"Nature is pleased with simplicity.
And nature is no dummy."

– Isaac Newton

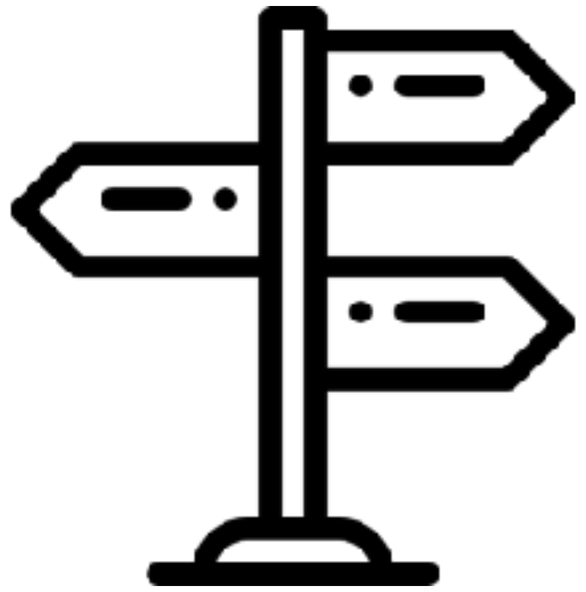
After the Falling Apple: Classical and Statistical Mechanics

Module II: Computations in the Physical World

"Nature is pleased with simplicity. And nature is no dummy."

– Isaac Newton

Guidance



Physics

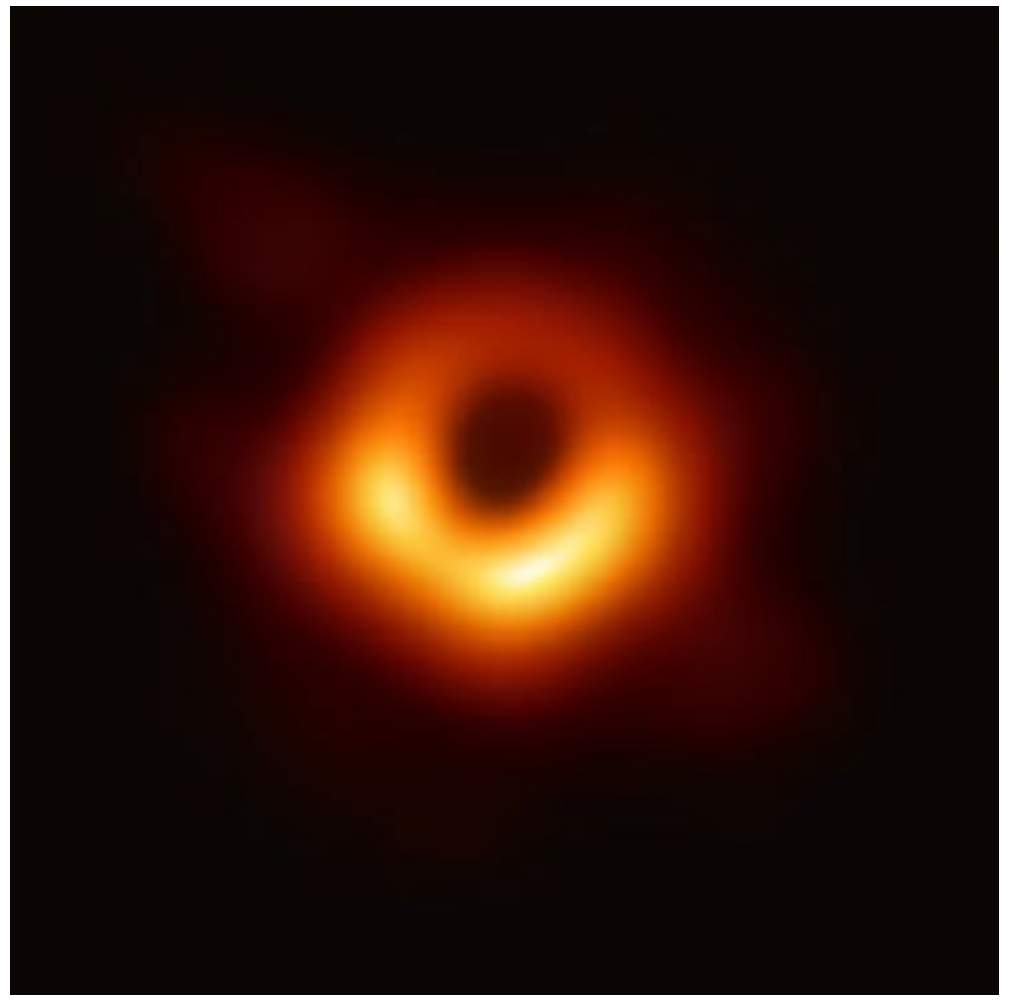
&

Computation

Tools

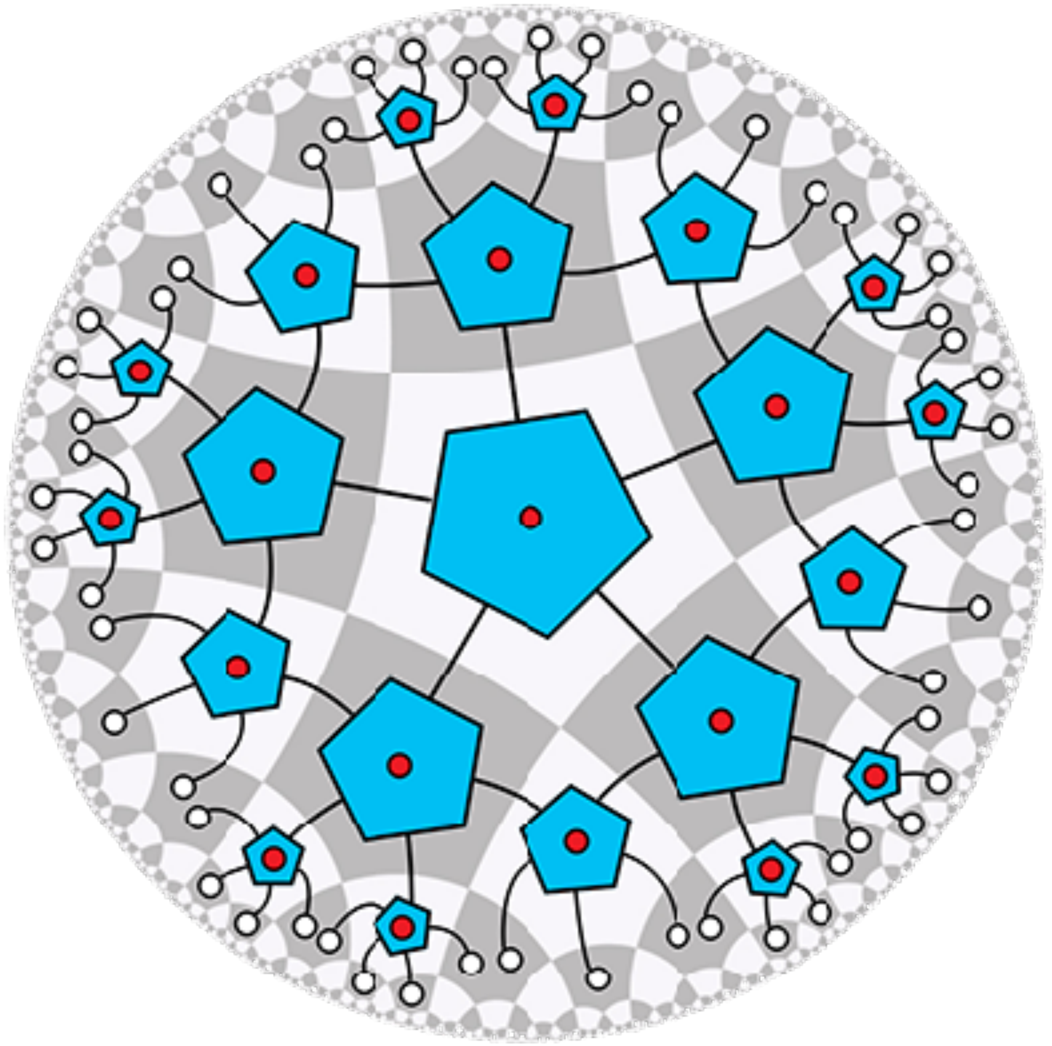
Why Physics?

Module II: Computations in the physical world



Constraints & Structures

Abstraction & Symmetry



I encourage you to focus on the different world views and postulates physicists used for studying reality!

What is Physics and Why Care?

"Physics is the natural science that studies matter, its fundamental constituents, its motion and behavior through space and time, and the related entities of energy and force."

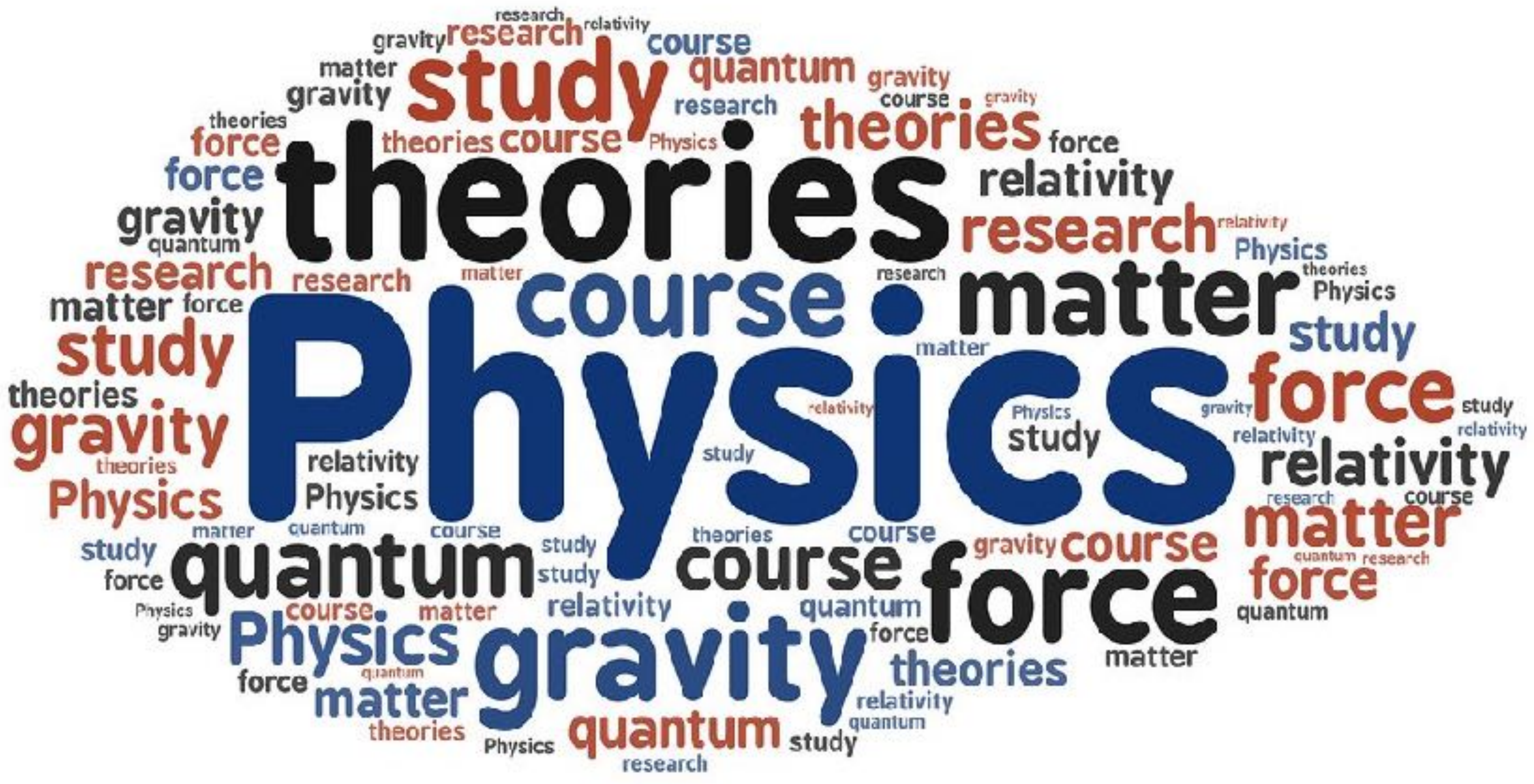
– Wikipedia

- Providing hardwares and methods to perform and implement computations.

- Physical laws themselves are doing certain computations.

Q: What are the computations in the physical world?

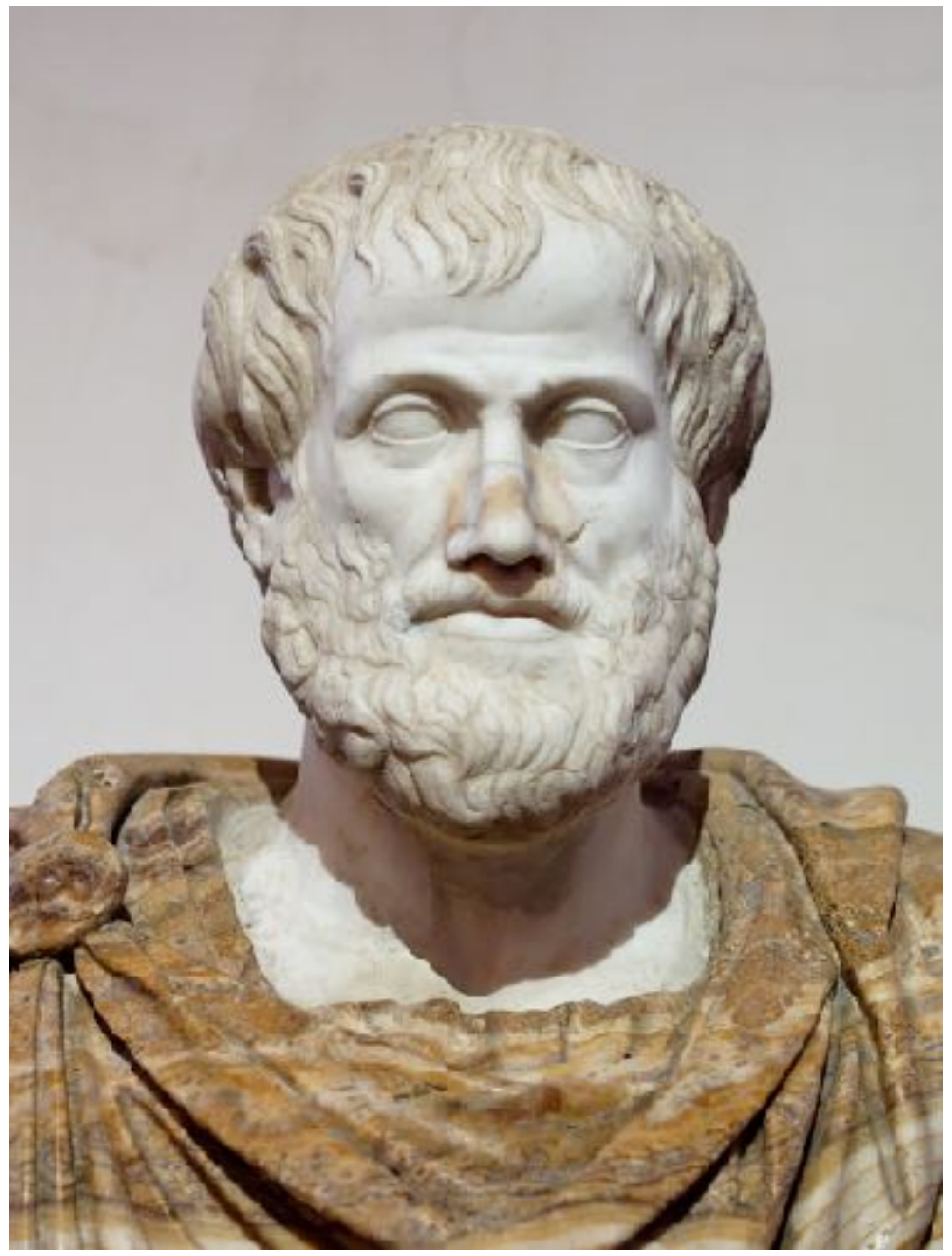
Q: Physics as constraints or guidances?



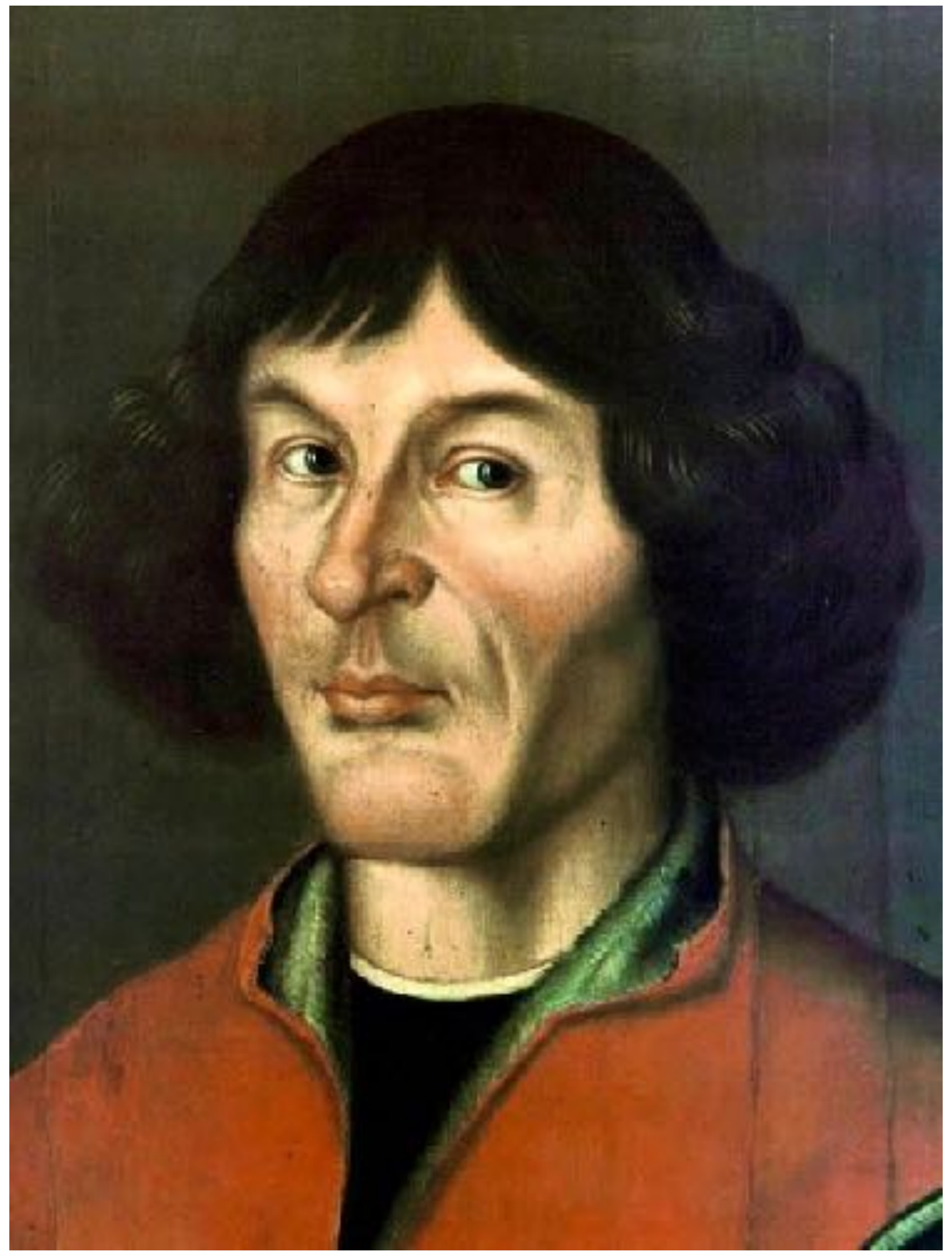
Pre-Newtonian Era

"If I have seen further, it is by standing on the shoulders of giants."

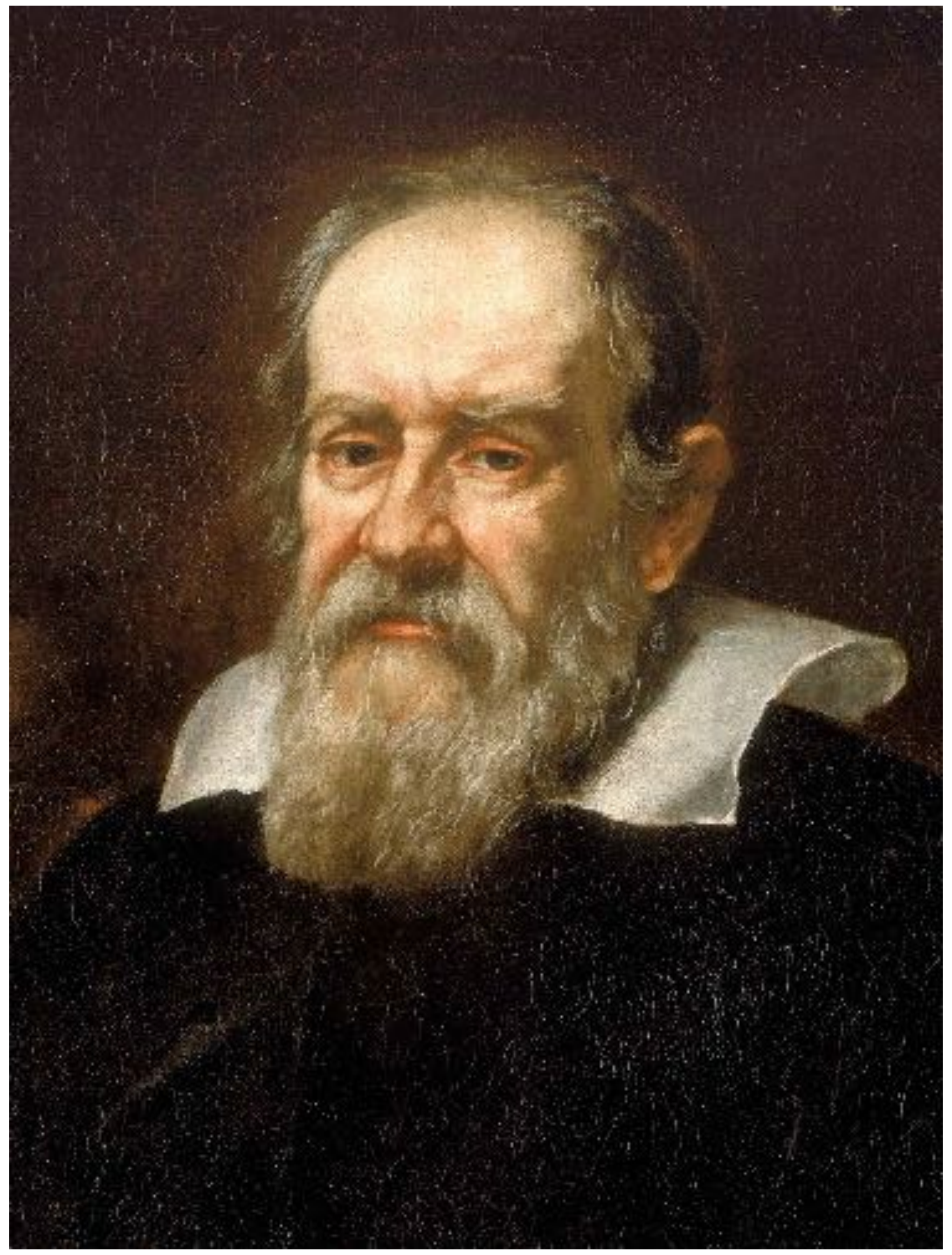
– Isaac Newton



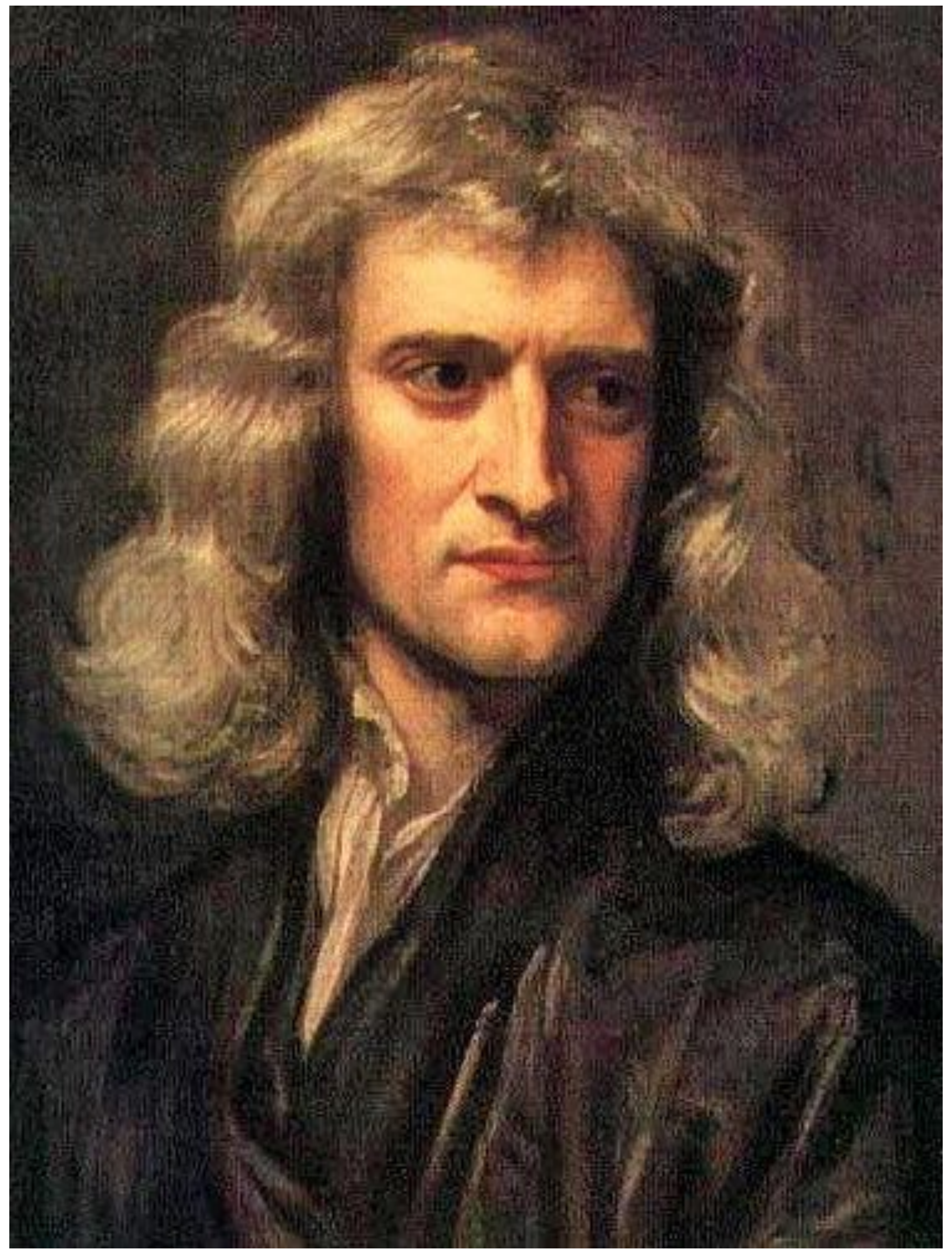
Aristotle 384BC-322BC



Copernicus 1473-1543



Galileo 1564-1642



Newton 1642-1727

Q: How did Newton differ from his ancestors?

Newton’s Laws

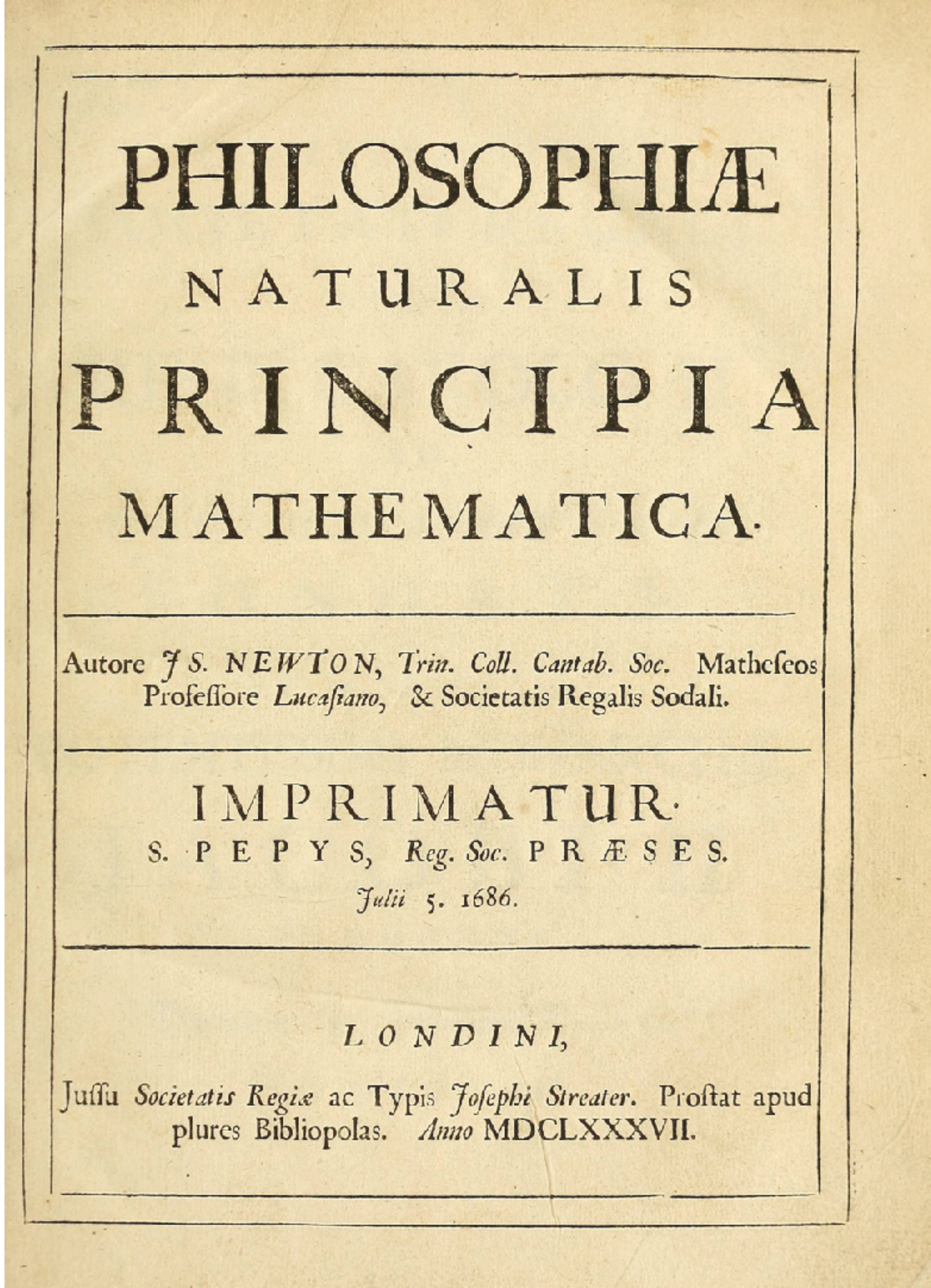
Axiomatization & Unification for the physical world

Law 1: The law of inertia

Law 2: $F = ma$.

Law 3: Action = Reaction.

A **deterministic** and **mechanical** model!



PHILOSOPHIÆ
NATURALIS
PRINCIPIA
MATHEMATICA.

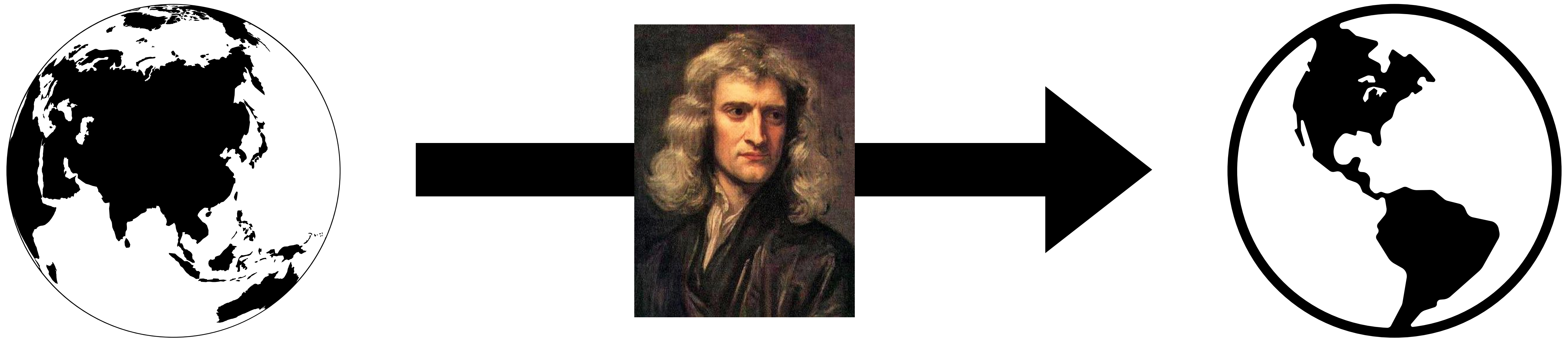
Autore *J S.* NEWTON, *Trin. Coll. Cantab. Soc.* Matheseos Professore *Lucasiano*, & Societatis Regalis Sodali.

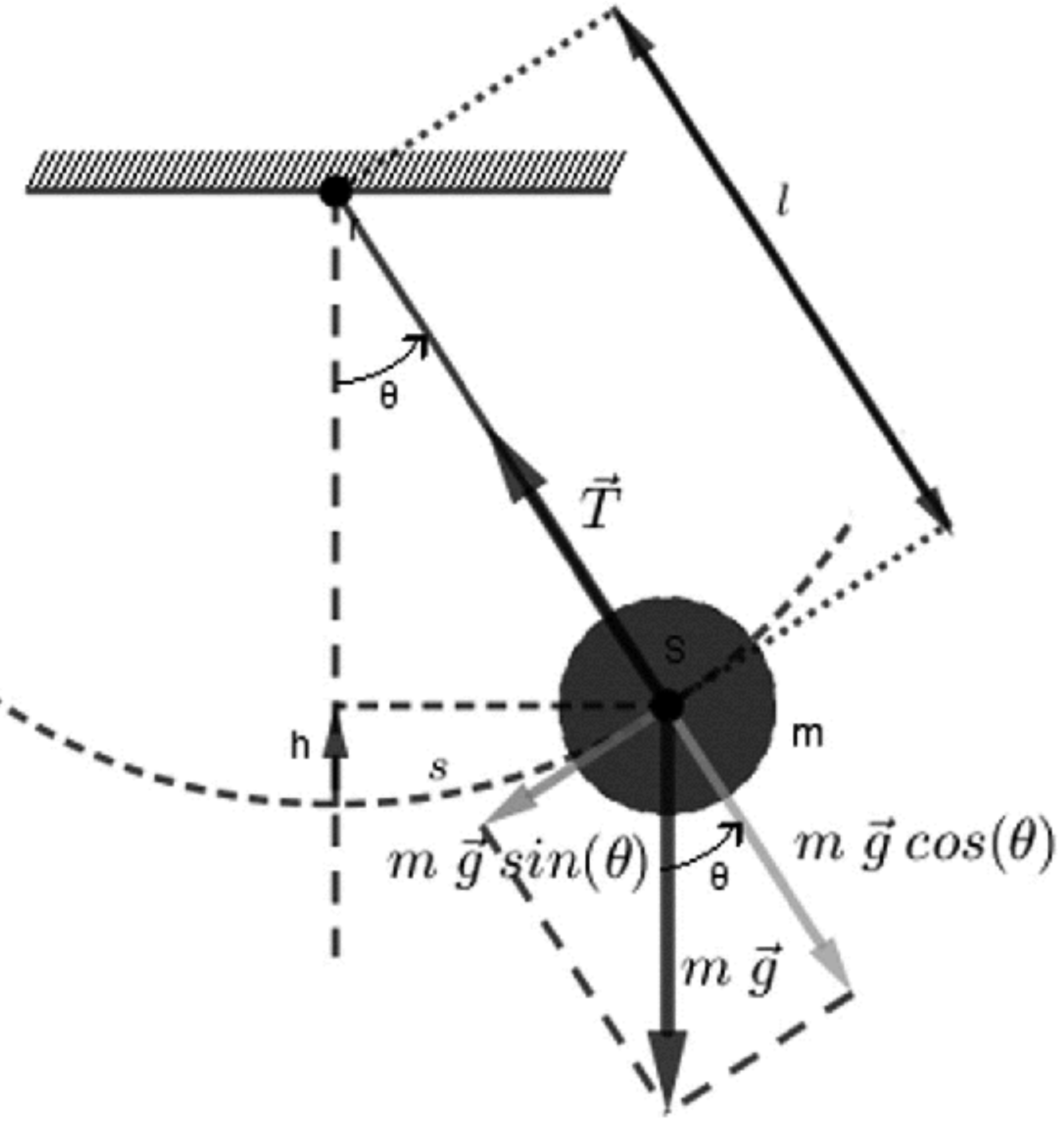
IMPRIMATUR.
S. PEPYS, *Reg. Soc.* PRÆSES.
Julii 5. 1686.

LONDINI,

Jussu *Societatis Regiæ* ac Typis *Josephi Streater*. Prostat apud plures Bibliopolas. *Anno* MDCLXXXVII.

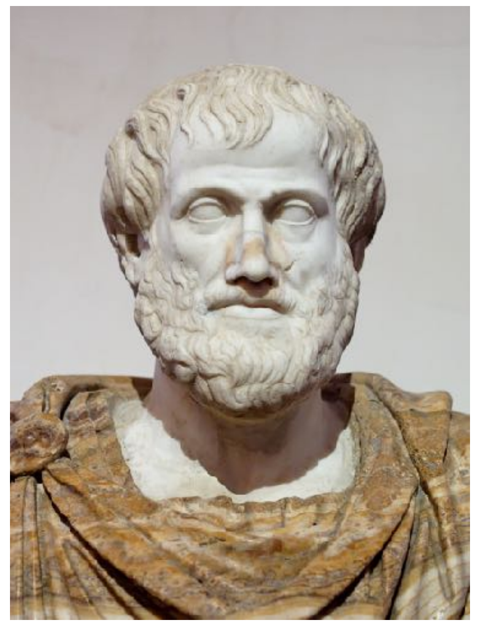
Computational Aspects of Newton’s Laws

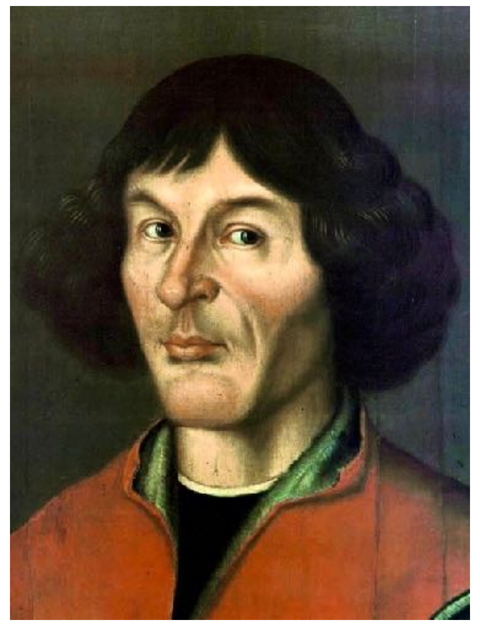


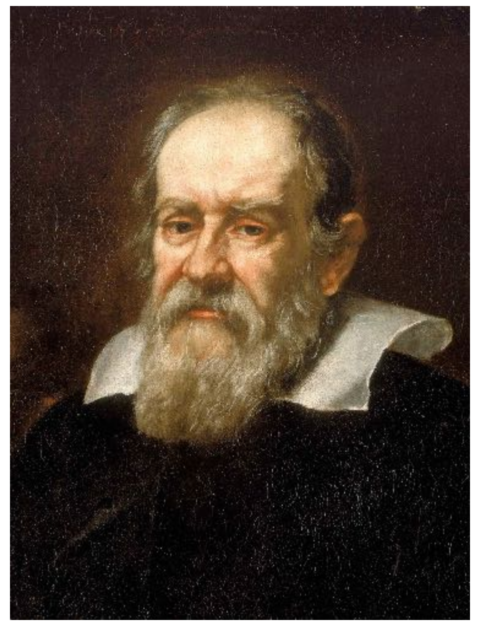


- Newton’s laws provide a computational model for the physical world.
- What’s the underlying computation/algorithmic idea?
- Are Newton’s laws the end of story?

After the Falling Apple







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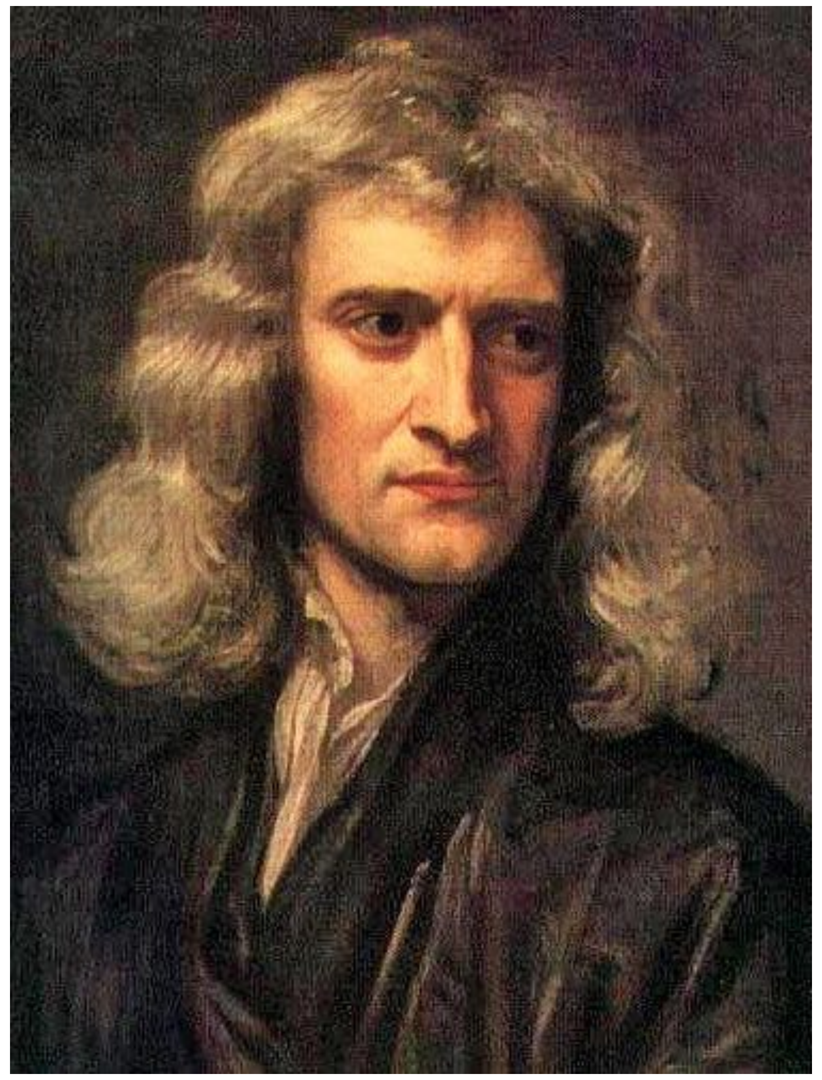

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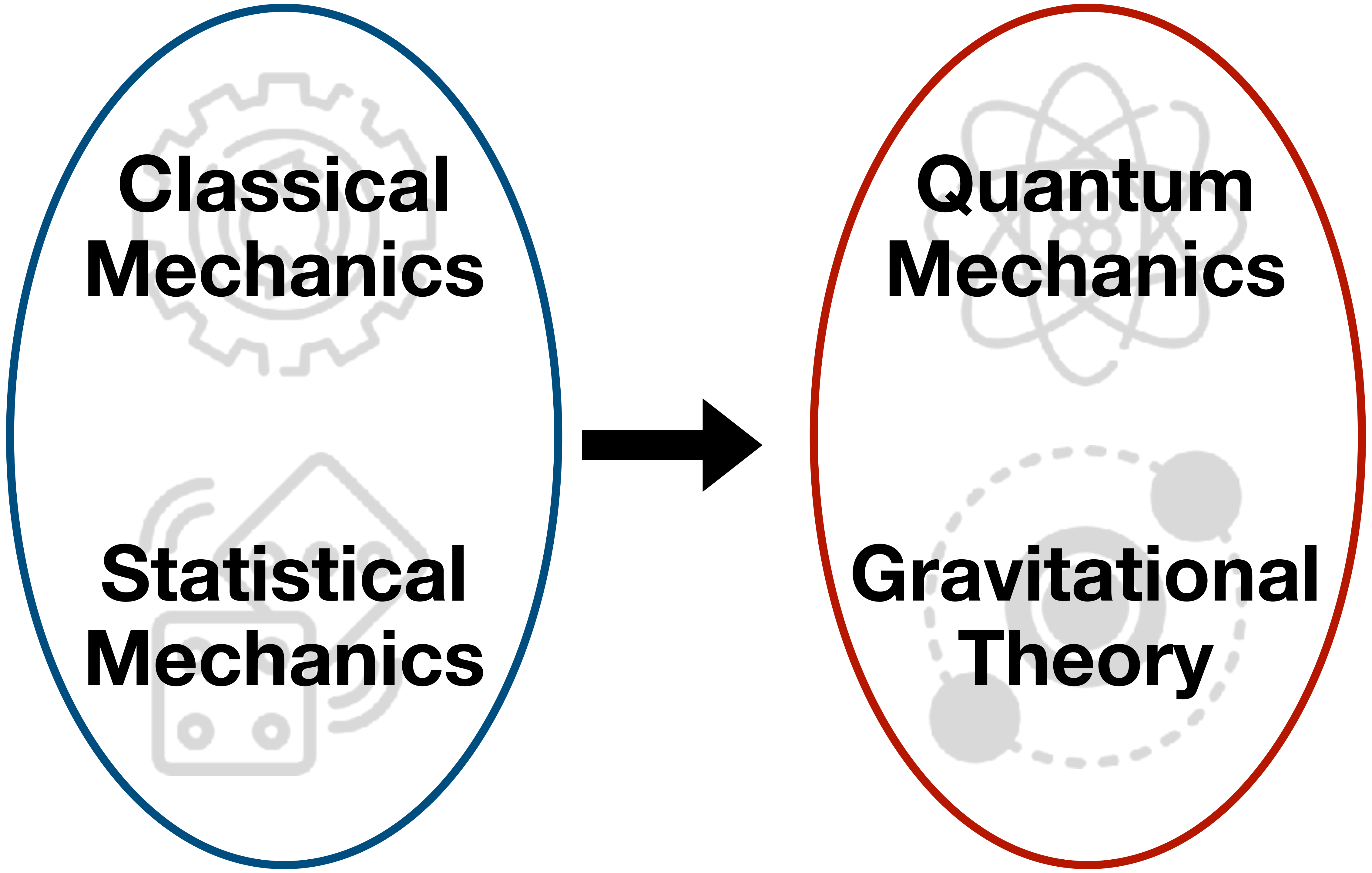


Q: What are the computation views?

Q: Computational/Algorithmic insights?

This lecture

Next lecture

Classical Mechanics and Computation

"In classical physics, science started from the belief – or should one say, from the illusion? – that we could describe the world, or least parts of the world, without any reference to ourselves."

– Werner Heisenberg

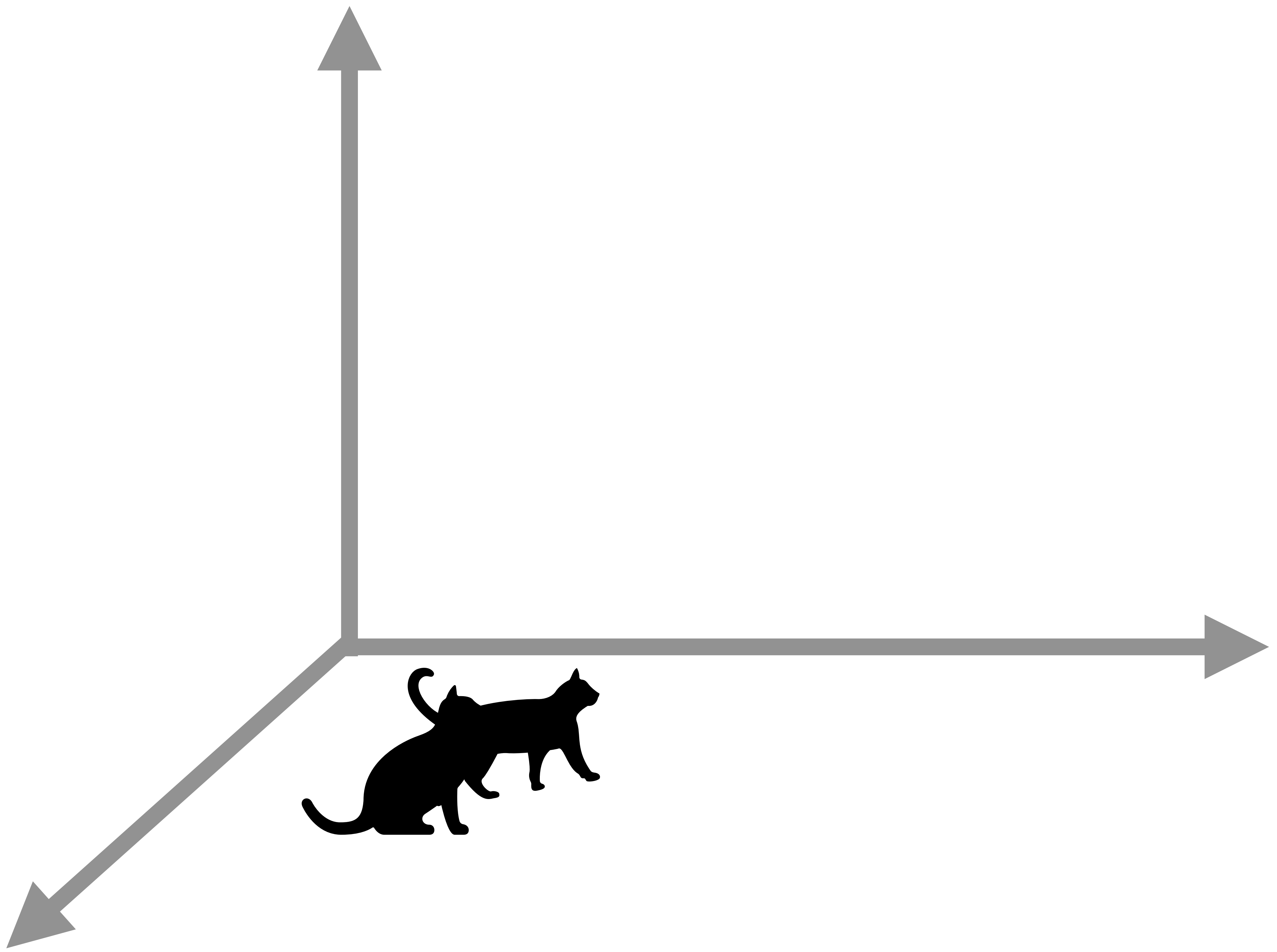
Newton's Mechanics as Evolution in an Euclidean Space

Newton's Laws

Law 1: The law of inertia

Law 2: $F = ma.$

Law 3: Action = Reaction.



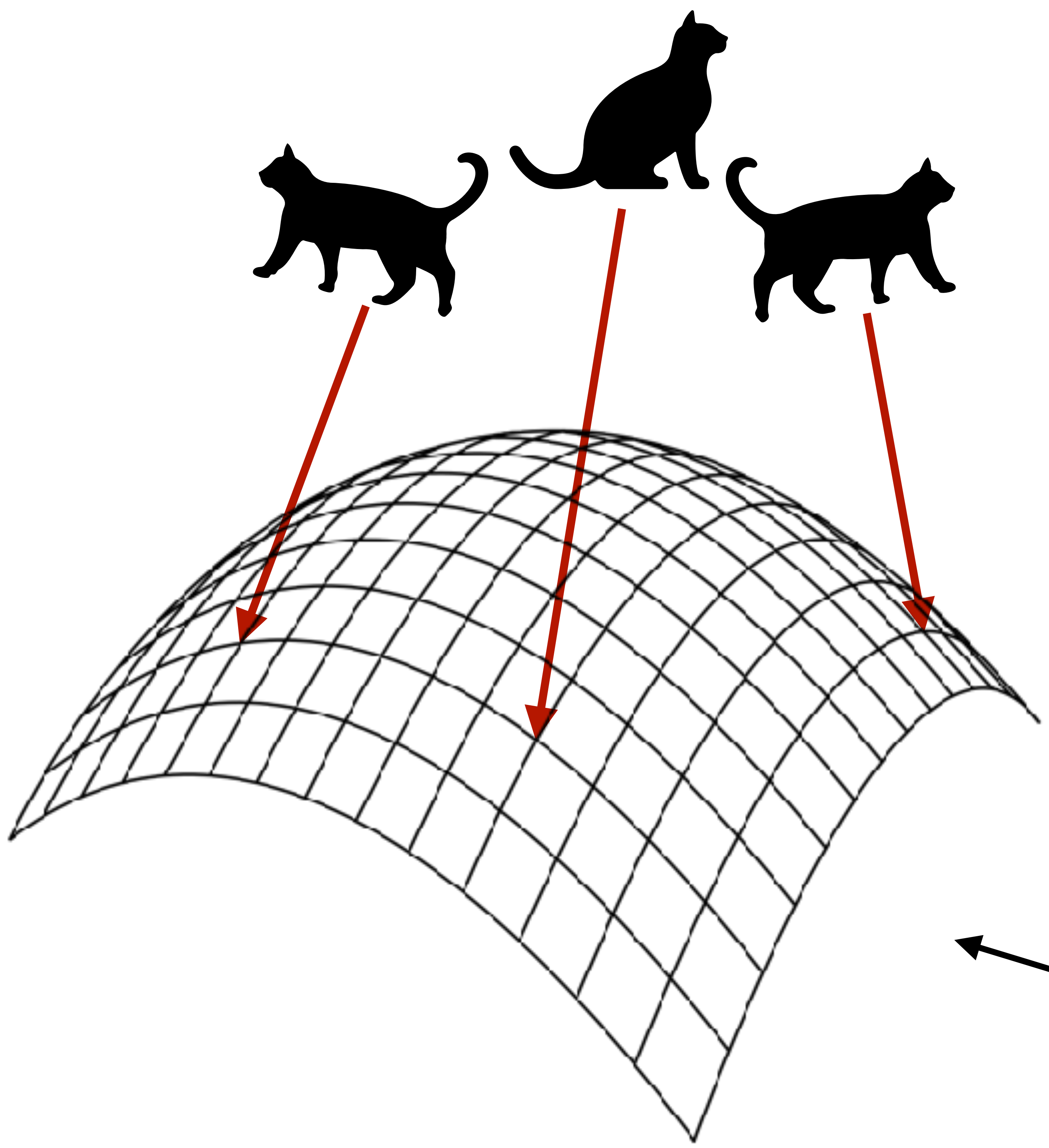
More structure and geometry in the physical world!?

Configuration Space and Phase Space

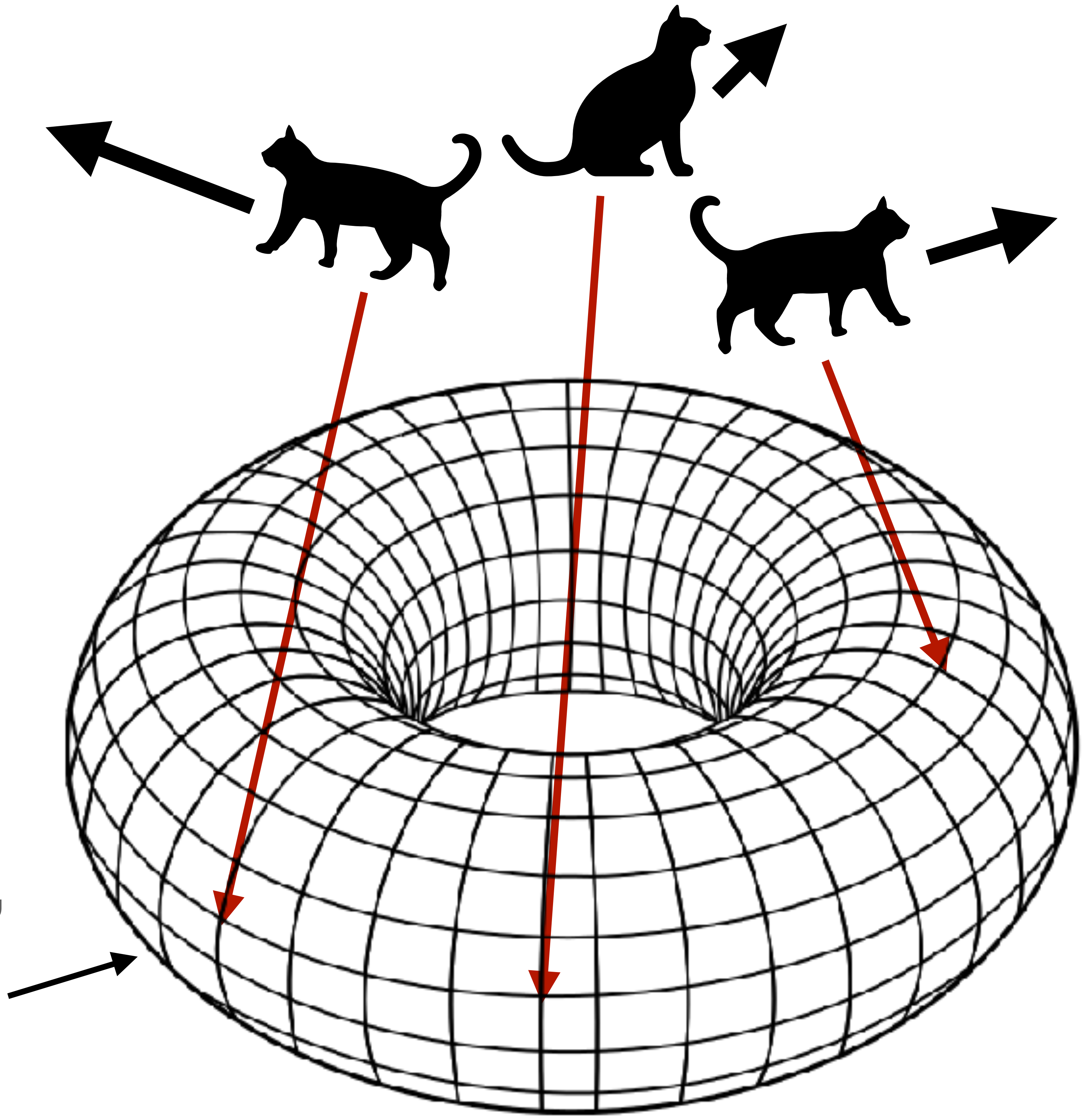
A switch of world view from Newton's Euclidean space

Postulate

Everything in the system is together modeled as a state on a manifold.



High-dimensional "manifold"
(Different formulations have different manifolds)



Configuration space

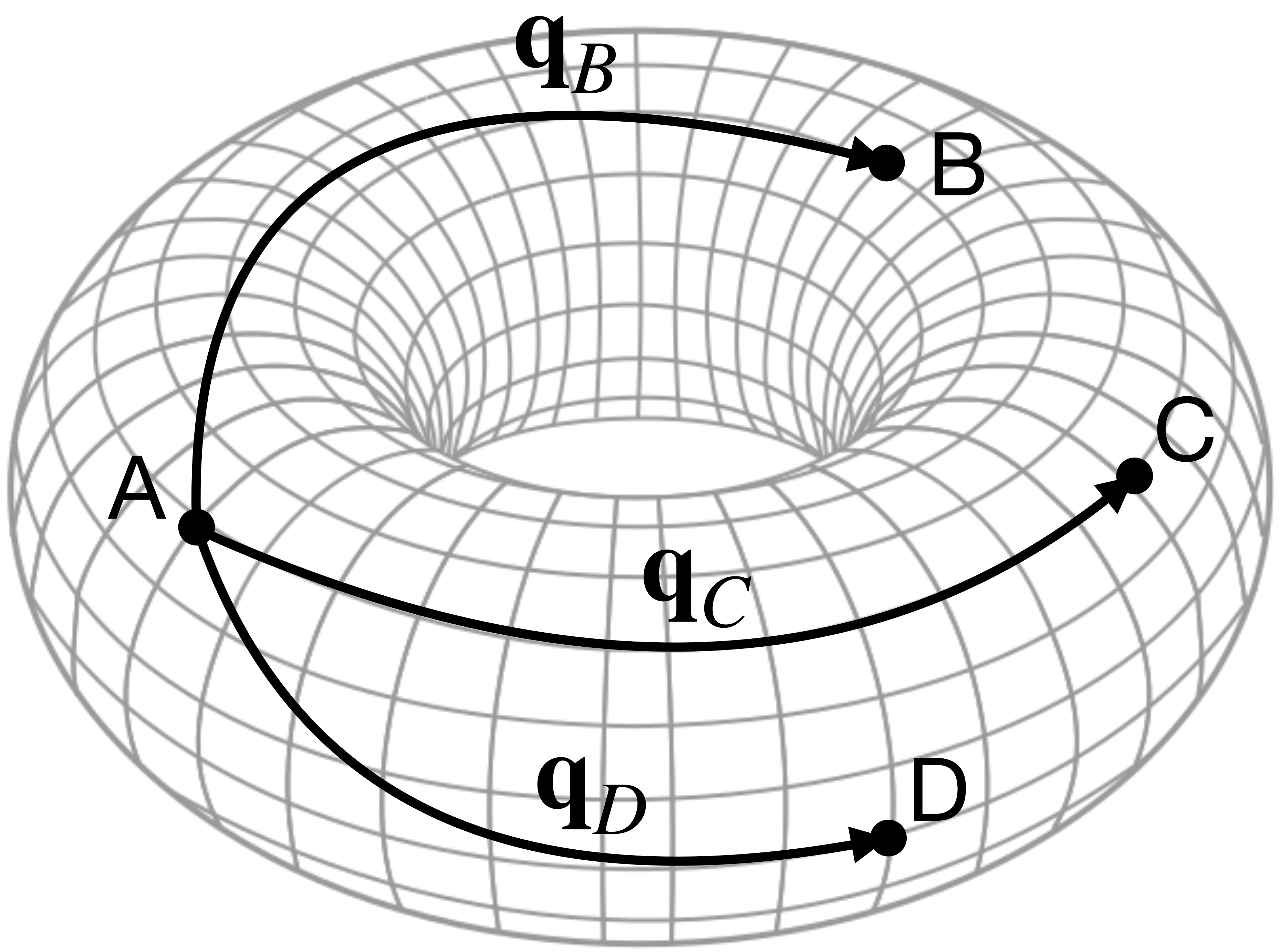
(Embedding of all the possible "configurations")

Phase space

(Embedding of "configurations" + additional properties, e.g., velocities/momenta)

Dynamics of System = Evolution in Phase Space

Which path to take in the phase space?



Q: Start from A, end at B,C, or D?

Principle of Stationary Action

Informally, the trajectory of the state will be the one that costs the least "*energy*".

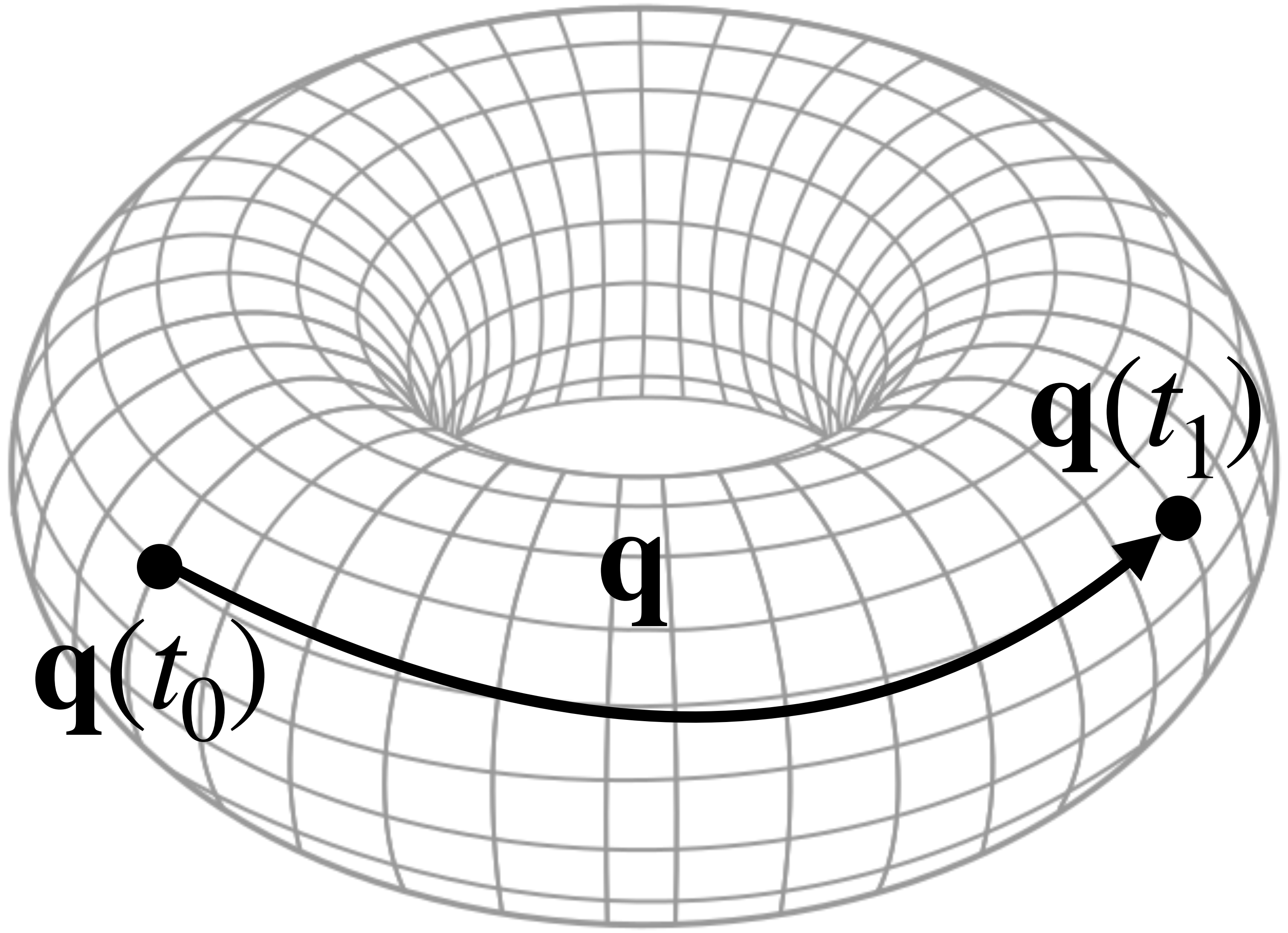
Formally, the "*action*" of a trajectory $\mathbf{q}$ of in the phase space is defined as

$$\mathcal{S}[\mathbf{q}] = \int_{t_0}^{t_1} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)dt$$

where $L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)$ is the *Lagrangian* and $L =$ kinetic energy - potential energy.

* Here we focus on Lagrangian mechanics while there exist lots of other formulations (e.g., Hamiltonian mechanics).

Classical Mechanics as Optimization



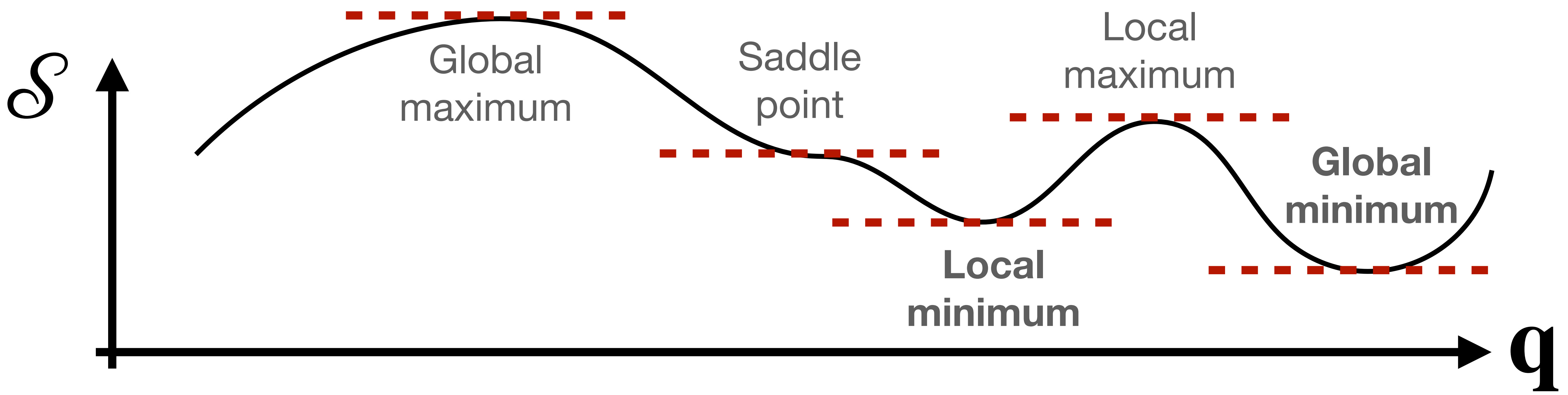
Principle of Stationary Action

The trajectory $\mathbf{q}$ will be the one that minimizes

$$\mathcal{S}[\mathbf{q}] = \int_{t_0}^{t_1} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)dt\,.$$

Principle of least action $\Rightarrow$

The physical reality locally minimizes the total action



Q: How to find the minimizer? **A:** Euler-Lagrange equations: $\dfrac{\partial L}{\partial \mathbf{q}} = \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{\mathbf{q}}}$.

* Here we focus on Lagrangian mechanics, other formulations (e.g., Hamiltonian mechanics) and more mathematical details will be covered in advanced sections.

Chaos and Unpredictability

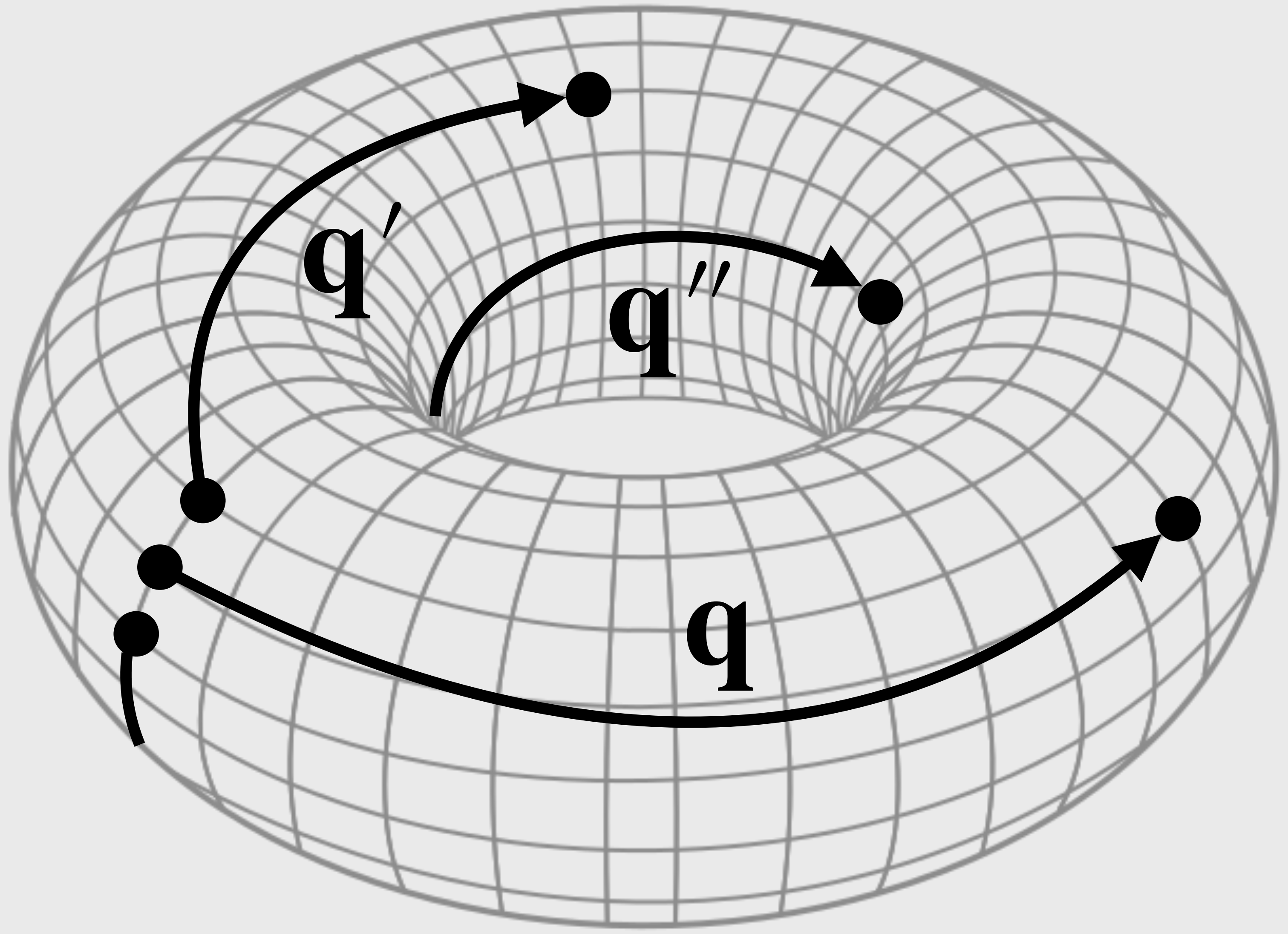
- Although the theory of classical mechanics gives extremely elegant models…
- The precision for measuring the initial configurations matter a lot!
- The dynamic is computable (given known initial configuration), but unpredictable (due to the imprecision in measurement)!

Q: When is the optimization view useful?

Q: How to handle chaotic cases?

Chaotic Phenomenon

A minor difference in the initial configuration can result in extremely different evolution.

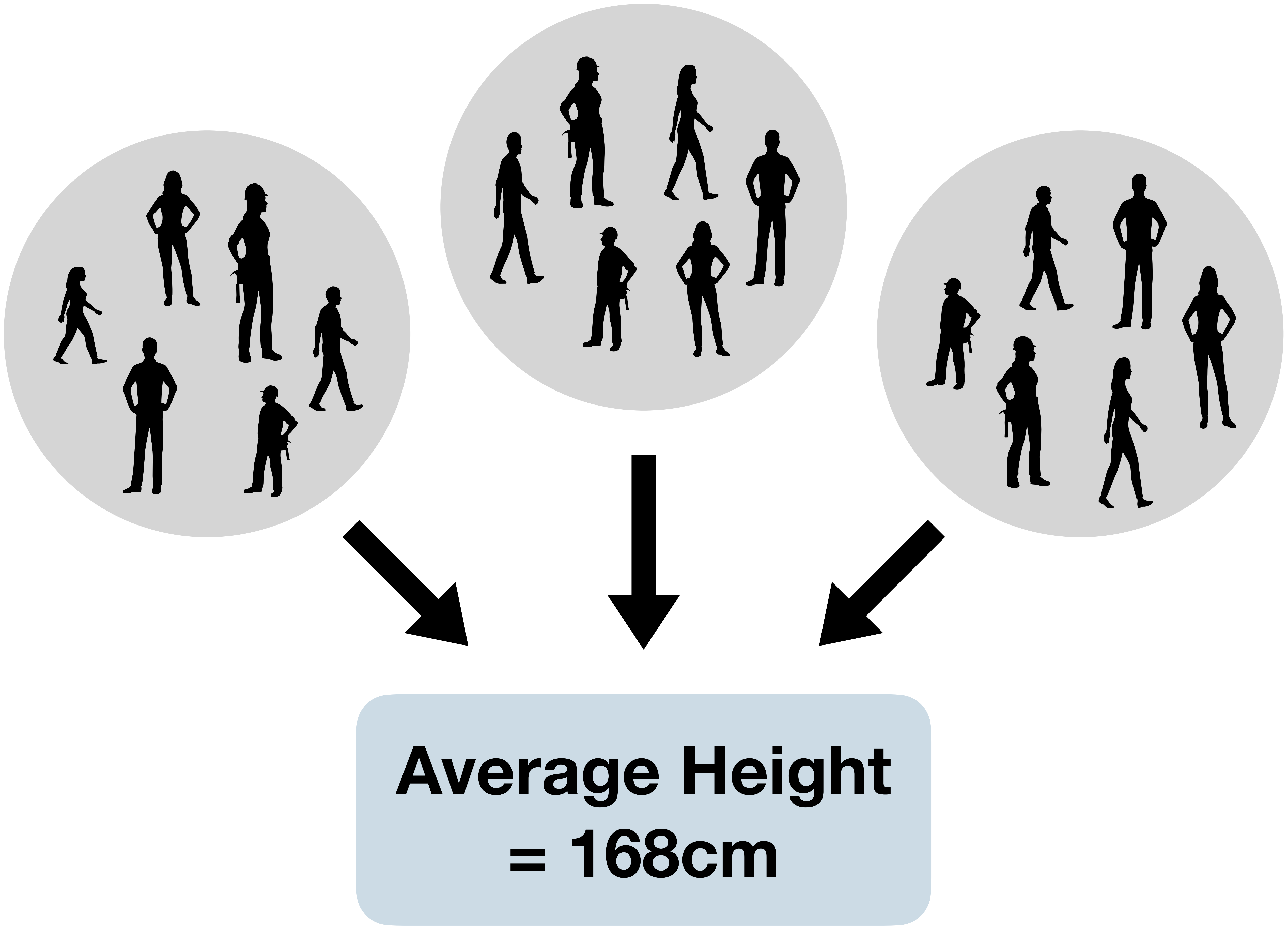


Statistical Mechanics and Computation

"Statistical mechanics is extremely easy and it's extremely hard. It's subtle. It's fulled of surprises. It's fulled of the applications of very simple formulas which then yield extremely surprising and powerful results."

– Leonard Susskind

Microstate and Macrostate



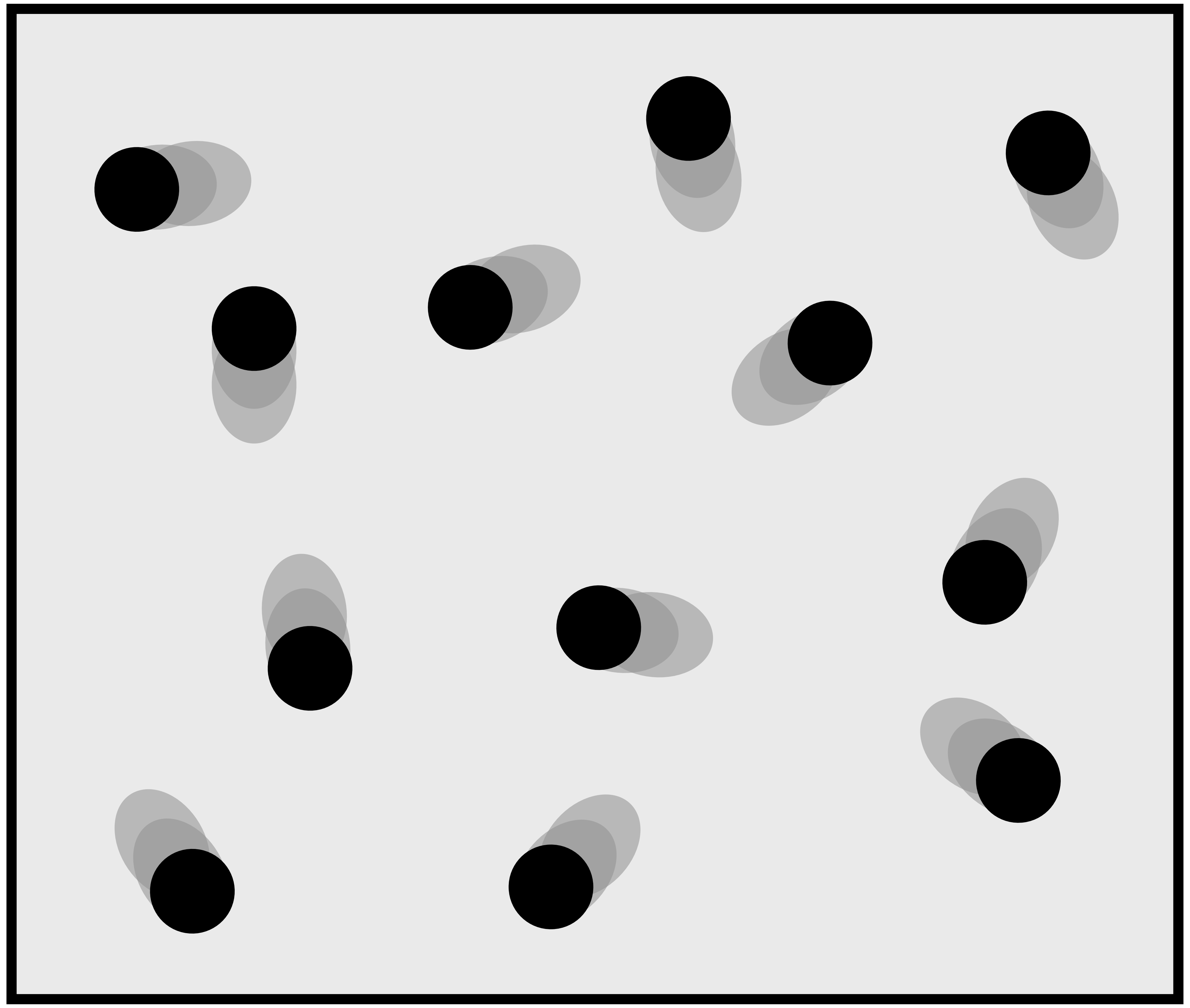
Microstate: A state in the configuration/phase space for all particles in the system.

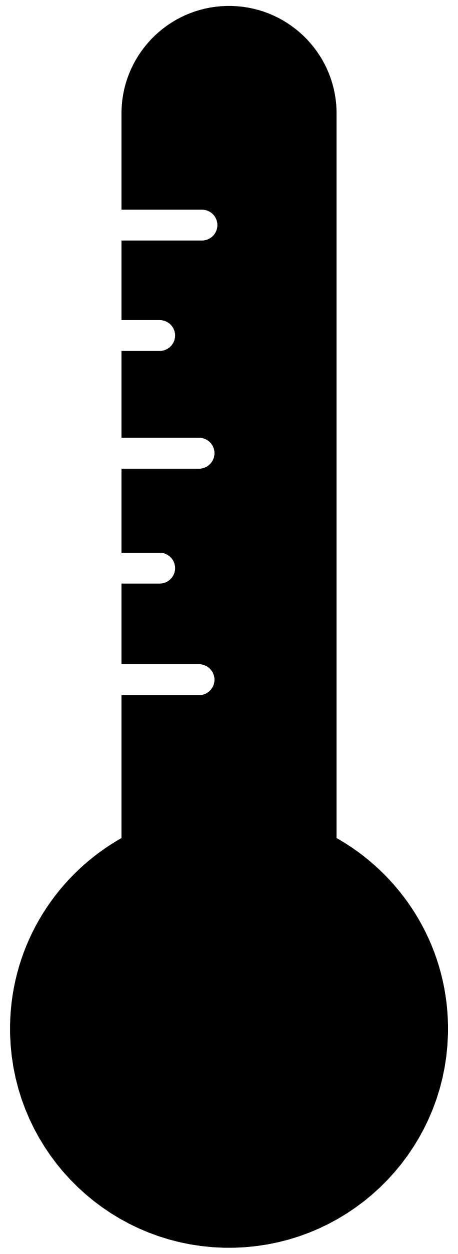
Macrostate: A statistical summary of a microstate, e.g., average speed, average energy.

- In practice, we can only measure the macrostate.

- A macrostate might correspond to multiple microstates!

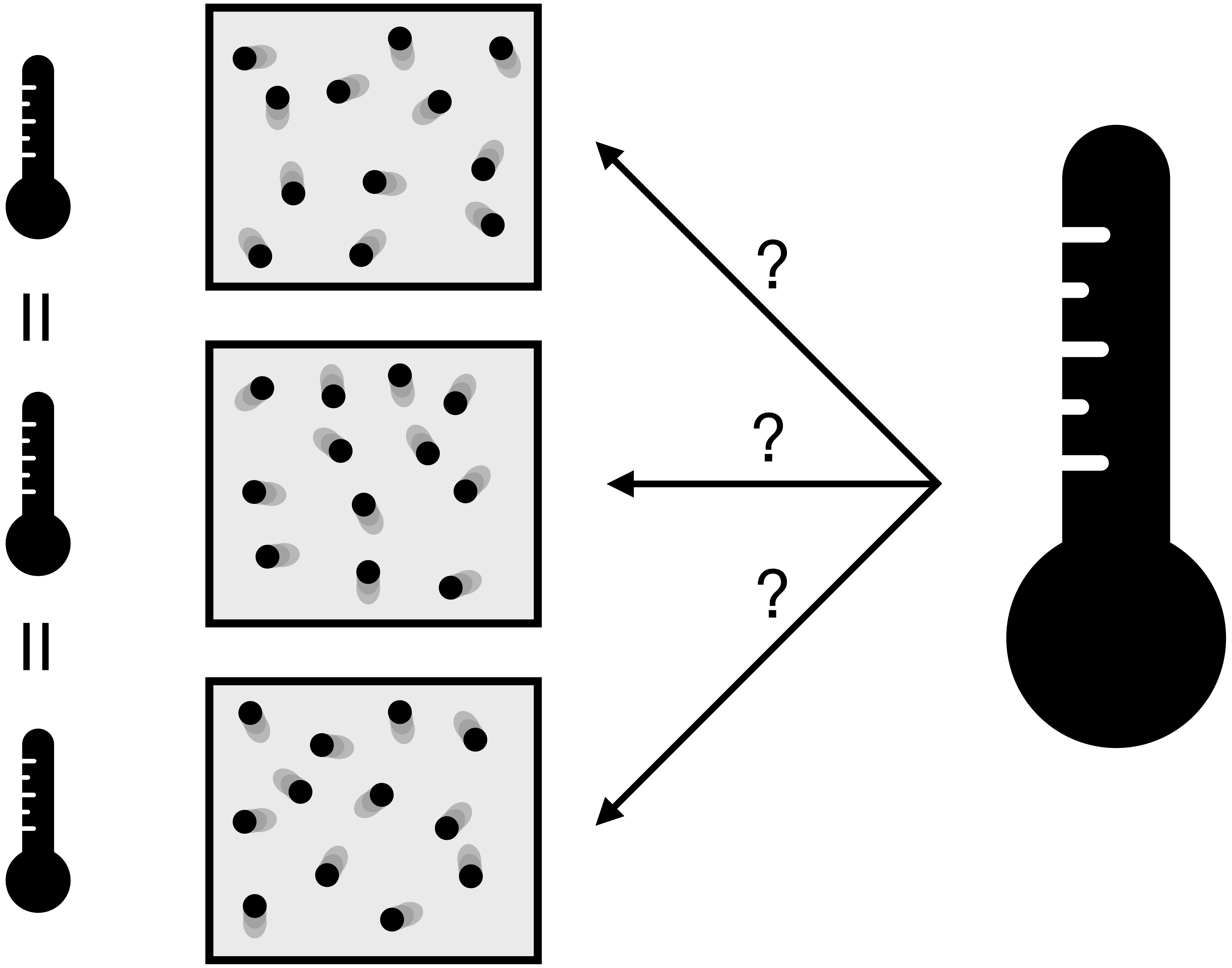
Example: Thermodynamics





Microstate **Macrostate**

A Priori Probability of a Microstate?



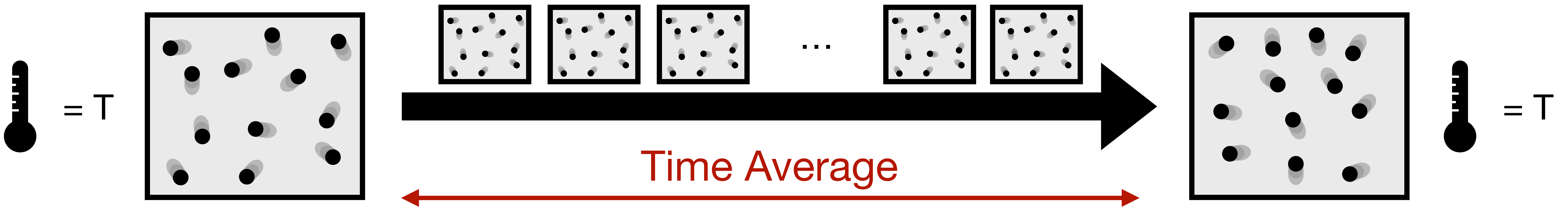
Q: Given a macrostate, what can we infer about the underlying microstate?

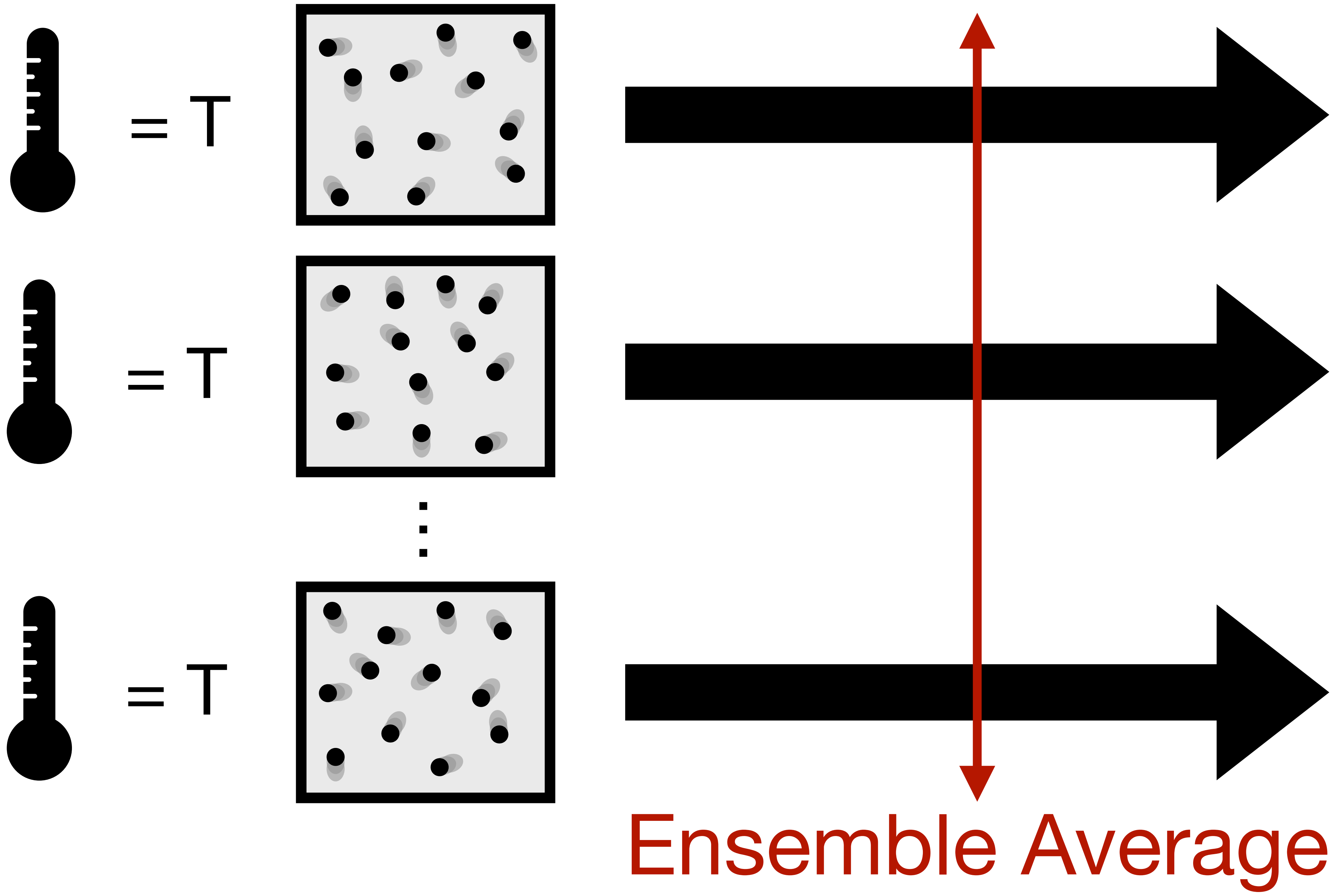
A: There’s no definite answer, only “a priori probabilities”.

Q: What do we mean by “probability” here?

How to Study Microstates from a Macrostate

Time average & Ensemble average



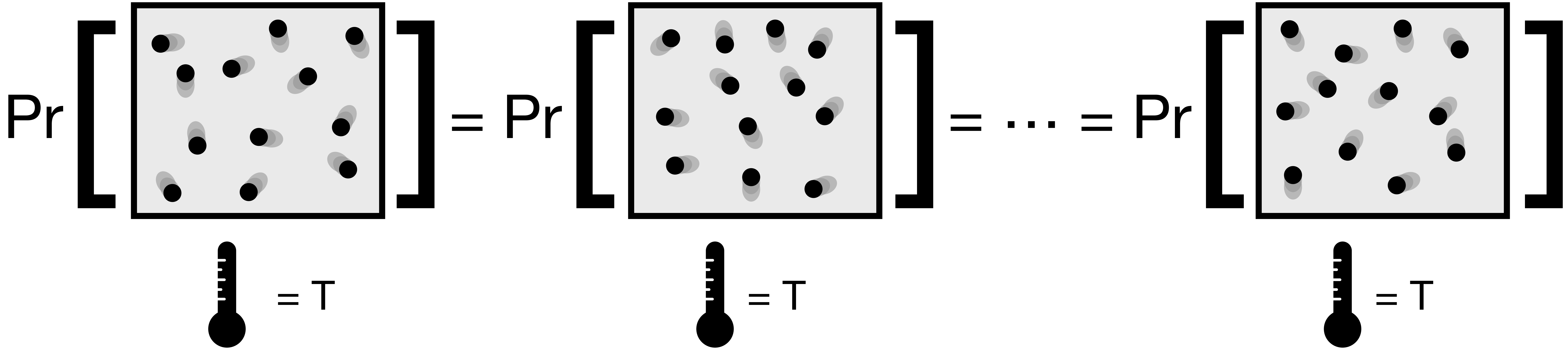


Ergodic Hypothesis

In an isolated system that reaches equilibrium, **the time average is equal to the ensemble average.** In particular, we say the system is ergodic.

The Postulate of Equal *a Priori* Probabilities

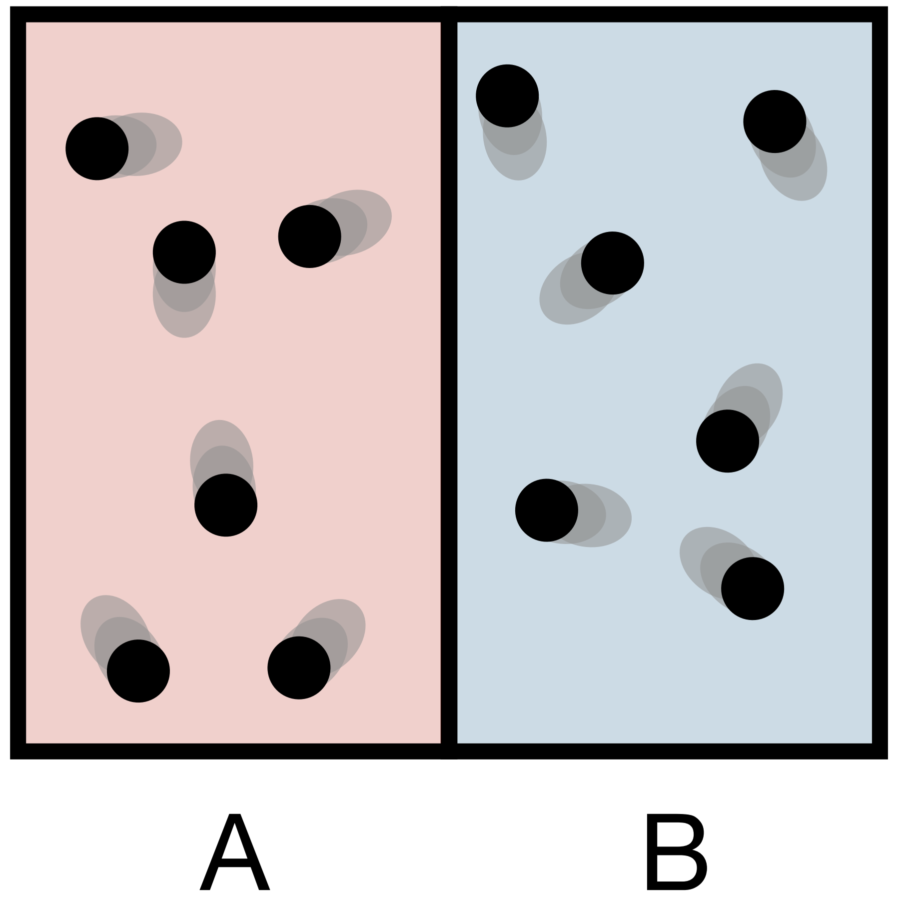
In an isolated system that reaches equilibrium, given a fixed macrostate…



When looking at a subsystem, given a fixed macrostate…

Q: What's the distribution of a macrostate in subsystem A?

A: Boltzmann distribution!



* Another way to see the postulate of equal *a priori* probabilities is thinking of it as a consequence of the second law of thermodynamics.

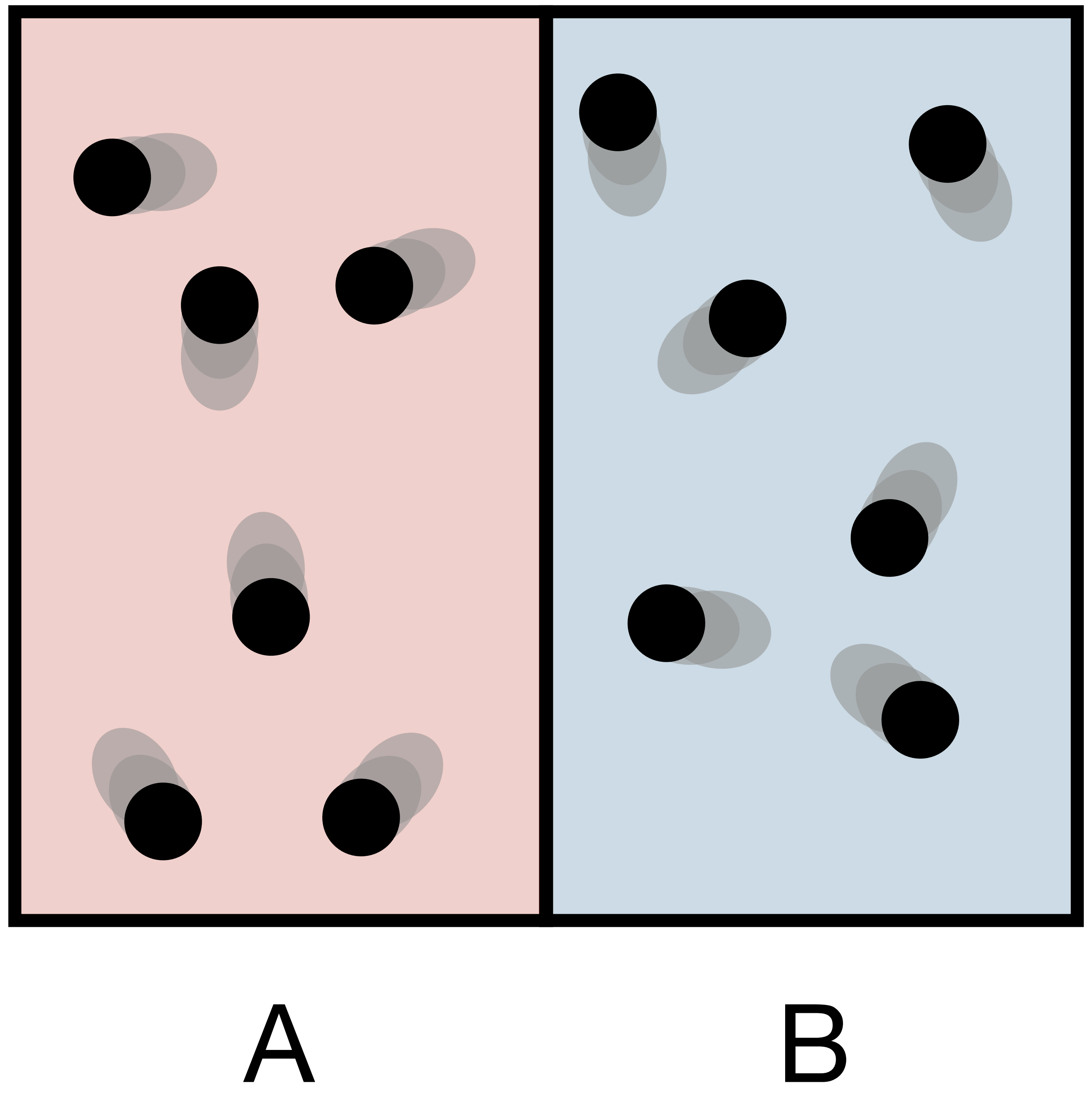
Boltzmann Distribution and Partition Function

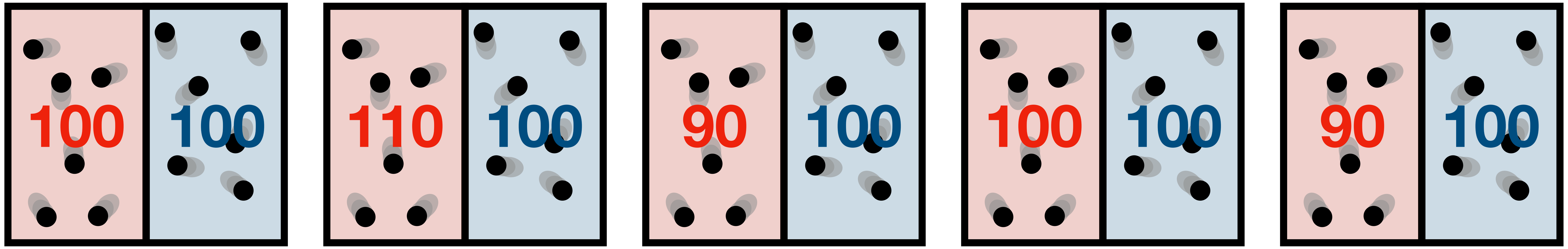
Derived from the postulate of *a priori* probabilities
+ marginalize subsystem B.

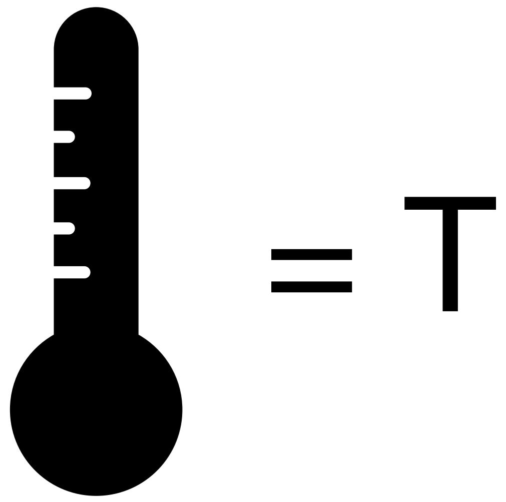
$$\Pr[\text{energy of A} = E] = \frac{\exp(-E/T)}{Z(T)}.$$

Concretely, this means a specific microstate with energy E

Partition function, a normalizing constant which contains lots of information about the whole system.







* Think of subsystem B being much larger than A.

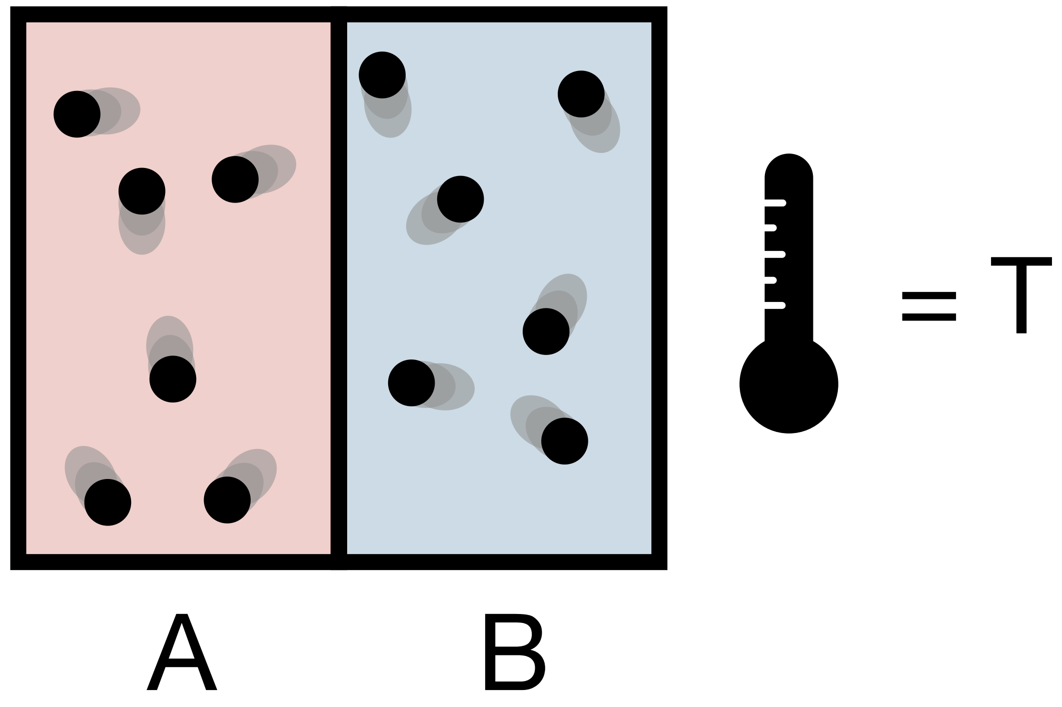
Statistical Mechanics as Computation

Optimization & Sampling & Counting

Simone
(Jan. 14
2pm-3pm ET)

“Simulated Annealing”

$$\Pr[\text{energy of A} = E] = \frac{\exp(-E/T)}{Z(T)}.$$



Optimization: Microstate with *lower* energy has higher probability!

Sampling: Start with a random microstate and lower the temperature.

Counting: The partition function $Z(T)$ encodes the number of microstates!

* More mathematical details in advanced sections.

Jump Back to Turing Machine

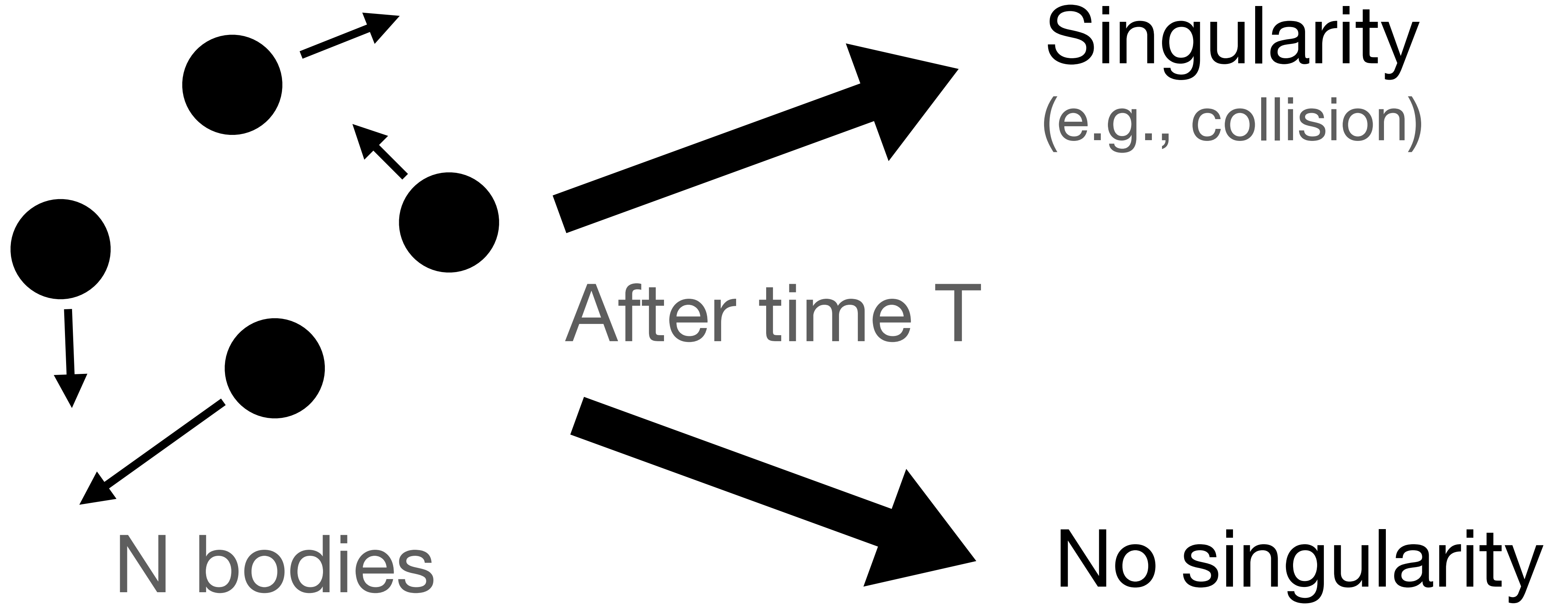
Can Turing Machine Simulate Classical Mechanics?

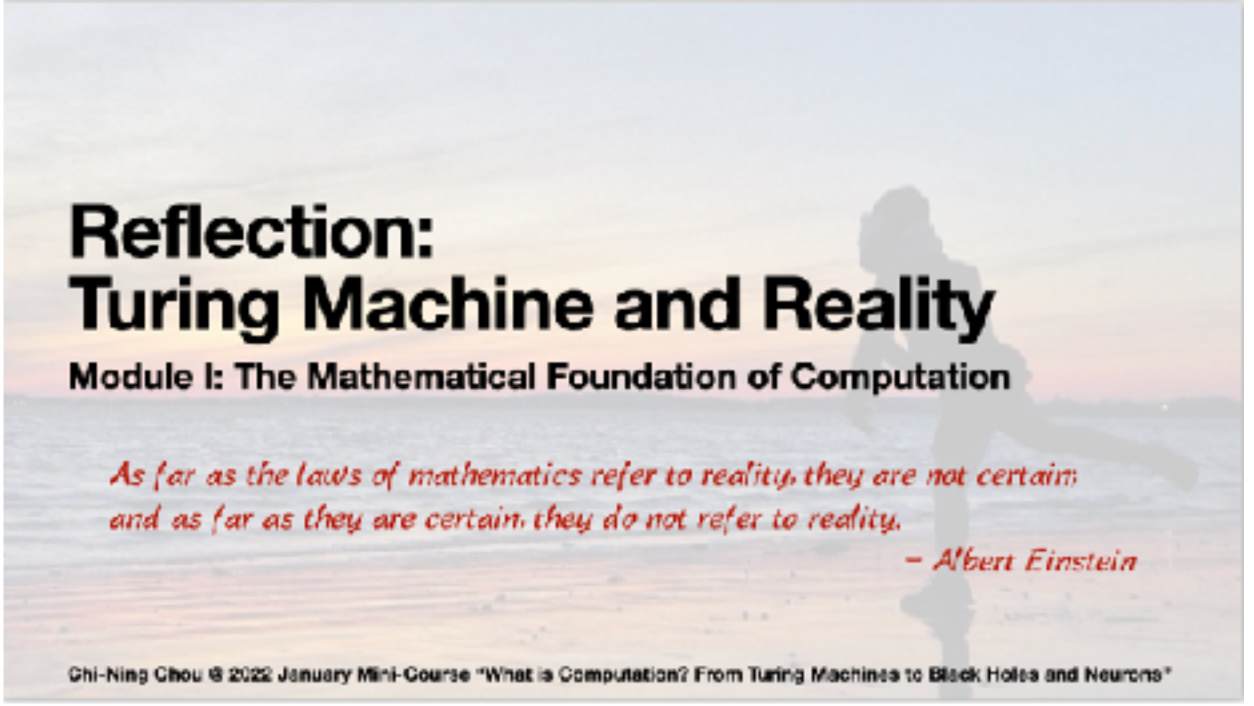
Extended Church-Turing Thesis

All feasible computation in the physical world can be done by a Turing machine efficiently.

Q: Can we identify some computational problems in classical mechanics that cannot be efficiently computed by a Turing machine?

Andrew Chi-Chih Yao





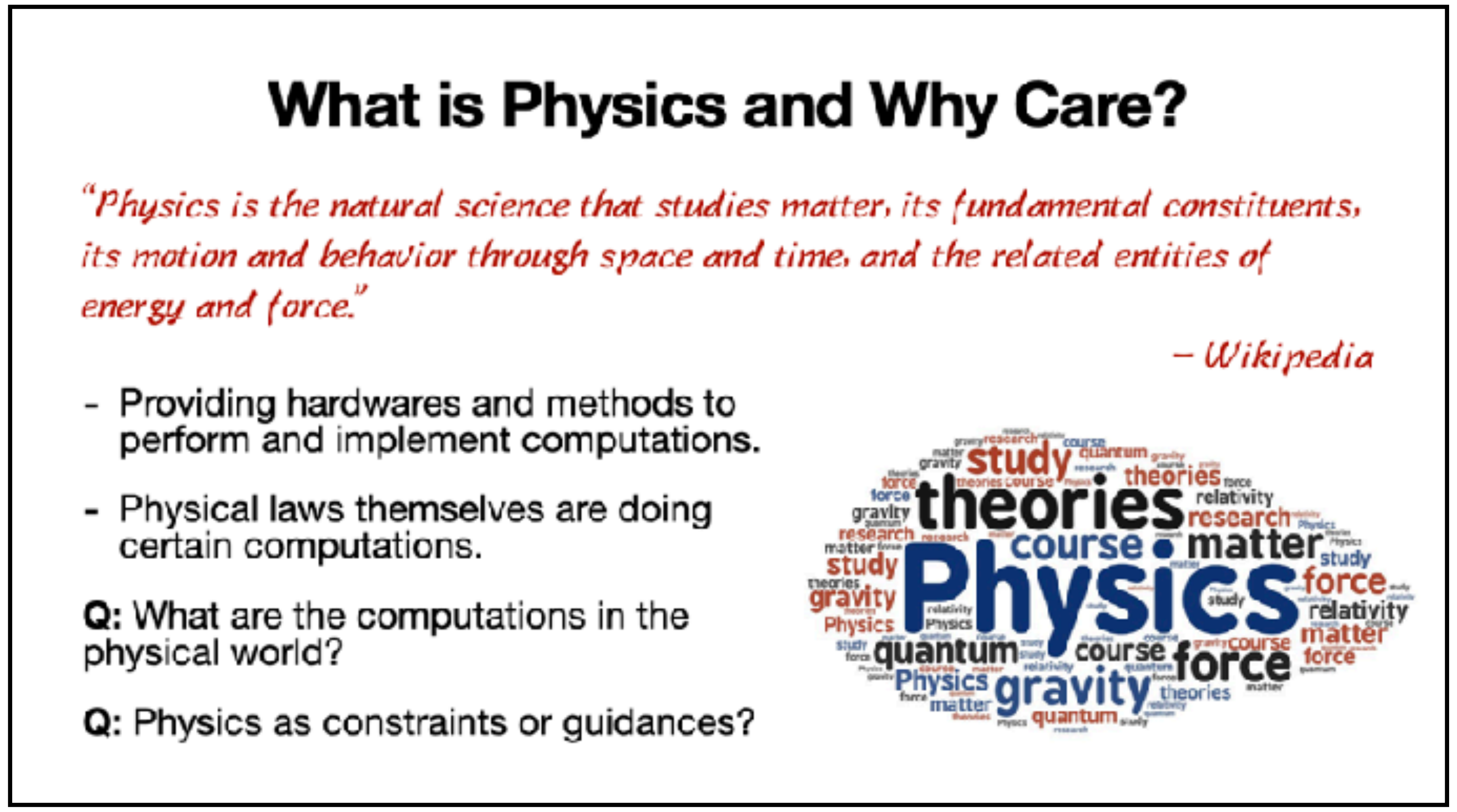
Lecture I.c

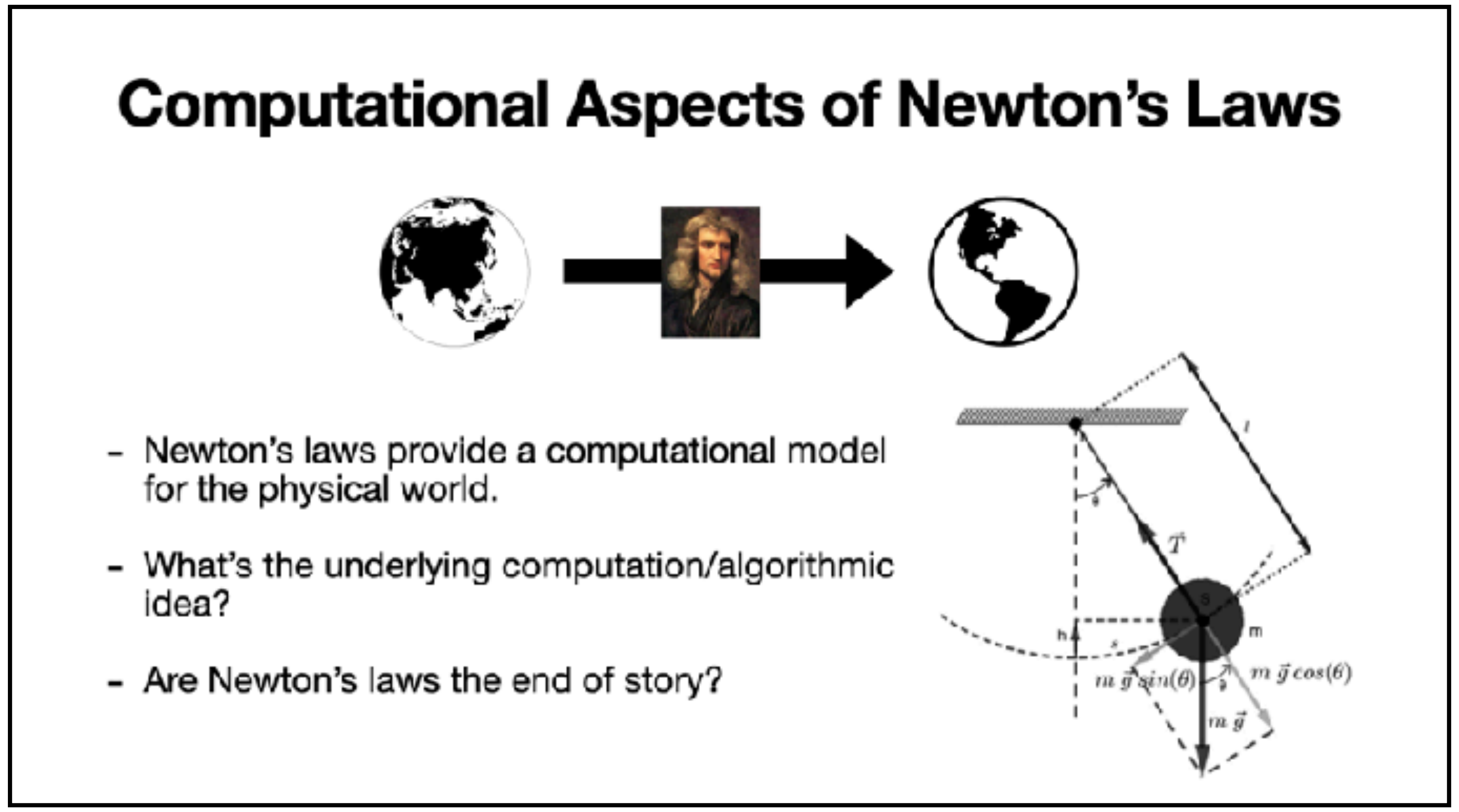
(Jan. 17 10am-11am ET)

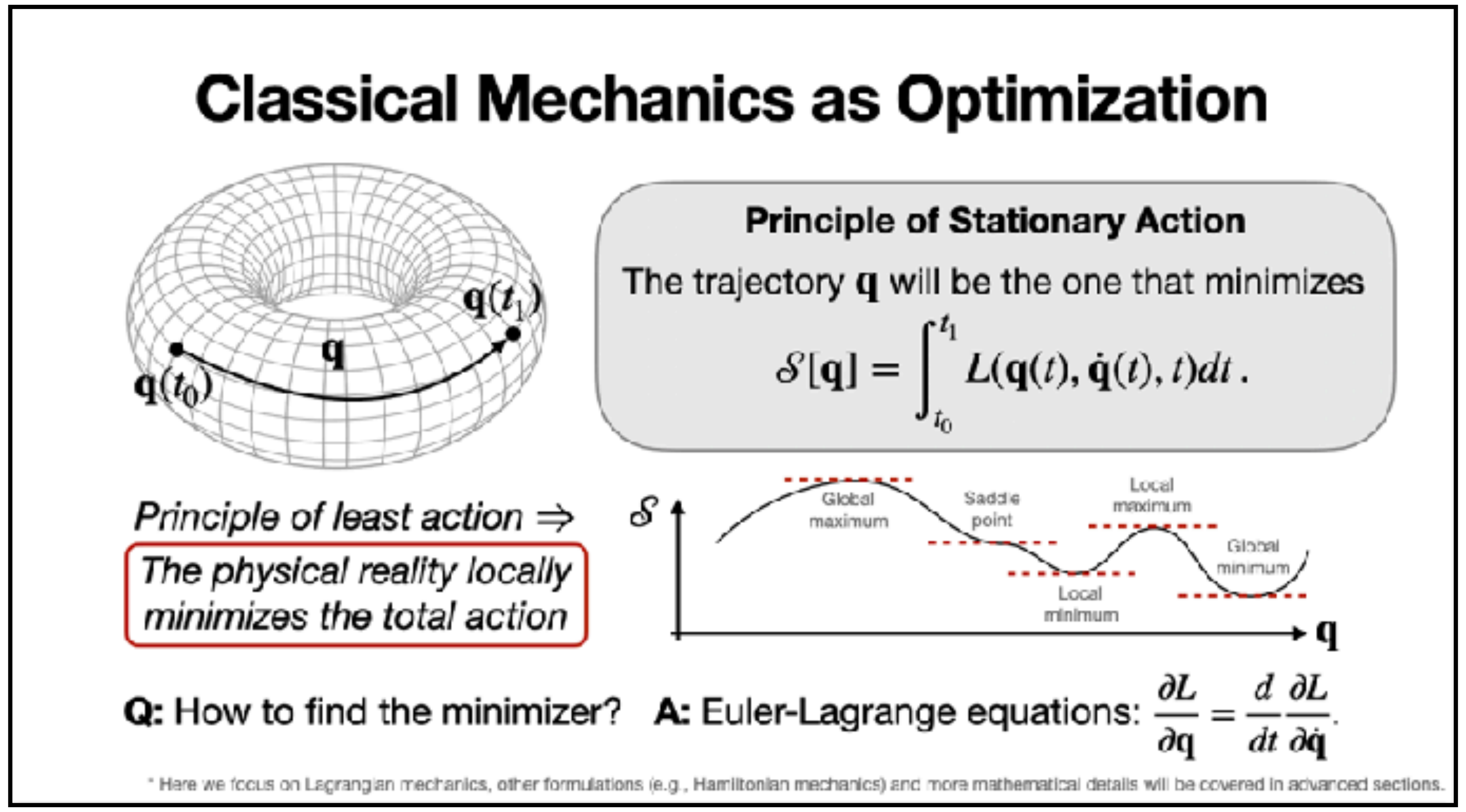
* Yao credited the original idea to [Smith 1993].

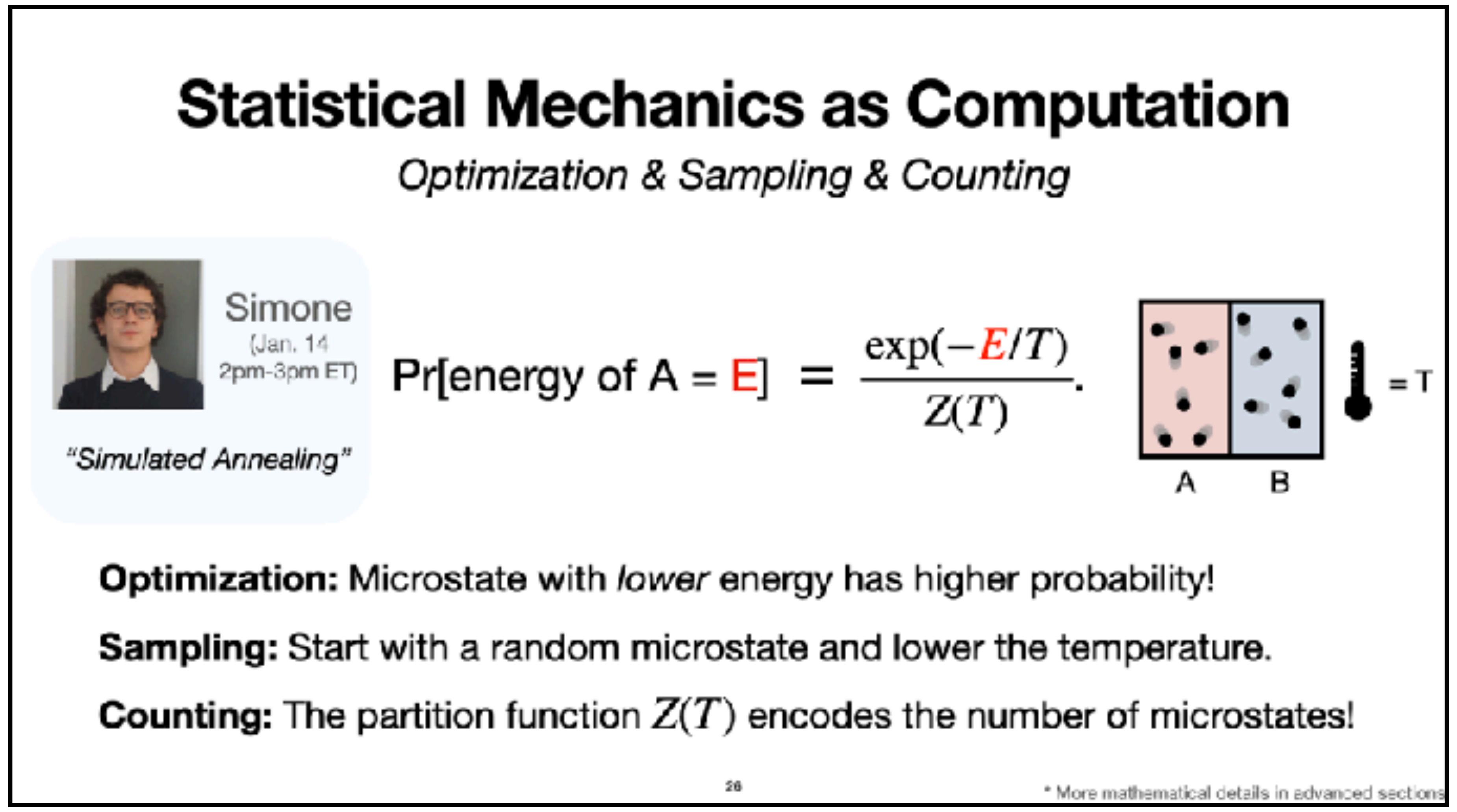
Summary

Key Concepts









Guest Speakers for Module II

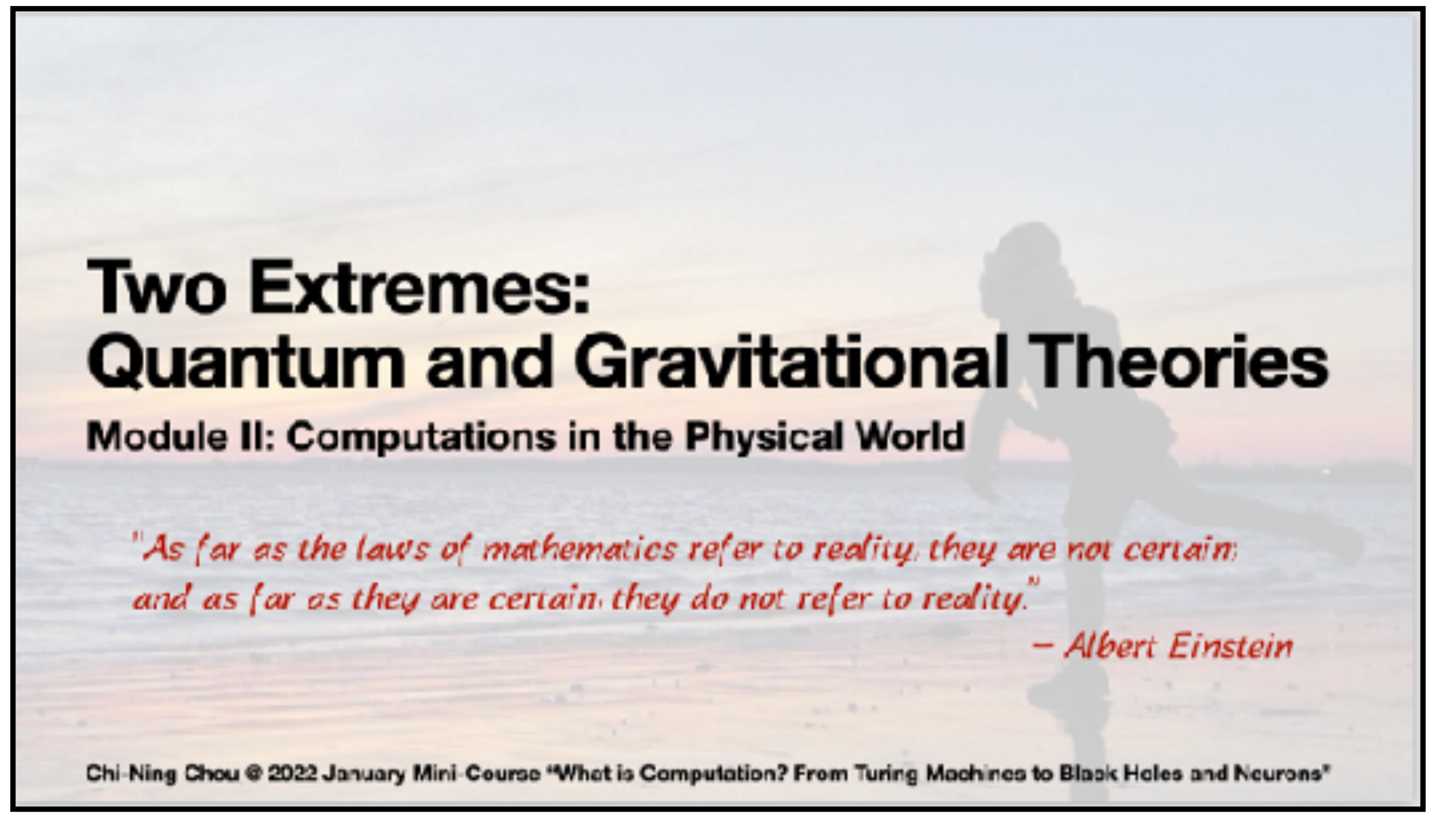
"Quantum Correlation: the Resource to Make Quantum Machine More Powerful"

Xun Gao
(Jan. 13 11am-12pm ET)

"Quantum Machine Learning from Algorithms to Reality"

Khadijeh Sona Najafi
(Jan. 14 11am-12pm ET)

Next



Lecture II.b
(Jan. 13 10am-10:50am ET)

Erick
(Jan. 13
2pm-3pm ET)

"Information Geometry"

Simone
(Jan. 14
2pm-3pm ET)

"Simulated Annealing"

Check them out on the calendar!

Food for Thought

Q: Do you think the physical world we are living in is deterministic?

Q: What's the "additional structure" of phase space?

Q: Can you come up with some examples of ergodicity in daily life?

Q: Can you come up with some examples of **not** having ergodicity in daily life?

Exercise

- What's the underlying "algorithmic idea" of the stationary action principle?
- Try to derive the Boltzmann distribution from the postulate of equal *a priori* probabilities!
- Try to figure out clearer the connection between partition function and counting problem.

References

Articles:

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- Gualtiero Piccinini and Corey Maley. “Computations in Physical Systems.” Stanford Encyclopedia of Philosophy, 2010, link.

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- Mezard, Marc, and Andrea Montanari. Information, physics, and computation. Oxford University Press, 2009, link.

Advanced Books:

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- Sakurai, Jun John, and Eugene D. Commins. “Modern quantum mechanics, revised edition.” (1995): 93-95, link.

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