

The online experience so far...

Expectations!!!

**What students have
actually felt!**

How to attend Online Class :

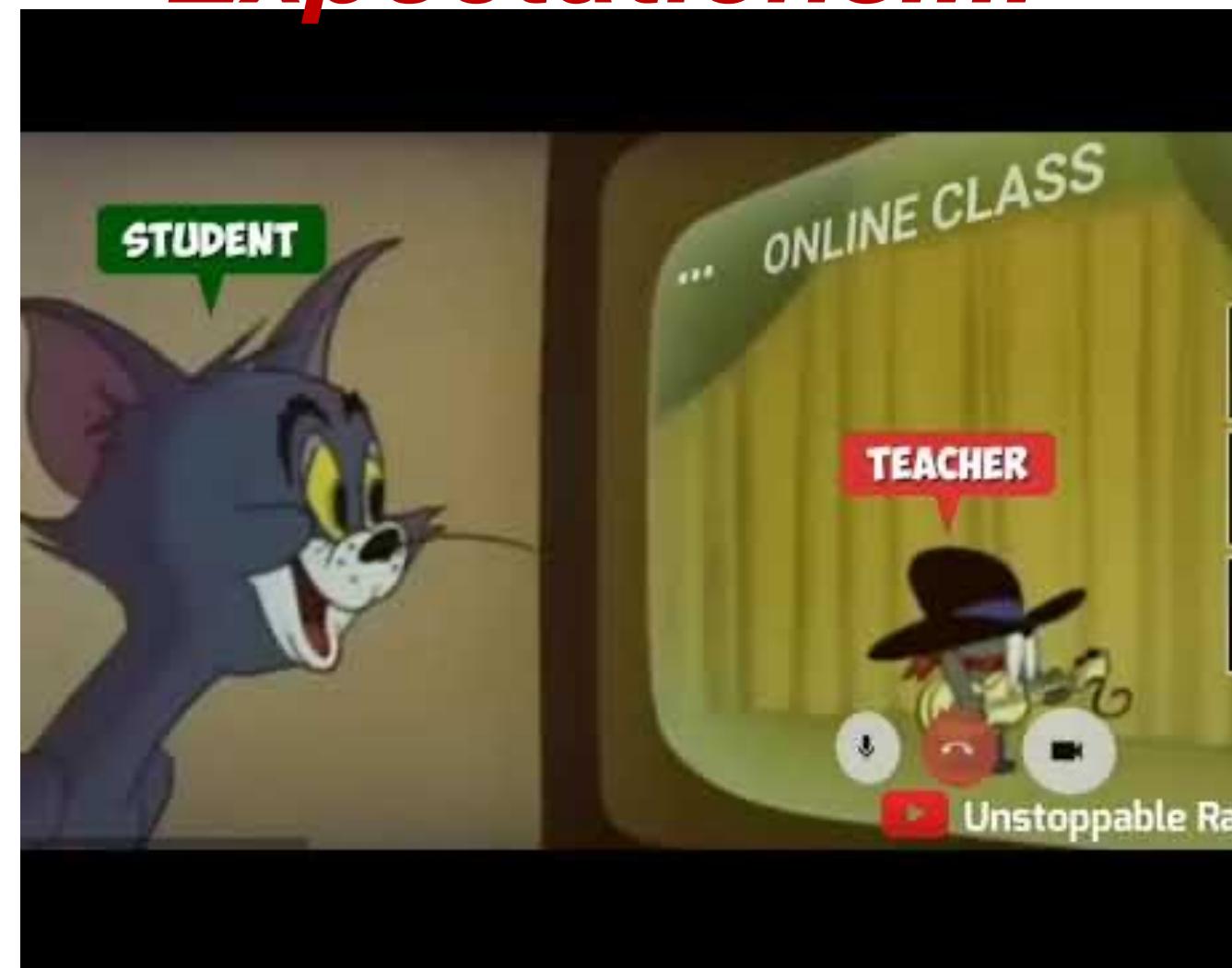
Step 1 :

Step 2 :

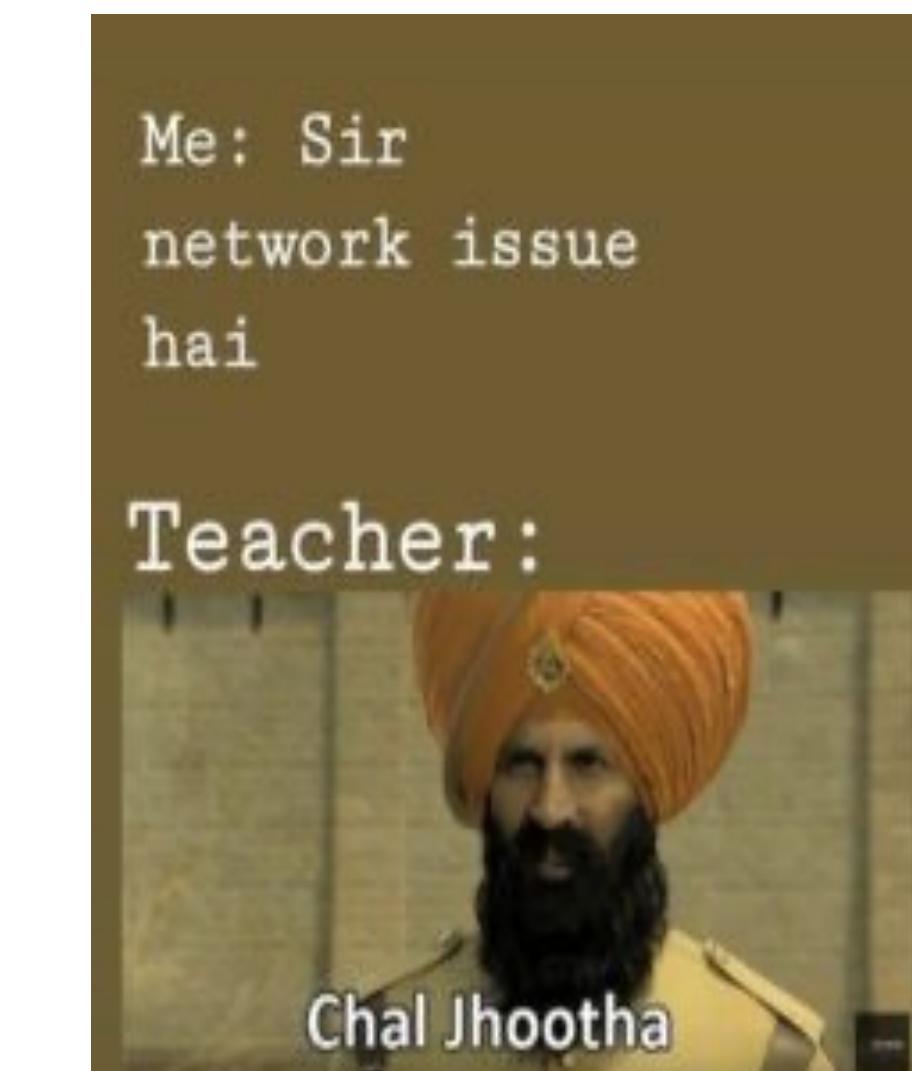
Step 3 :



Me during online classes



When the teacher asks us a question
online and no one knows the answer
Me :



Me: Sir
network issue
hai

Teacher:

Chal Jhootha

**What Teachers have
actually felt!**

"HOW WAS ONLINE TEACHING?"



Teacher In Offline Class



Teacher In Online Class



What COVID era has taught us?



We got connected to
ourselves



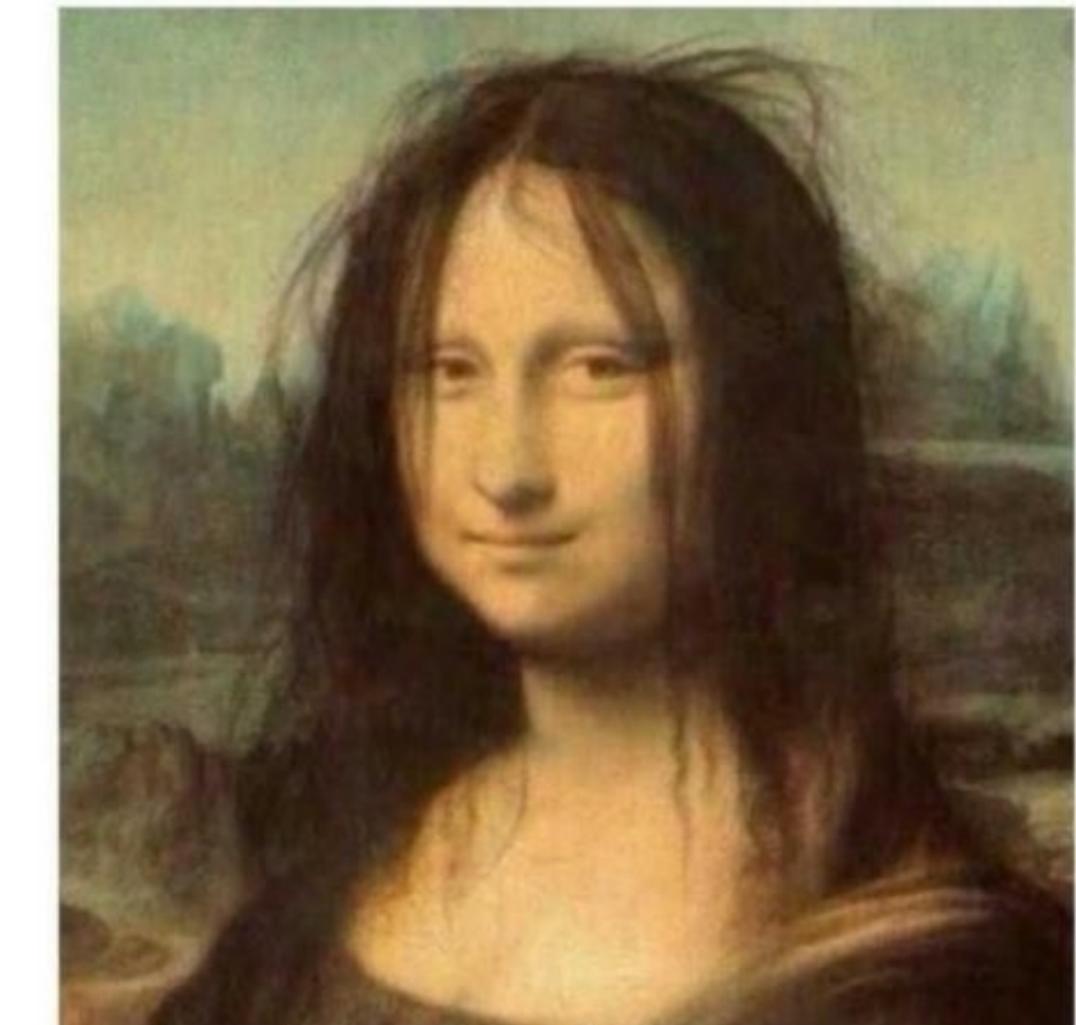
We found out our hidden talents and hobbies



We got closer to our families

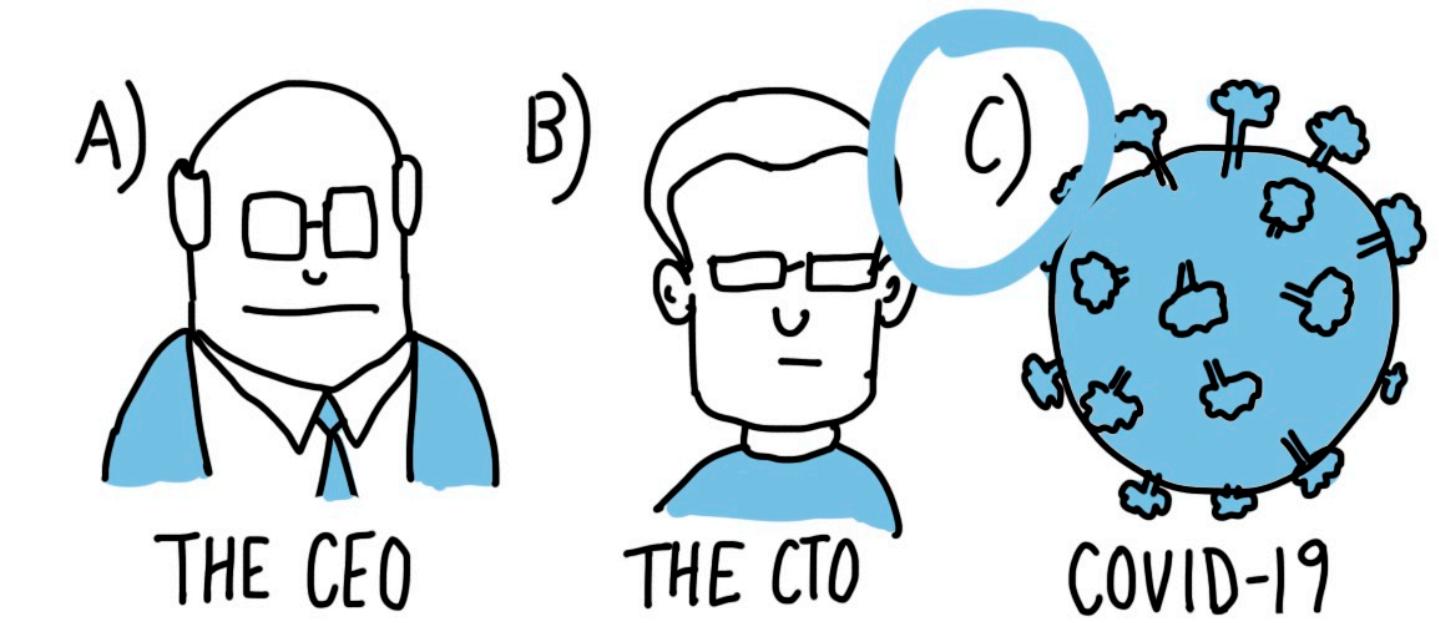
Travel agents: "Yeah, we're good!" 😂

Thanks for your patience during this trying time!



We got more patient

WHO LED THE DIGITAL TRANSFORMATION
OF YOUR COMPANY ?



We got more DIGITAL

Welcome to the Offline lectures!

Lecture 33

Computational modeling of materials- An introduction

Textbooks:

- Computational Materials Science: J. Gunn Lee
- Understanding Molecular Simulations: D. Frenkel and B. Smit
- Molecular Modelling Principles and Applications: Andrew Leach

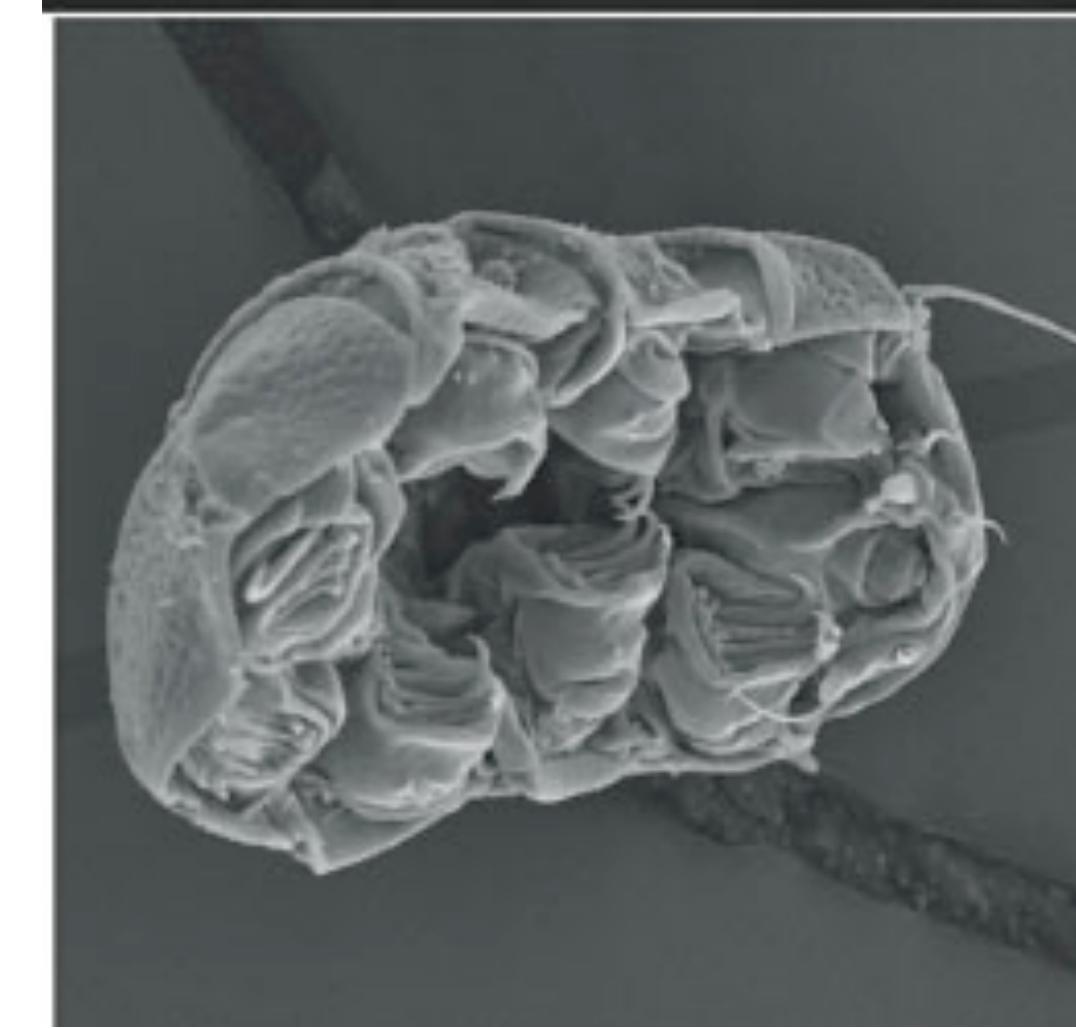
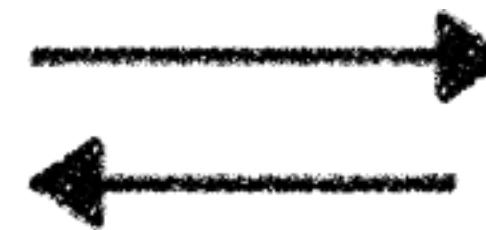
Prof. Divya Nayar
Department of Materials Science and Engineering
divyanayar@mse.iitd.ac.in

What we will cover in three lectures?

- Introduction to computational materials science
- Molecular modeling: the basics
- Multiscale modeling
- Molecular simulations methods: molecular dynamics
- Examples of simulations of materials

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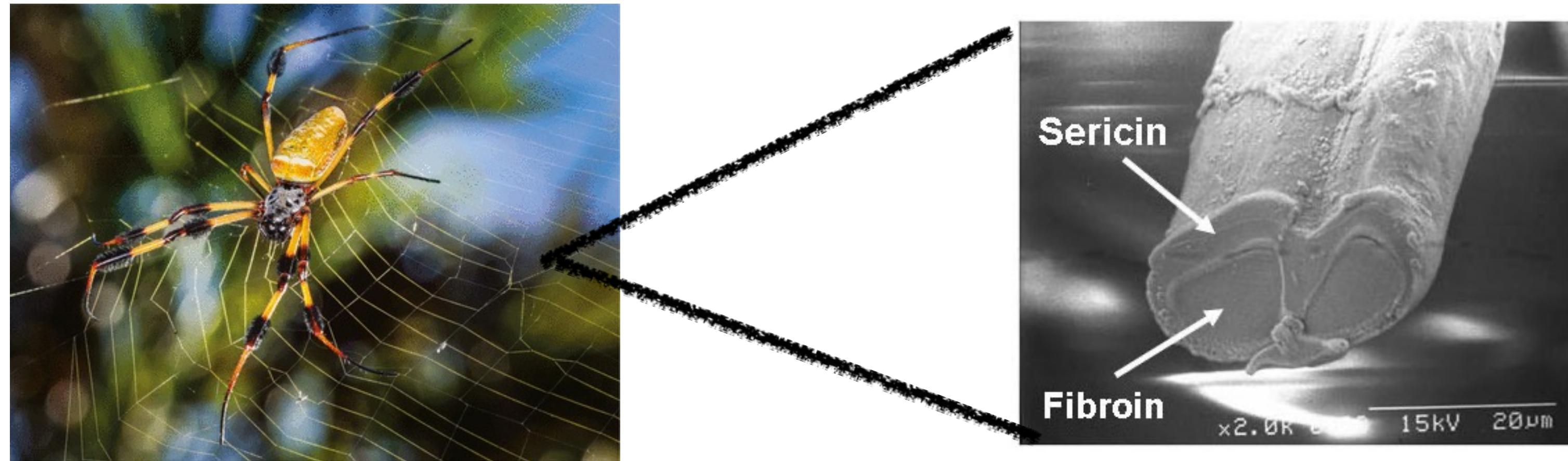
Tardigrade: Water Bear



Microscopic animals that can survive extreme conditions:
high altitudes, deep sea, exposure to radiation including space!

Can survive in dehydrated state for several weeks because of sugar present in cells !

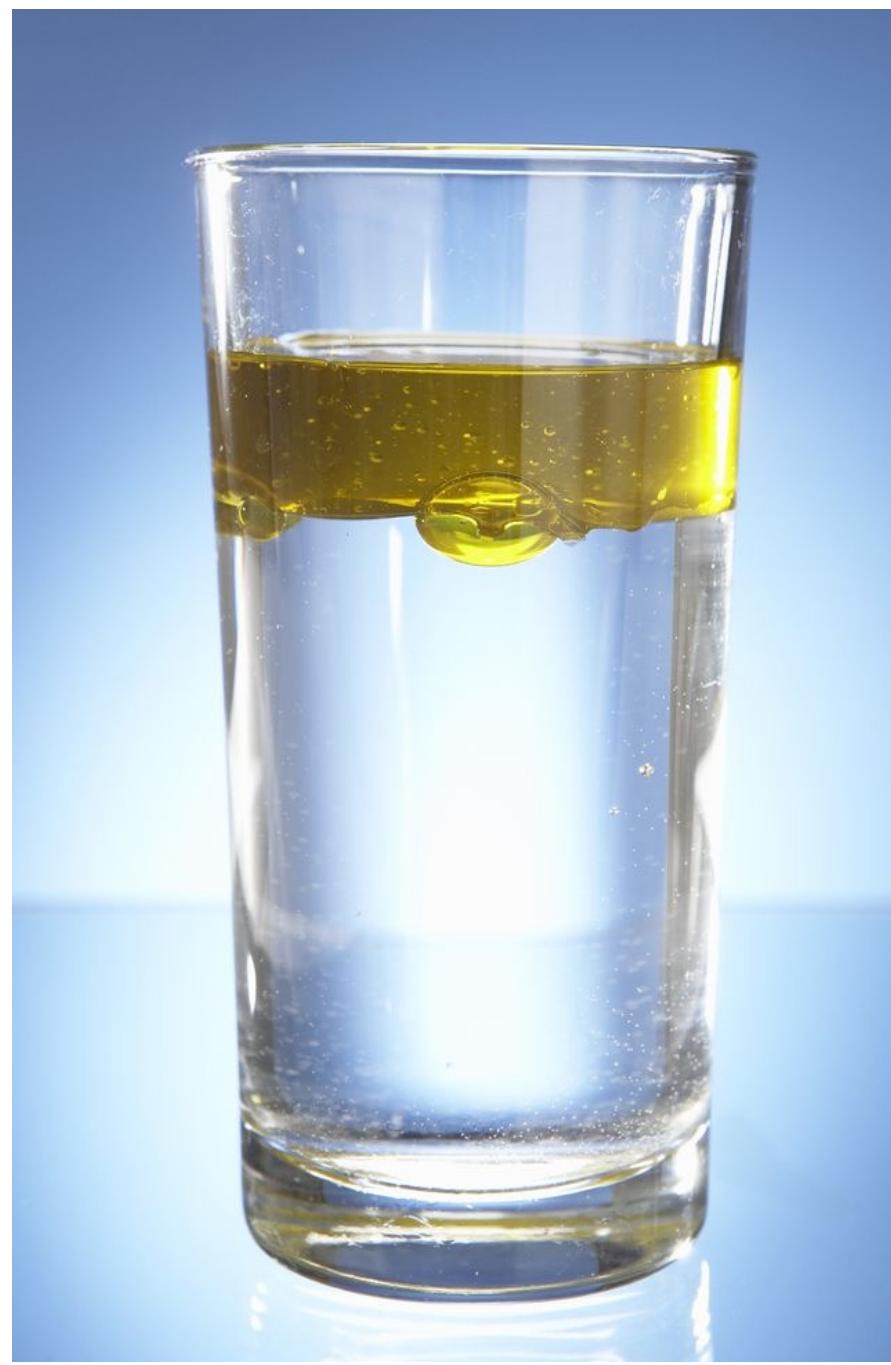
Can we understand how sugar protects this organism?



Spider Silk: tensile strength
5 times more than steel !

Protein called Fibroin
(fibril structure)

Can we design materials with the strength of spider silk ?



Water and oil don't mix!

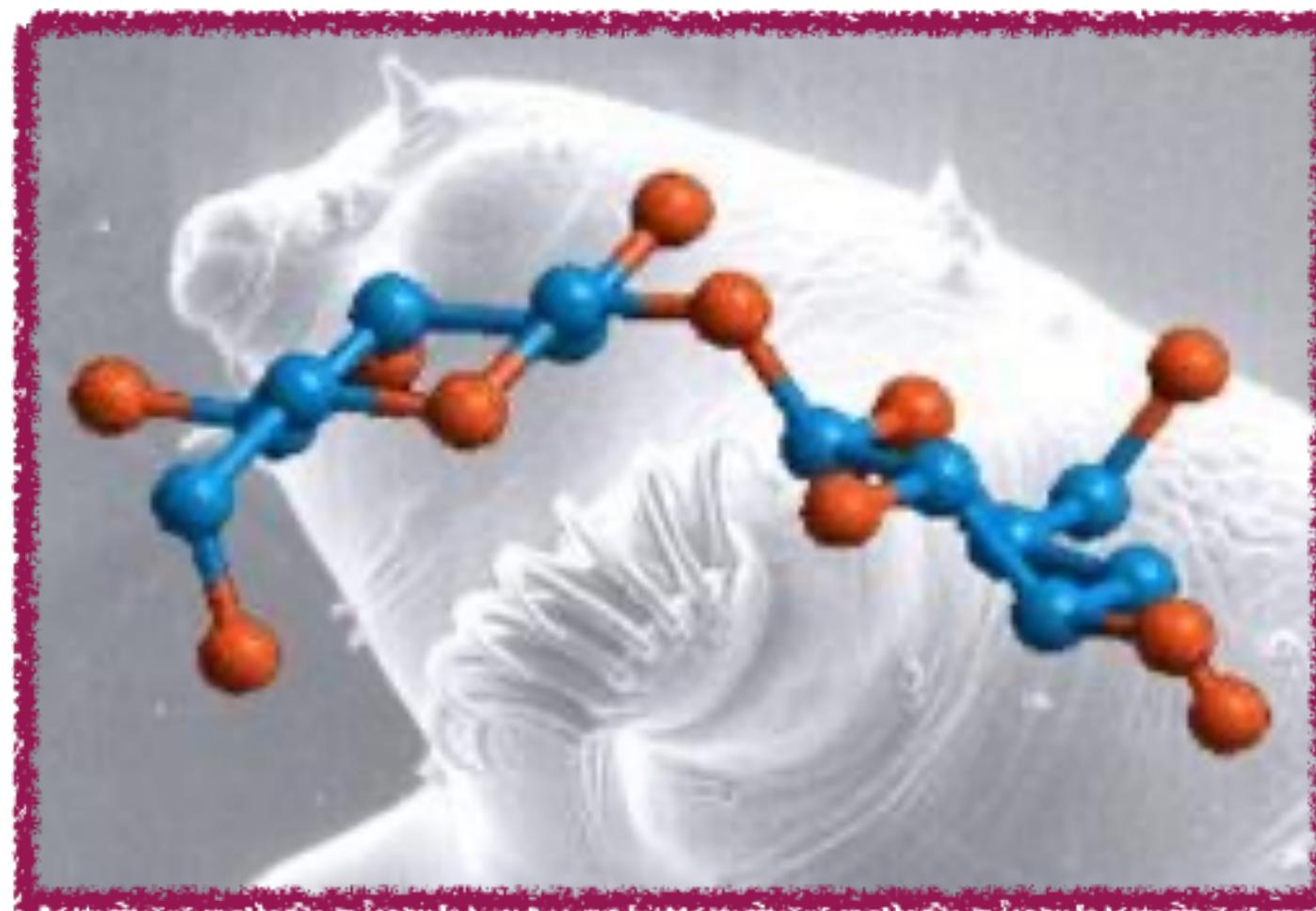


Yet water clogs natural (methane) gas pipelines under sea by forming solid hydrates

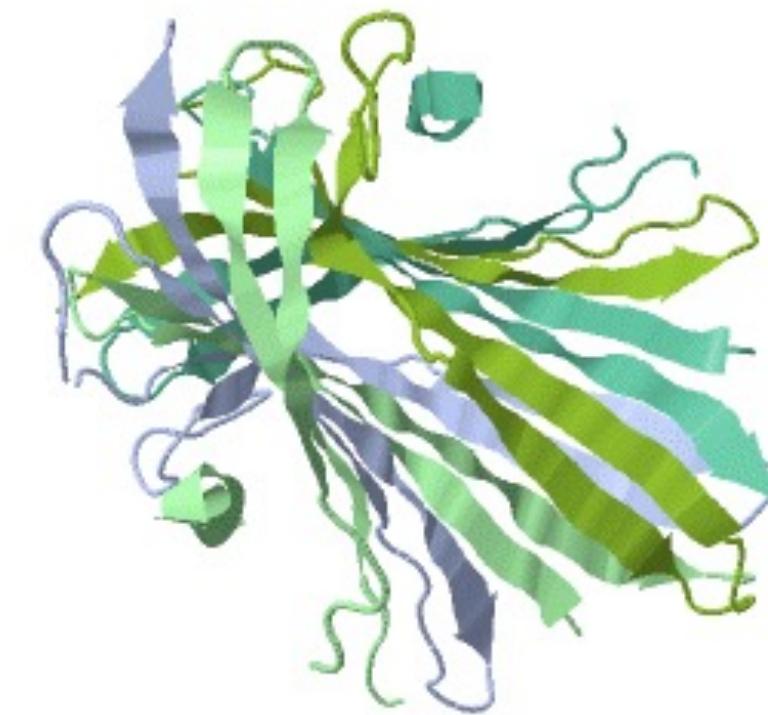
Why water does not mix with oil in one case but forms solid hydrates in natural gas pipelines in the other case?

Computational Experiments!

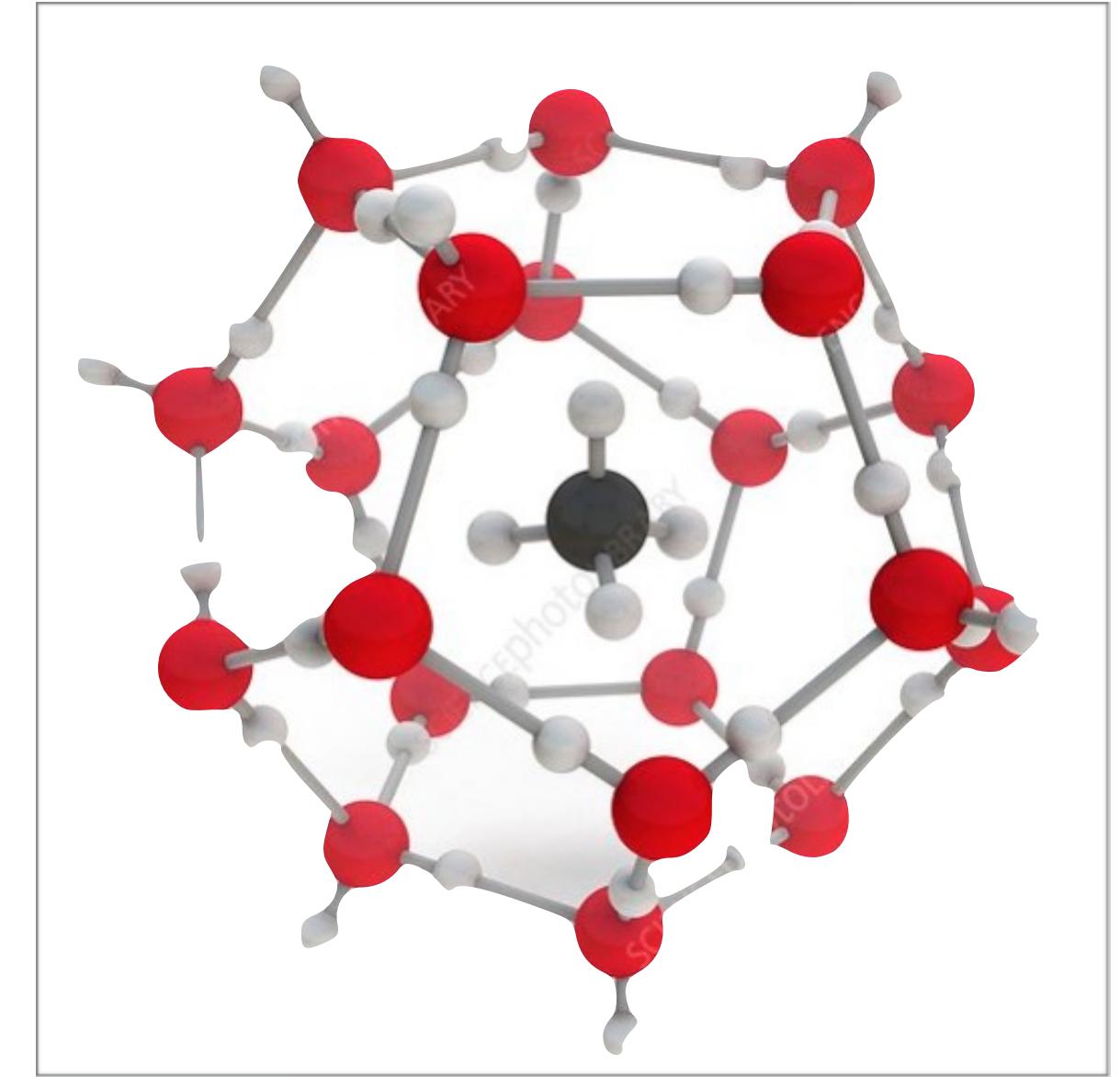
Molecular Modeling



Trehalose sugar



Fibroin protein



Methane gas hydrate

<https://proteopedia.org/wiki/index.php/Fibroins>

<https://www.chemistryworld.com/news/water-trapped-in-a-sugar-crystal/3004284.article>

<https://www.sciencephoto.com/media/568364/view/methane-hydrate-molecule-artwork>

Computational Materials Science

Modeling and Simulations: *Not just an extra tool!*

- Can act as a bridge between theory and experiments
- Can help in validating a theory
- Can help in understanding problems under extreme conditions where experiments are not feasible
- Can provide additional insights into experiments
- Can help in designing and predicting new materials: motivating new experiments

Three pillars of science



The Nobel Prize in Chemistry 2013
Martin Karplus, Michael Levitt, Arieh Warshel

The Nobel Prize in Chemistry 2013



© Harvard University
Martin Karplus

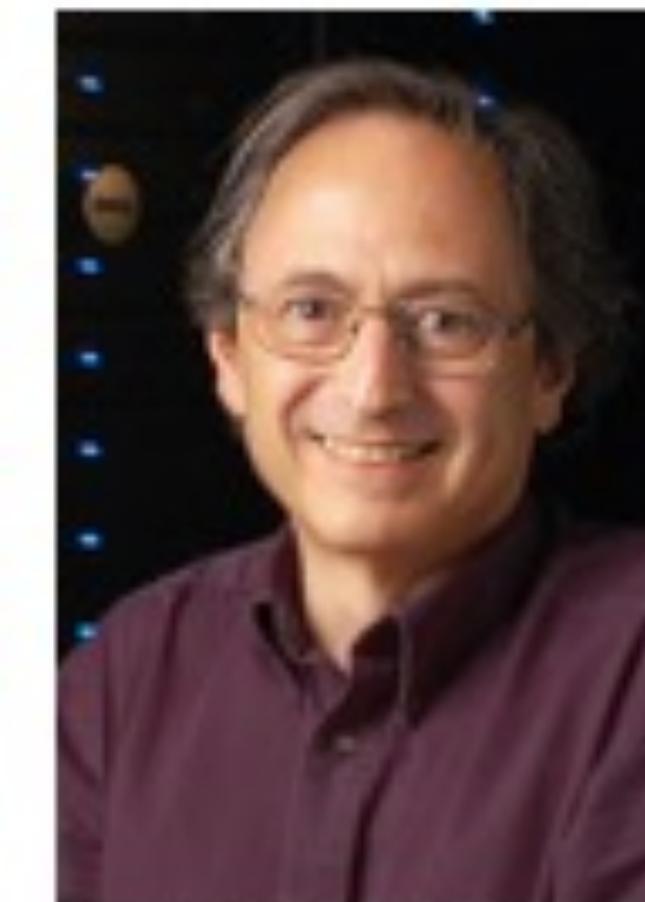


Photo: © S. Fisch
Michael Levitt



Photo: Wikimedia Commons
Arieh Warshel

The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel "for the development of multiscale models for complex chemical systems".

The ingredients

Computer, Programming, Models, Simulation...



Ada Lovelace
(1815-1852)

Ada Lovelace broke gender barriers like never before and went on to discover computer programming 175 years ago, an industry still dominated by men.

ADA LOVELACE FIRST COMPUTER PROGRAMMER

The Analytical Engine

Lovelace's program turned a complex formula into simple calculations that could be encoded on punched cards and fed into Charles Babbage's Analytical Engine, a mechanical computer that he designed but never built. She published it in 1843, a century before the modern computer age.

$$\frac{x}{e^x - 1} = \frac{1}{1 + \frac{x}{2} + \frac{x^2}{2 \cdot 3} + \frac{x^3}{2 \cdot 3 \cdot 4} + \&c.}$$

"I want to put in something about Bernoulli's Number, in one of my Notes, as an example of how an explicit function may be worked out by the engine, without having been worked out by human head and hands first."

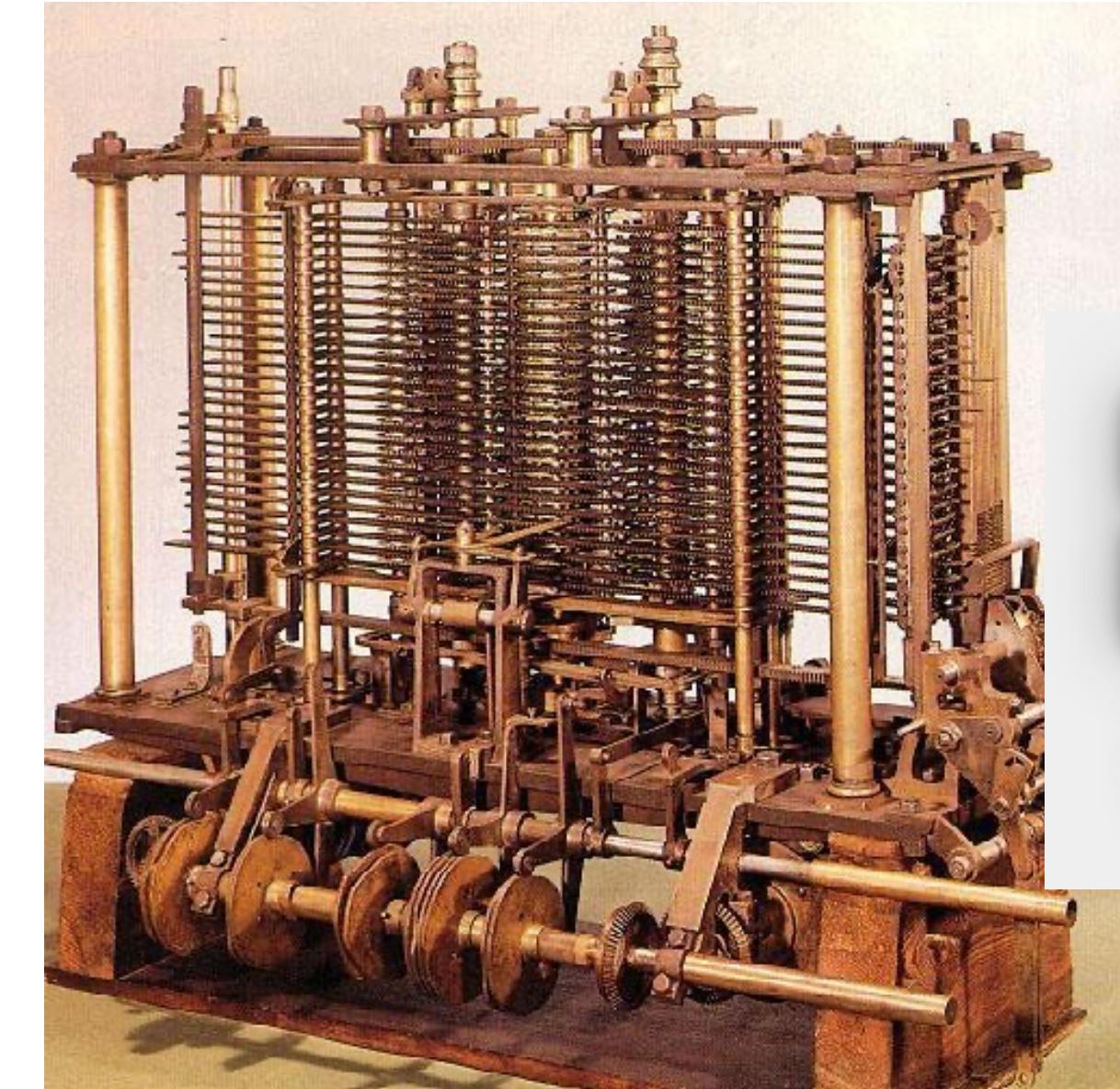
A Universal Computer

Lovelace did more than write the first computer program. She was also the first person to realise that a general purpose computer could do anything, given the right data and instructions.

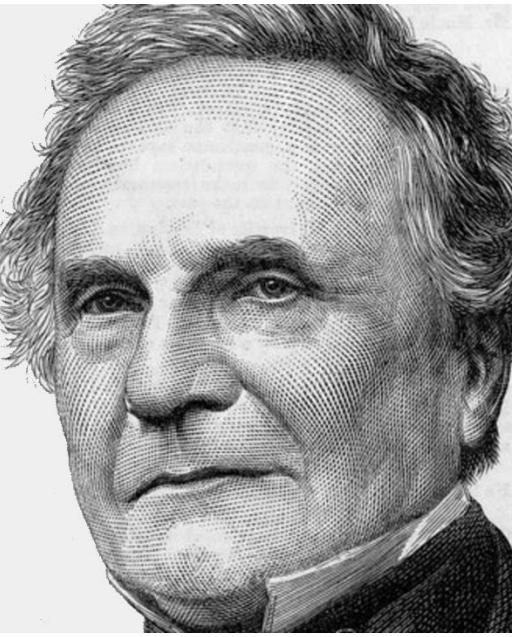
"The Analytical Engine weaves algebraic patterns just as the Jacquard loom weaves flowers and leaves."

Augusta Ada King, Countess of Lovelace
Born: 10 December 1815
Died: 27 November 1852

Ada Lovelace Day
FindingAda.com

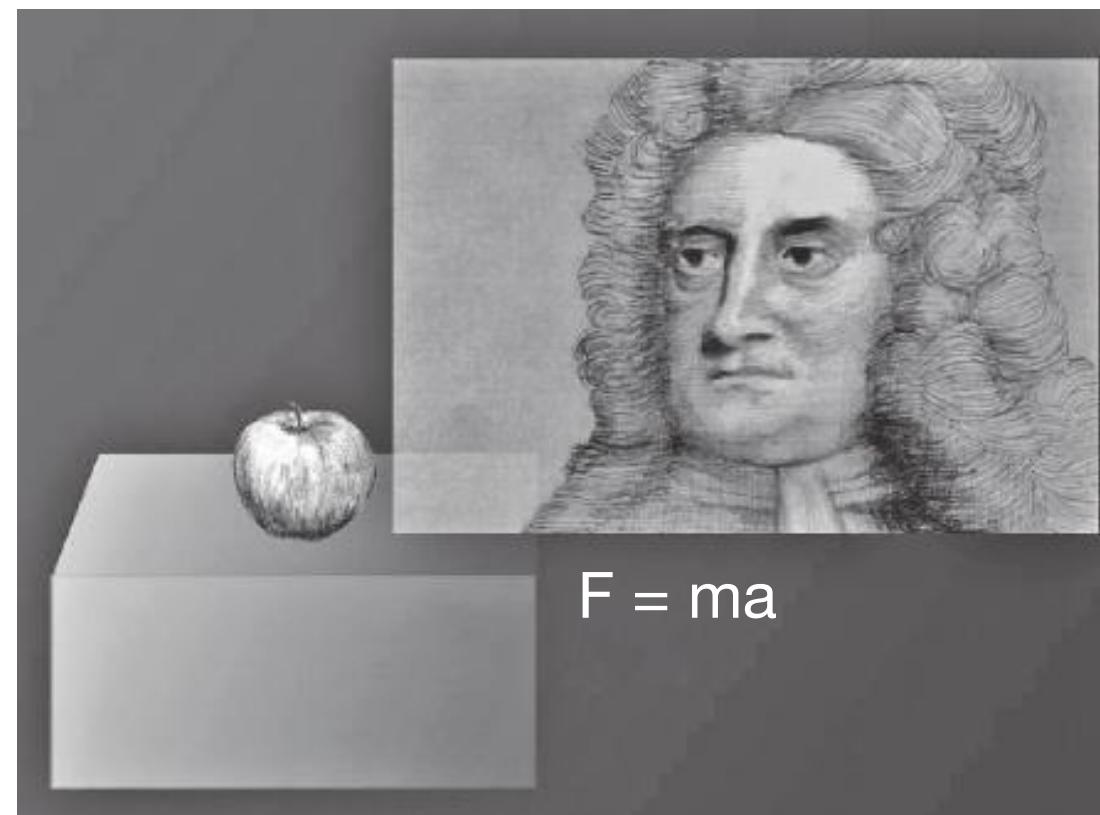


CHARLES
BABBAGE
1791-1871

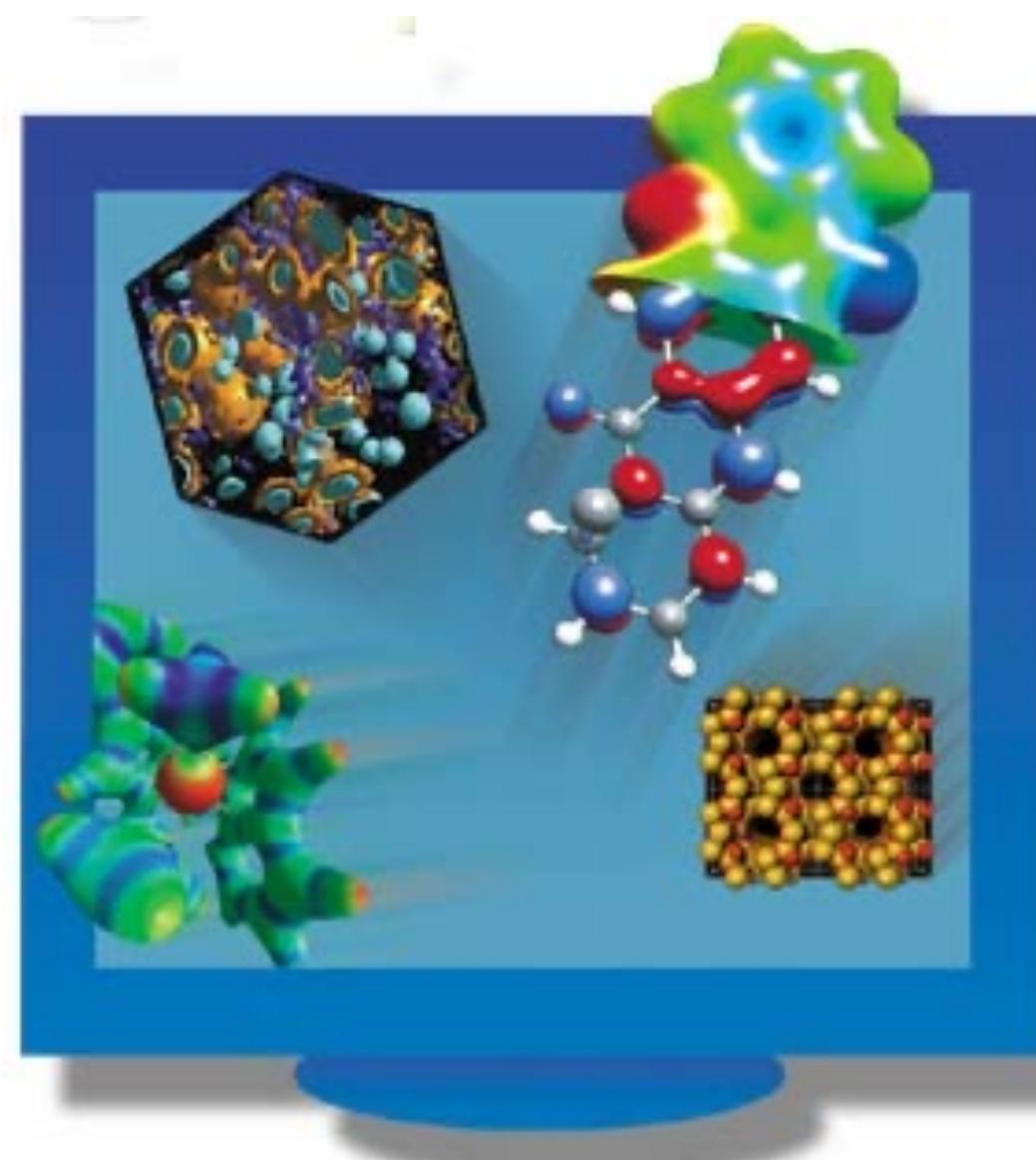


Analytical Engine: First computer

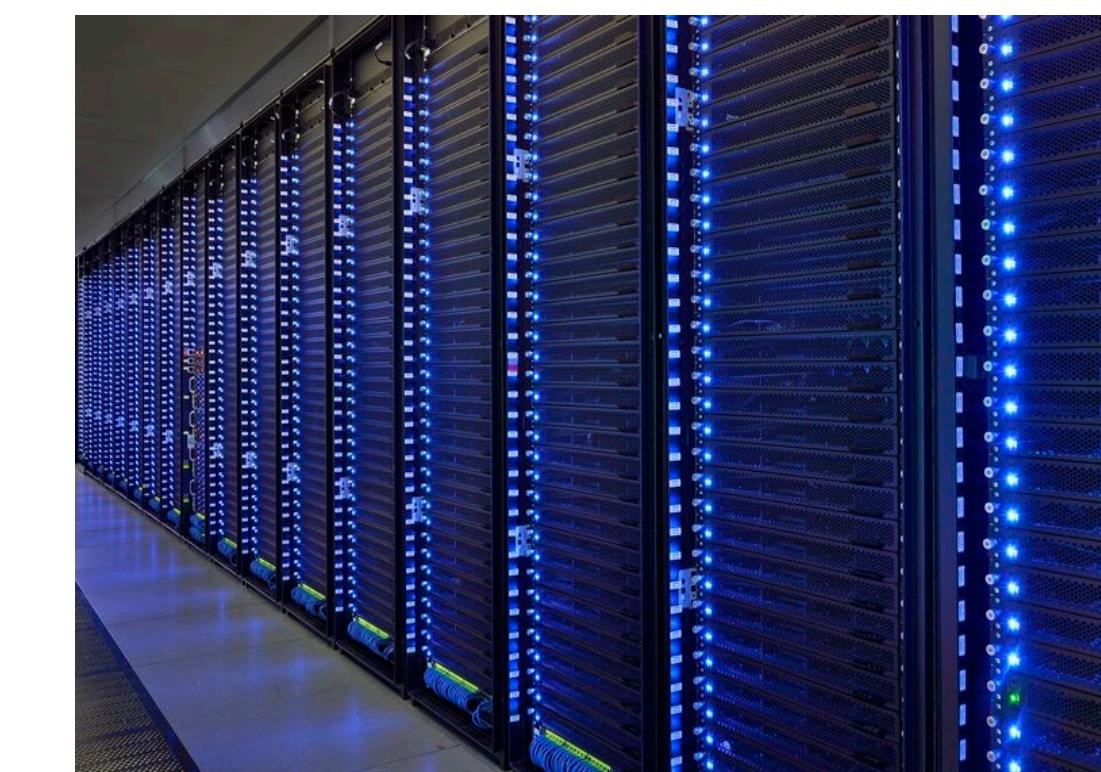
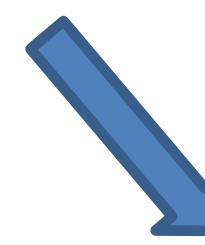
Computational Materials Science



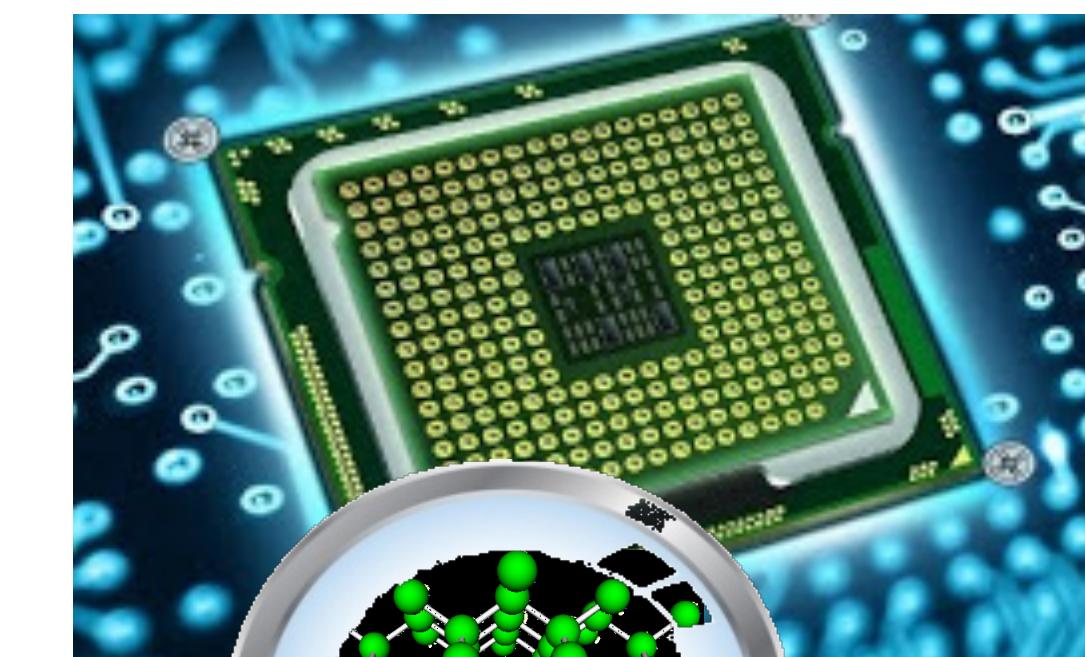
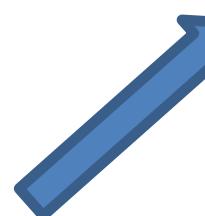
Theory



Modeling and simulations



High Performance Computing

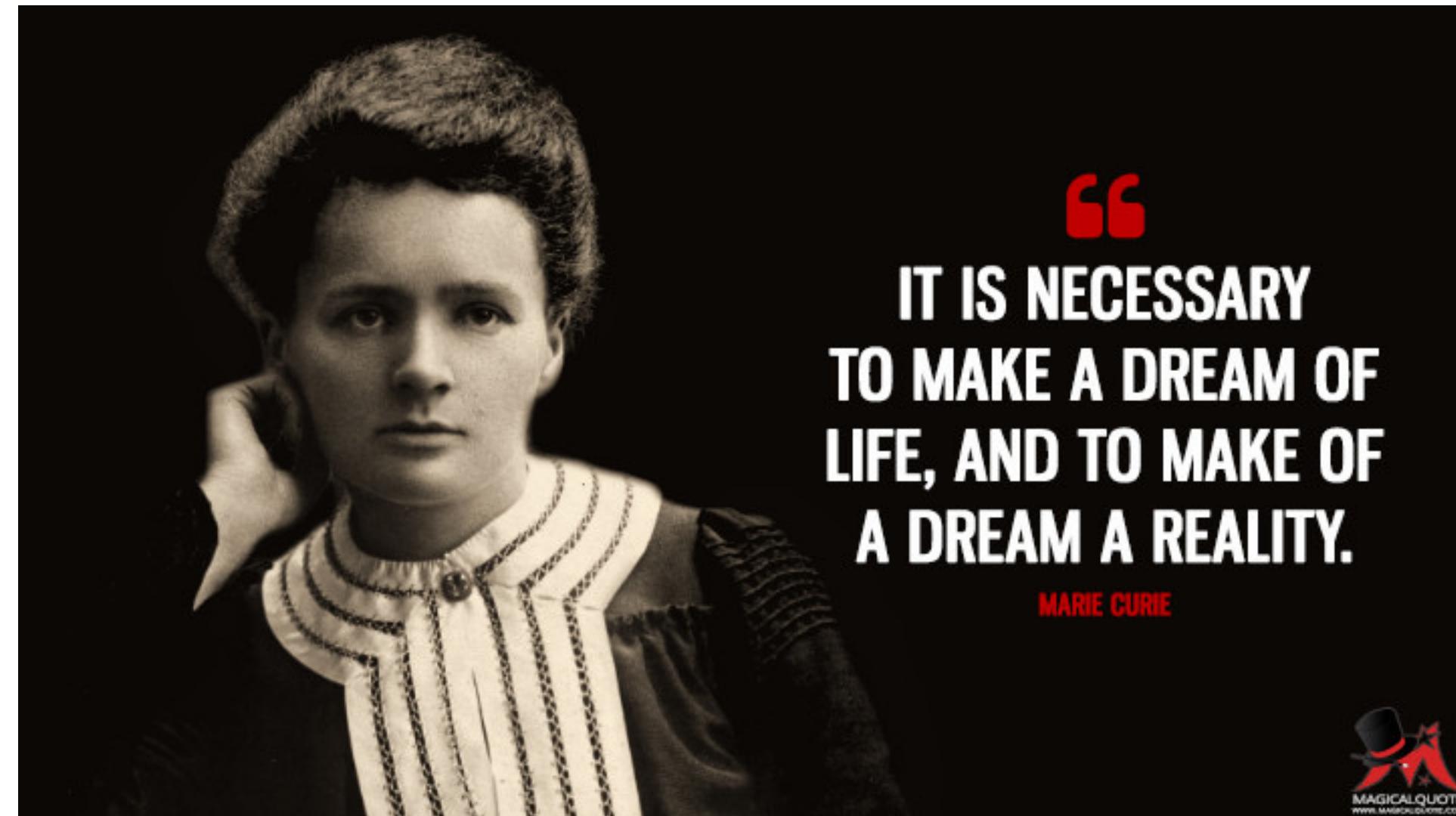


Computational microscope !



Dream

Decipher, Design, Discover... *Develop*



A computational experiment

The Recipe

- Define the problem
- Make a MODEL (that represents the real system properly)
- Select the relevant rules (THEORY)
- Write a code or use a software to do the job
- Run the SIMULATION
- Analyze the data produced

What is *modeling* in computational “experiments”?

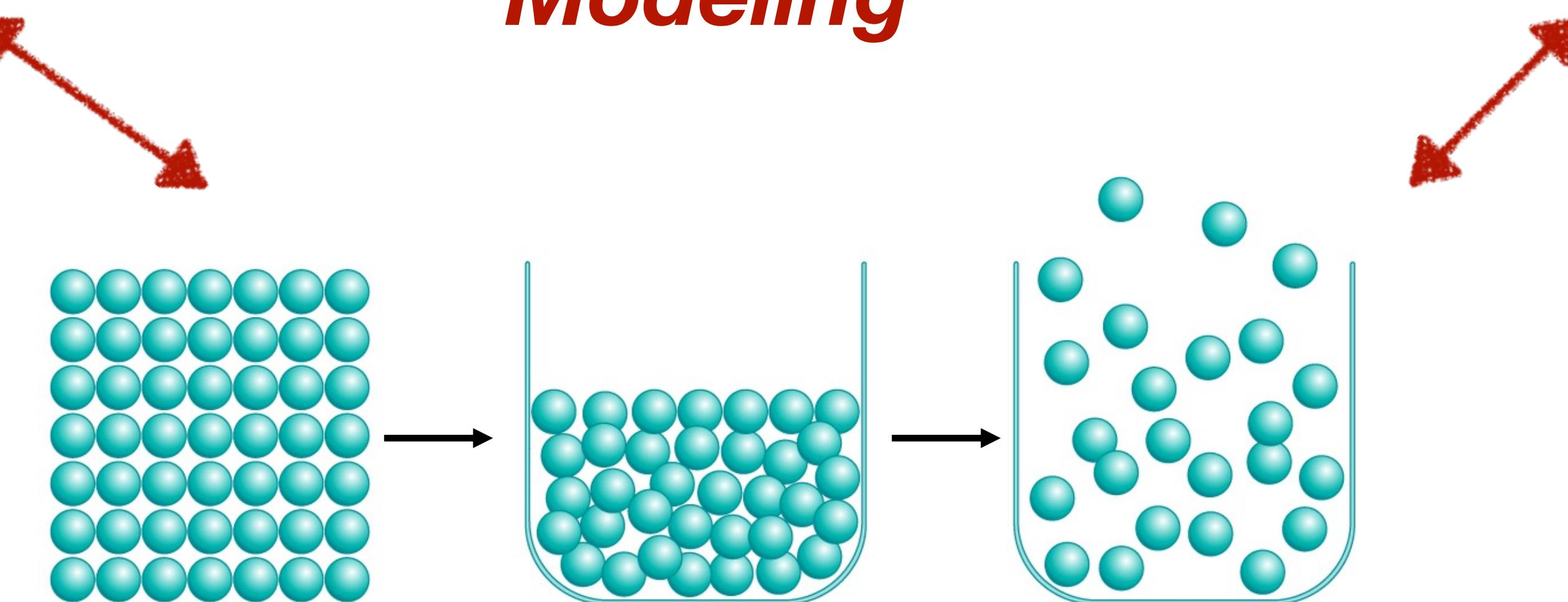
A model describes the *nature* of the system

Even if it may not describe the system completely

Experiment



Modeling



Theory

Latent heat of fusion and
Vaporisation

Create a *model* to study the pollution levels in different areas of Delhi

Whole city

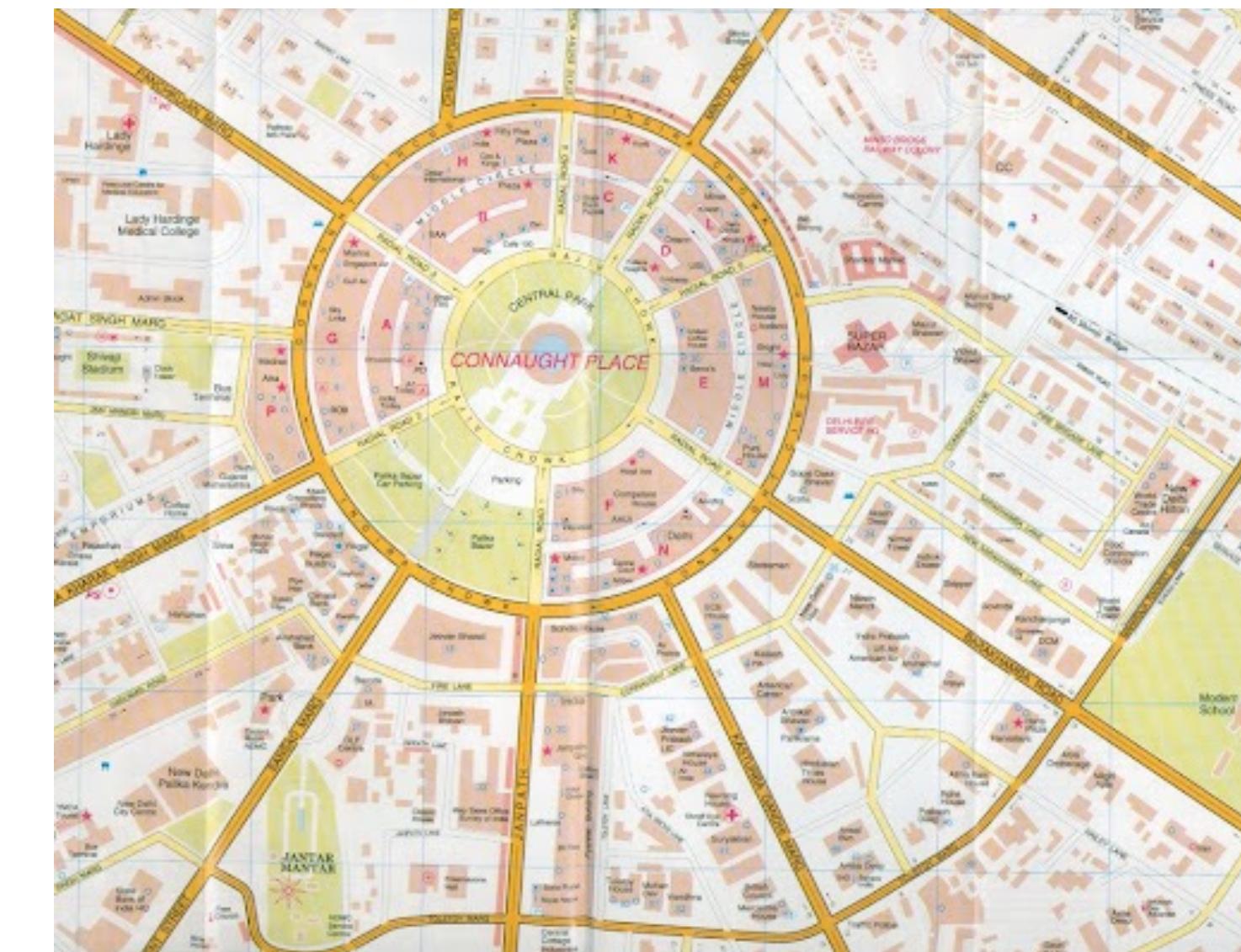


Study the map of the whole city

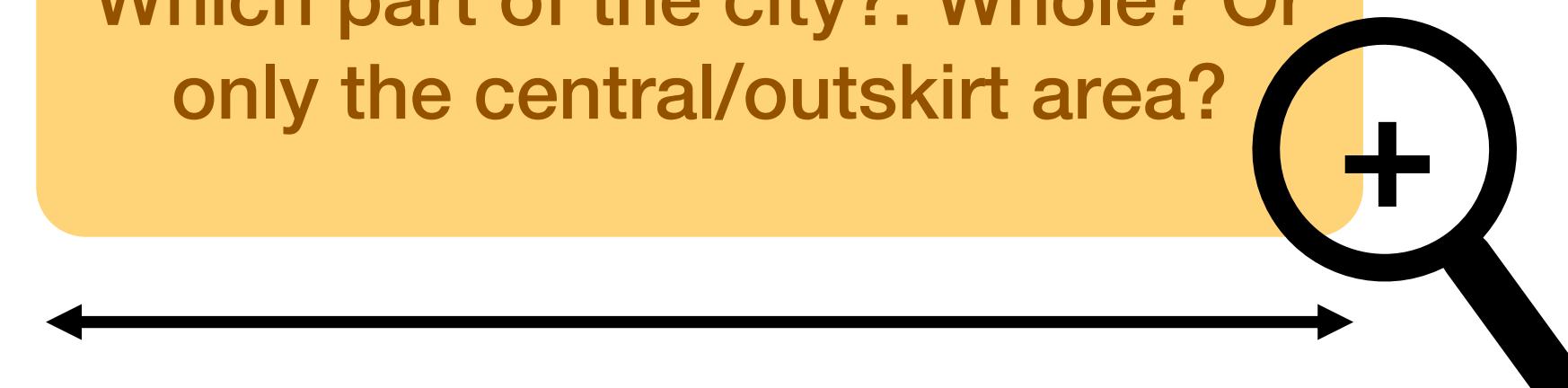


Scale!

A busy area of the city e.g. Connaught Place

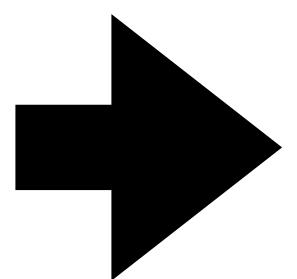


Which part of the city?: Whole? Or only the central/outskirt area?



Pollution levels in the *whole* city

The BIG Picture



The Scale



Create a model of
Delhi

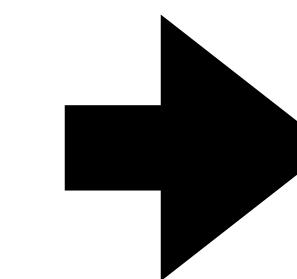
Study the map of the
city

Google images

The Details



Major regions of Delhi:
S, N, E, W



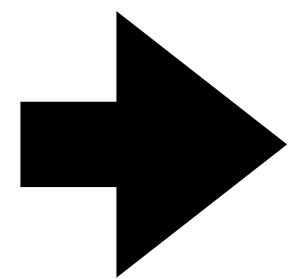
The Connections



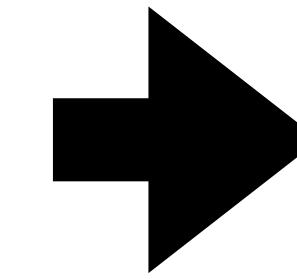
Roads, Metro...

Pollution levels in a part of the city

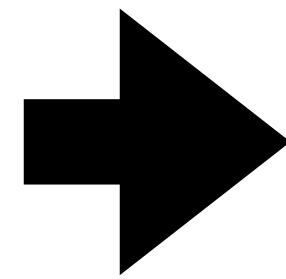
The BIG Picture



The Scale

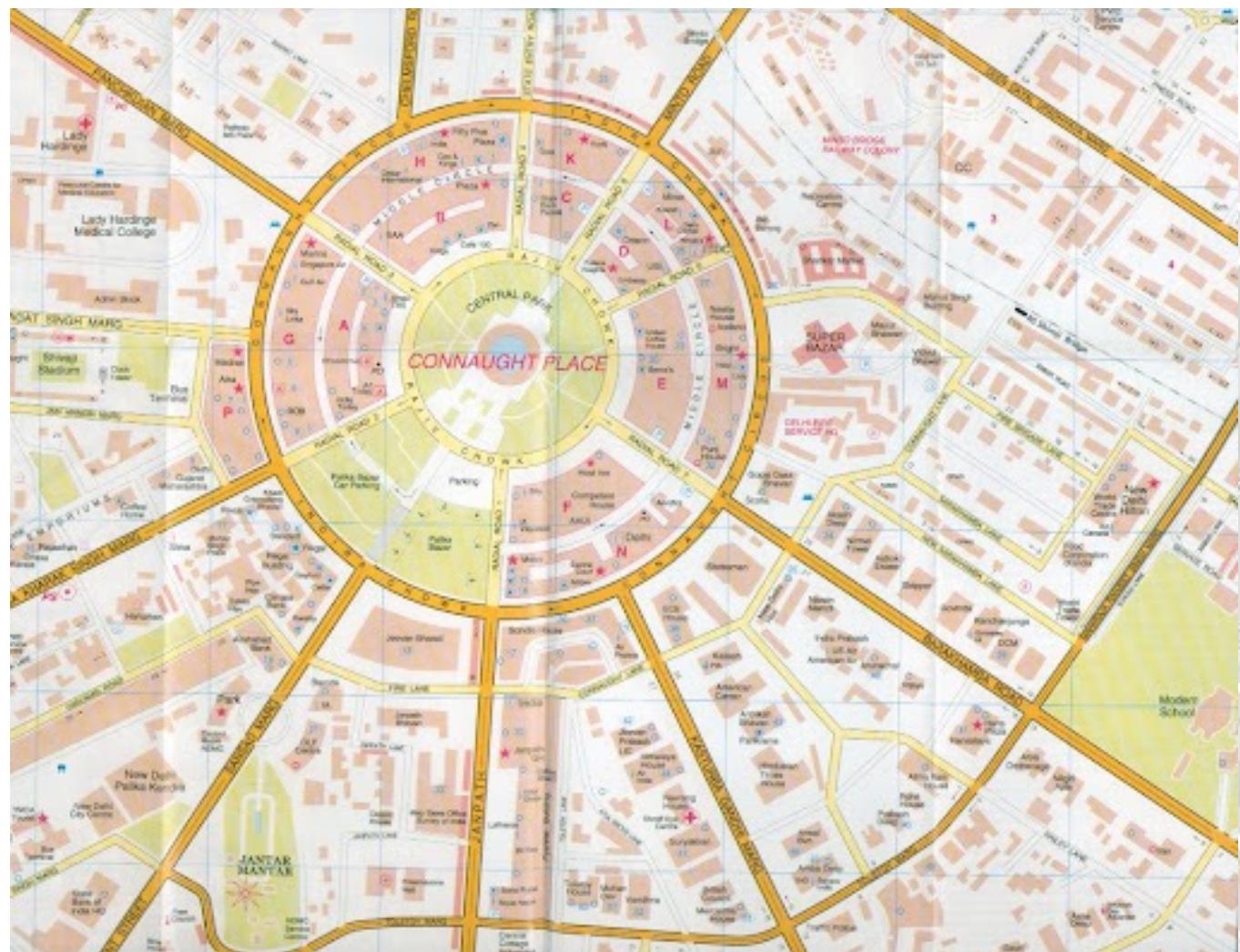


The Details



The Connections

Create a model of a commercial area of Delhi



Which part of the city?: Whole?
Or only the central/outskirt area?

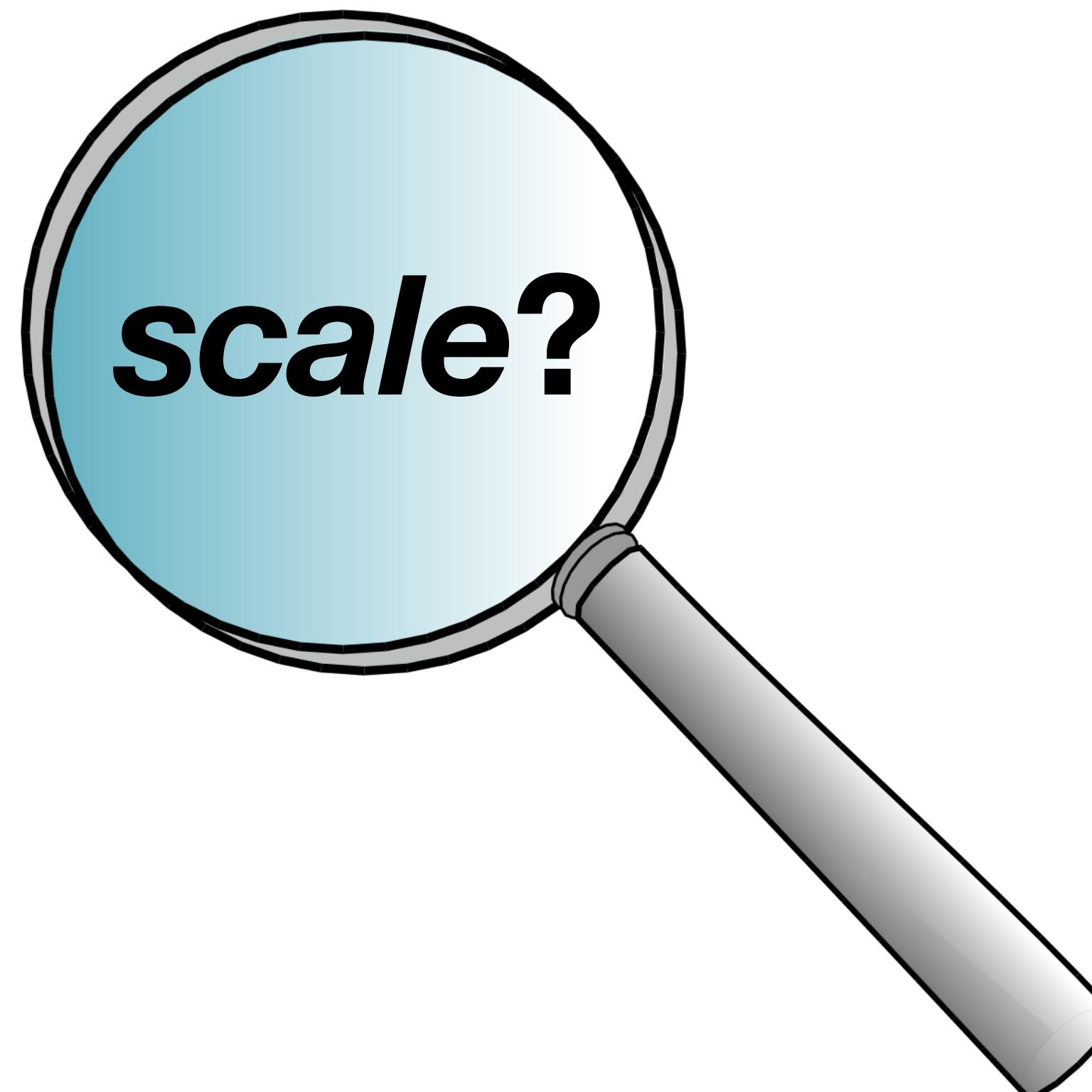


Buildings, blocks, roads, parks, shops, restaurants

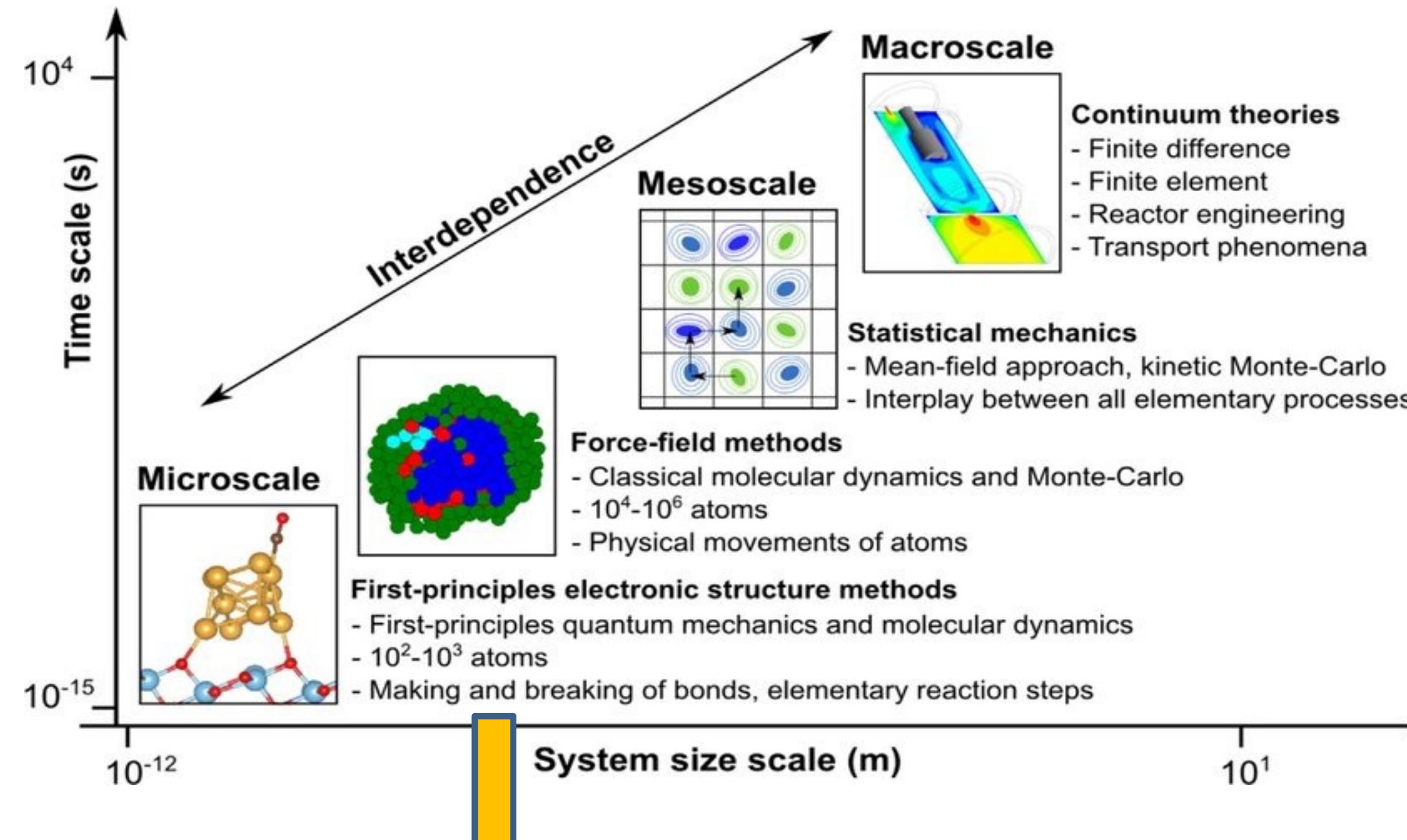


Distance between the buildings, area of parks, length of roads

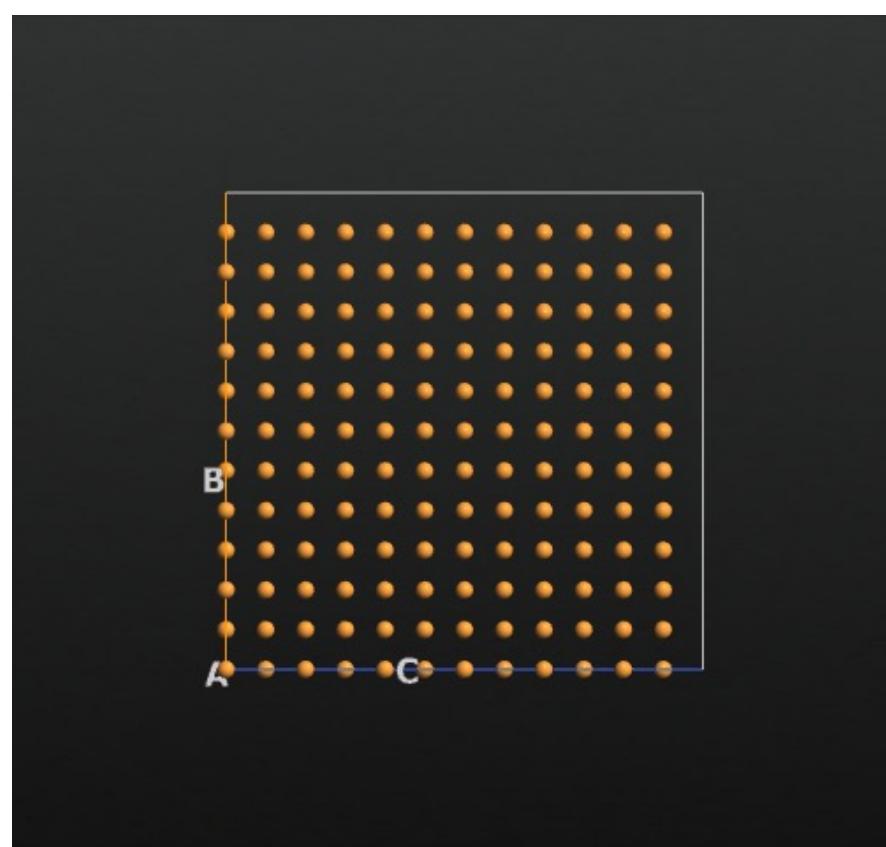
How to determine the magnification



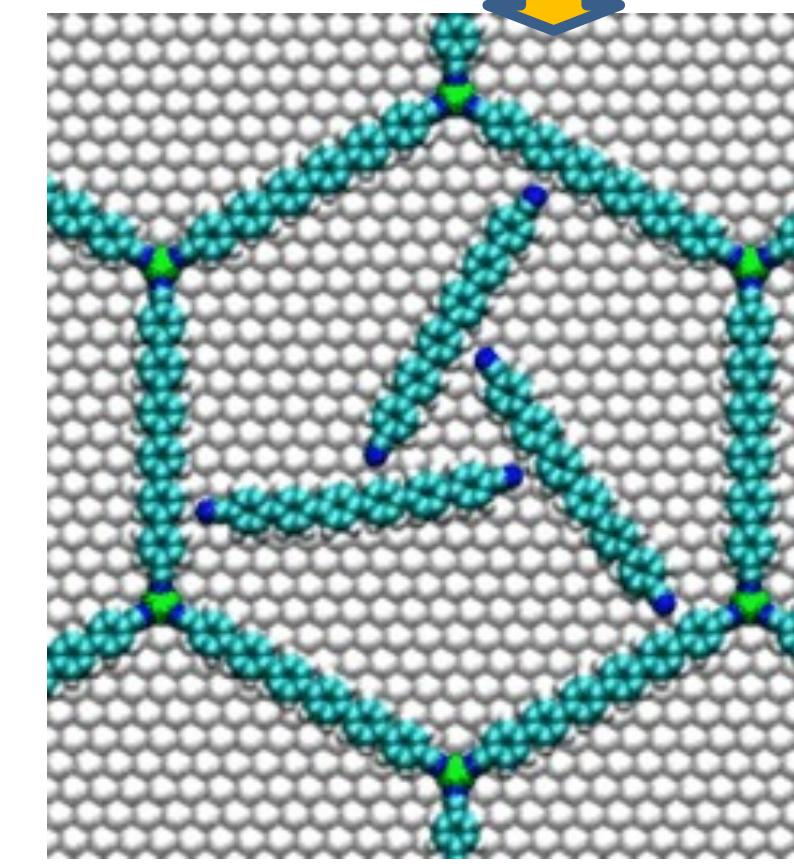
Materials modeling at different length scales



<http://dx.doi.org/10.1016/B978-0-12-409547-2.14273-8>



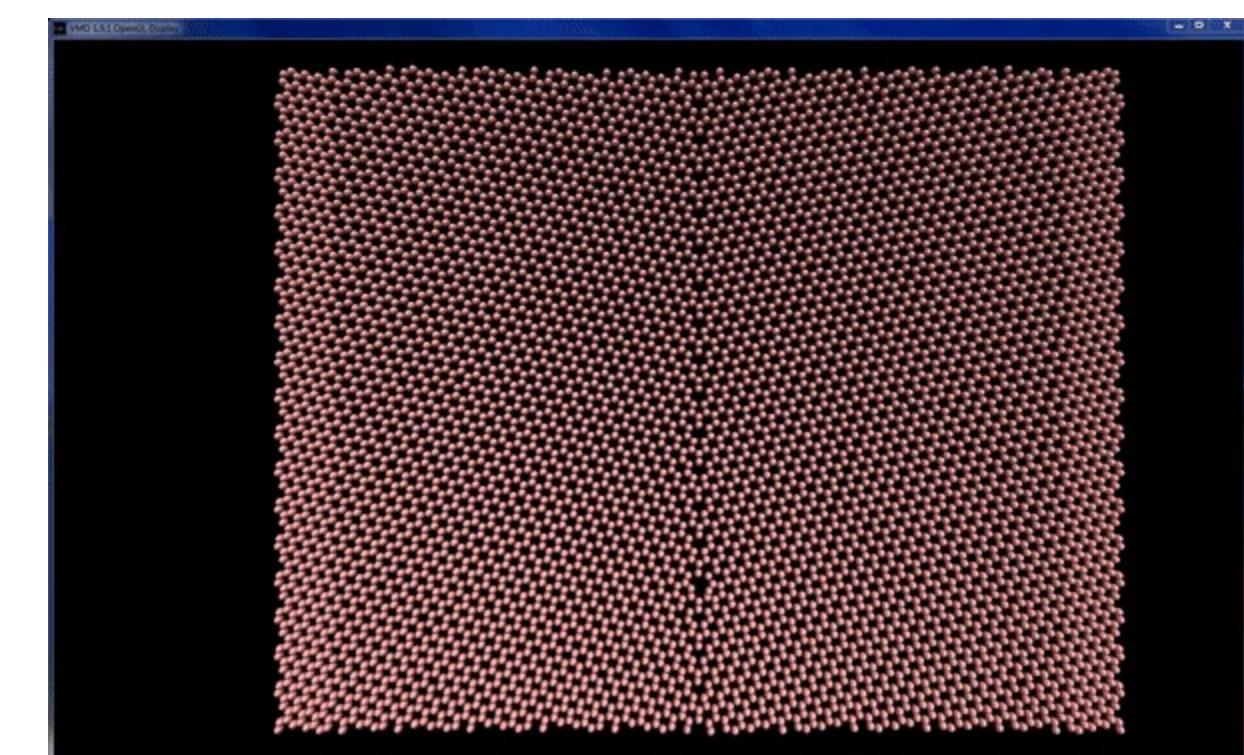
Melting of Cu



Molecular motor in a nanopore

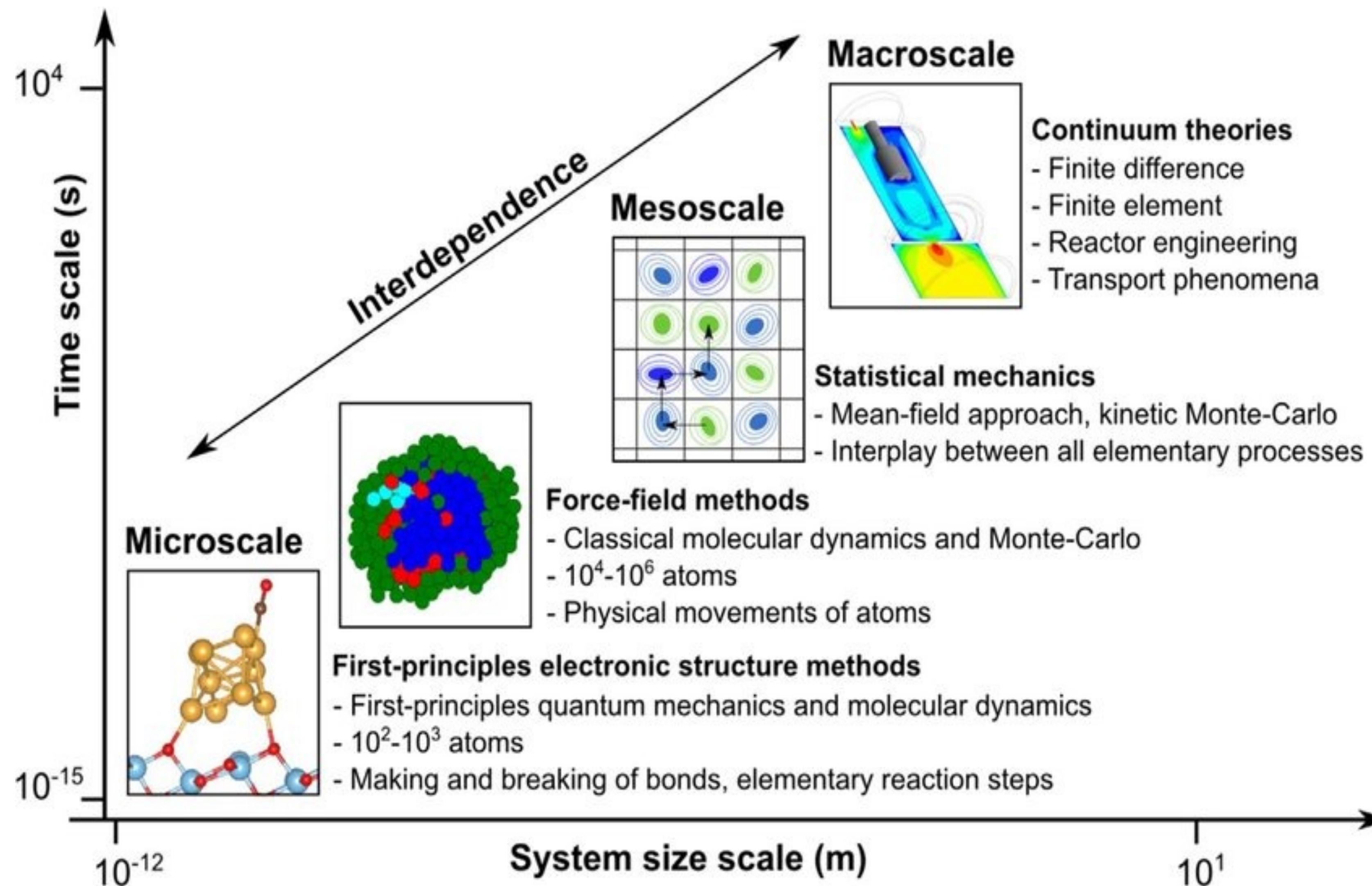


Polymers growth on a surface



Graphene grain boundary failure

Materials Multi-scale modeling (M³)



Create a model to study the behaviour of water

River



(kms)



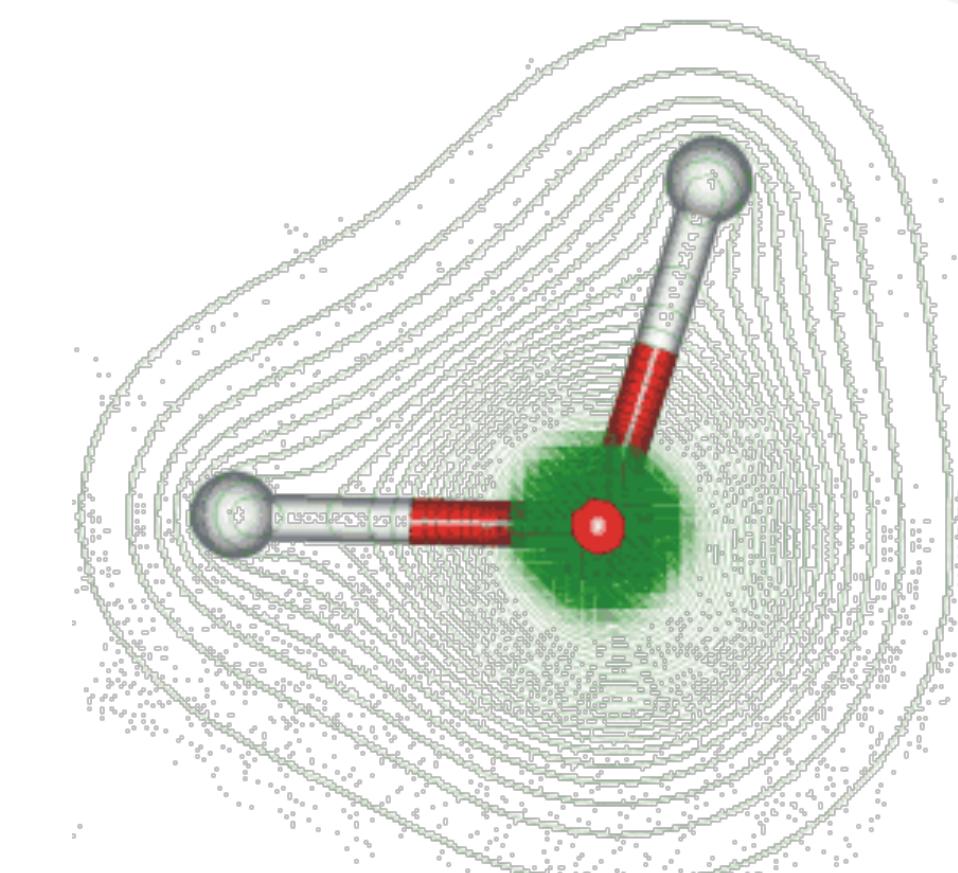
Water pipes
(Meters)



Glass of water
(Many molecules)
(Nanometer= 10^{-9} m)



Scale!



Electron density in a water
molecule (picometer= 10^{-12} m)



Google images

https://water.lsbu.ac.uk/water/water_molecule.html

