

# Computational Microscopy

bridging the gap between simple models and complex reality

Group Leader

Weria Pezeshkian ([weria.pezeshkian@nbi.ku.dk](mailto:weria.pezeshkian@nbi.ku.dk))

## Current members

Neda Rahmani



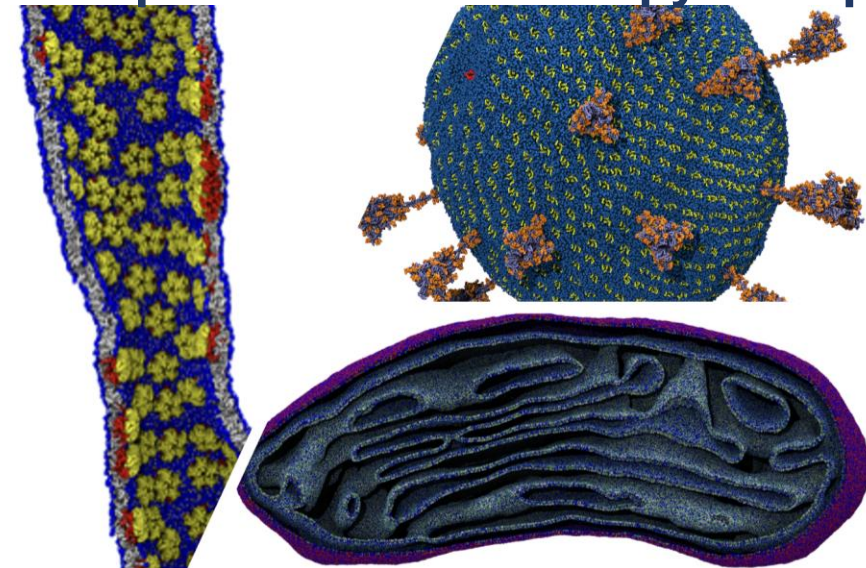
Fabian Schuhmann



Adrià B. Vidal



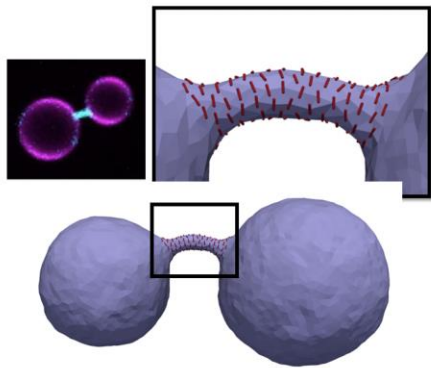
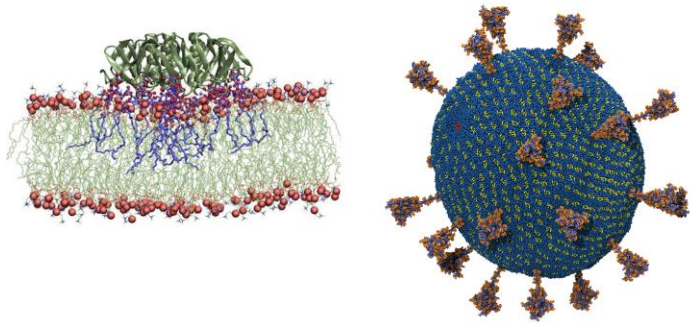
## Computational Microscopy Group



# Research topics

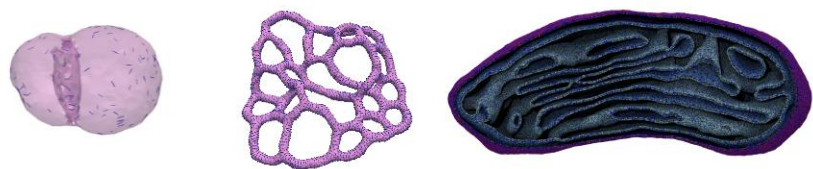
# Development

virial and toxic particles

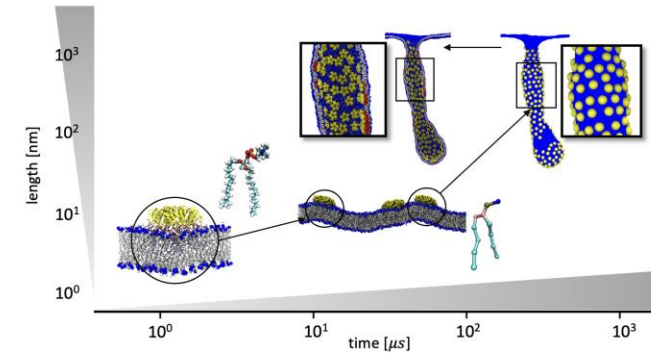


cell division

emergence of intracellular forms



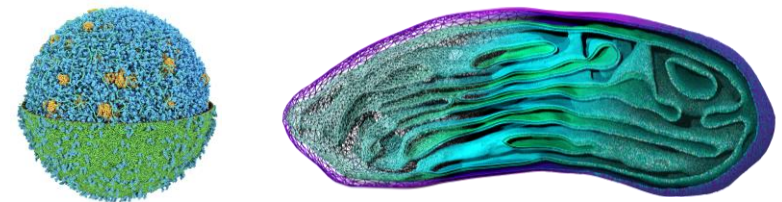
multiscale simulations scheme



**FreeDTS:** mesoscale simulation software



**TS2CG:** structure builder for next generation MD simulations



Computational  
Microscopy

# Why is important

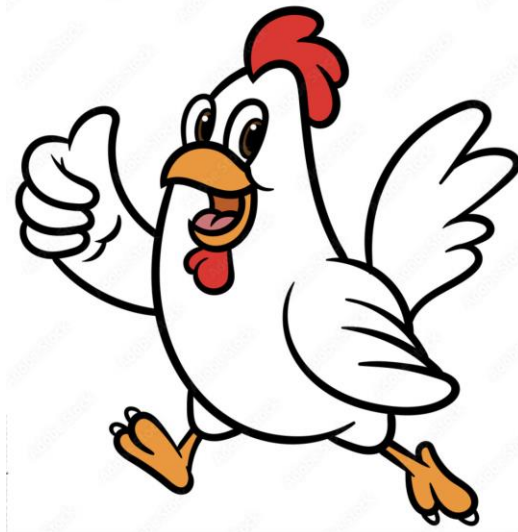
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Scientific knowledge emerges from results by different methodologies.

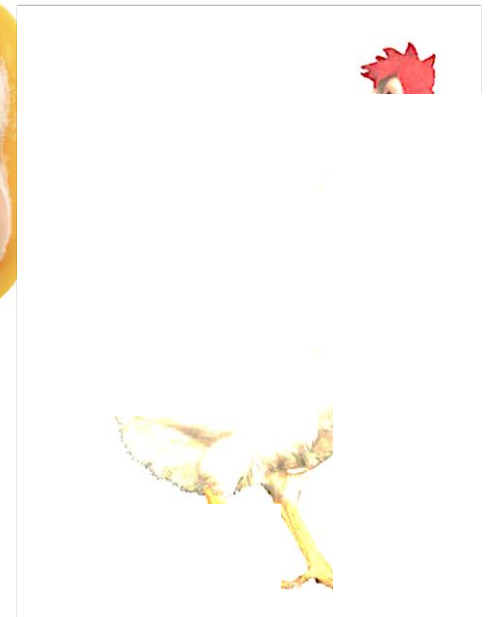
**chicken**



**simulation**



**experiment**



# Division of artificial cells

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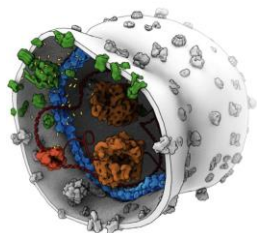


<https://www.syntheticcell.eu/>

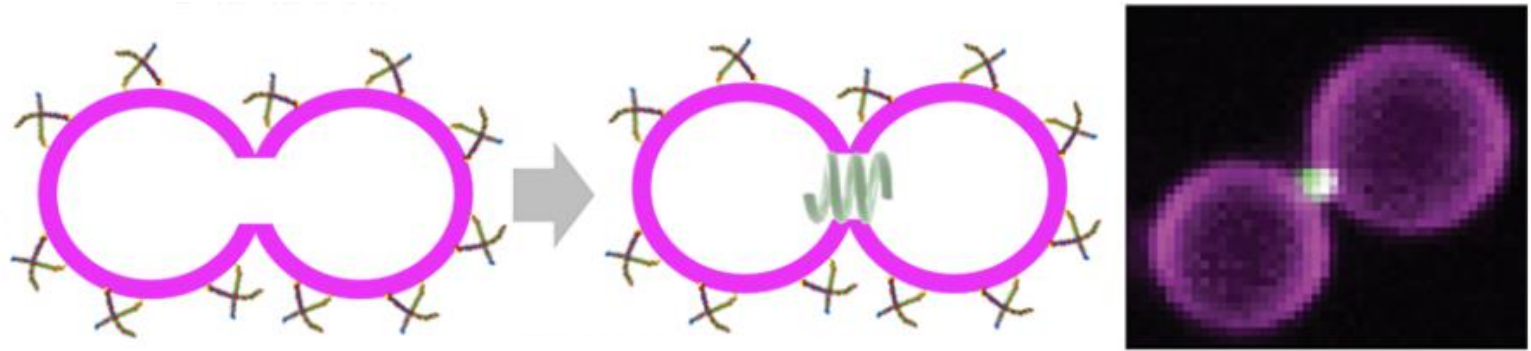
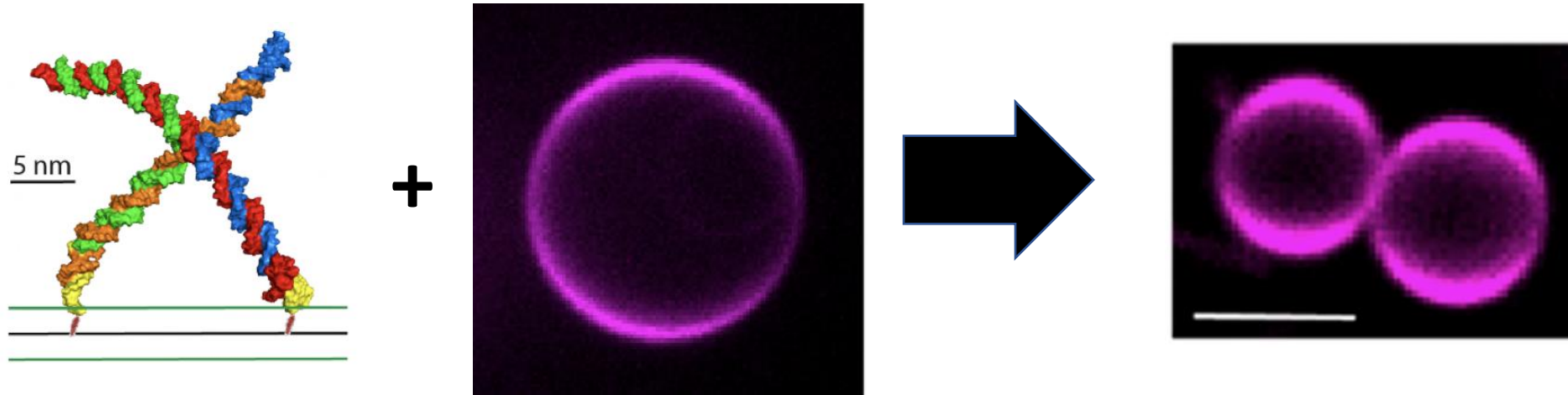


European Synthetic Cell Initiative

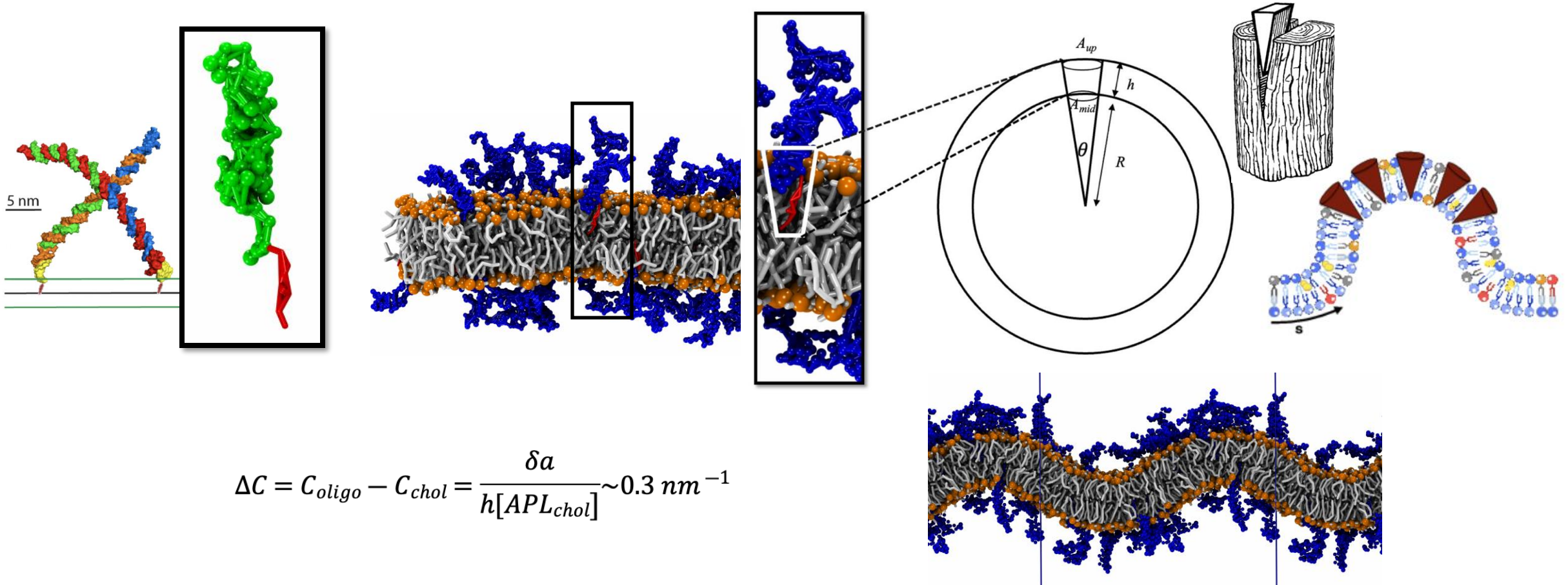
*Nature is our next technology*



# Division of an artificial cell

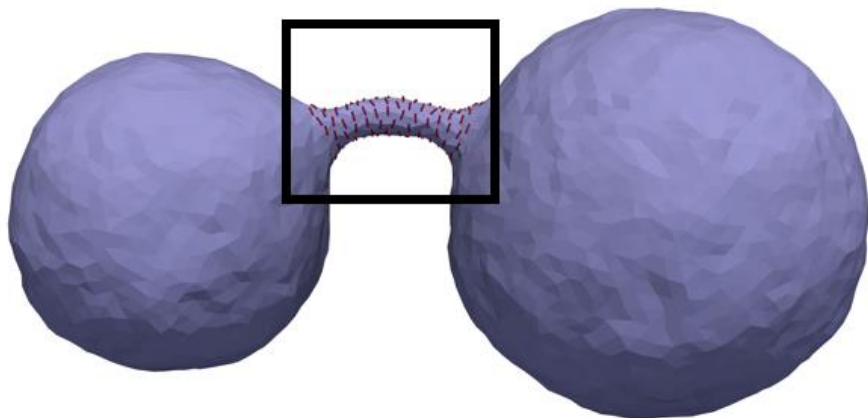
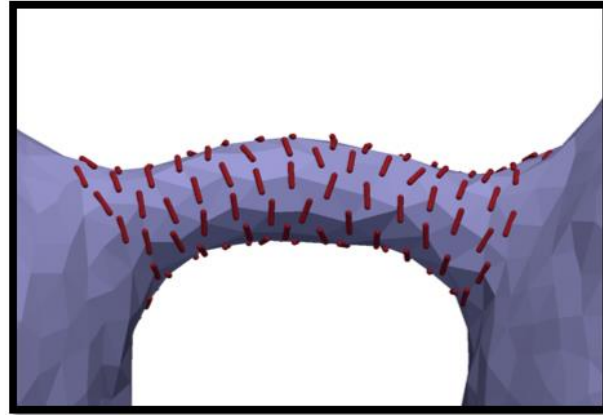
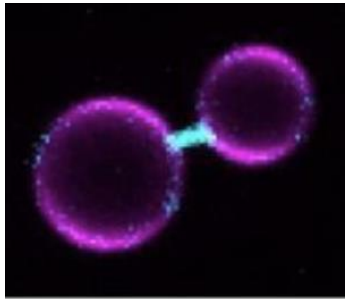


# Shaping membranes

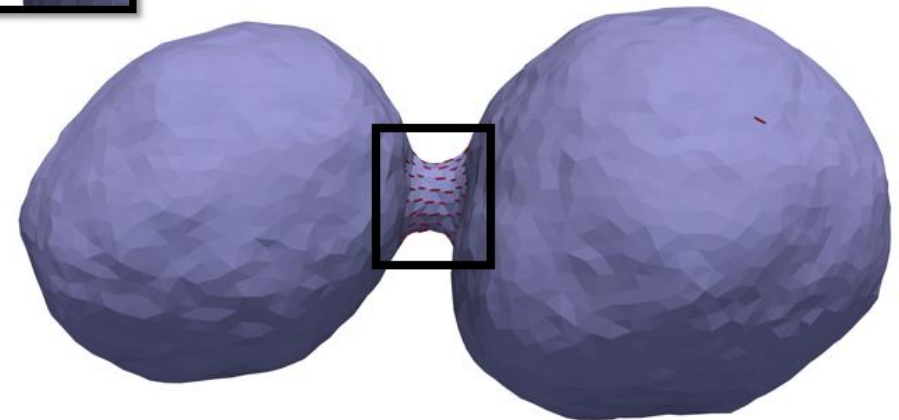
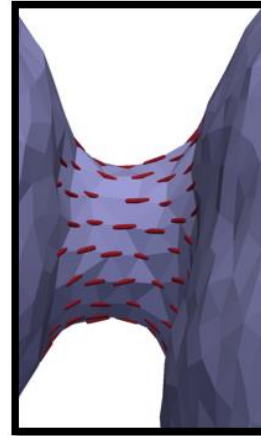


# Recruitment of enzymatic proteins

negative curvature: binding from inside



positive curvature: binding from inside



# NBIA MSc Day 2023: Non-equilibrium statistical mechanics

## Karel Proesmans

Group members:



Jonas Berx



Prashant Singh



Dana Kamp

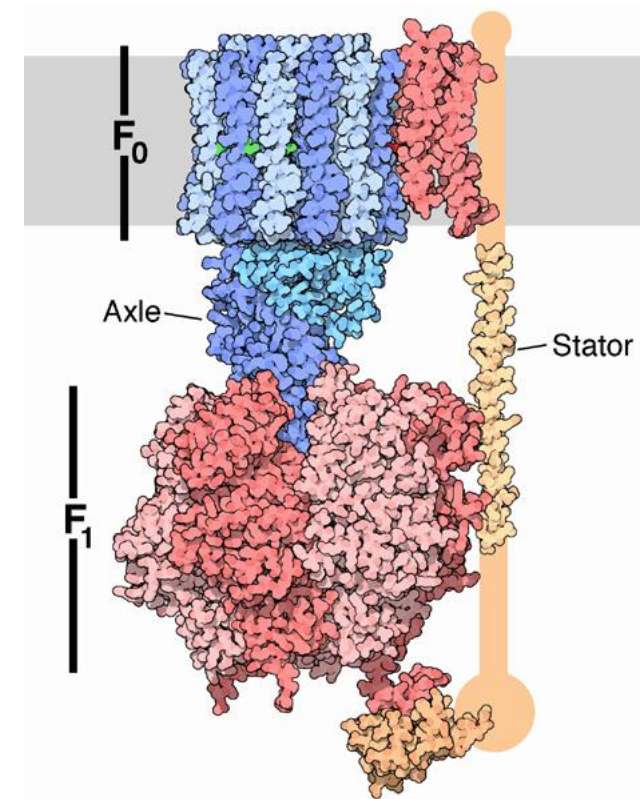


# Introduction: non-equilibrium statistical mechanics and stochastic thermodynamics

Classical thermodynamics:  
steam engine



Stochastic thermodynamics:  
ATP synthase



# Introduction: stochastic thermodynamics

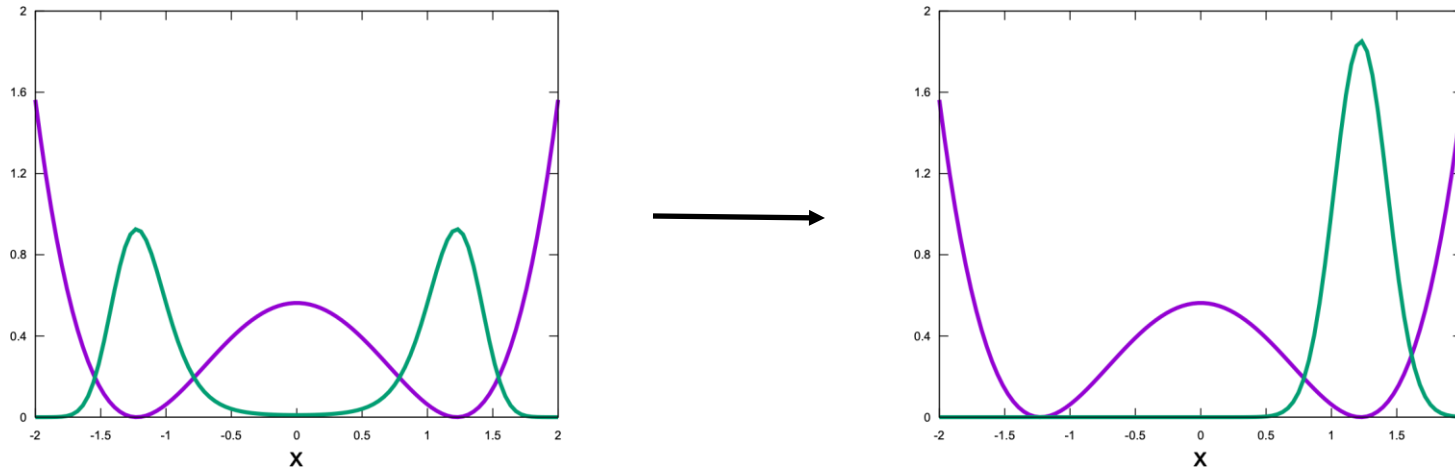
Classical thermodynamics:  
Second law

$$\Delta S \geq 0$$

Stochastic thermodynamics:  
Fluctuation theorem

$$\frac{p(\Delta S)}{p(-\Delta S)} = e^{\frac{\Delta S}{k_B}}$$

# Possible projects: Machine learning optimal bit erasure



- Landauer limit:

$$W \geq k_B T \ln 2$$

- Limits under limited control (electronic+biological applications)
- Machine-learning based methods

# Possible projects: optimal protocols

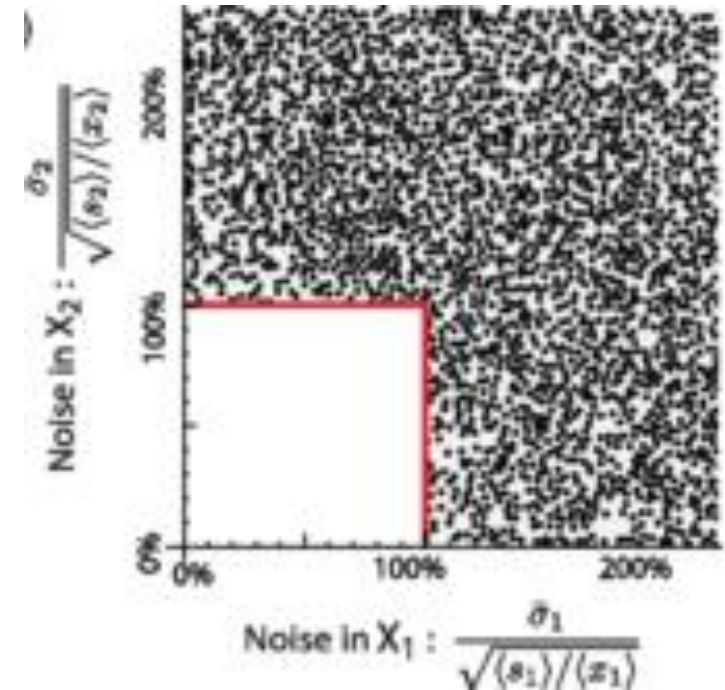
- Derive new no-go theorems for thermodynamic processes
- Example:

$$x_1 \xrightarrow{f(x_2)} x_1 + b_1,$$

$$x_2 \xrightarrow{g(x_1)} x_2 + b_2,$$

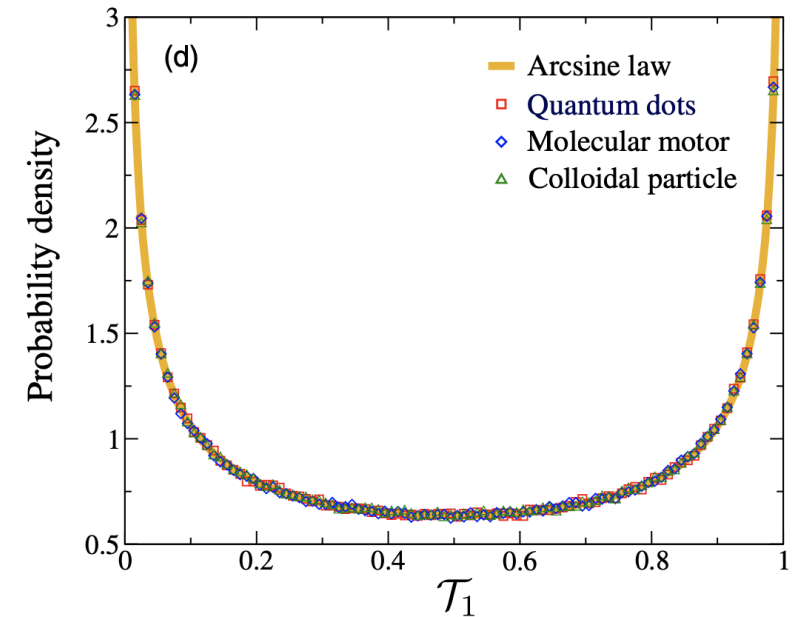
$$x_1 \xrightarrow{x_1/\tau_1} x_1 - 1,$$

$$x_2 \xrightarrow{x_2/\tau_2} x_2 - 1.$$



# Possible projects: arcsine laws for chemical reaction networks

- Arcsine laws
- Applications to chemical reaction networks



Questions?