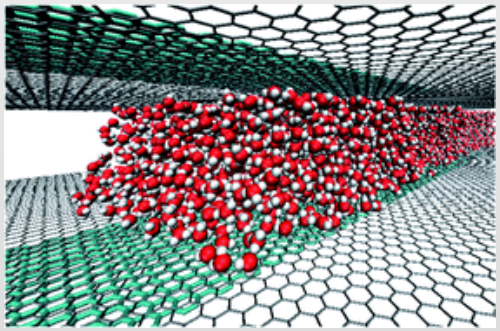
2. Advanced grid methods for complex geometry

3. Simulating complex states of matter

4. Data Analysis and Learning

On Fields, Particles and Probabilities

FIELDS: based on the CONTINUUM assumption: granular/molecular aspects can be ignored. Typically modelled by **Partial Differential Equations (PDE's)**. Apparently the most economic description but often faces formidable computational complexity due to the four main barriers:
NON-LINEARITY+COMPLEX GEOMETRY+NON-LOCALITY +HIGH DIMENSIONS.
Other representations may prove more efficient;
(**PARTICLES, PROBABILITY DISTRIBUTIONS**).



AC274 covers more than PDE's!

Modern physics reveals new states of matter besides the traditional triad **Gas/Liquid/Solid**: Amorphous (foams, emulsions, gels, colloids), and of course Quantum Materials, but also Active Matter (biomaterials, animal flocks) including Social Systems

The unifying conceptual framework is: **STATISTICAL MECHANICS**

Statistical Mechanics

Four basic levels to describe matter: (all covered by AC274)


MACRO

Continuum Fields

$$\partial_t u + (u \cdot \nabla) u = -\frac{\nabla P}{\rho} + \nu \Delta u$$

MESO

Probability distribution functions

$$\partial_t f + (\boldsymbol{v} \cdot \nabla) f = -\frac{1}{\tau}(f - f^{(eq)})$$

MICRO

Particles (atoms/molecules)

$$\frac{d^2 r_i}{dt^2} = -\sum_{j>i} \nabla V_{ij}$$

QUANTUM

Complex Fields

$$i\hbar \partial_t \Psi = H\psi$$

Continuum Fields and PDE's


VE
RI
TAS
HARVARD

The Physics of Fluids

Why are fluids important ?

Pervasive!

The heroes: Navier-Stokes

(L. Navier, 1785-1836))

(G. Stokes, 1819-1903)

The Navier-Stokes equations

$$\partial_t \rho + \nabla \cdot (\rho \vec{u}) = 0$$

Mass conservation

$$\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u}\vec{u} + \overleftrightarrow{P}) = \vec{f}$$

Momentum conservation

$$\overleftrightarrow{P} = p\overleftrightarrow{I} - \overleftrightarrow{\sigma}$$

$$p = f(\rho, T)$$

Equation of State
(Ideal/Nonideal)

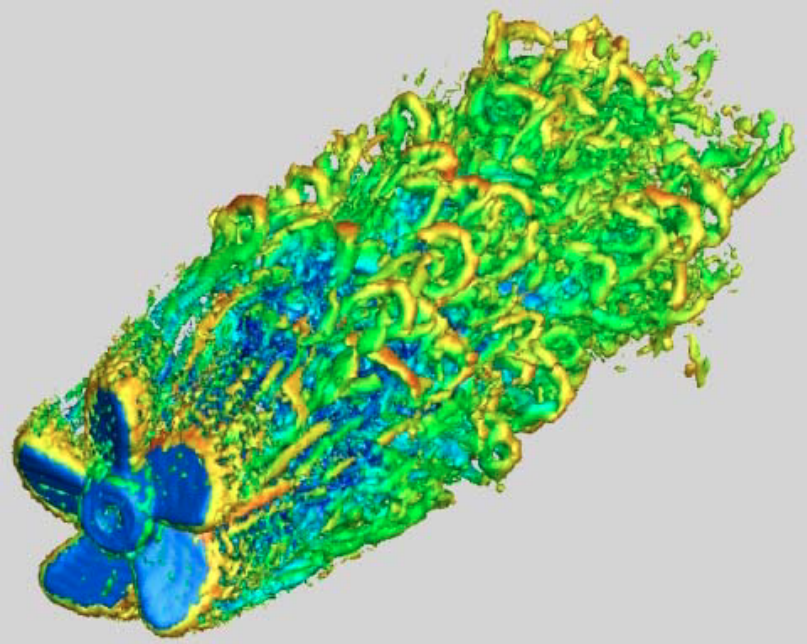
$$\overleftrightarrow{\sigma} = \lambda(\nabla \cdot \vec{u})\overleftrightarrow{I} + \mu[\vec{\nabla}\vec{u} + (\vec{\nabla}\vec{u})^T]$$

Stress-Strain Constitutive Relation
(Newtonian/Non-Newtonian)

Pandora's box

The NSE's look innocent but they are not!

TURBULENCE!



The physics is not as much in the equations as it is in their solutions !!!

NEW physics from OLD Equations!

(Covered by AC274, both in simulation and data analysis)

Solid/Wave Mechanics

How materials deform under stress (RHEOLOGY)

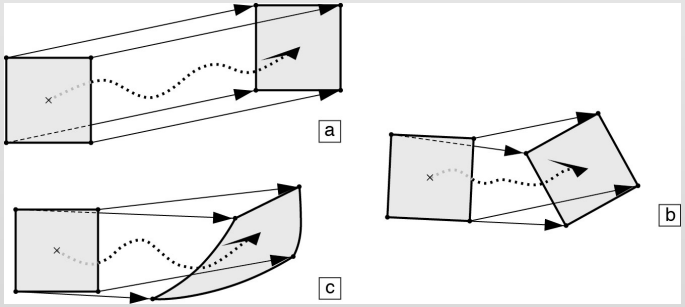
Displacements from the equilibrium configuration, **wave-propagation**

$$\xi(x,y,z) = r(x,y,z) - r_{eq}(x,y,z)$$

Obey a large set of Newton Equations:

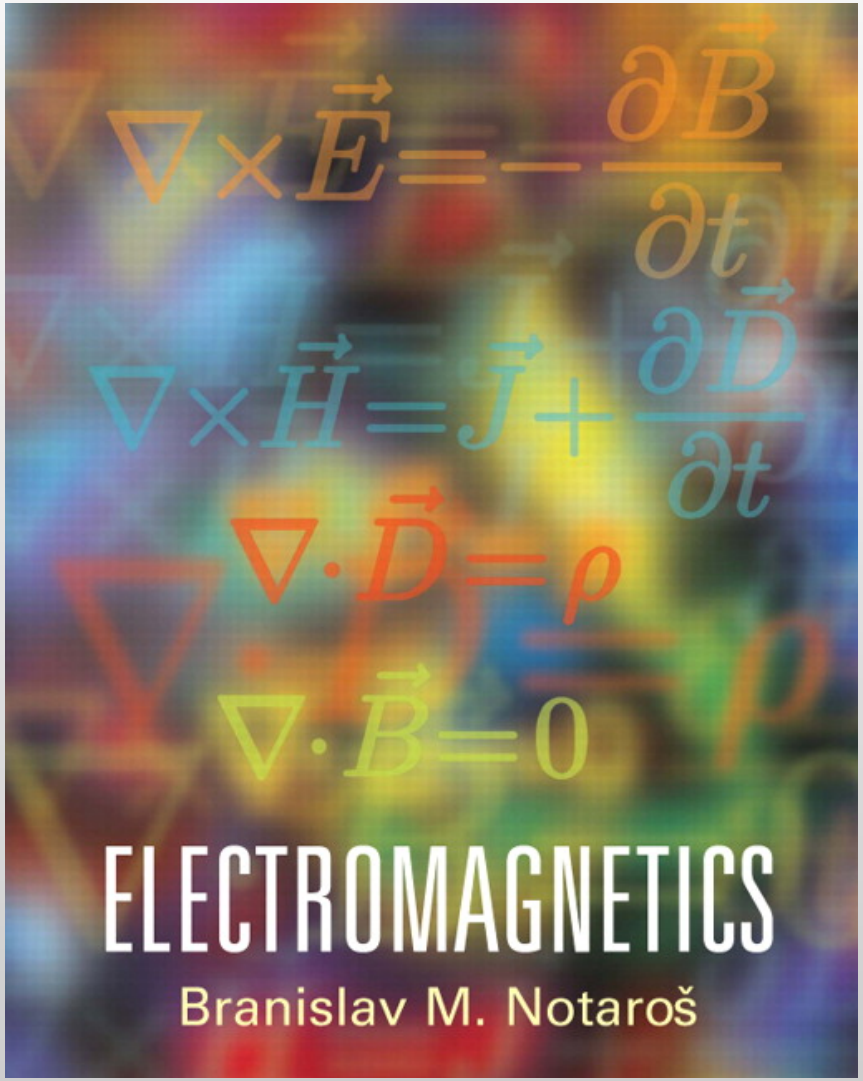
$$M\ddot{\xi} = -K(\xi)\xi + F_{ext}$$

Inertia Stiffness External Load

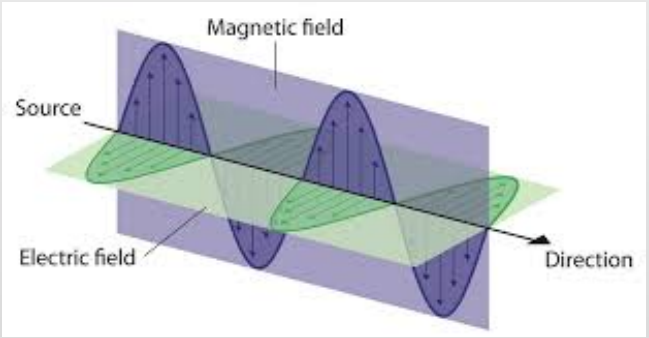


Challenge: **Large (non-linear) deformations**

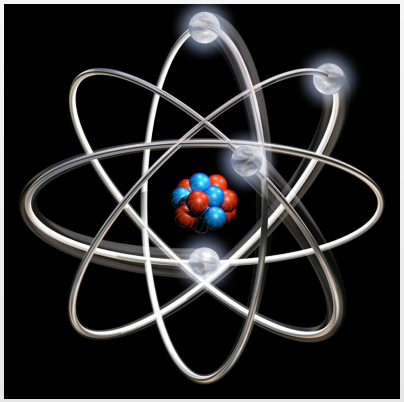
Electromagnetics



How em waves interact
with and propagate with matter
LIGHT-MATTER physics



Quantum Physics



Quantum physics is the language we speak with Nature, paramount for applications and modern technology.
It deals with COMPLEX WAVEFUNCTIONS and PROBABILITIES

It comes in many forms:

Single body (quantum mechanics)
Many-body (quantum chemistry/biology)
Quantum field theory (hep, condmat, exotic materials)
Quantum computing, entanglement …

AC274 will cover the basics (QM + many-body)

The hero

Schrödinger's Equation

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V(\mathbf{r},t)\psi(\mathbf{r},t)$$

i is the imaginary number, $\sqrt{-1}$.

$\hbar$ is Planck's constant divided by 2π: 1.05459×10^{-34} joule-second.

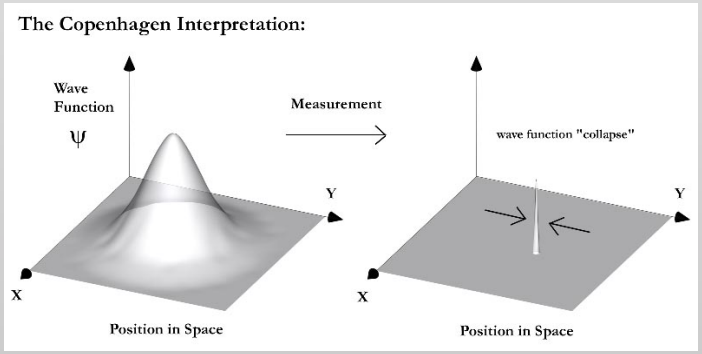
$\psi(\mathbf{r},t)$ is the wave function, defined over space and time.

m is the mass of the particle.

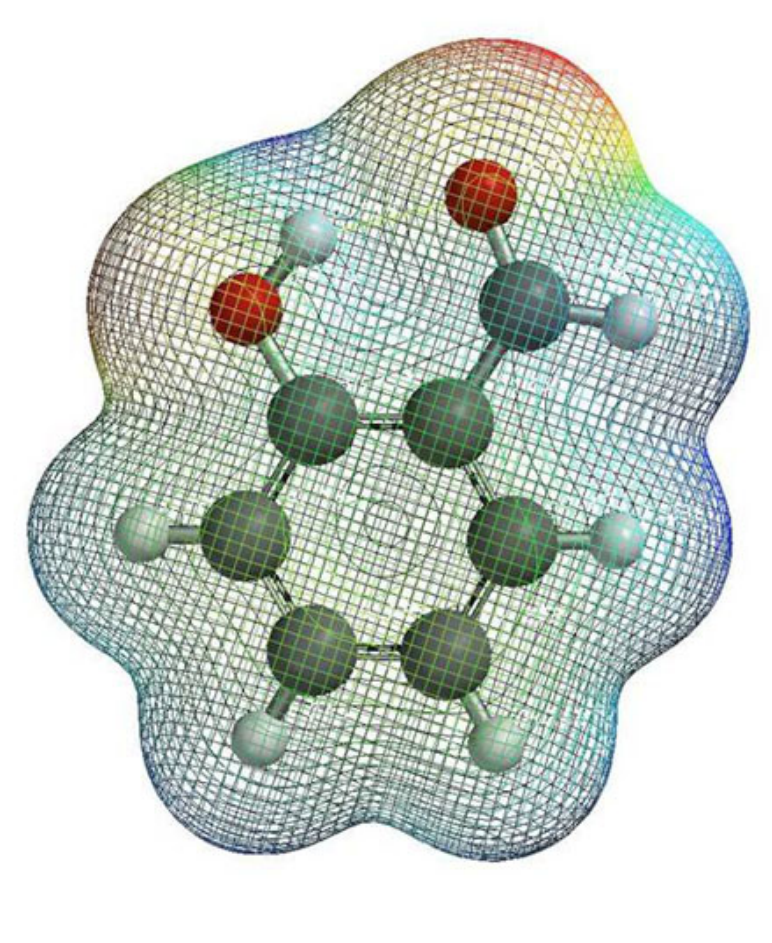
∇^2 is the Laplacian operator, $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$.

$V(\mathbf{r},t)$ is the potential energy influencing the particle.

Erwin Schroedinger (1887-1961)



Computational Chem/Bio



Molecules and Biomolecules

N=Nuclei+Electrons

The N-body wavefunction

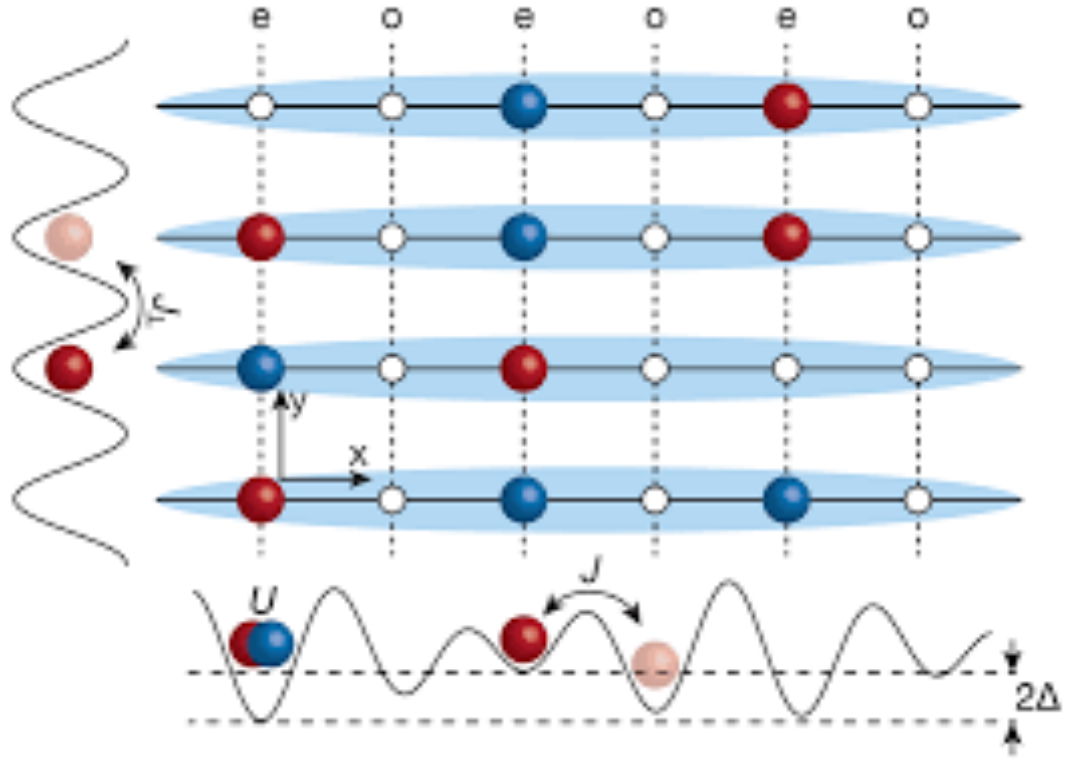
$$\Psi(\vec{r}_{1,},\vec{r}_{2,},\ldots\vec{r}_{Nel,};\vec{R}_1,\vec{R}_2,\ldots\vec{R}_{Nuc})$$

Lives in 3N-dimensional space!

N~10^5: Ungriddable!
The kingdom of particle methods (MonteCarlo)

Quantum Field Theory

Each lattice site i=1,2 … N hosts a quantum field, then **send N to infinity!**



Promising Quantum Computing platforms

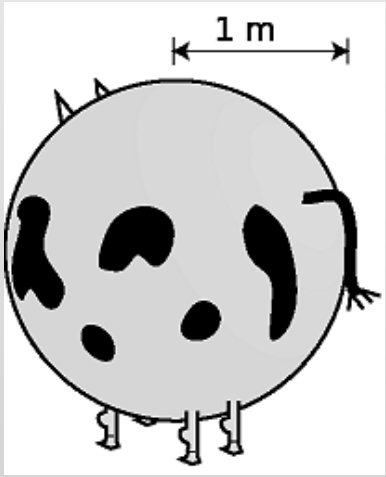
Complex geometries

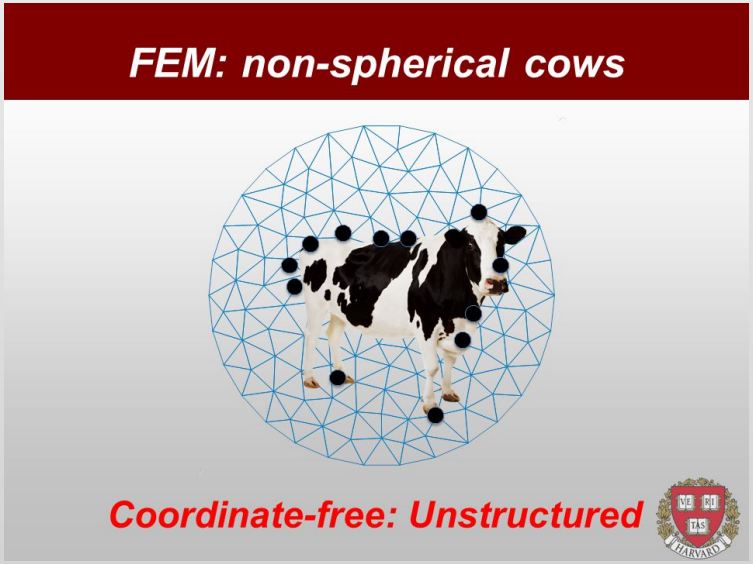
Non-spherical cows

Field theory and PDE's are subject to BOUNDARY CONDITIONS

Analytics is often at loss with complex geometries,
No smoothness!

Form-Function paradigm



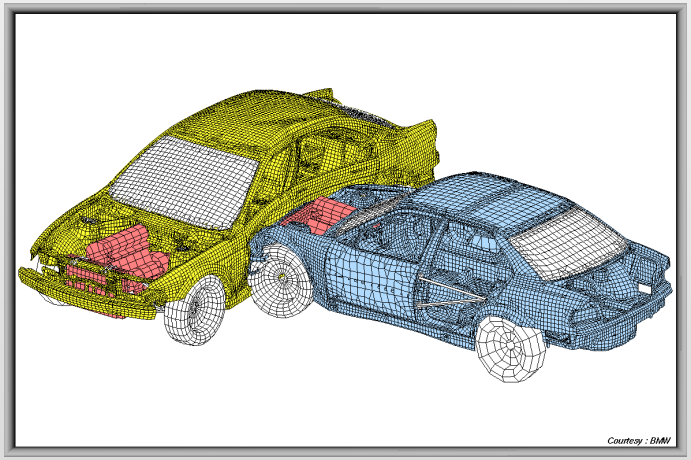


Major methods: **Finite Volumes and Finite Elements**

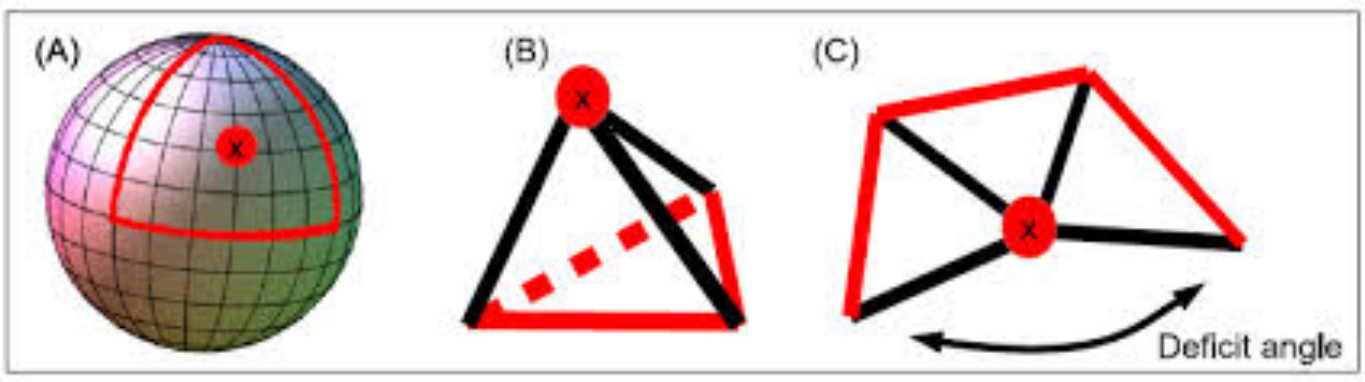
Finite Volumes/Elements

Computing without coordinates: Unstructured Data

From engineering to quantum gravity!



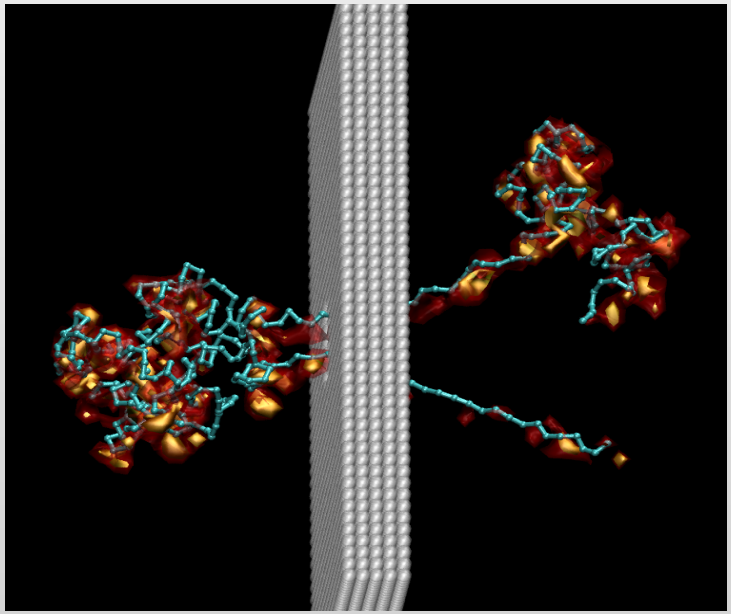
(Tullio Regge, 1931-2014)



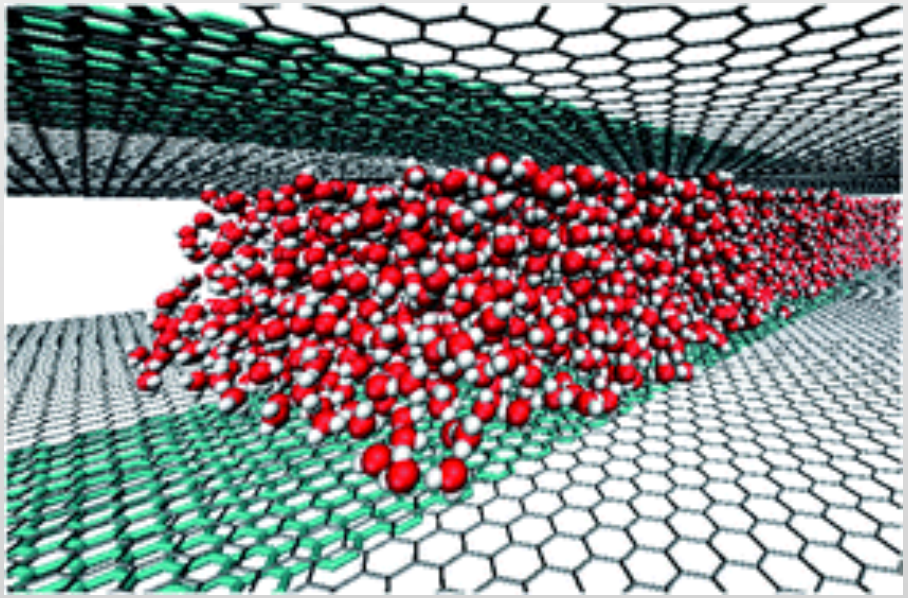
From fields to Particles: PDE's to ODE's

Molecular physics

Under the drive towards increasing miniaturization, micro and nanofluids are becoming more and more important in modern science. Granular nature of matter is exposed: **thermal fluctuations**



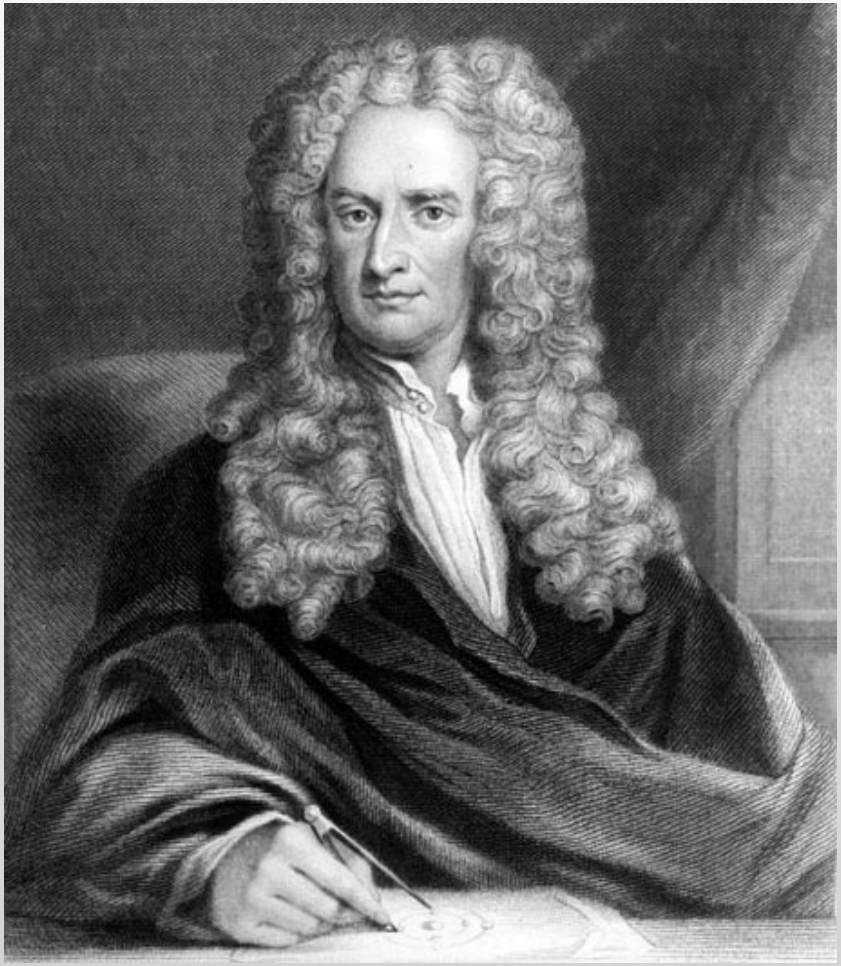
DNA Translocation



Water flow in nano-ribbons

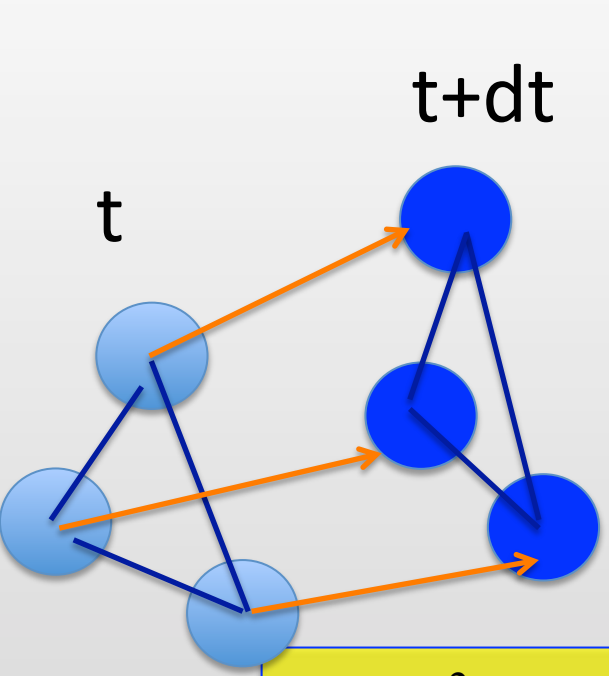
(See Lectures on Lattice Boltzmann and Molecular Dynamics)

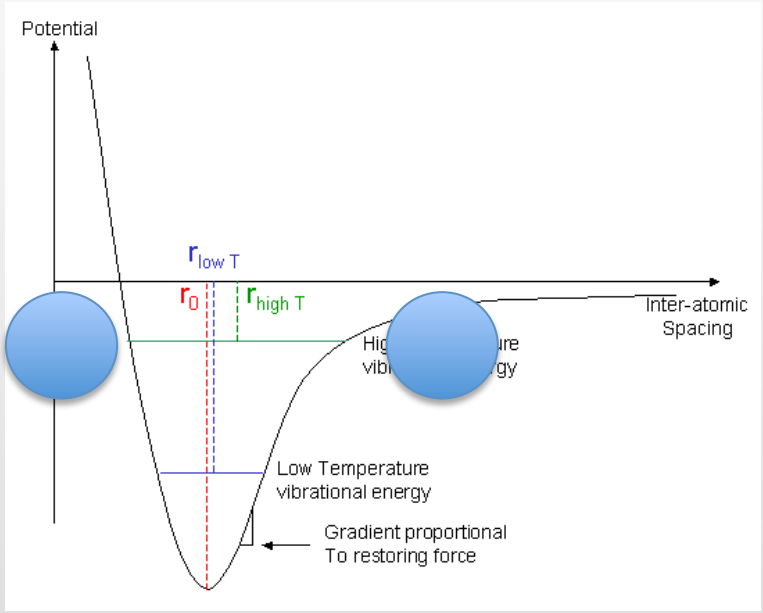
The hero



Isaac Newton (1642 – 1727)

Molecular Dynamics



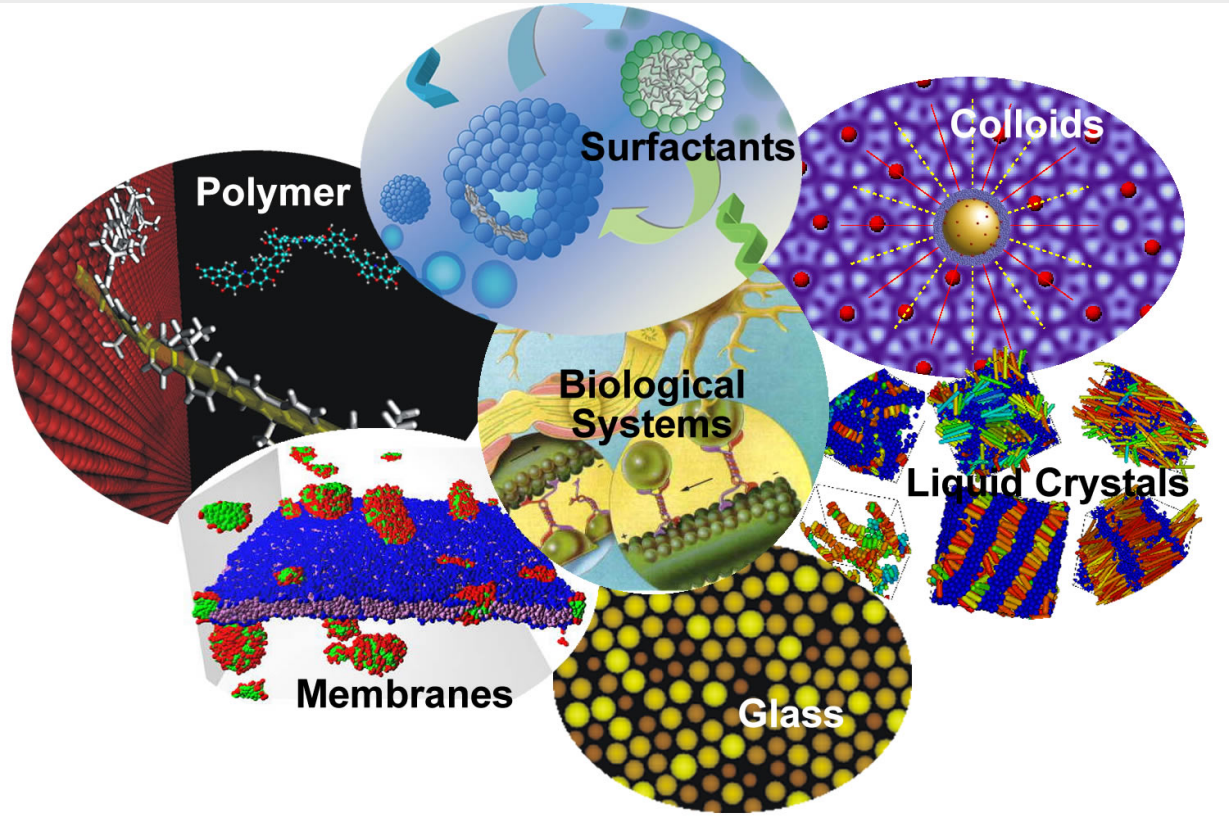


$$m\frac{d^2\vec{r}_i}{dt^2} = -\sum_{j>i}^{N}\nabla_i V_{ij} + \sum_{k>j>i}^{N^2}\nabla_i V_{ijk} + \dots$$

"Just " a huge bag of ODE's: but the bag is **Avogadro-huge** and the time-integration goes on for billions/trillions time-steps. Femtoseconds to seconds: the **TIME-GAP** problem

Complex states of matter

Molecules with *internal structure*, interferes with external motion, very complex rheology



An ocean of applications
In Material Science,
Biology, Medicine…
you_name_it…

Boltzmann kinetic theory

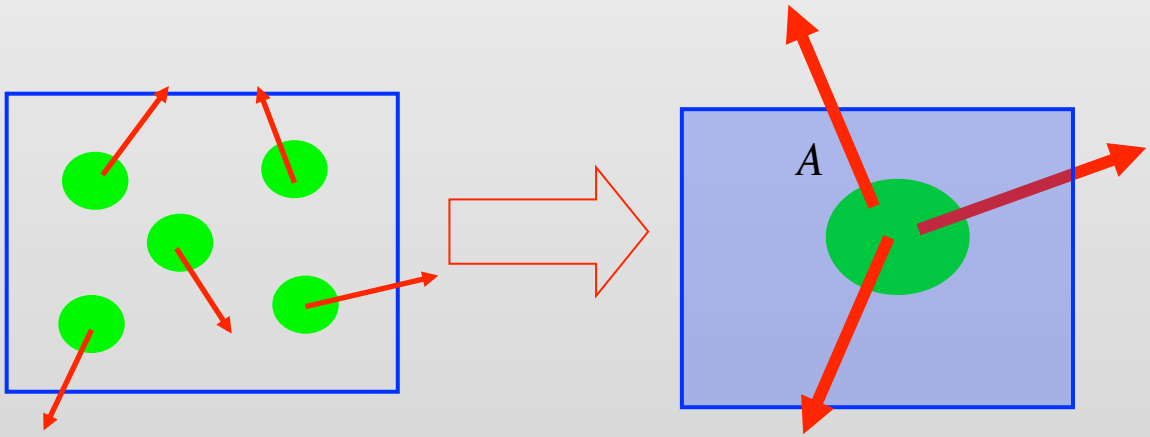
"The man who trusted atoms"

Ludwig Boltzmann (1844-1906)

Boltzmann: Probability Distribution Function

The **average** number of molecules around r at time t with velocity v

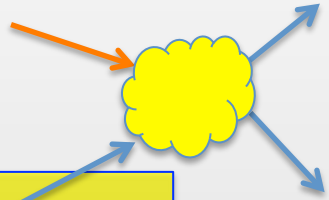
$$\Delta N = f(\vec{r}, \vec{v}; t)\Delta\vec{r}\,\Delta\vec{v}$$



f lives in a 6-dimensional world (phase-space)

The Boltzmann equation

Fluid in 6-dim phase-space:



$$\partial_t f + \vec{v} \cdot \nabla_r f + (\vec{F}/m) \cdot \nabla_v f = C(f, f)$$

$$\frac{d\vec{r}}{dt} = \vec{v} \qquad m\frac{d\vec{v}}{dt} = \vec{F}$$

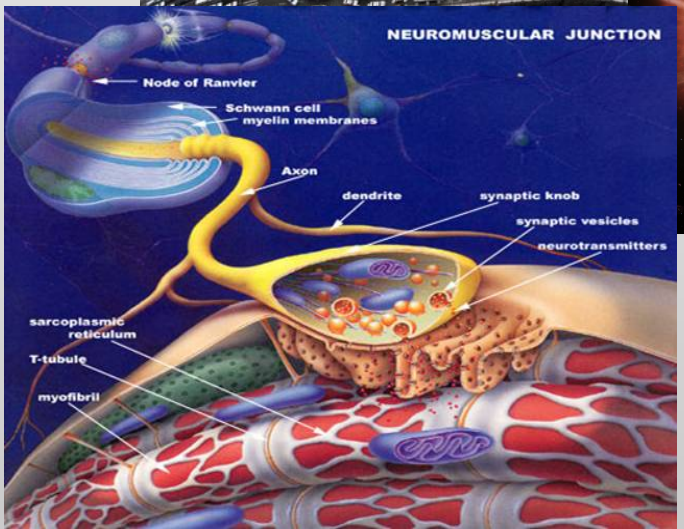
Collisions

A very tough computational cookie!
6+1 dimensional, nonlinear, integro-differential…

Usually solved by Monte Carlo, but many simplified models (see Lattice Boltzmann)

The Boltzmann equation

Transport in dilute media far from local equilibrium



Neutron transport

Gamma rays transport

Shuttle re-entry

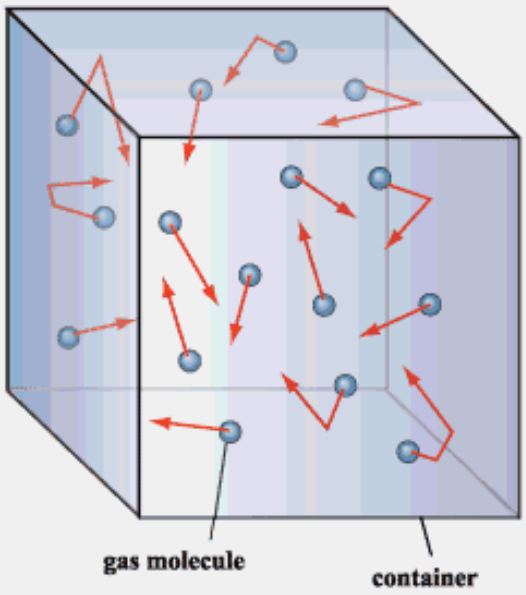
Electron flows

Traffic flows

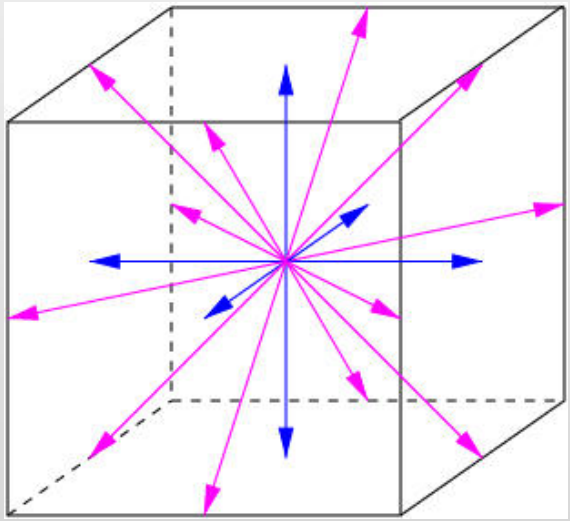
Lattice Boltzmann: Platonic hydrodynamics

$$f(x,v;t) = \sum_{i=0}^{b} f_i(x,t)\delta(v - c_i) \qquad i = 0, b$$

Triple infinity to just 19!

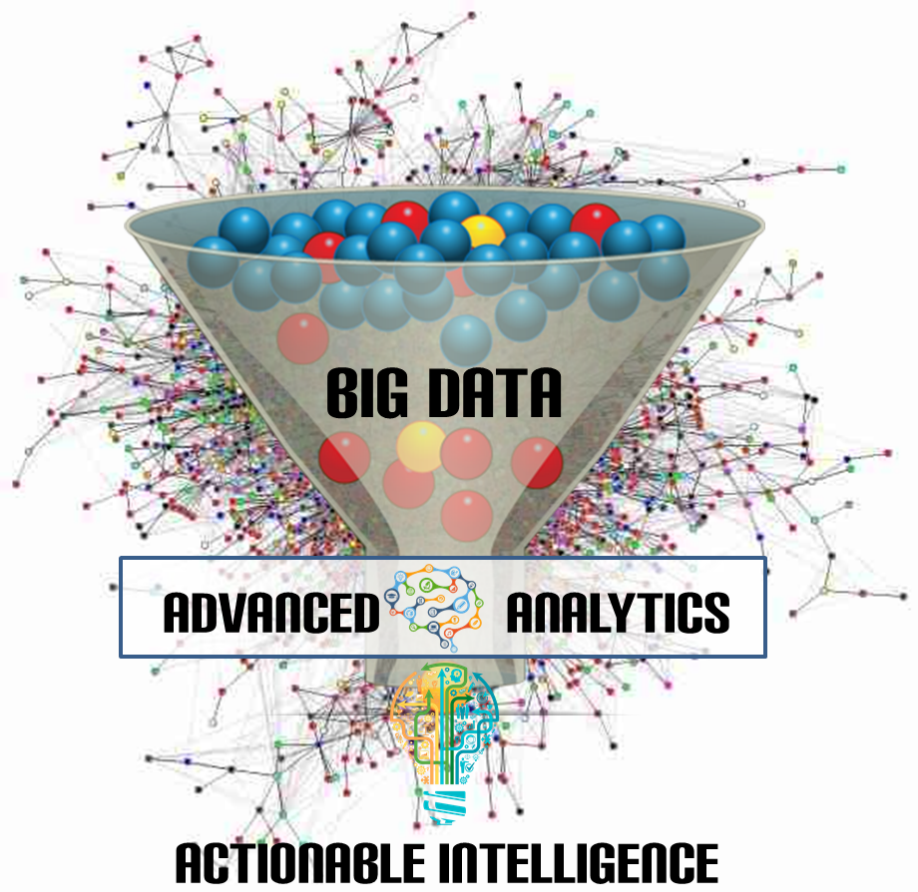


Magic speeds!



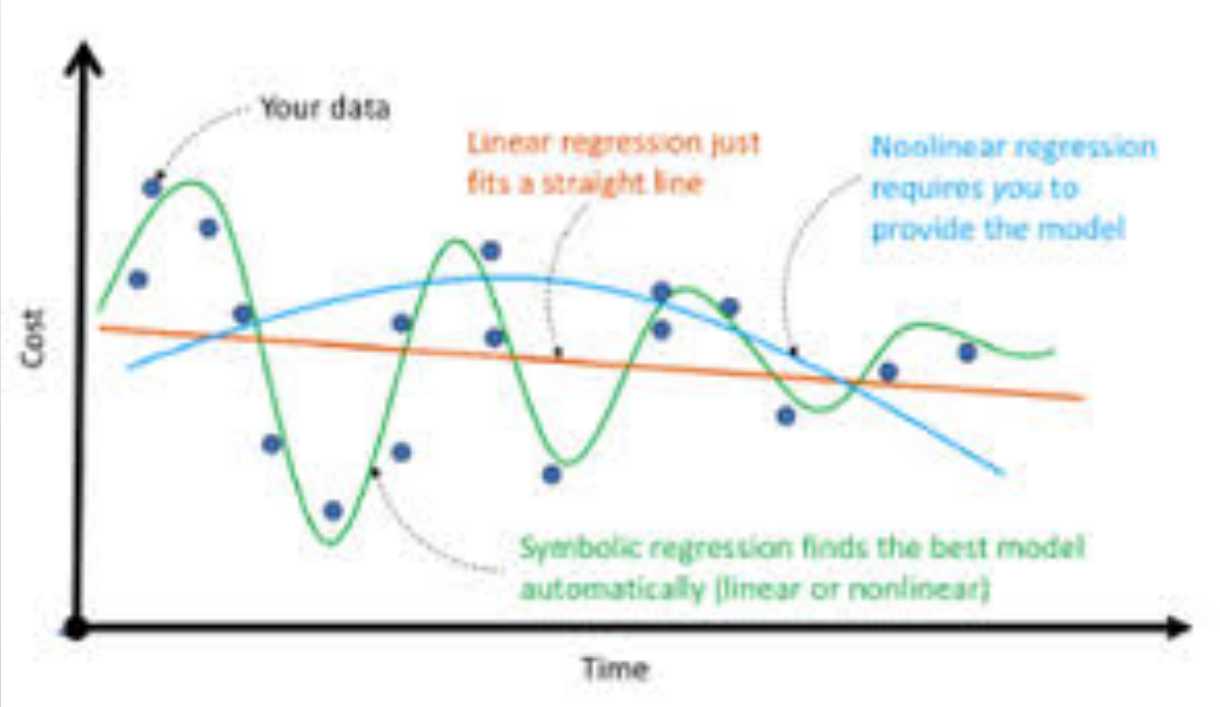
Continuum spacetime --> Crystal

Data Science



Numerical and Symbolic regression

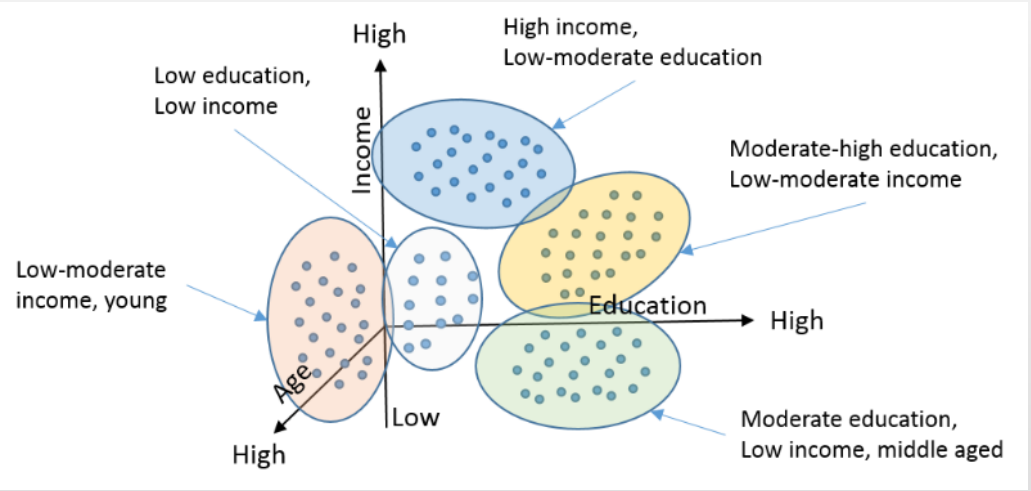
Numerical regression: best (linear or nonlinear fit)
Symbolic regression: finds the best model by searching symbolic space of equations (algebraic, ODE's, PDE's …).
Goes more and more into AI territory (**Machine Learning**)



DS for decision-making

Classify (A,E,I) and give a score:

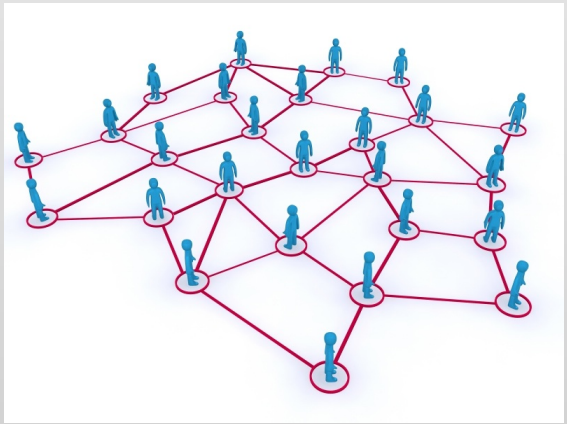
$$s_i = f(A_i, E_i, I_i)$$



Decision:

Fix a bar and filter 0,1 = NO/YES

$$y_i = sign(s_i - s^*)$$



Identify a few qualifiers (order parameters in physics parlance) and **cluster** the data accordingly.

Decision-making: each individual gets a score and produces a binary (yes/no) output beyond a given score threshold.

The binary output is the **DECISION:**

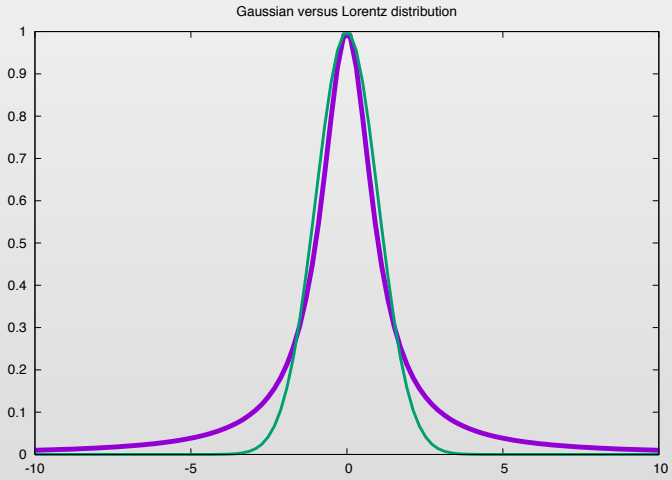
(SOCIAL/PSYCHO PHYSICS…)

Sentiment Analysis:

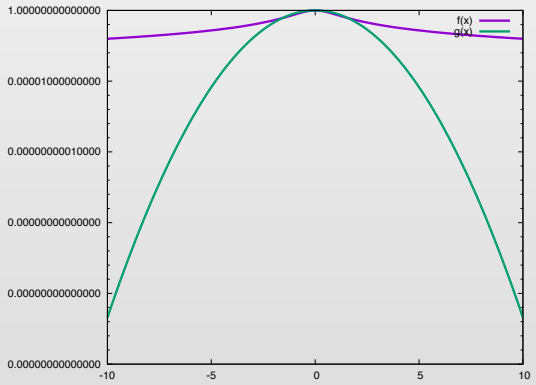
(steer and manipulate?

Wild fluctuations and rare events

Outliers (**rare events**) are heavily suppressed in the Gaussian world.
But the real world (complex systems) is hardly gaussian!



x



x

$$I = \int_{-\infty}^{+\infty} p(x) i(x)\, dx$$

If p(x) does not decay fast enough, the overall Intensity I
Is dominated by rare (small p) but intense (high i) events; divergent!

Turbulence
Weather
Earthquakes
Finance
…

The Gauss distribution exp(-x^2/2) has finite moments at *all orders*
The Lorentz distribution 1/(1+x^2) has infinite variance

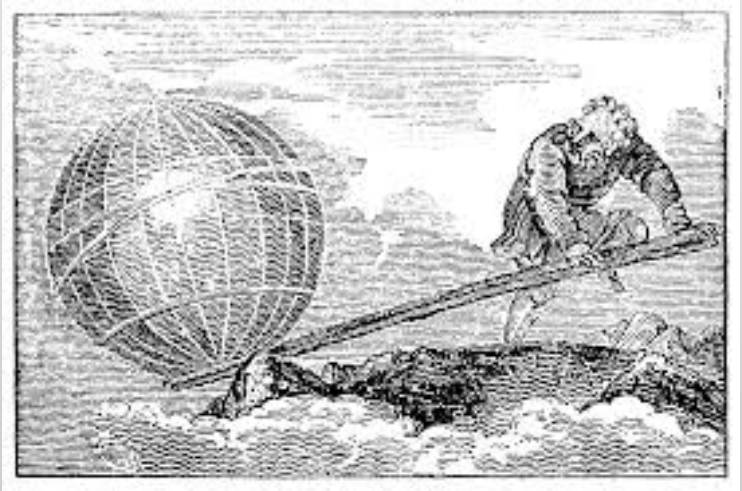
Why is Bigdata so sexy?

1. Extracting **patterns/trends** from Big Datasets can be MUCH faster than modeling/simulating the phenomena which produce the data

2. It applies to **all disciplines**, including those allegedly not math-friendly (too complex to be modeled)
   Biology, Medicine and esp Social, Communications and … Marketing…

The Grand-Question:

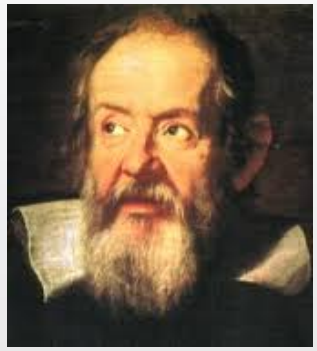
Is BigData the
i) New Archimedes lever?
ii) The graveyard of Theory?
iii) The End of Insight?



See Chomsky vs Norvig, Strogatz…

The end of Insight?

Is Bacon defeating Galileo?



Predict/Control/(Manipulate) without theoretical underpinning/understanding?

But…is it all blue-sky?

Big-Data depends on EXTRA-polation (from in_sample to out_of_sample).
Highly complex and/or singular behavior does not converge in the
for any reasonable N, **in fact ML can be much slower/less accurate than modeling!**
Bogus correlations, Overfitting, ….

Can ML help with Quantum Gravity or Turbulence?
Not yet: Till then, down-toning and cooperation is healthier
AC274: examples of ML-assisted simulations in materials and turbulence

Summary

Computational Physics provides a third effective avenue for scientific exploration
Driven by hw advances and even more so, by methodological breakthroughs

Traditionally targeted to **continuum fields** (PDEs), is getting more and more
into **complex states of matter,** including **quantum, active matter and social systems**
More general mathematical structures (*fields, particles, probabilities*,
New synergies between Computational Modeling and Data Science
are key to future applications involving complex systems in science and society.

AC274 will help grasping this exciting
forefront of modern science:

ENJOY!

References

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(https://www.amazon.com/Fundamentals-Engineering-Numerical-Analysis-Parviz/dp/0521711231)
Excellent for grid methods (especially finite differences)

T. Pang, *Computational Physics, Cambridge U. P., 4° ed., 2010*
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Nice coverage of a very broad range of topics in classical and quantum physics

S. Succi, *The lattice Boltzmann Equation, Oxford Univ. Press, 2001*
(https://www.amazon.com/Boltzmann-Numerical-Mathematics.../dp/0198503989)
Lattice Boltzmann method for fluids and beyond

Y. Abu-Mostafa et al, *Learning from Data, AMLbook.com, 2012*
(https://www.goodreads.com/book/show/15706459-learning-from-data)
Nice introduction to Data Science and Machine Learning

End of the lecture