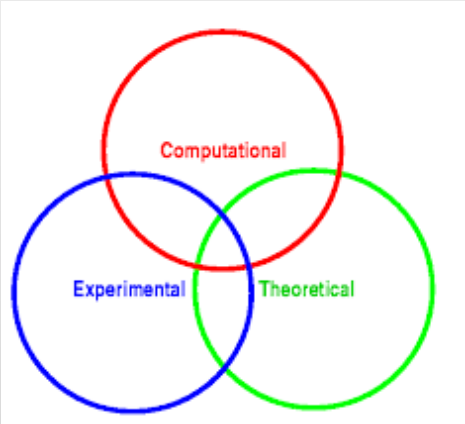
AC274: Computational Physics

The third avenue of scientific investigation



Sauro Succi,

IAC Rome and IACS Harvard

What is Computational Physics?

Solving physics problems using computers

The art of filliing the daunting gap between the degrees of available to Mother Nature and those affordable by our most poweful computers …

The Avogadro syndrome:

- 10^23 molecules in a cc of water vs ~ 10^16 bits in the largest computers.
- Our best computers can simulate a few billions computational molecule over milliseconds at most: 1 computational molecule ~ sqrt(Avogadro) molecules.

YET IT WORKS!

WHY? Because Nature is ***Redundant***, ***Hierarchical*** and (often) ***Detail Insensitive***:

Hence: broad scope for Mathematical MODELS

The Pillars of Computational Physics

The two pillars of computational physics:

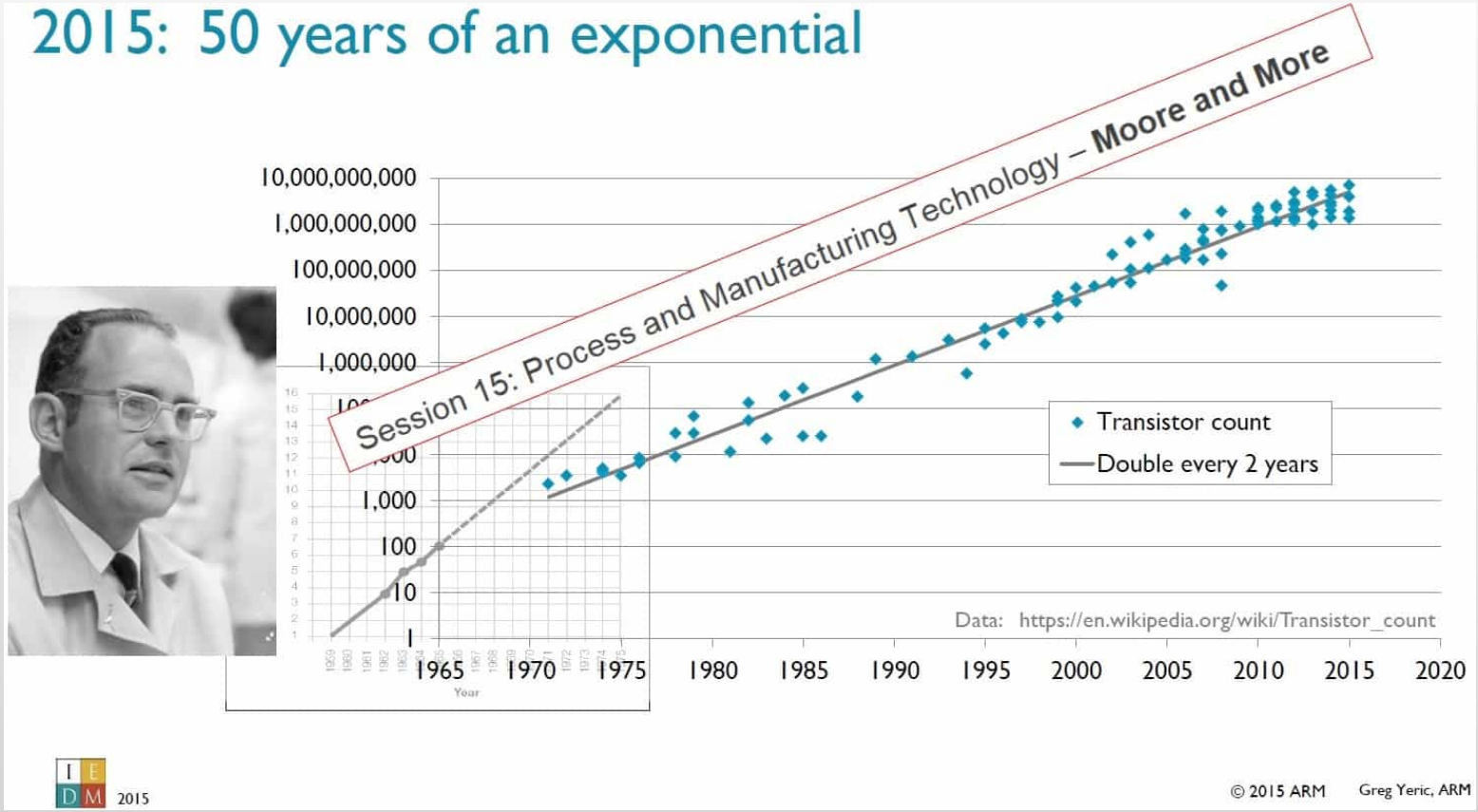
Computers (hw)

Algorithms (sw)

HW: Spectacular progress over the last 50 yrs: the compute power has **doubled every 2 yrs** (Moore's law): over a million in five decades!

SW: No less spectacular, see next slides…

Moore's law



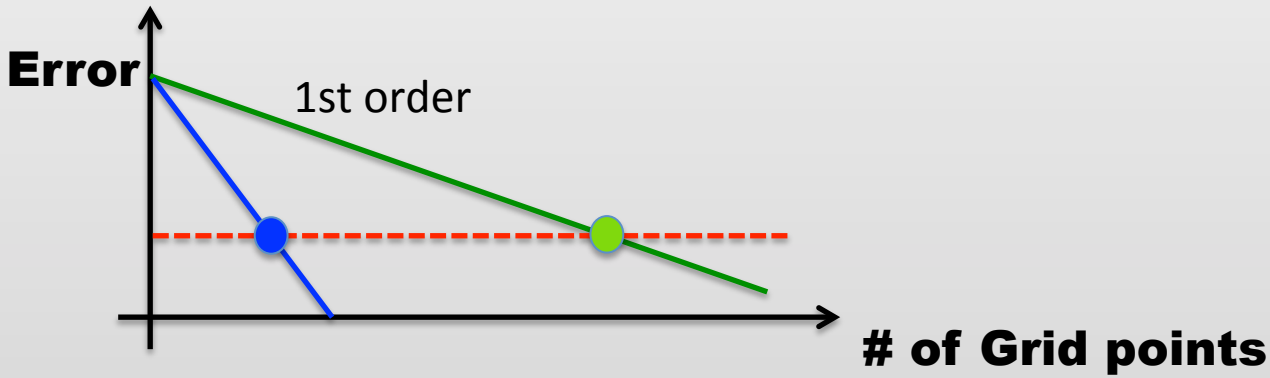
With the same trend in automotive, today we would drive faster than light!

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

Methods of Computational Physics

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!!!



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 (-:)

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:

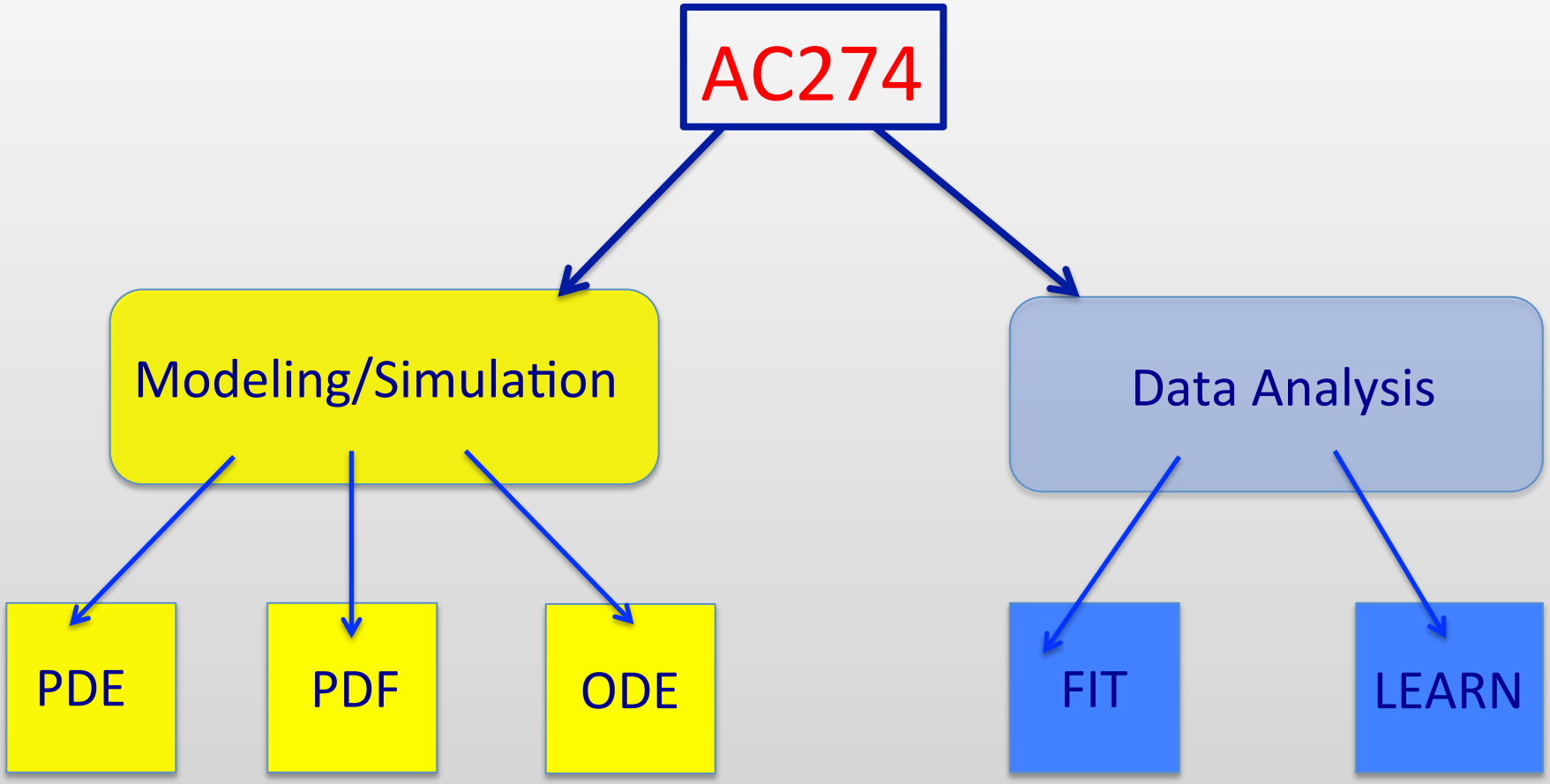
1. Grid methods for classical and quantum fields

2. Complex states of matter (fluids, solids, amorphous)

3. Active states of matter (psycho/social physics)

4. Learning from data

AC274: Plan of the course



Fluids
Solids
Quantum

Soft Matter

Active Matter
Social Systems

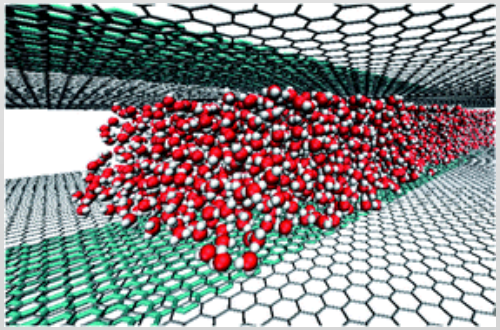
Regression,
Correlations,
Fractals…

Neural nets
Physics apps

Fields, Particles and Probabilities

FIELDS: based on the CONTINUUM assumption: granular/molecular aspects can be ignored. Typically modelled by **Partial Differential Equations (PDE's)**. This is apparently the most economic description but often faces formidable computational complexity due to the three main scarecrows:
NON-LINEARITY+COMPLEX GEOMETRY+HIGH DIMENSIONS.
Other representations may turn out to be 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 conceptual/mathematical framework: **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

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

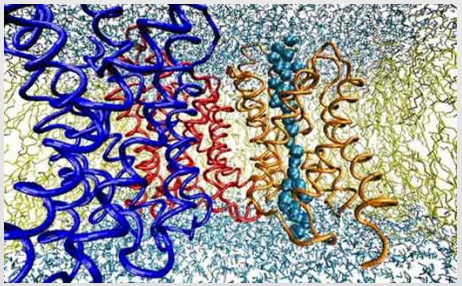
Complex states of matter

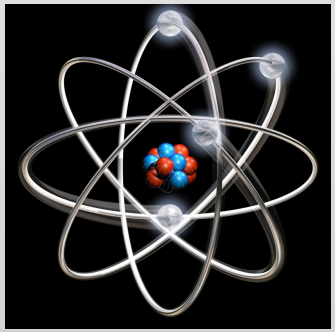
Emergence: Complex aggregate states of matter express genuinely new properties which cannot inferred from a microscopic description.

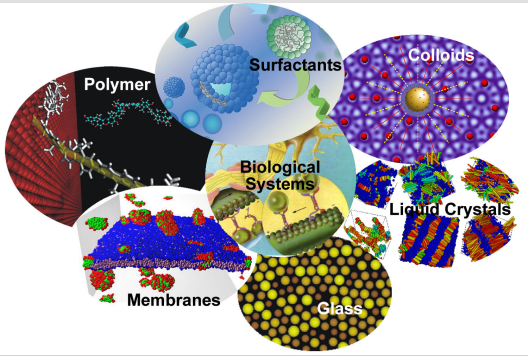
Gas, Solid, Liquid

Plasmas, Amorphous

Quantum materials







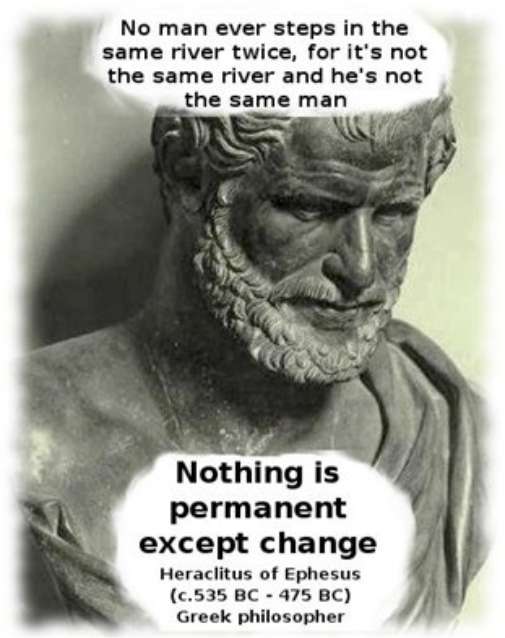
Let us proceed to illustrate how AC274 addresses all that…

Continuum Fields and PDE's

FLUIDS

πάντα ρεῖ

(Everything flows)
(Heraclitus)



A pervasive presence across virtually ALL human endeavours!

Modeling Matter in Motion (fluids across scales)

Why are fluids important ?

Pervasive!

The heroes: Navier-Stokes

(L. Navier, 1785-1836))

(G. Stokes, 1819-1903)

The Navier-Stokes equations

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

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

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

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

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

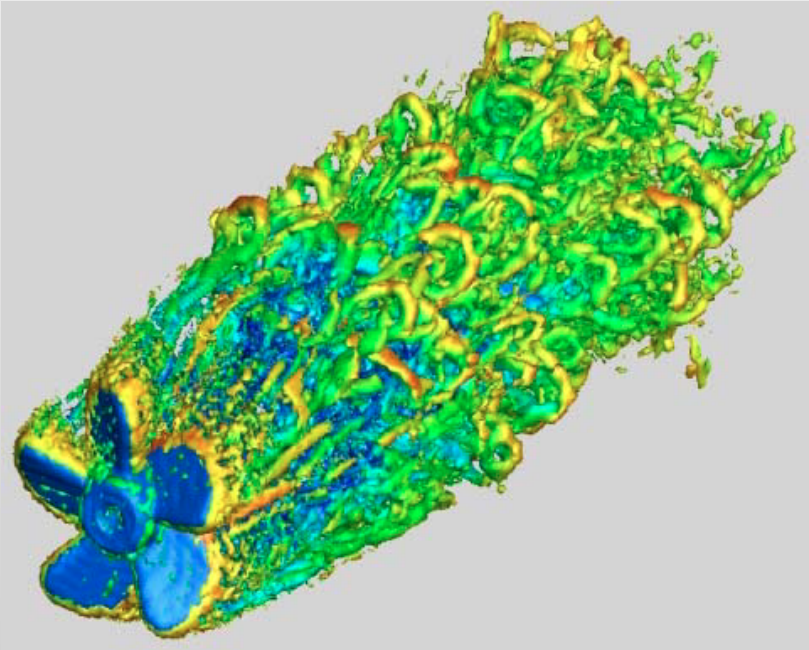
Equation of State
(Ideal/Nonideal)

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 in their solutions!!!

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

Solid Mechanics

How materials deform under stress (RHEOLOGY)

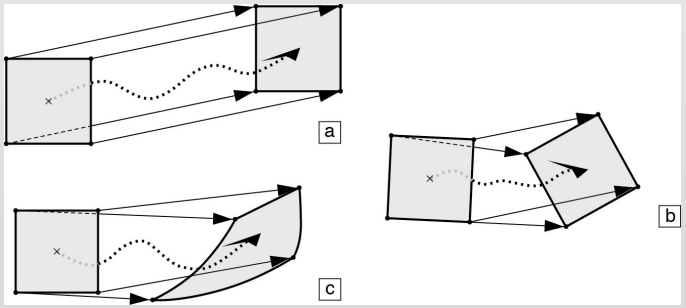
Displacements from the equilibrium configuration

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

Obey a large set of Newton Equations:

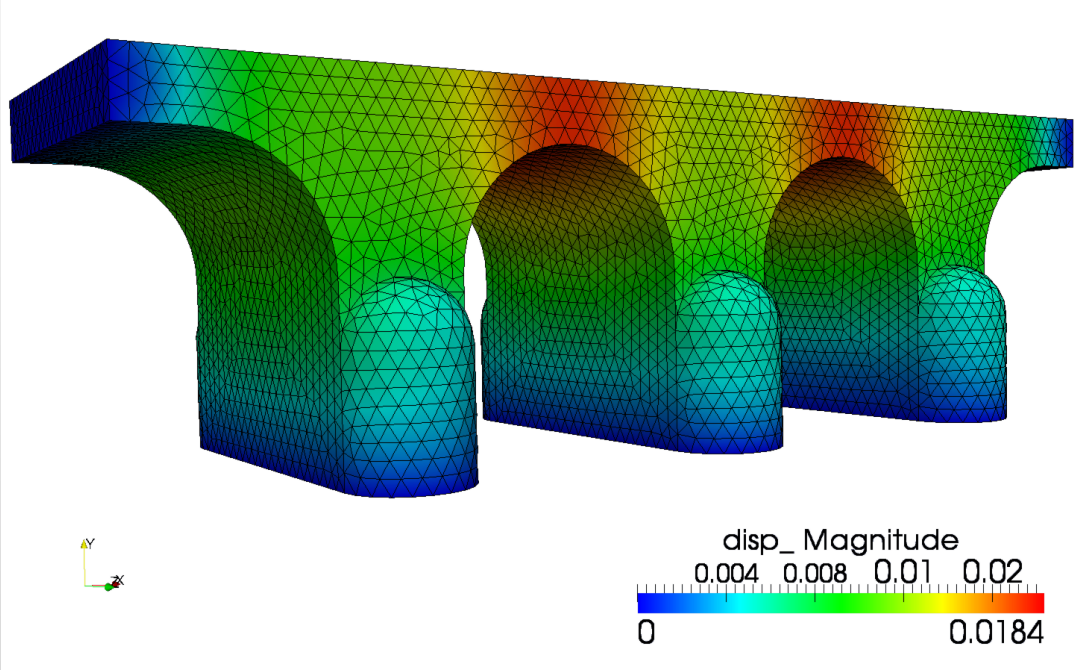
$$M\ddot{\xi} = -K(\xi)\xi + F_{ext}$$

Inertia Stiffness External Load



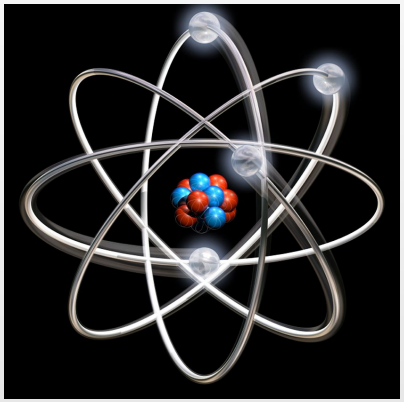
Challenge: **Large (non-linear) Deformations**

Solid Mechanics



Newton's F=ma for complex extended structures
The kingdom of the FINITE ELEMENT METHOD
(should definitely feature in the to p10…)

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 (single-body)

The hero

Erwin Schroedinger (1887-1961)

Quantum Mechanics

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.

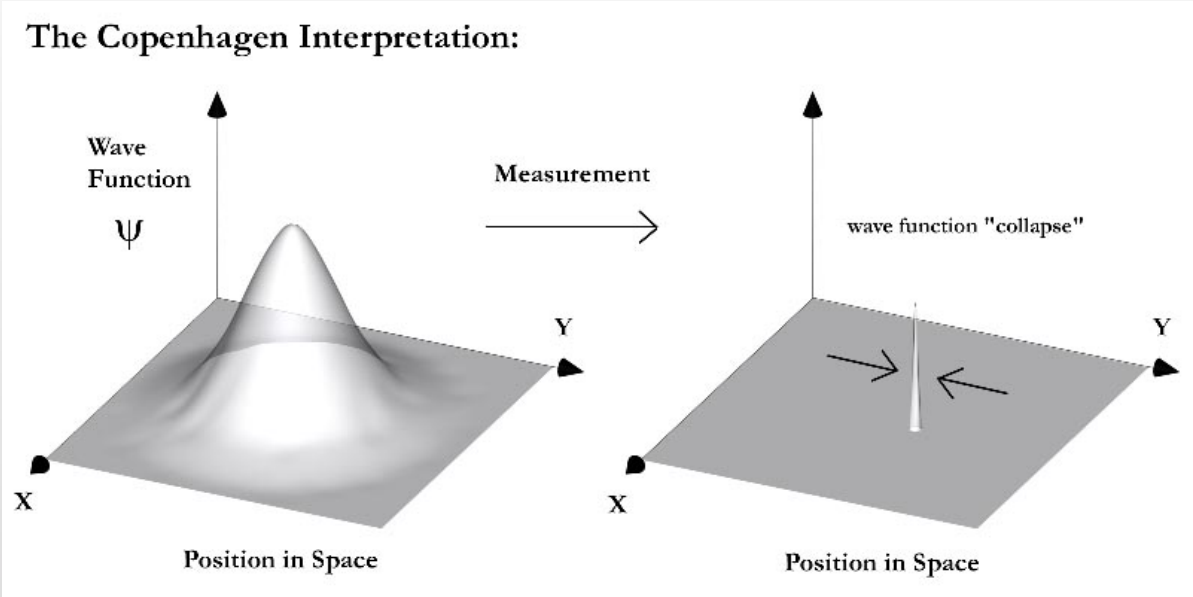
$\psi(\mathbf{r},t)$ is the wave function, defined over space and time.

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.

The quantum wavefunction

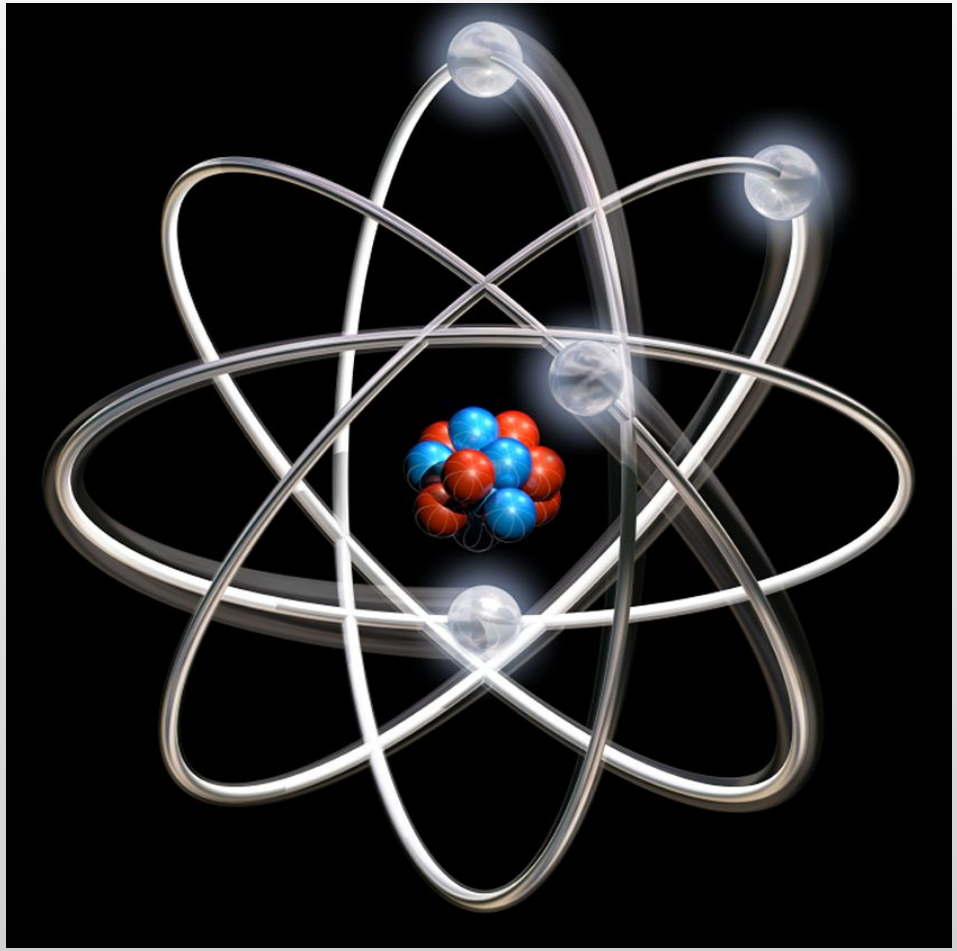


Probability to find the particle at poistion r at time t:

$$P(\vec{r};t) = |\psi^*(\vec{r};t)\psi(\vec{r};t)|$$

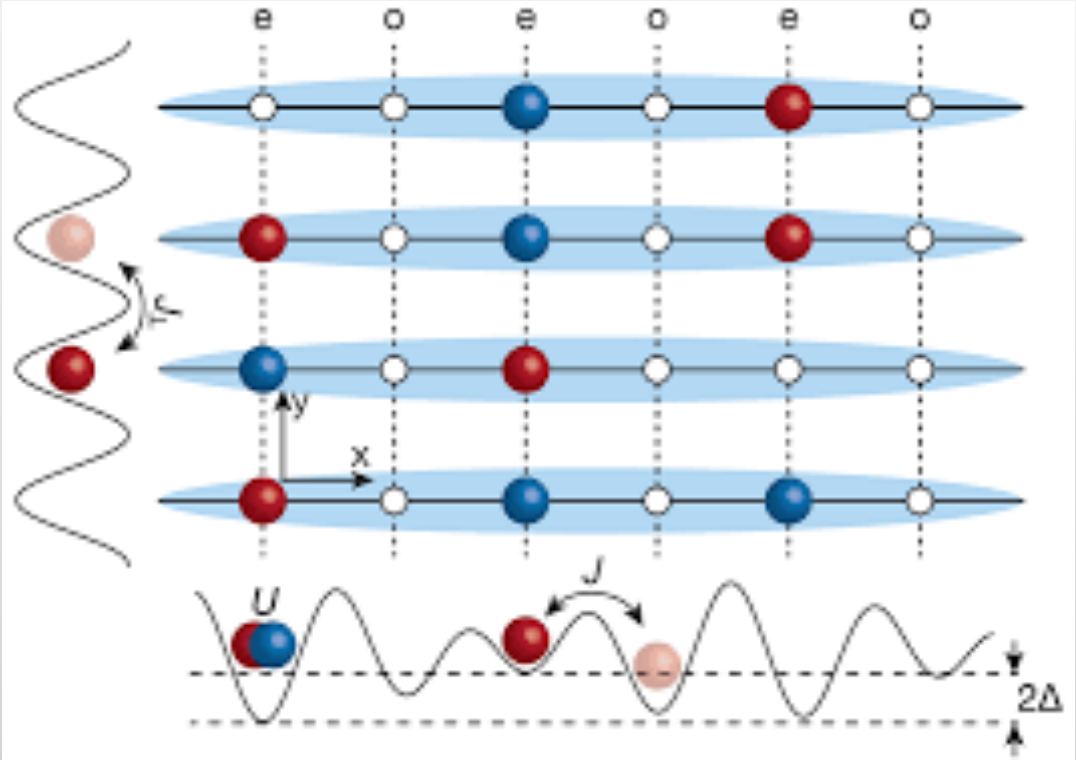
The amplitude tells the probability, the phase tells the velocity

Computational Chemistry



Quantum Field Theory

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

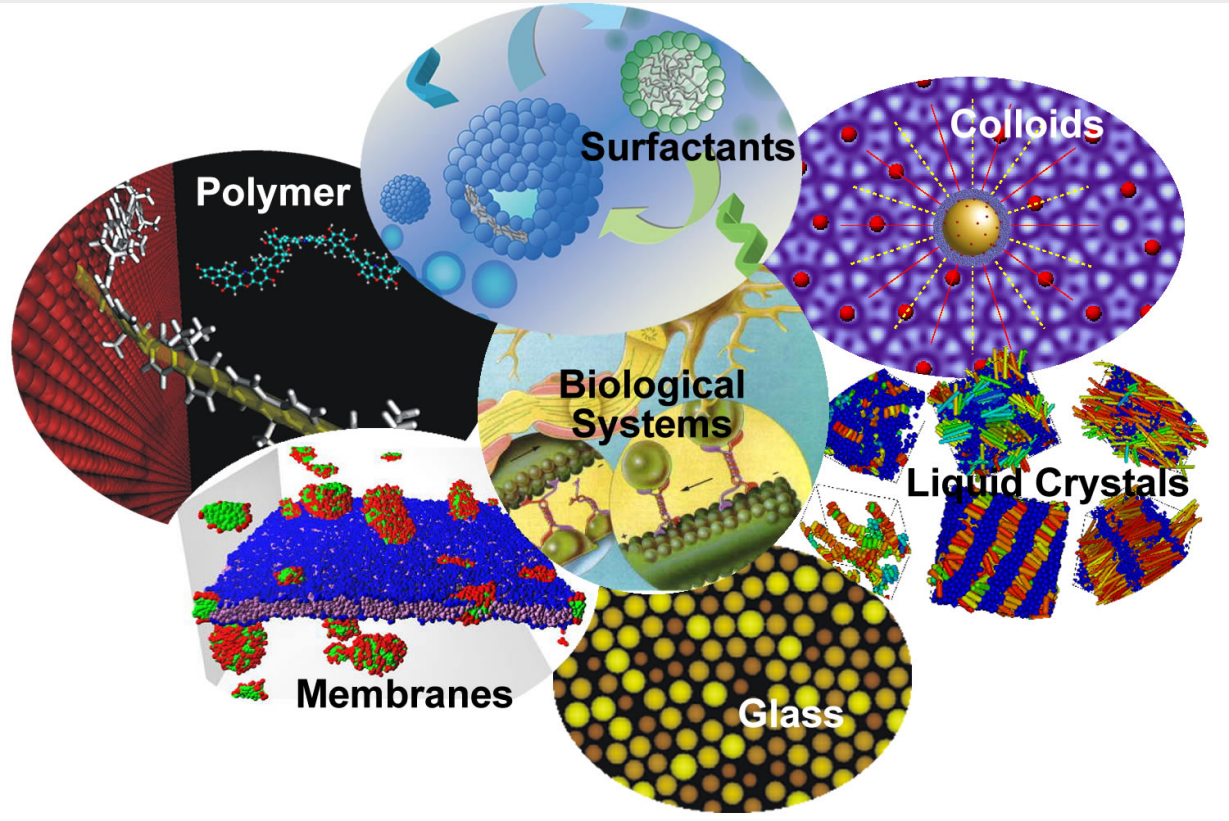


Promising quantum computing platforms

Physics beyond PDE's

Soft matter

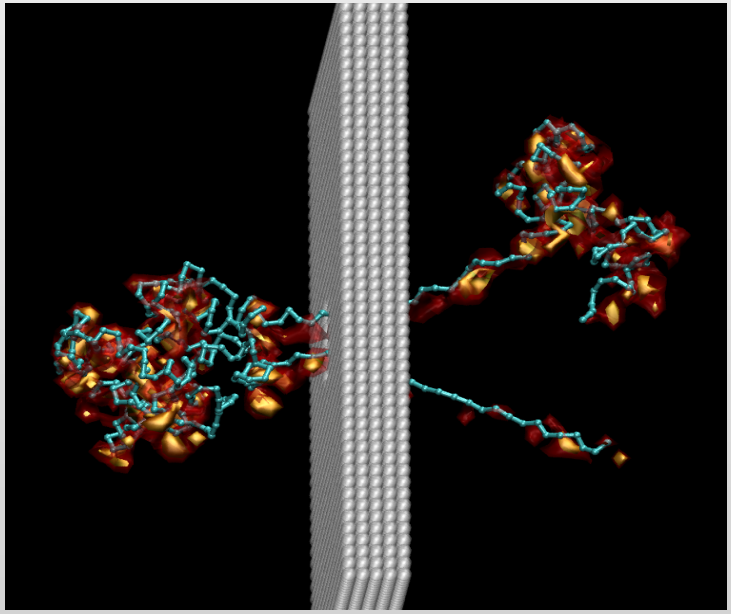
Molecules with internal structure, interferes with external motion, very complex rheology



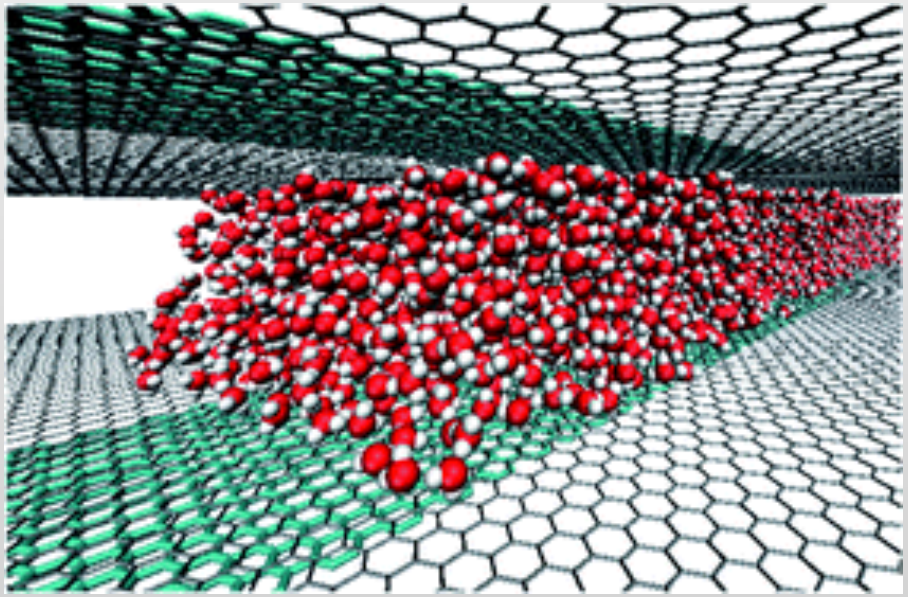
An ocean of applications
In Material Science,
Biology, Medicine…
you_name_it…

Molecular fluids

Under the drive towards increasing miniaturization, micro and nanofluids are becoming more and more important in modern science



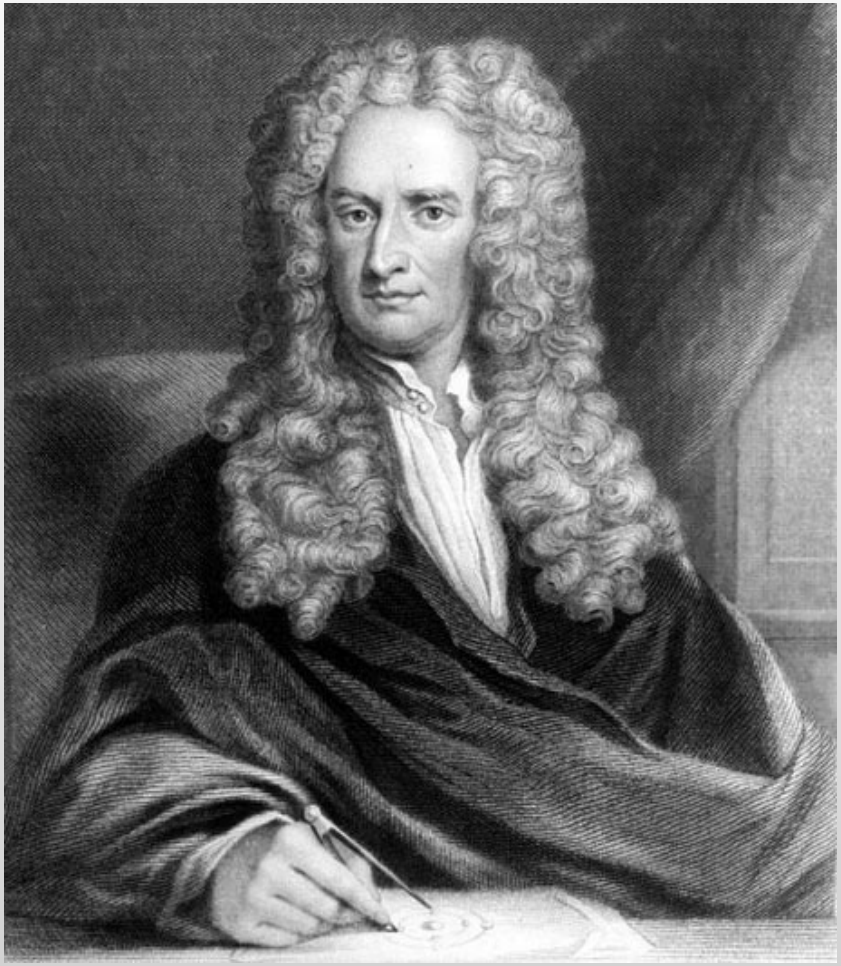
DNA Translocation



Water flow in nano-ribbons

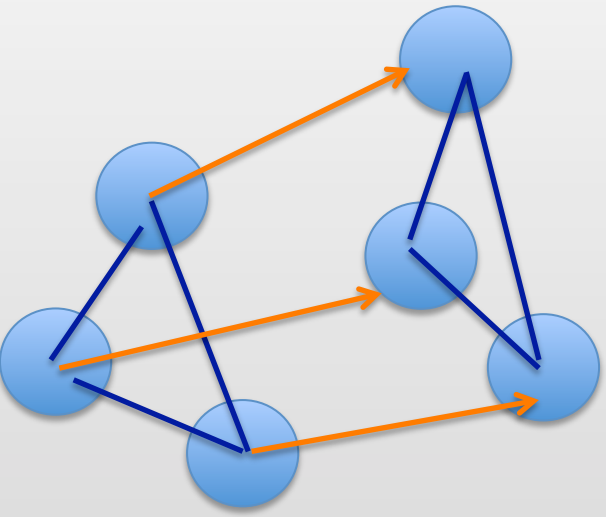
(See Lectures on Lattice Boltzmann)

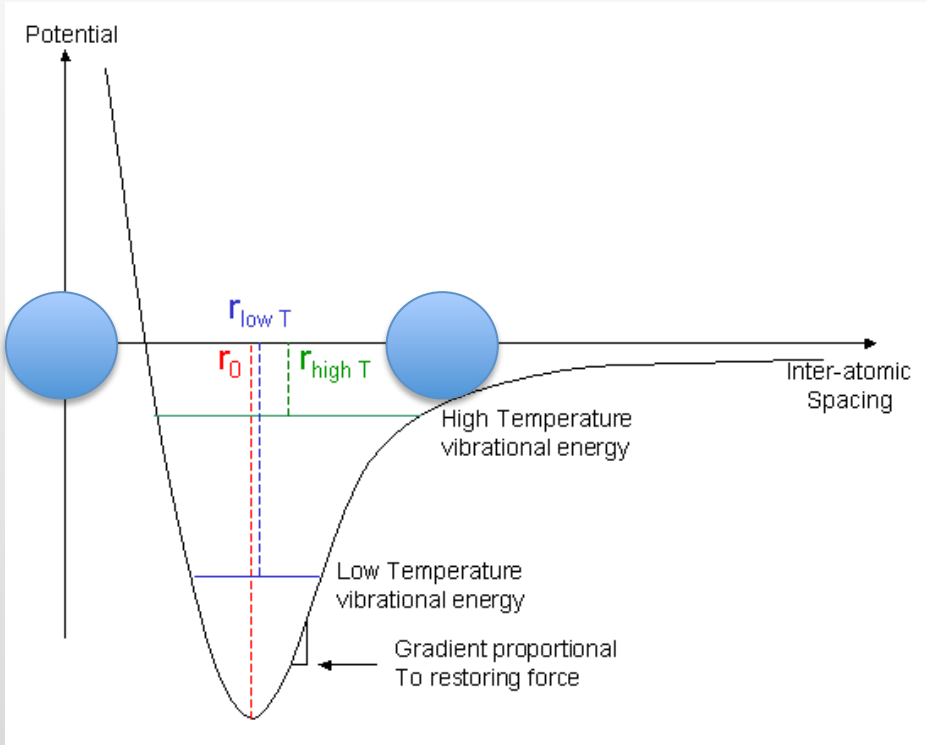
The hero



Isaac Newton (1642 – 1727)

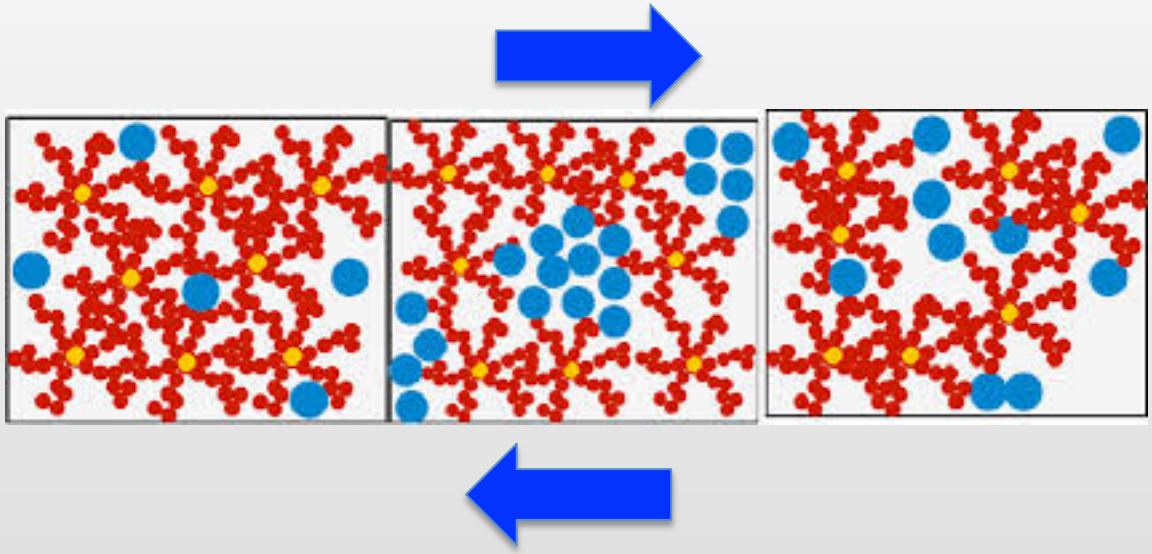
Molecular Dynamics





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

Mesoscale flows (soft-glassy flows)



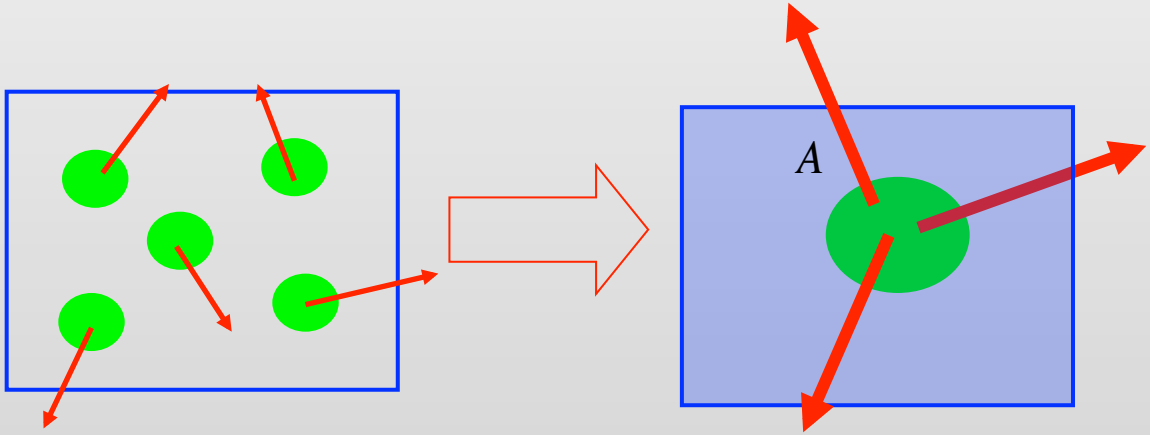
Internal dof (structure) couple with external ones (spacetime). This coupling "*breaks*" universality and fluid equations are no longer appropriate.

Boltzmann kinetic theory

Ludwig Boltzmann (1844-1906)

Boltzmann: Probability Distribution Function

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



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

The Janus nature of PDF

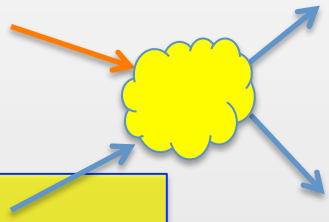
Kinetic Theory: half particles and half fields = fieldicles

Probability Distribution Functions

Extremely flexible for computational soft matter (see Lattice Boltzmann)

The Boltzmann equation

Fluid in 6-dim phase-space:



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

Collisions

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

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

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

The Boltzmann equation

Transport in dilute media far from local equilibrium

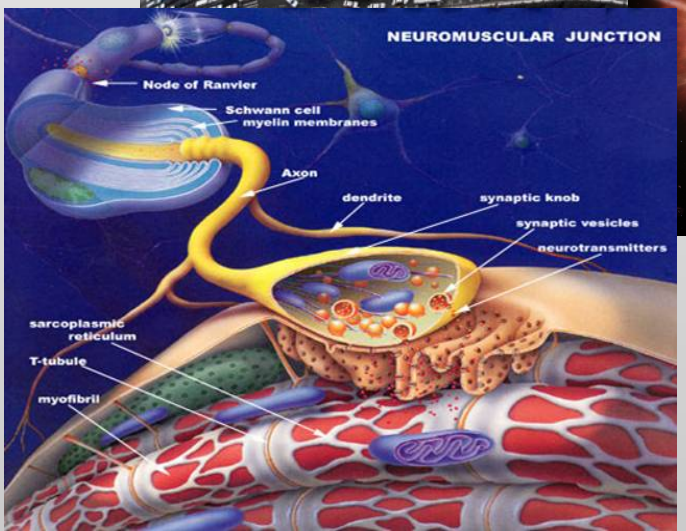
Neutron transport

Gamma rays transport

Shuttle re-entry

Electron flows

Traffic flows



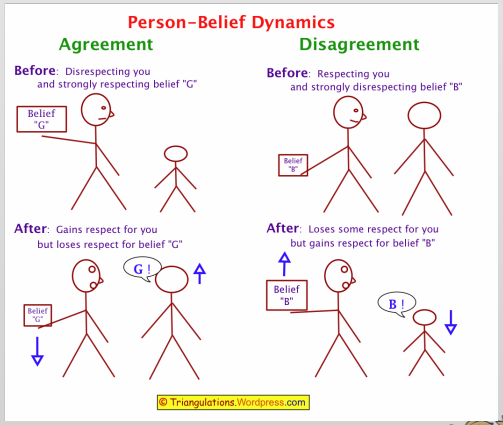
Active matter

Active states of matter

Agent-based models (Thinking Molecules): Computational Psycho-Physics:
The internal degrees of freedom (psycho) interact with the external ones. ADAPTIVE complexity: the systems learns from the environment and affects it (humans!). A new branch of statistical mechanics.

Flocks, herds, pedestrians, opinion dynamics:

Driven by Social Interactions



Psycho-physics

The motion of each agent is governed by "social" interactions:

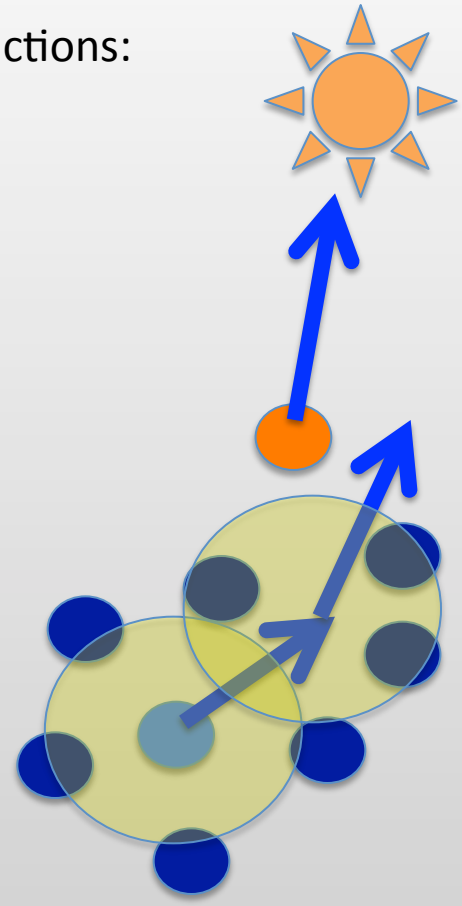
$$\vec{V}_i(t+dt) = p\vec{V}_i(t) + q\vec{V}_{ave}(t) + r\vec{V}_{lead}(t)$$

p Self-confidence

q Go-with-the flow: conformism

r Follow the leader

$$\vec{V}_{lead}(t+dt) = -kf(\vec{R}_{lead} - \vec{R}^*)$$



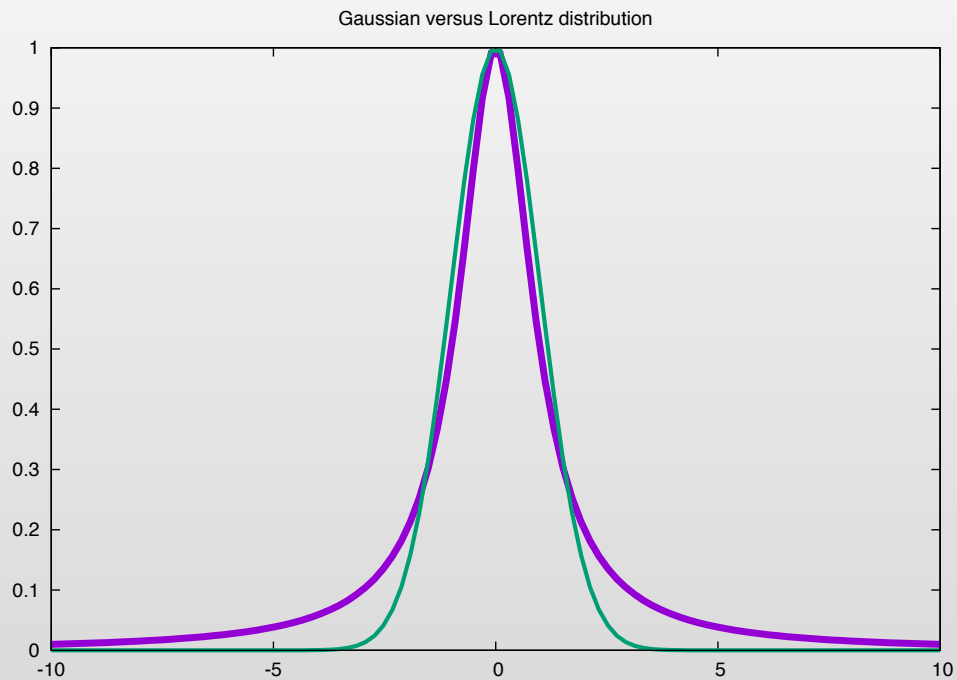
(See AC274 Lectures on Birds Flocking)

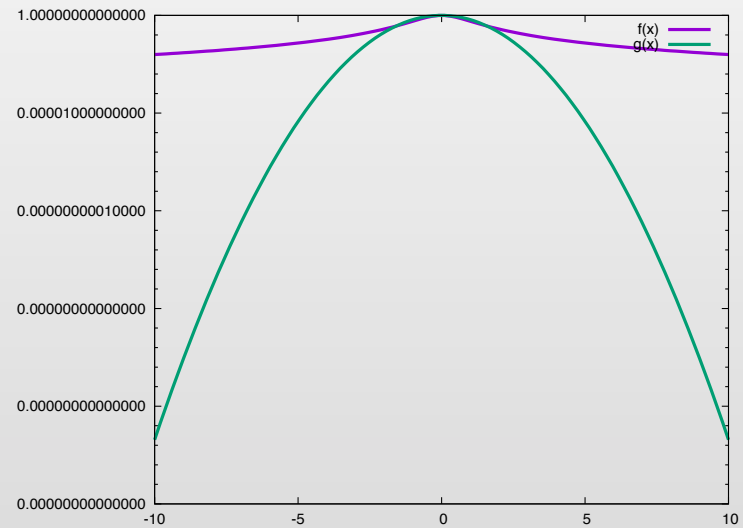
Predicting X-events

Extreme (X) events in complex systems occurr way more frequently than expected.
Non-linearity + psychological reinforcement (market crashes).
The consequences can be dire: **black swans**
Tornaodes, hurricanes, financial crashes…

Damage Risk =Probability*Severity

ProbDisFun (PDF)



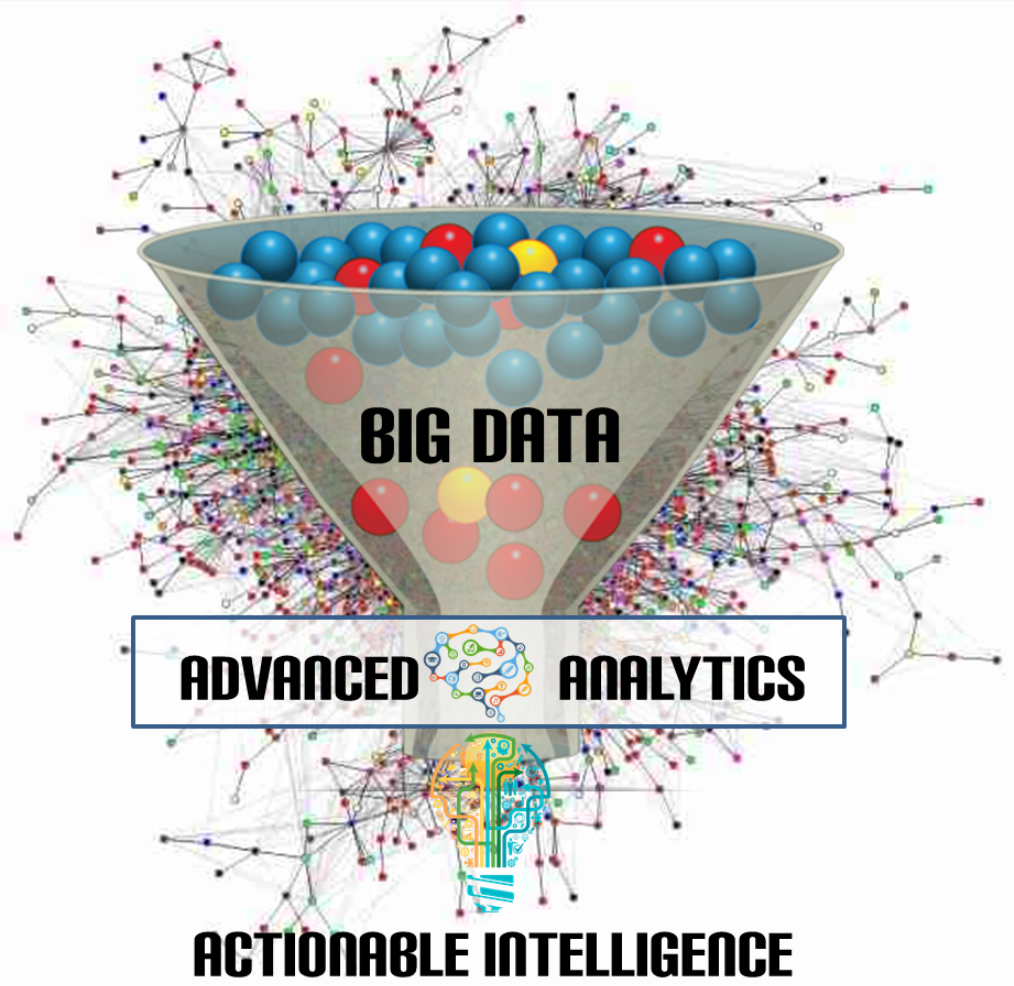


The Gauss distribution exp(-x^2/2) has all finite moments
The Lorentz distribution 1/(1+x^2) has infinite variance
(finite size fixes it, though…)

(AC274 shall cover this in the Active Matter and Data part)

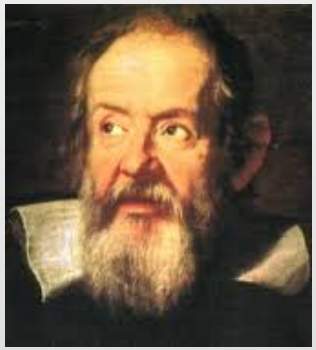
Data Science

Learning from (Big) data



Galileo vs Bacon

Computational physics consists of TWO basic stages:



G. Galilei
(1564-1642)

The G-part: MODEL&SIMULATIONS:
to produce data

The B-part DATA ANALYSIS:
to gain knowledge, ask questions,
Perform more simulations, in a self-reinforcing loop.

That's how computers become **TOOLS OF DISCOVERY**

Data Science

The escalation of Data Science

Fitting,

Mining,

Searching,

Clustering,

Training,

Learning,

Deep Learning

...

DS gets increasingly ambitious, from data fitting to AI

Francis Bacon (1561-1626)

Deduce trends and even physical laws from (big) data.

With big enough data, "any" law can be reconstructed

No need of "understanding" (Super-Bacon)

Extracting Trends: Data fitting

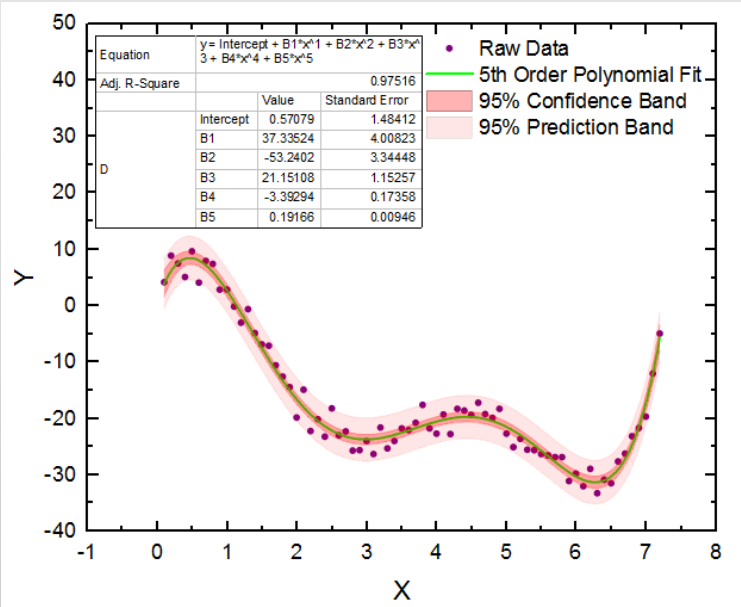
Given a set of input and output data {x_i, y_i}

$$D \equiv \{x_i, y_i\}, \quad i = 1, N$$

Choose a parameter-dependent model (trial) function

$$y^T = f(x; p) \quad p = p_0, p_1, \ldots p_M; \quad M << N$$

Such as to minimize the "distance-error" between y and y_trial

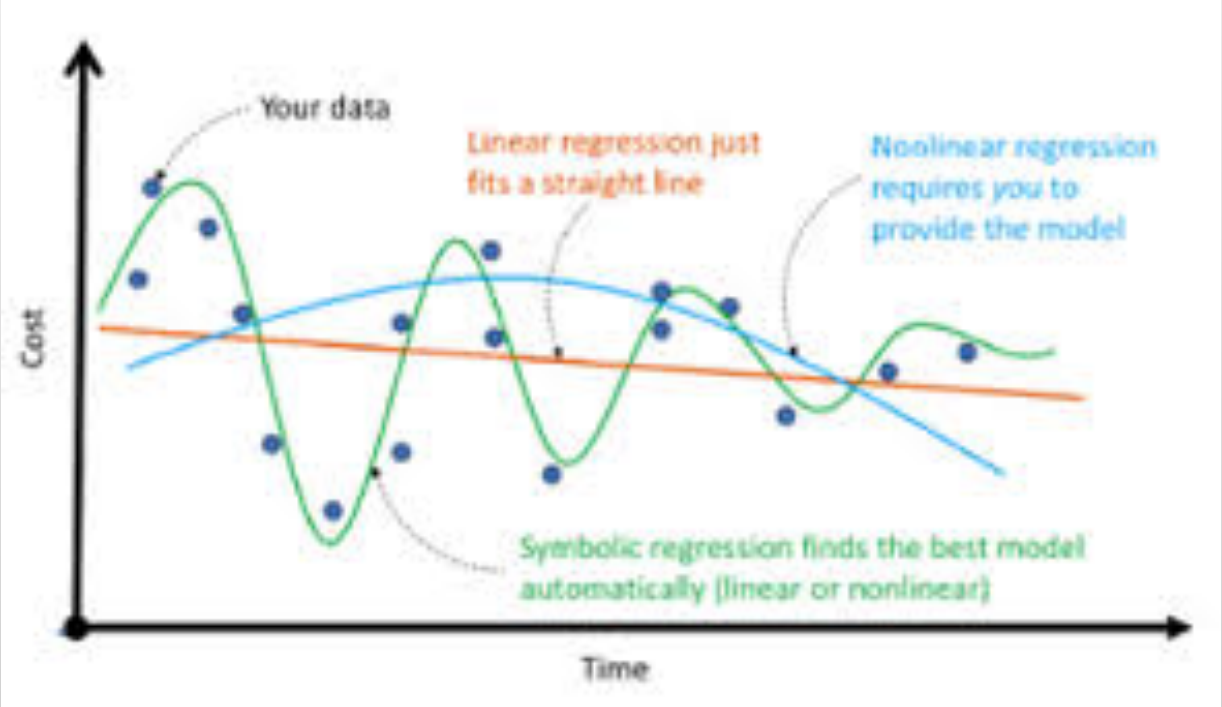


$$Min_{\{p\}}[\varepsilon(p)] \equiv dis\{y_i, y_i^T; p\}$$

A set of M<<N
Linear or non-linear equations
for the parameters p0, p1 pM.
Simplest: linear regression
y=a*x+b (M=2)

From Numerical to Symbolic regression

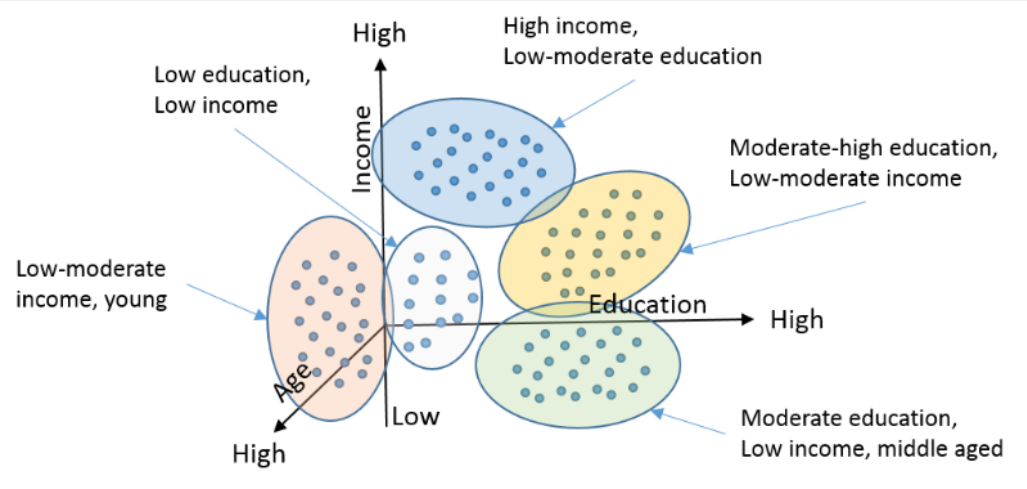
Numerical regression: best (linear or nonlinear fit)
Symbolic regression: finds the best model by searching symbolic space of equations (algebraic, ODE's, PDE's …).
Goes more and more into AI territory.



DS for Decision-making

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

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



Decision:

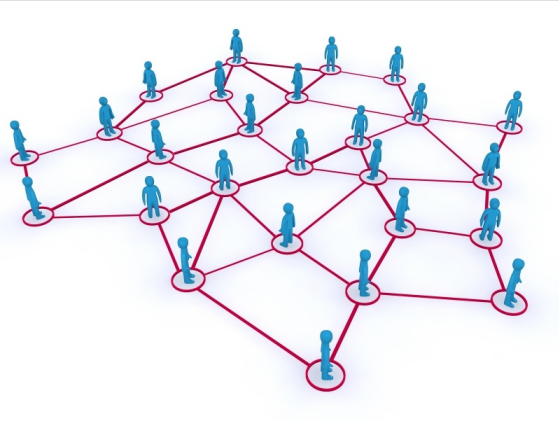
Fix a bar and filter 0,1 = NO/YES

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

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

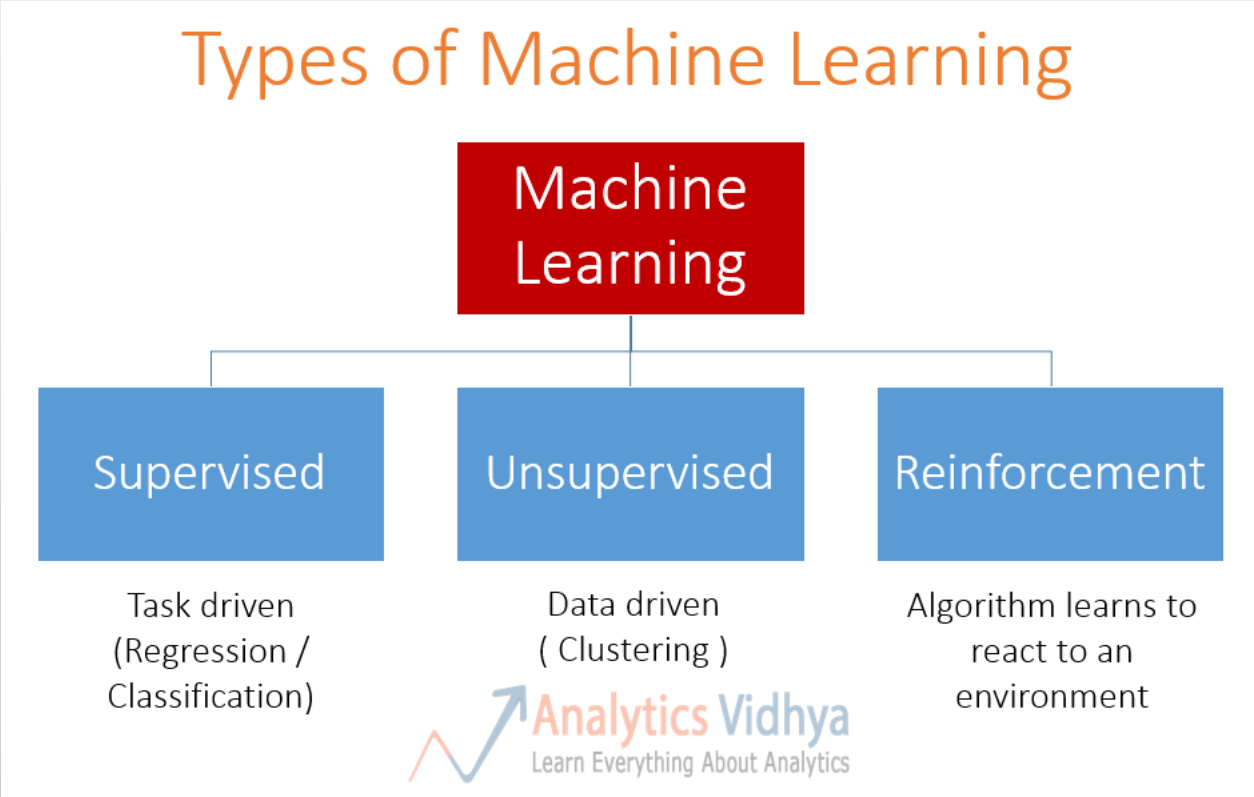


… Steer and manipulate?

Machine Learning

Learning: Train on data sample; extract the rule; predict out-of-sample data

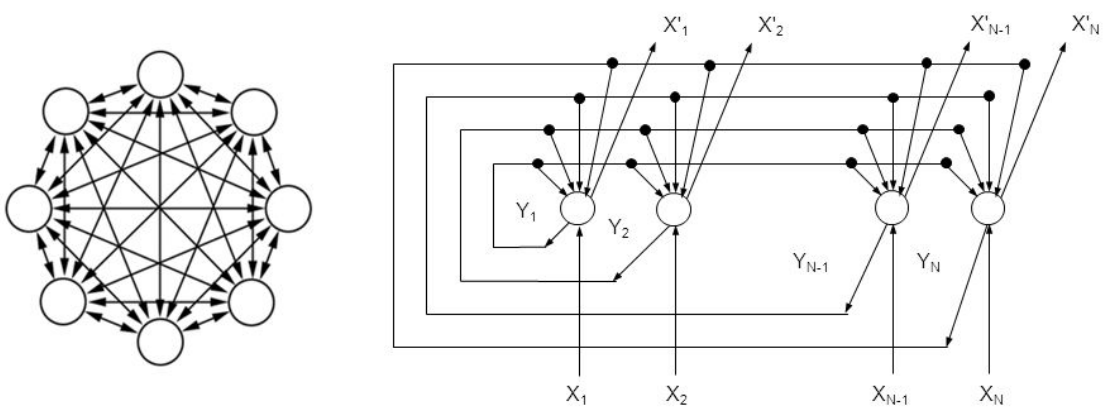
Supervised: receives the trial solution as an input
Unsupervised: no input, finds out by itself
Reinforced: no input, learns and improves the search strategy



The Hopfield neural network

Neuron=single bit {0,1}, fires above threshold: $V_i = sign(\sum_{j=1}^{N} W_{ij} V_j - V^*)$

Model of Hopfield



Features of structure:

- Every neuron is connected with all others
- Connections are symmetric, i.e. for all *i* and *j* $w_{ij} - w_{ji}$
- Every neuron may be Input and output neuron
- Presentation of input is set of state of input neurons

IDEA:

"Brain"= configuration of N "digital neurons".

Brain functions = special patterns minimizing the energy function E=H{V}. Realizes a content-addressable memory.

LEARNING:

Change the Wij so that the Network achieves local minima on the presented examples

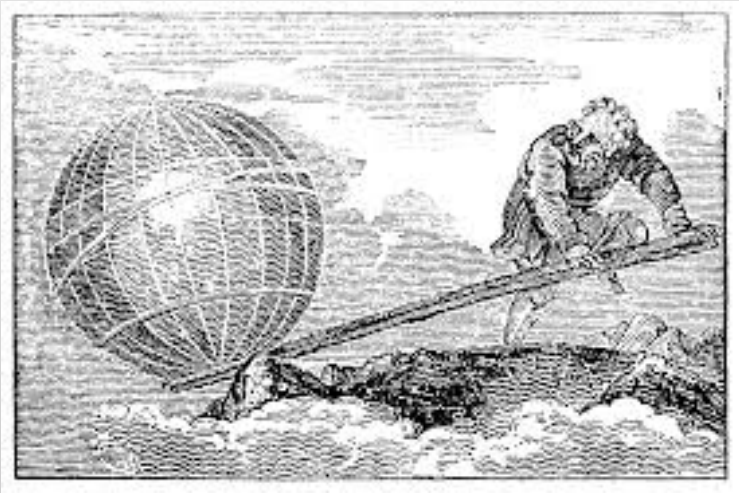
Why is Big data so sexy?

1. Reading off trends from Big Datasets can be MUCH faster than simulating them

2. It applies to all disciplines, including those allegedly not math-friendly ones (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 Chomosky vs Norvig, Strogatz…

The end of Insight?

Super-Bacon defeating Galileo, or maybe Popper…

Predict/Control/Manipulate without theoretical underpinning/understanding?

But… how big is big enough?

A theory/model predicts NEW facts by INTRA-polation;
Big-Data success depends on EXTRA-polation (out_of_sample).
Highly complex and/or singular behavior does not converge in the limit N to infinity for any reasonable N, **in fact ML can be much slower/less accurate than modeling!**

Can ML derive Einstein Equations or Turbulence Models?
NO: Till then, down-toning and cooperation is healthier (examples of ML-assisted simulations in AC274…).

ML-assisted simulation

PRL **114,** 108001 (2015) PHYSICAL REVIEW LETTERS week ending 13 MARCH 2015

Identifying Structural Flow Defects in Disordered Solids Using Machine-Learning Methods

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(Received 25 September 2014; published 9 March 2015)

We use machine-learning methods on local structure to identify flow defects—or particles susceptible to rearrangement—in jammed and glassy systems. We apply this method successfully to two very different systems: a two-dimensional experimental realization of a granular pillar under compression and a Lennard-Jones glass in both two and three dimensions above and below its glass transition temperature. We also identify characteristics of flow defects that differentiate them from the rest of the sample. Our results show it is possible to discern subtle structural features responsible for heterogeneous dynamics observed across a broad range of disordered materials.

DOI: 10.1103/PhysRevLett.114.108001 PACS numbers: 45.70.-n, 61.43.-j, 62.20.F-, 83.50.-v

(See AC274 lectures by Prof. E. Kaxiras)

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 **active matter and social systems** which require more general mathematical structures (*particles, probabilities*, thinking molecules…). New synergies between modeling and data learning
Are key to future applications involving complex systems in science and society

AC274 will convey a flavor of all this:

ENJOY!

End of the lecture