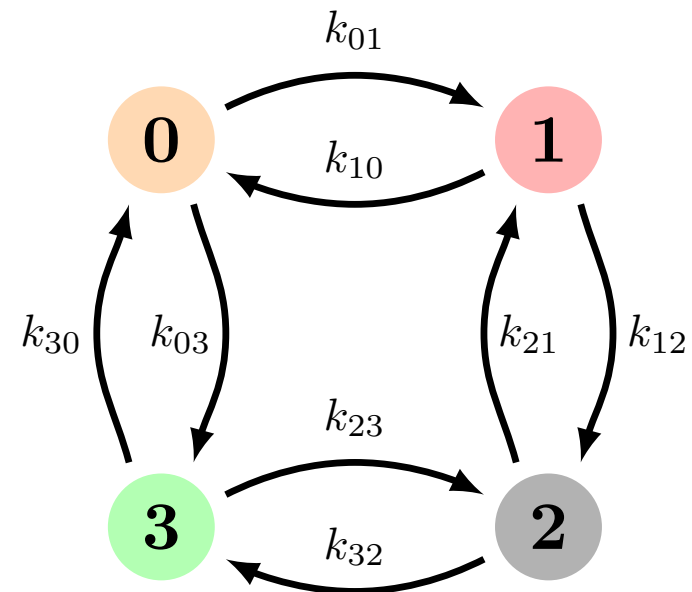
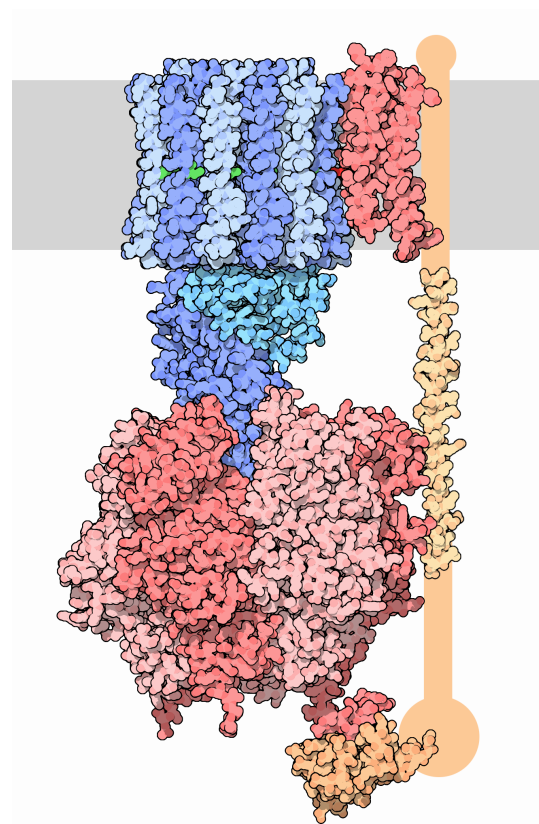


Molecular machinery

Quantifying the energetic cost of controlling nanoscale biological systems



CAP Congress 2019

Steven Large


Department of Physics, Simon Fraser University

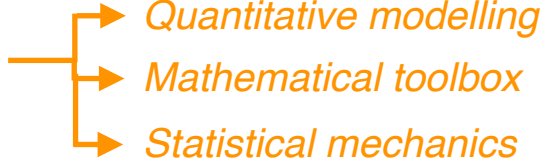
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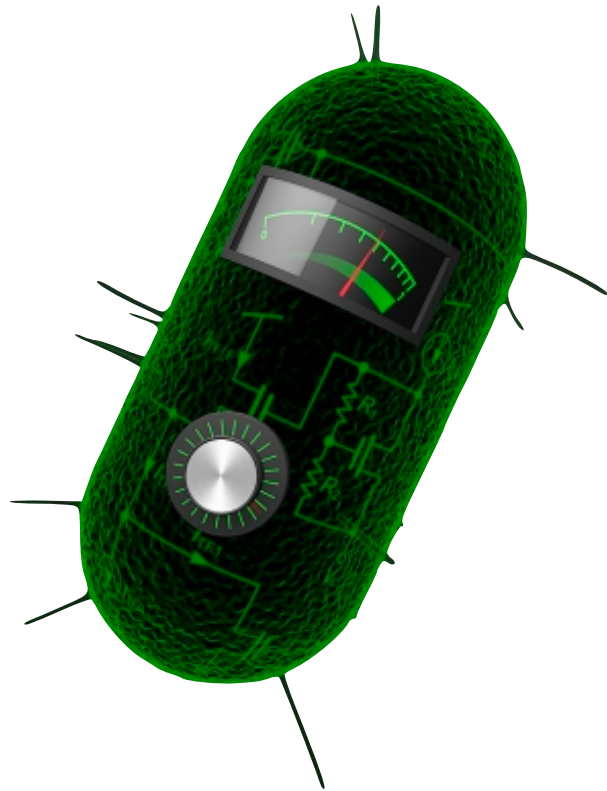
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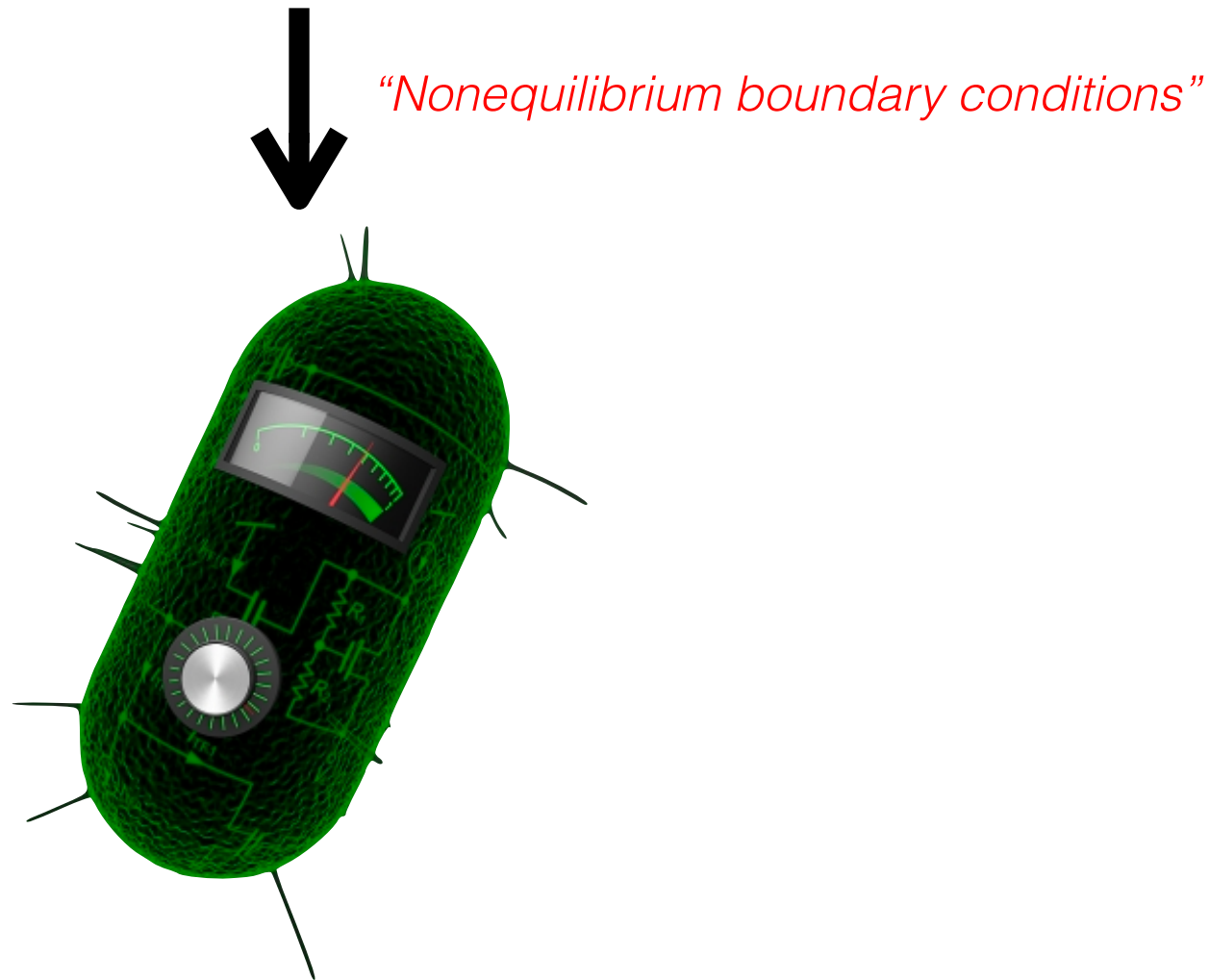
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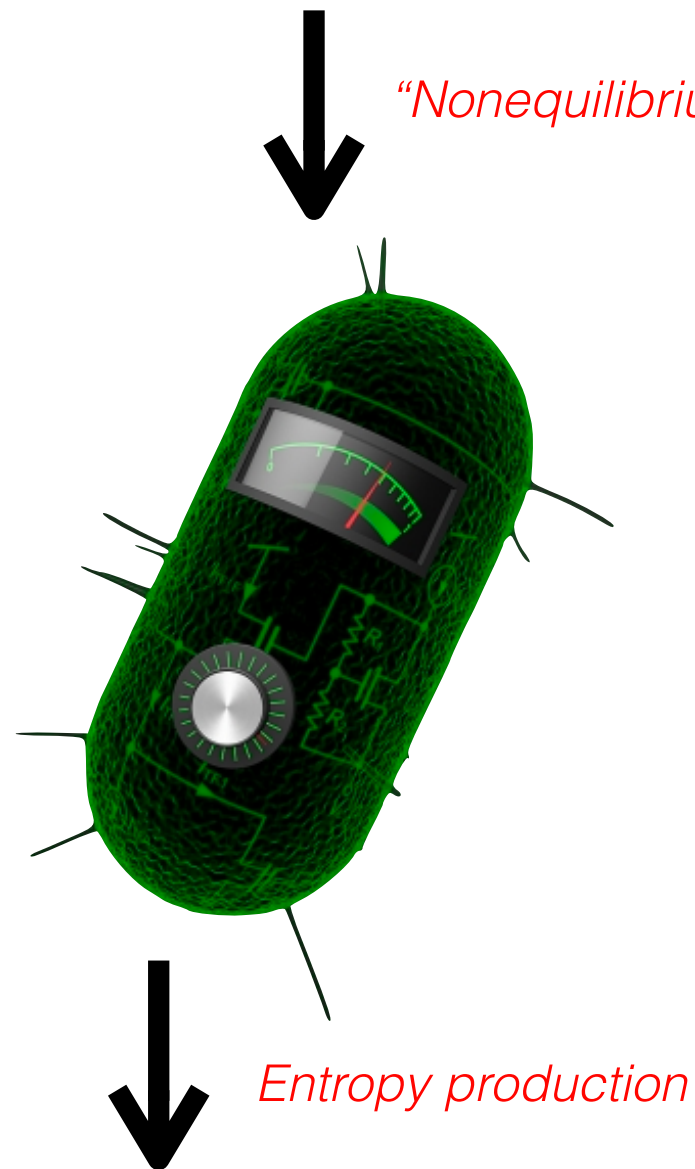
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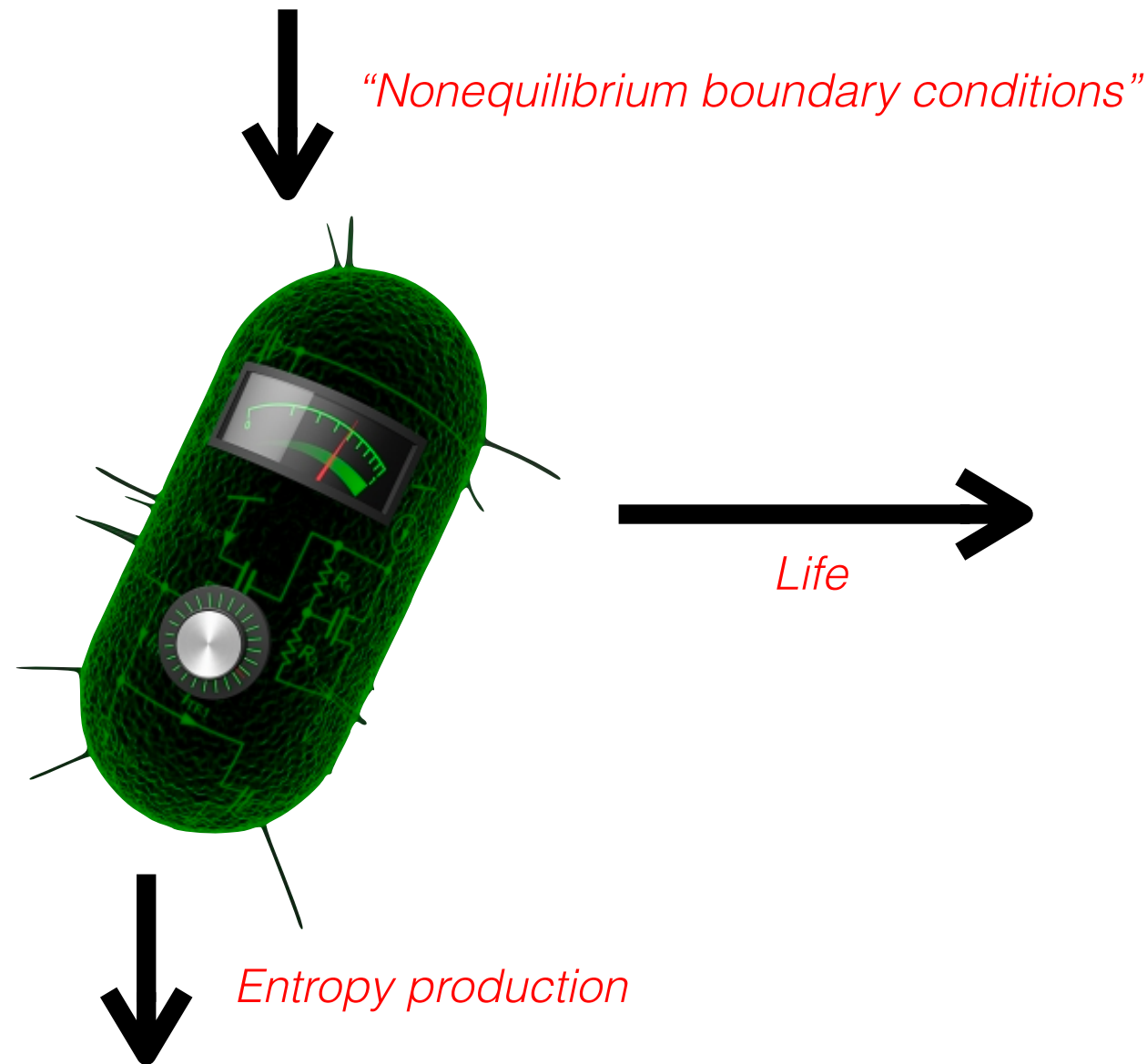
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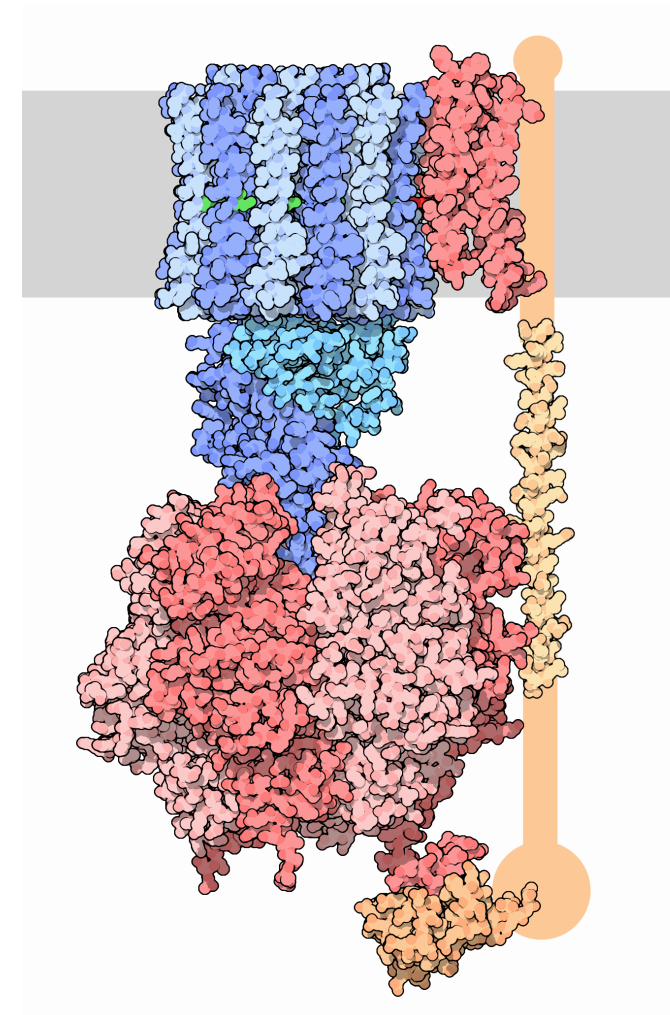
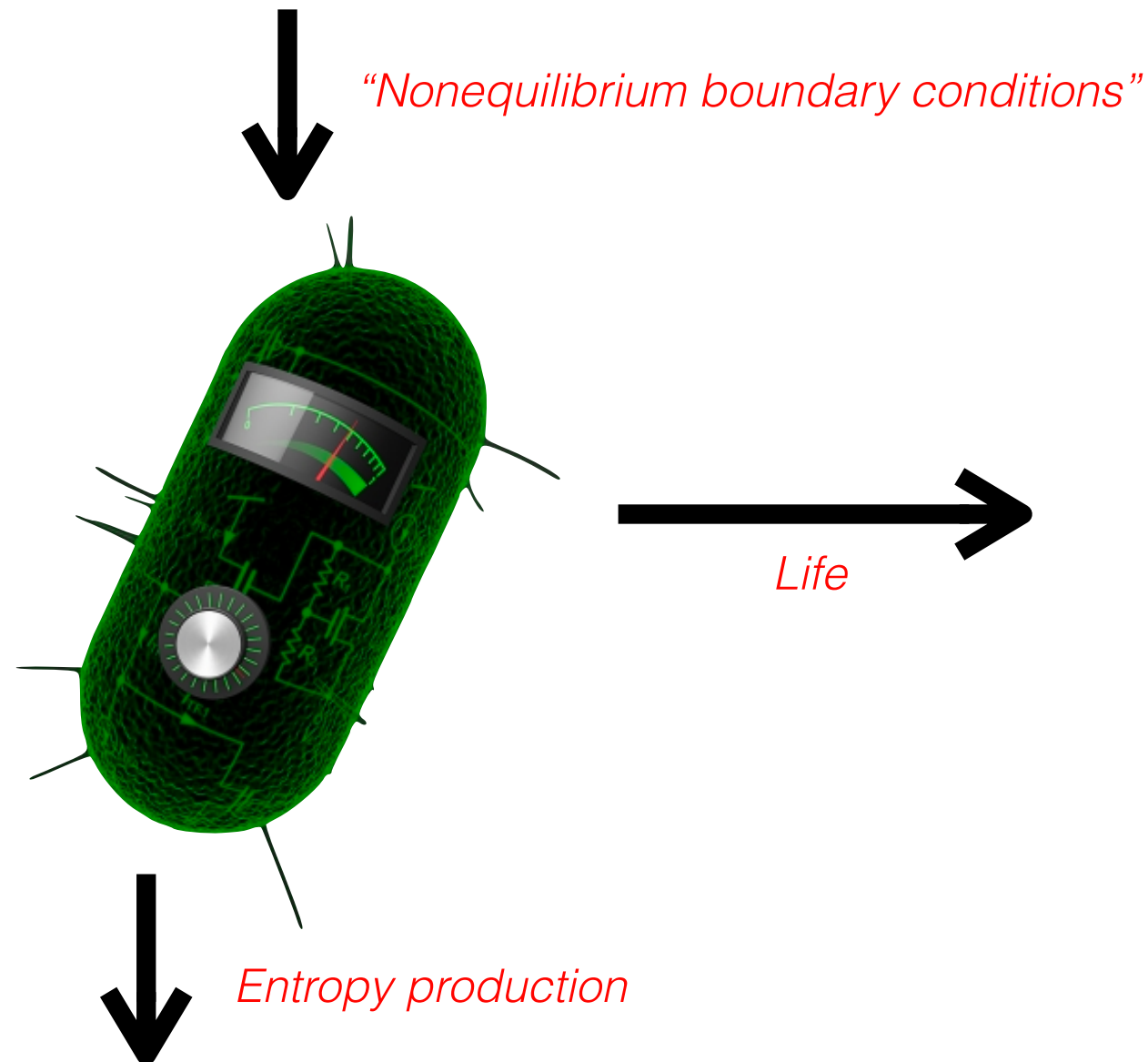
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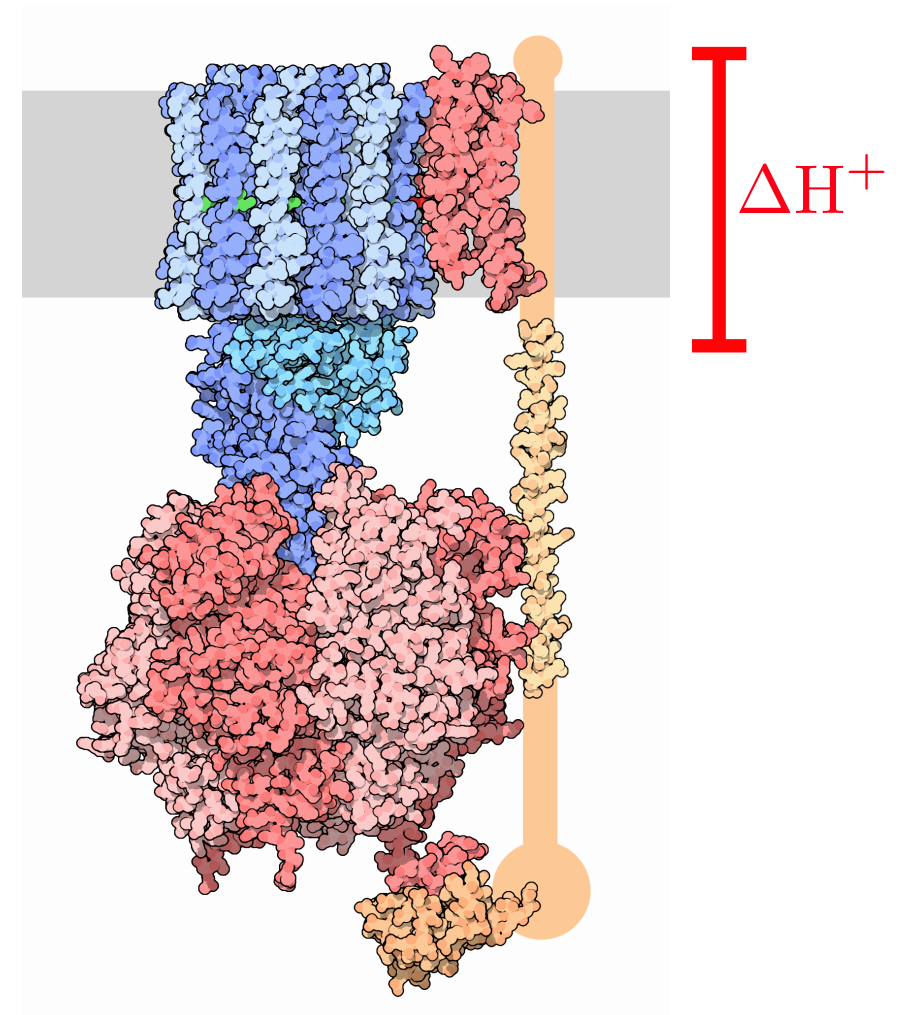
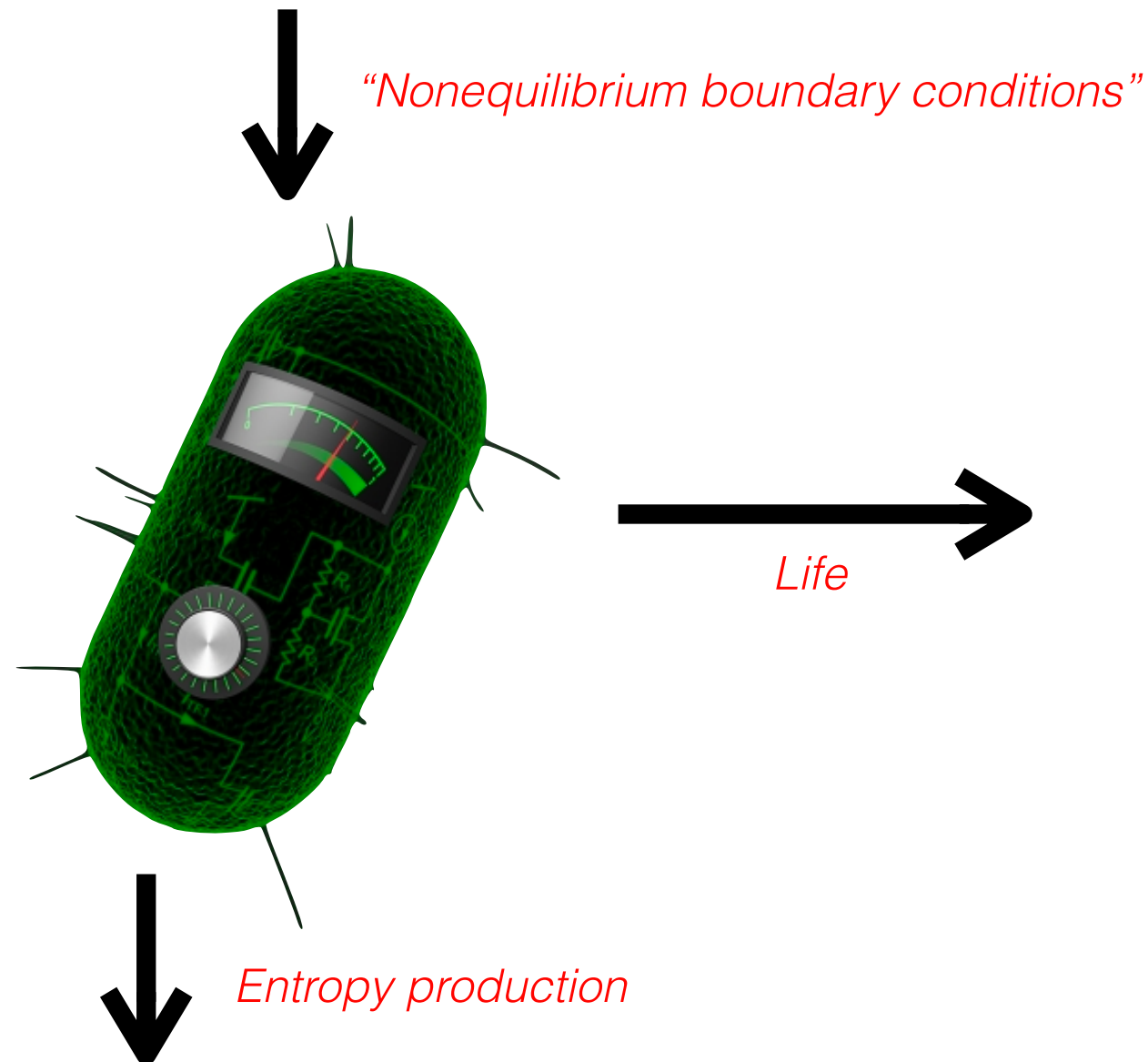
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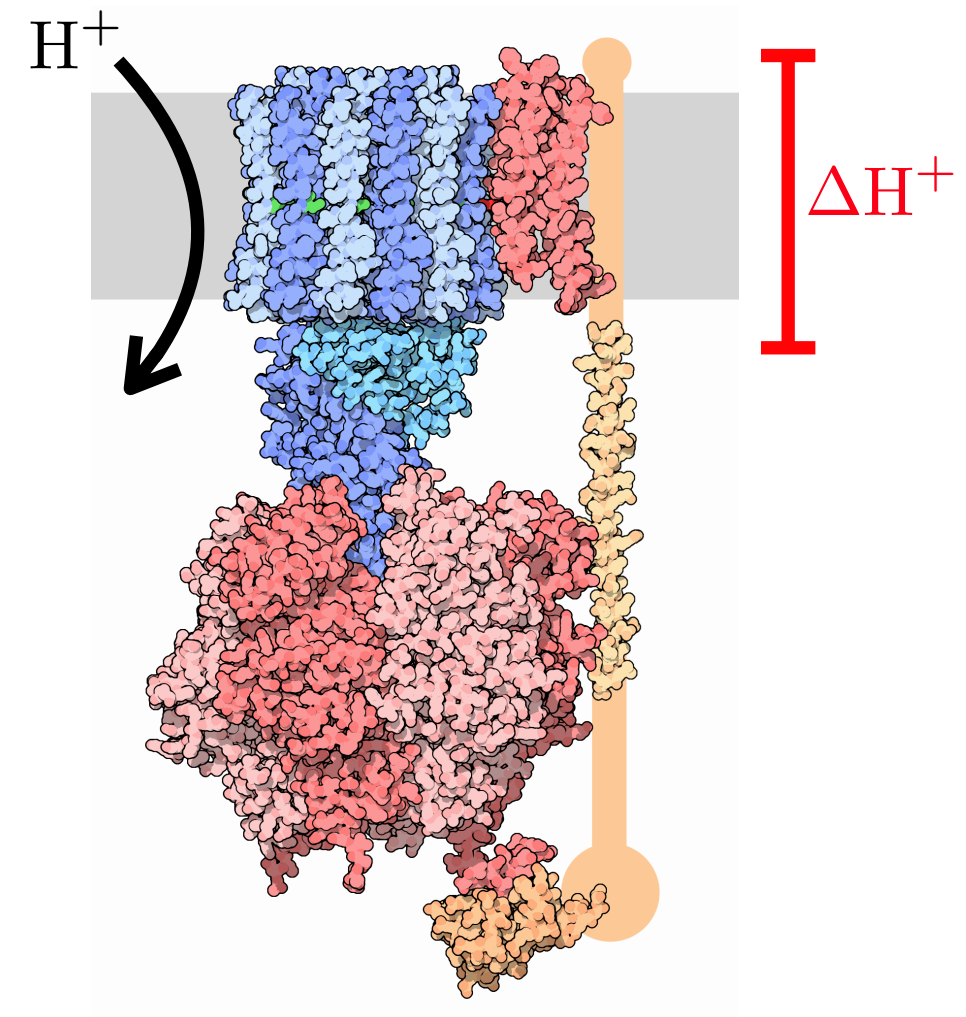
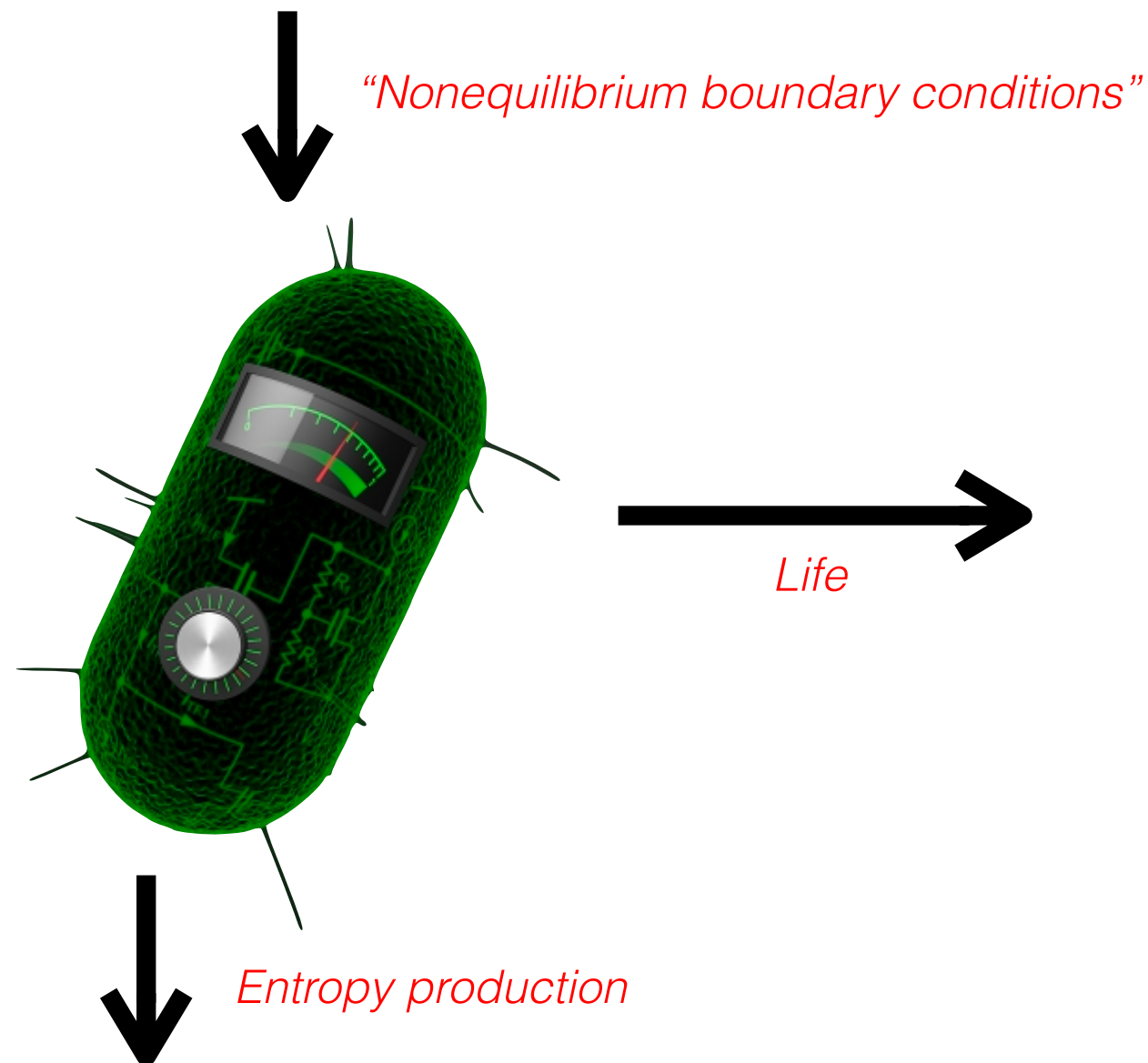
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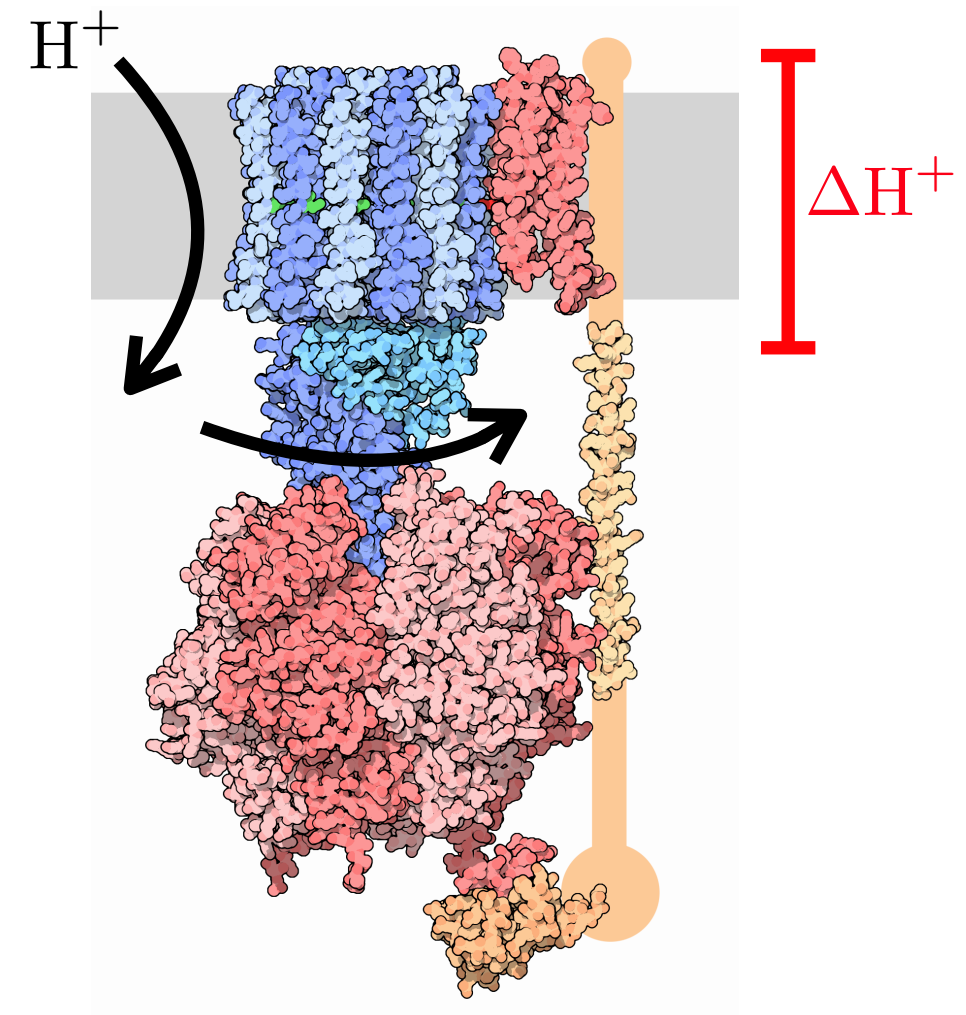
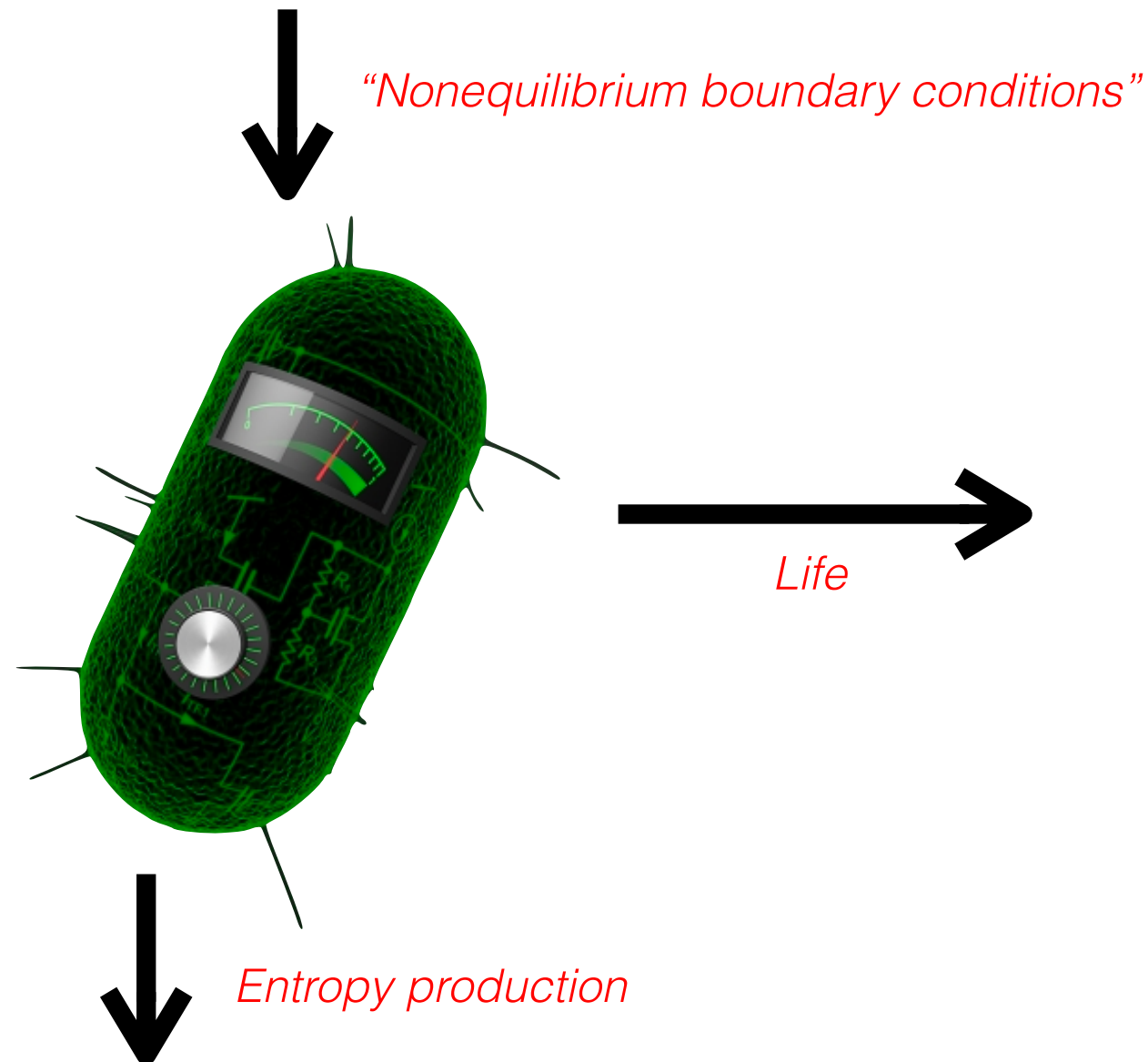
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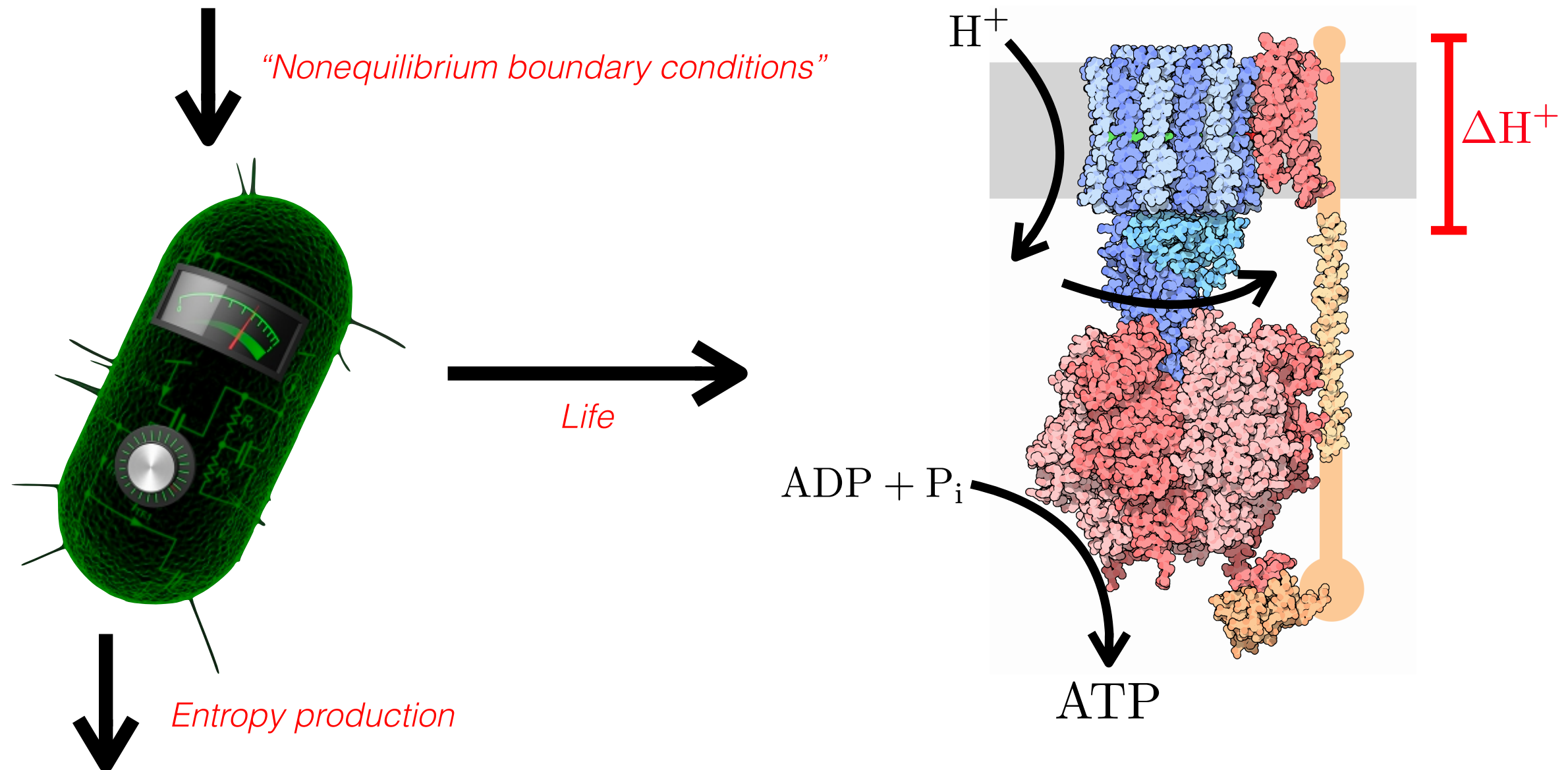
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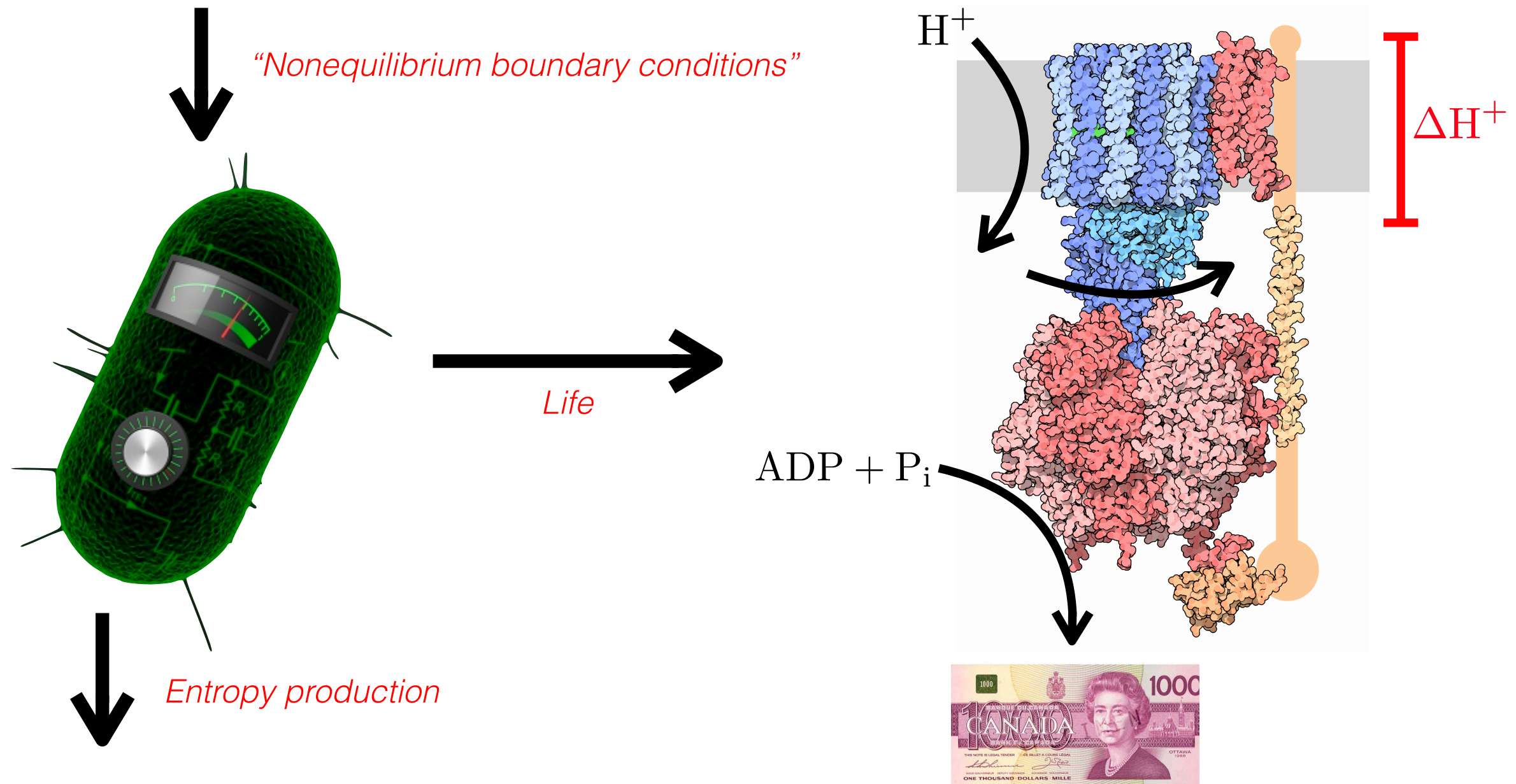
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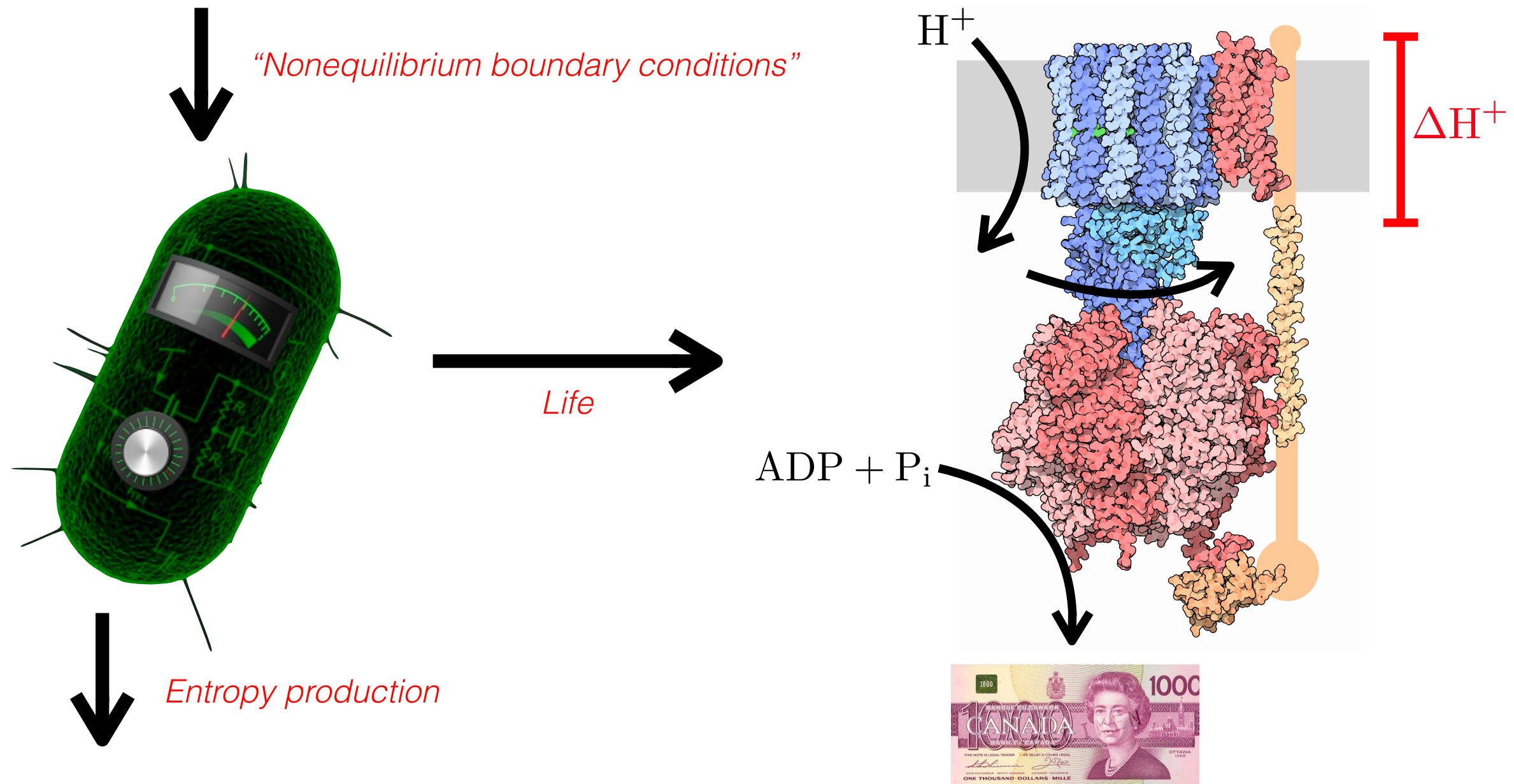
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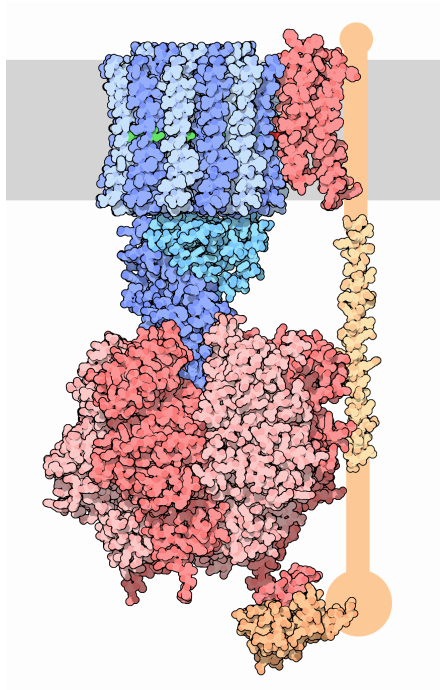
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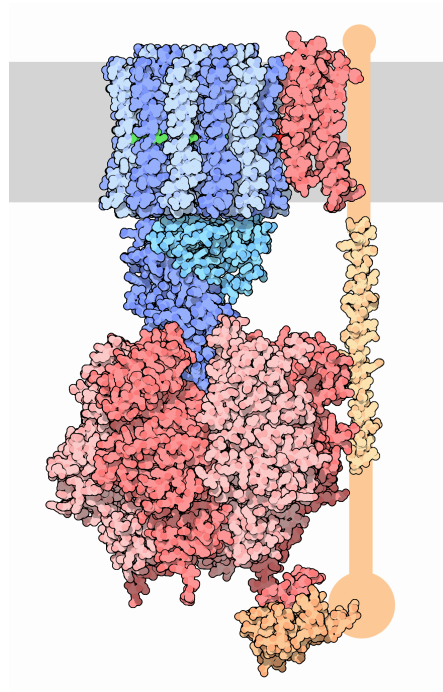
- Quantifying flows of **energy** (and other things) in nanoscale systems is a central challenge to understanding microscopic physics of biological systems

- How can we formulate a mathematical description of a nonequilibrium system?

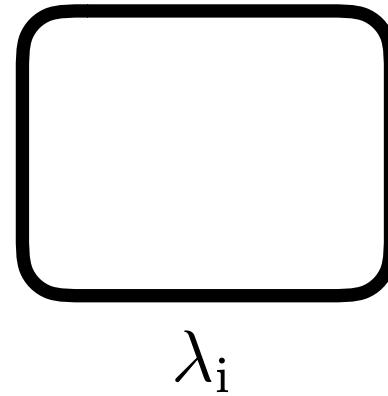
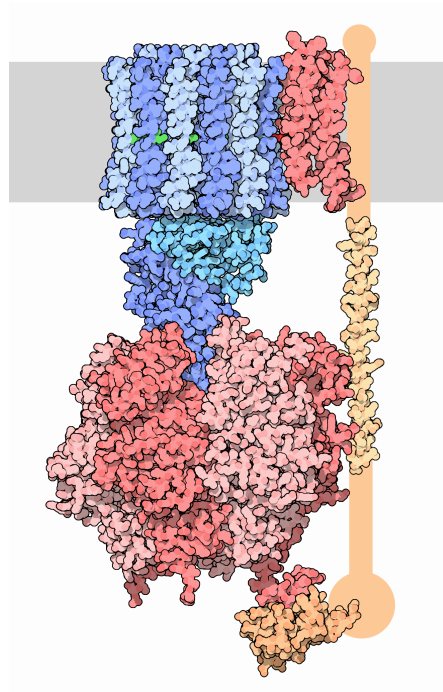
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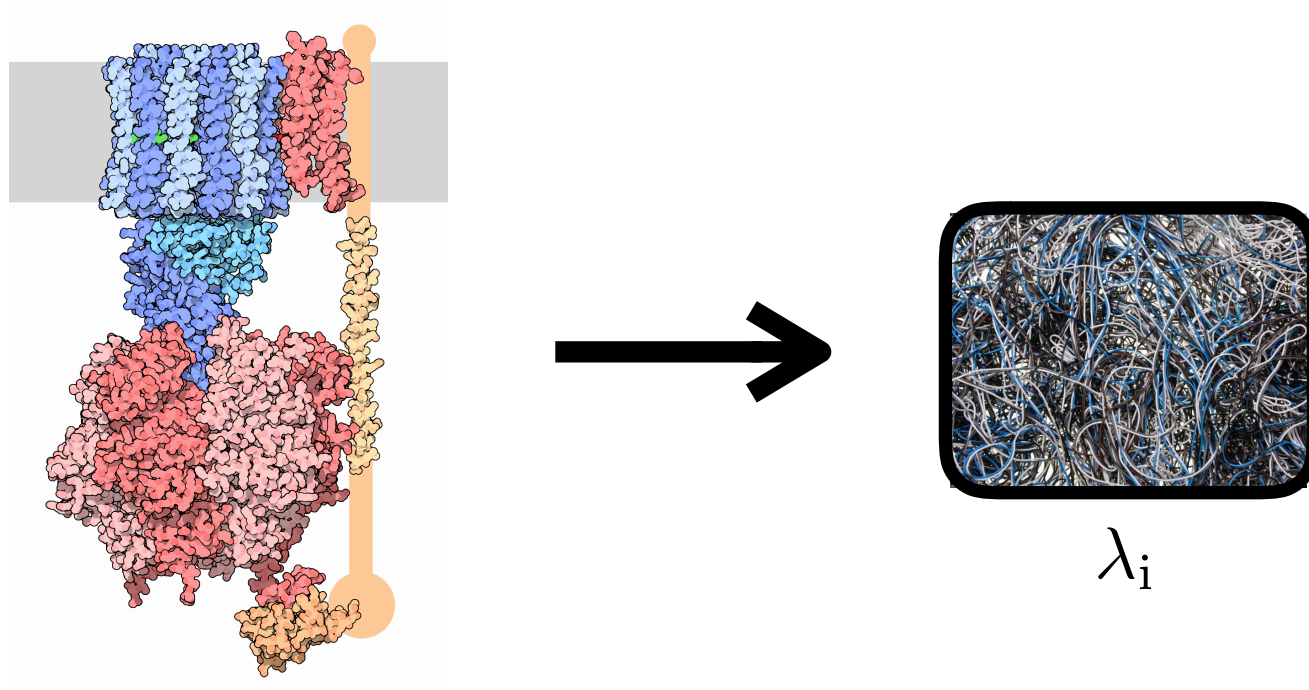
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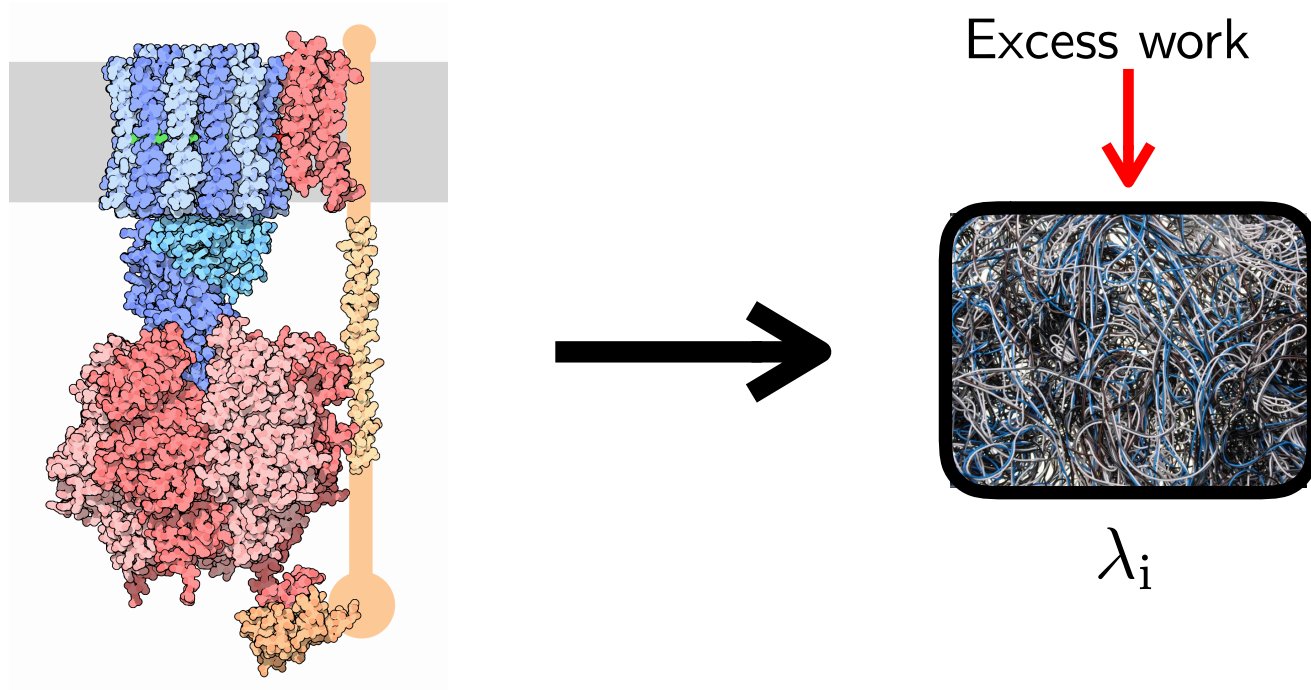
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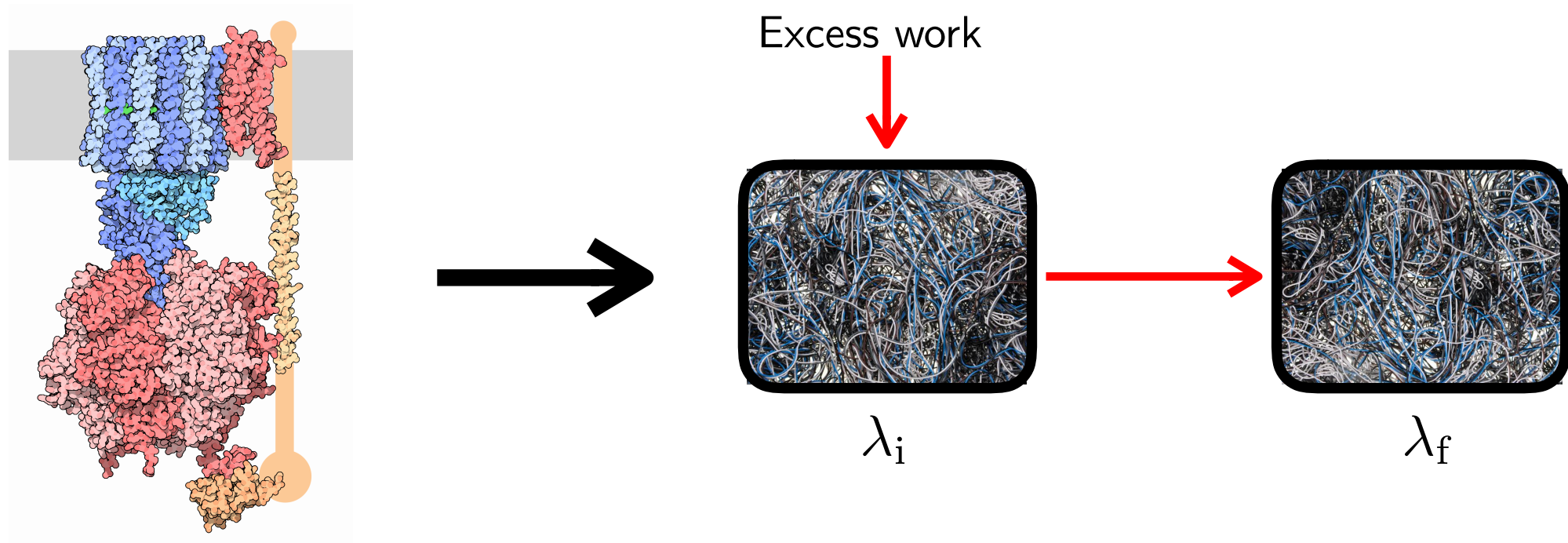
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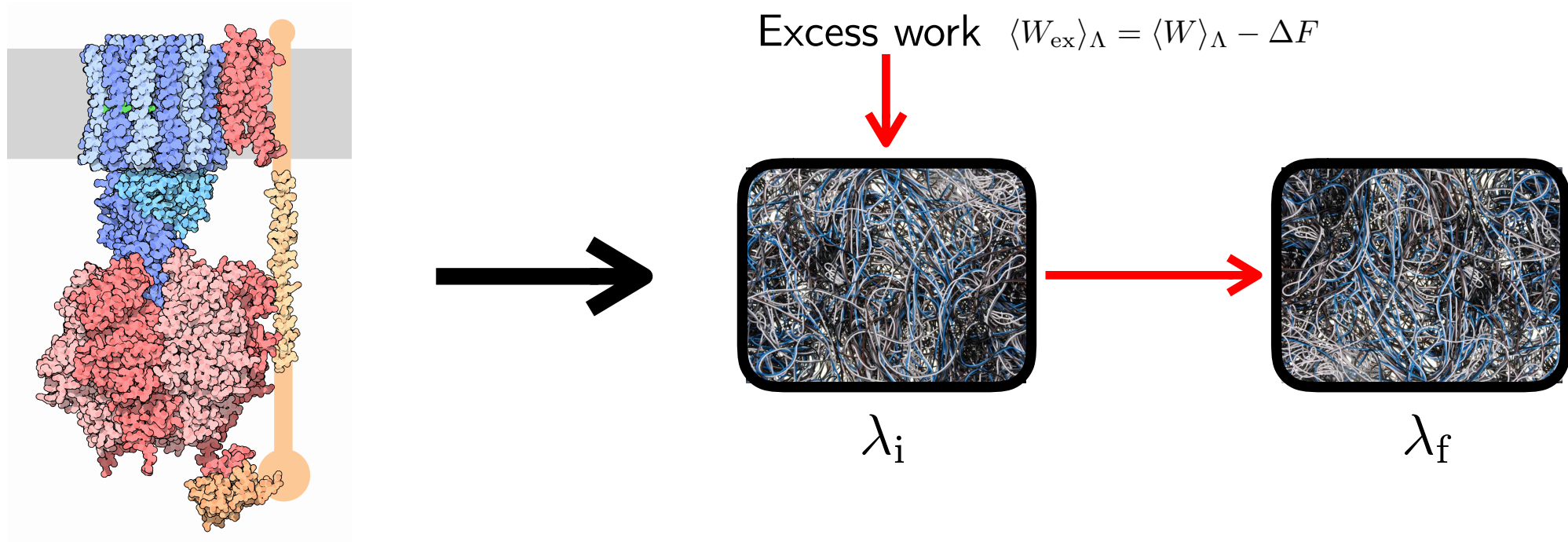
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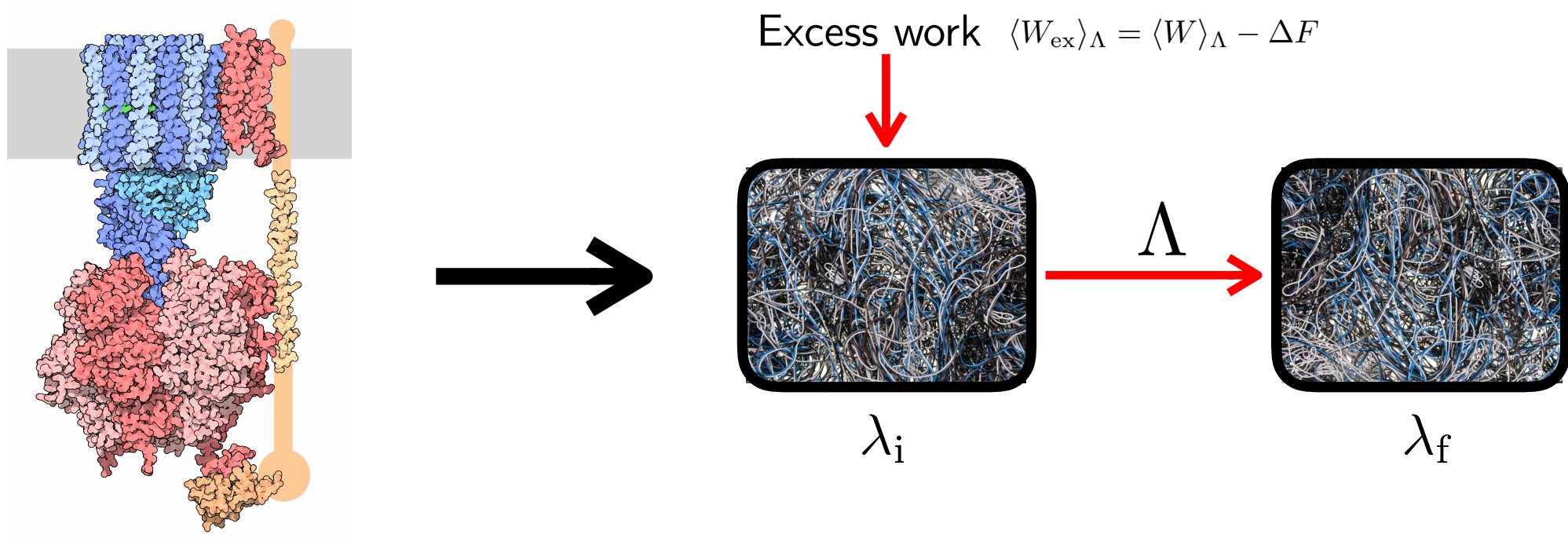
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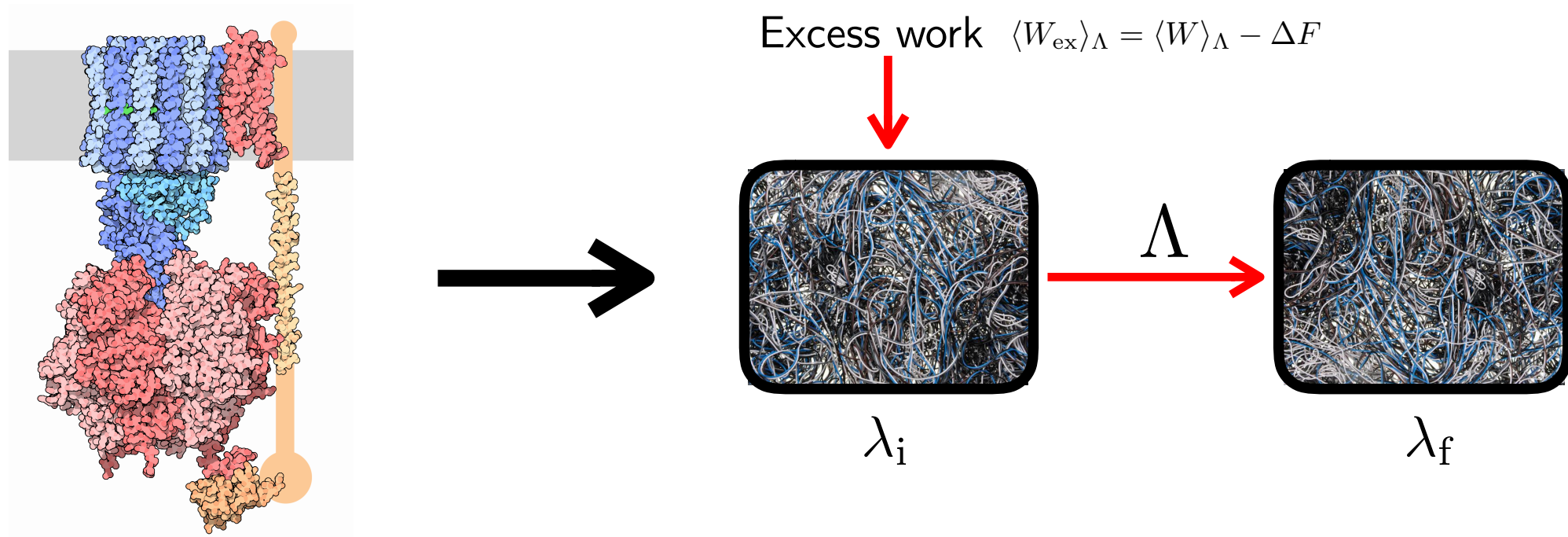
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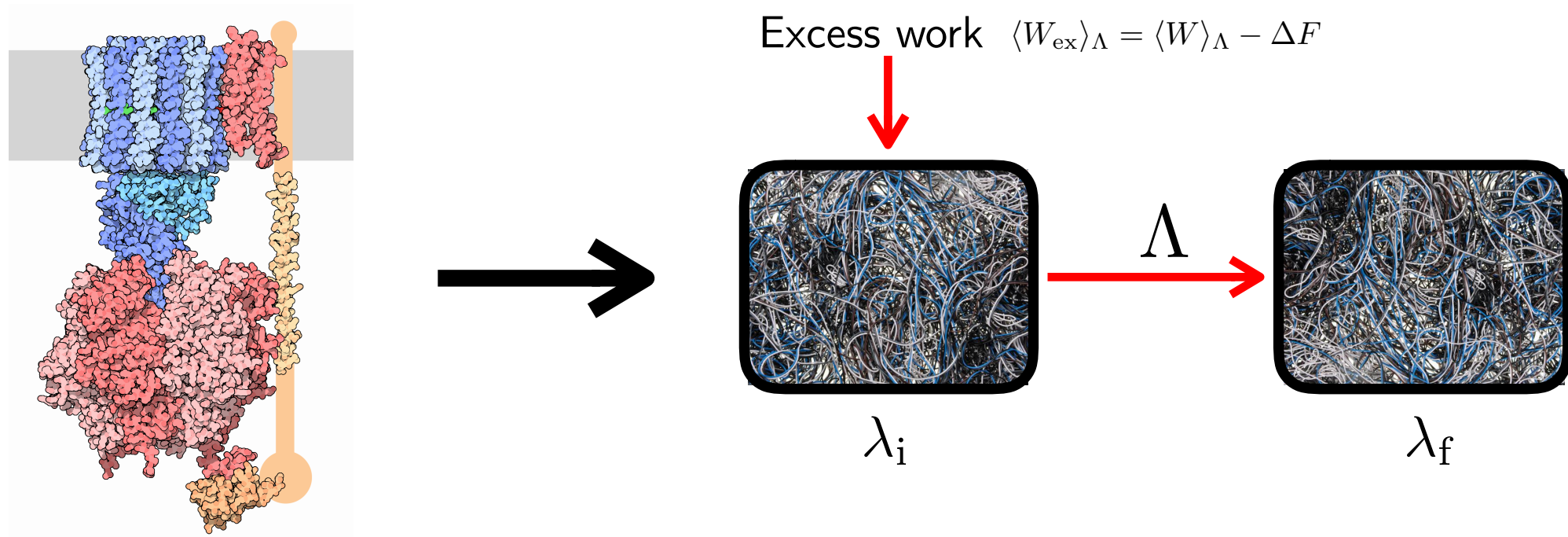


- How can we formulate a mathematical description of a nonequilibrium system?



- Average excess work required depends on the particular control protocol

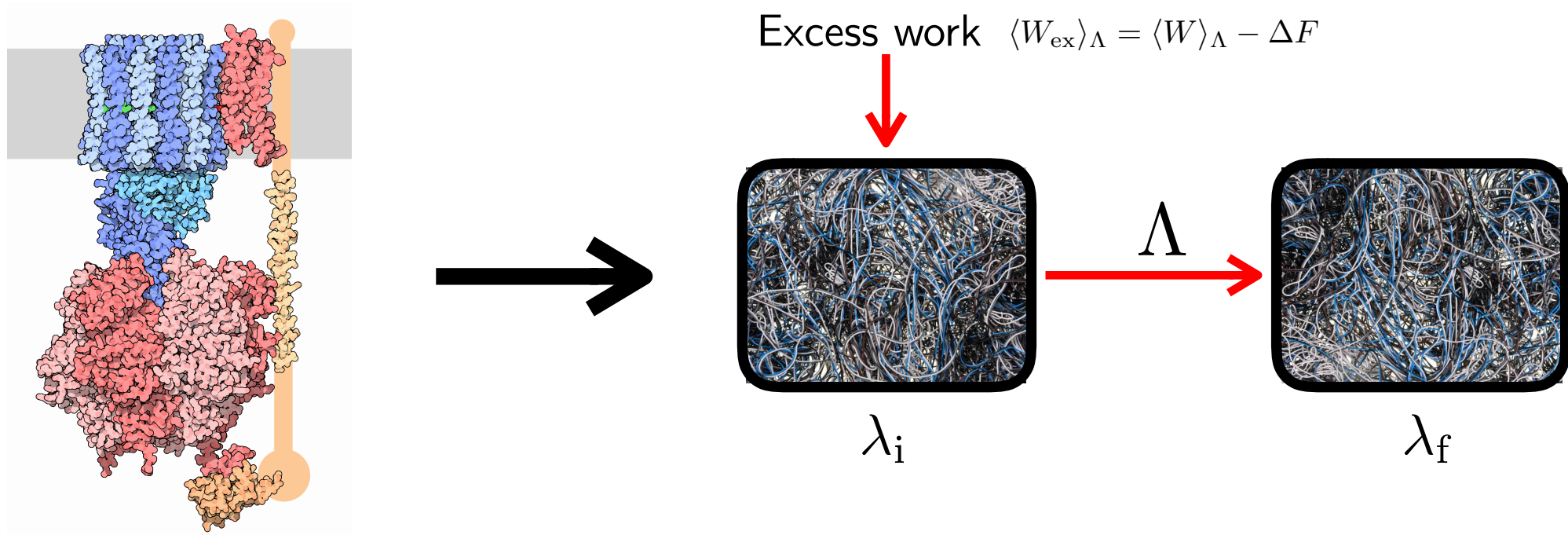
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- Average excess work required depends on the particular control protocol

$$\langle W_{\text{ex}} \rangle_{\Lambda} = \int_0^{\tau} \dot{\lambda}^2 \zeta(\lambda) dt$$

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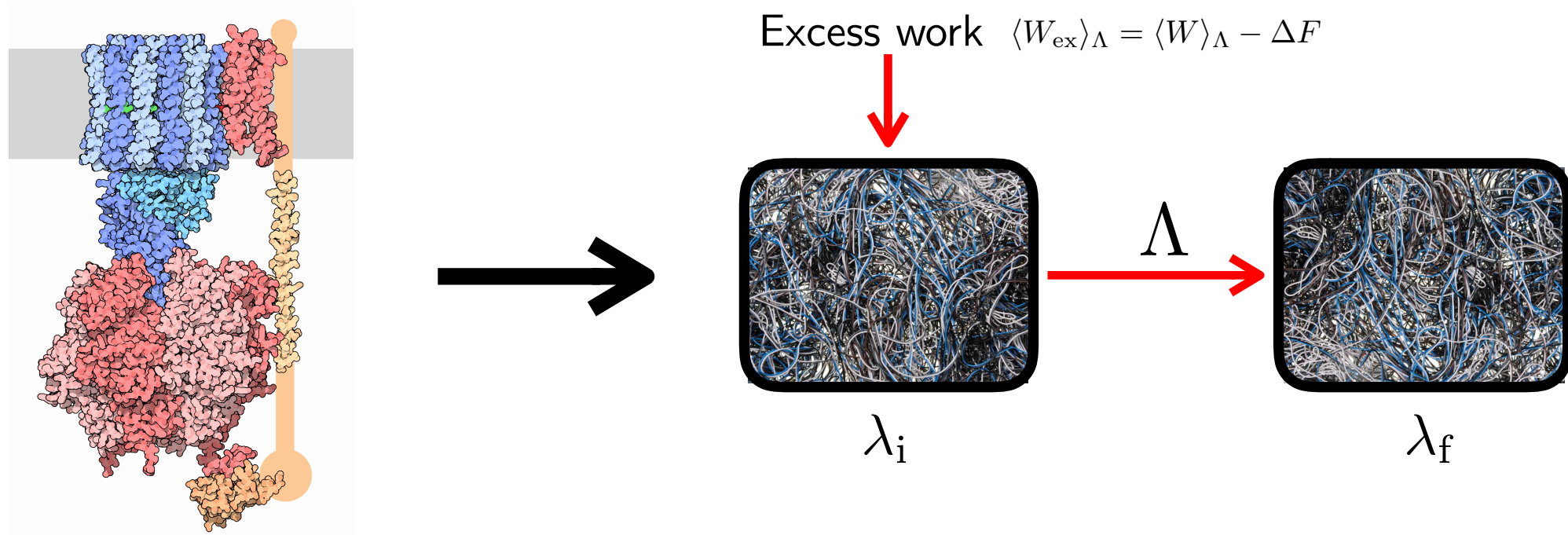


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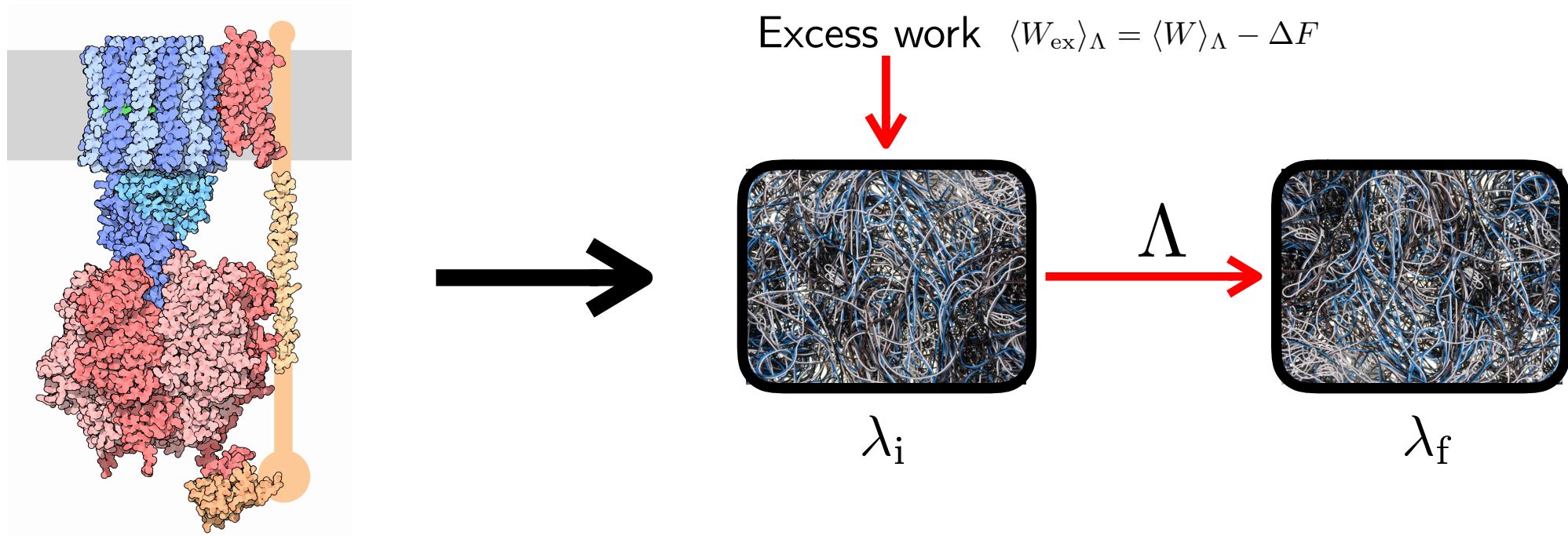
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Average excess work

Protocol duration

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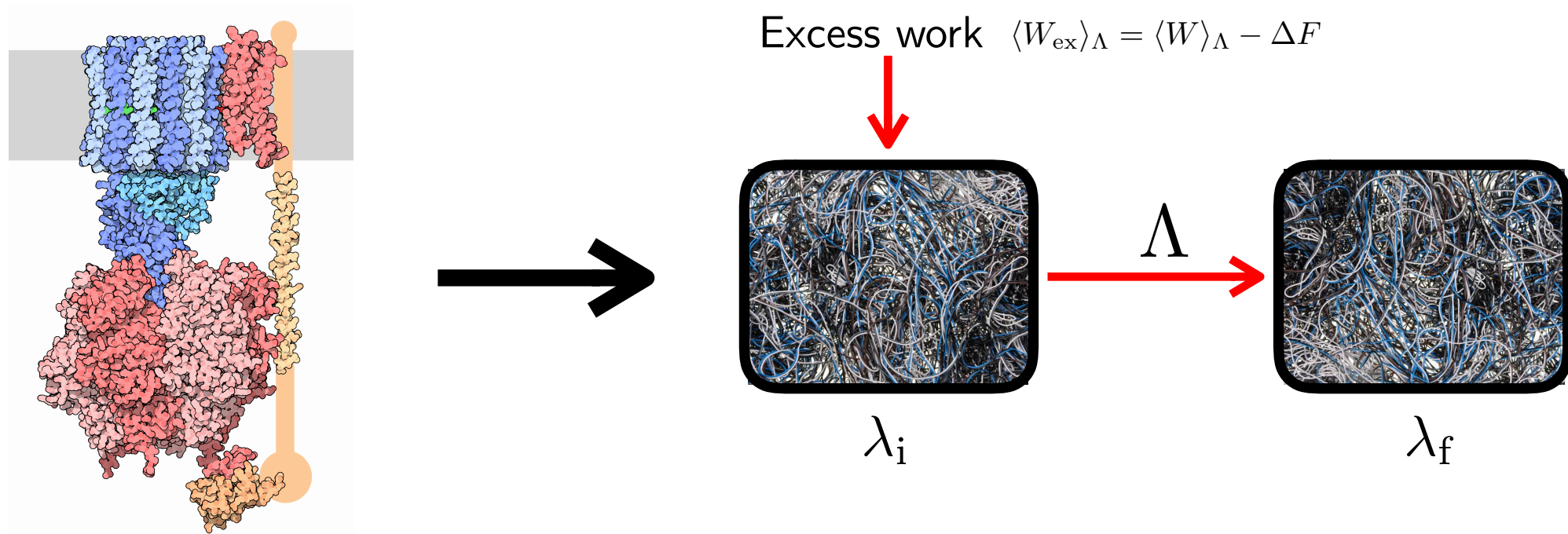
Average excess work

Protocol duration

Control protocol velocity

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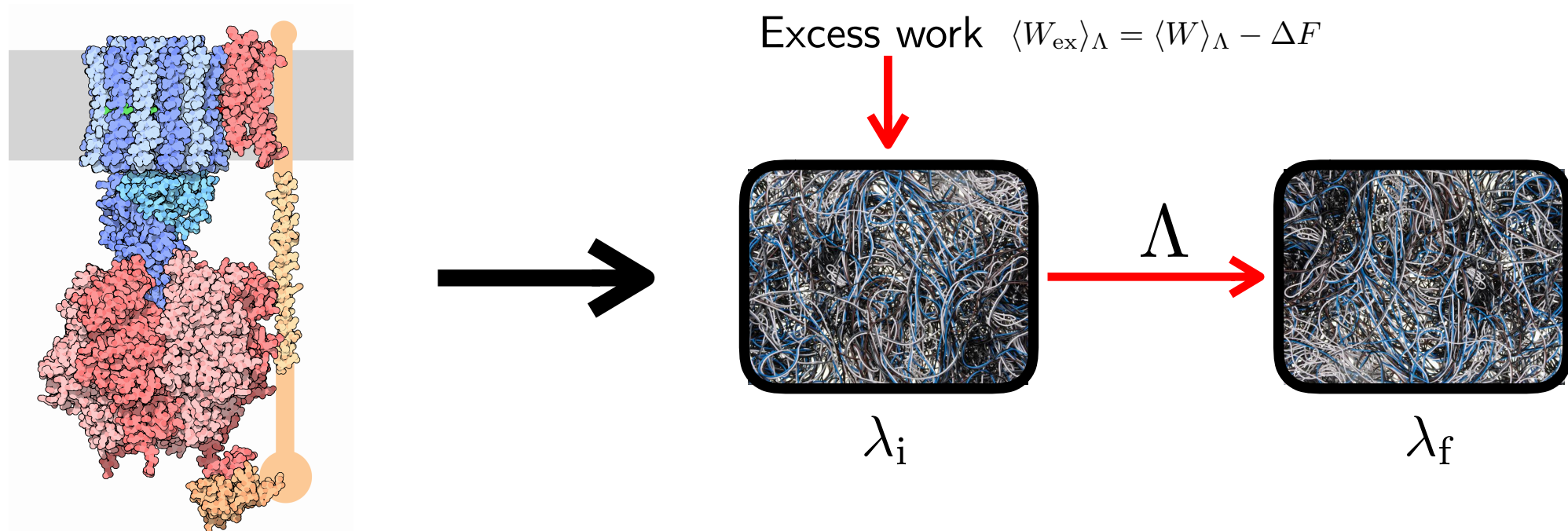
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Protocol duration

Control protocol velocity

Generalized friction

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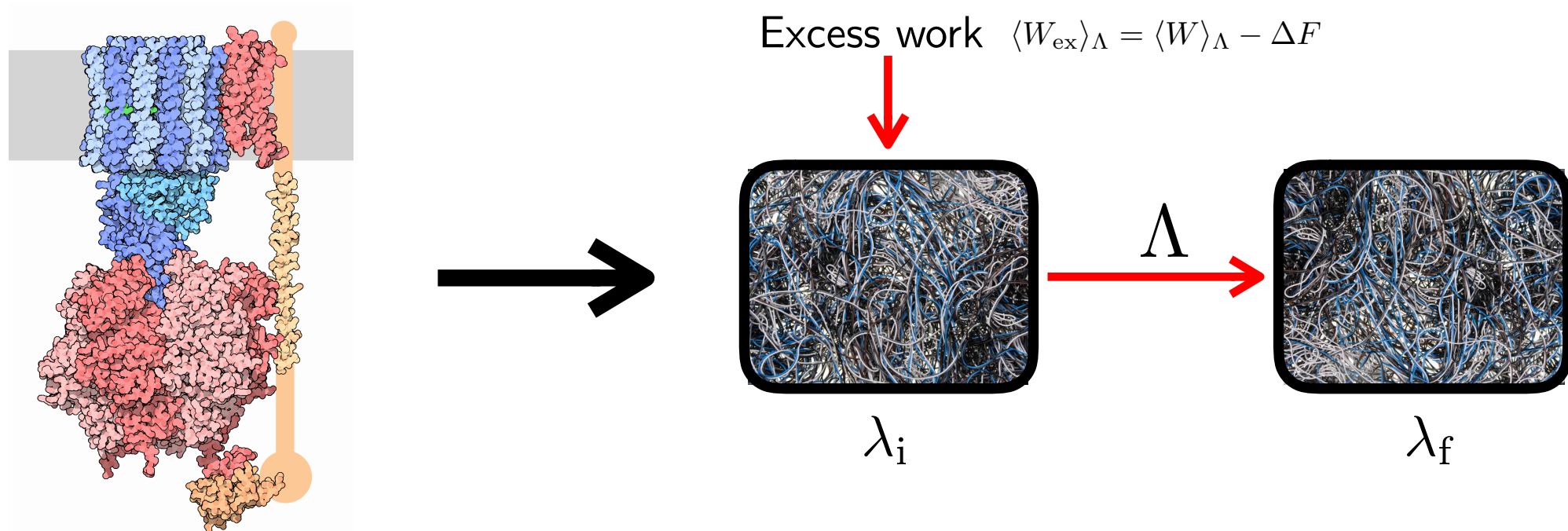
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Control protocol velocity

Generalized friction

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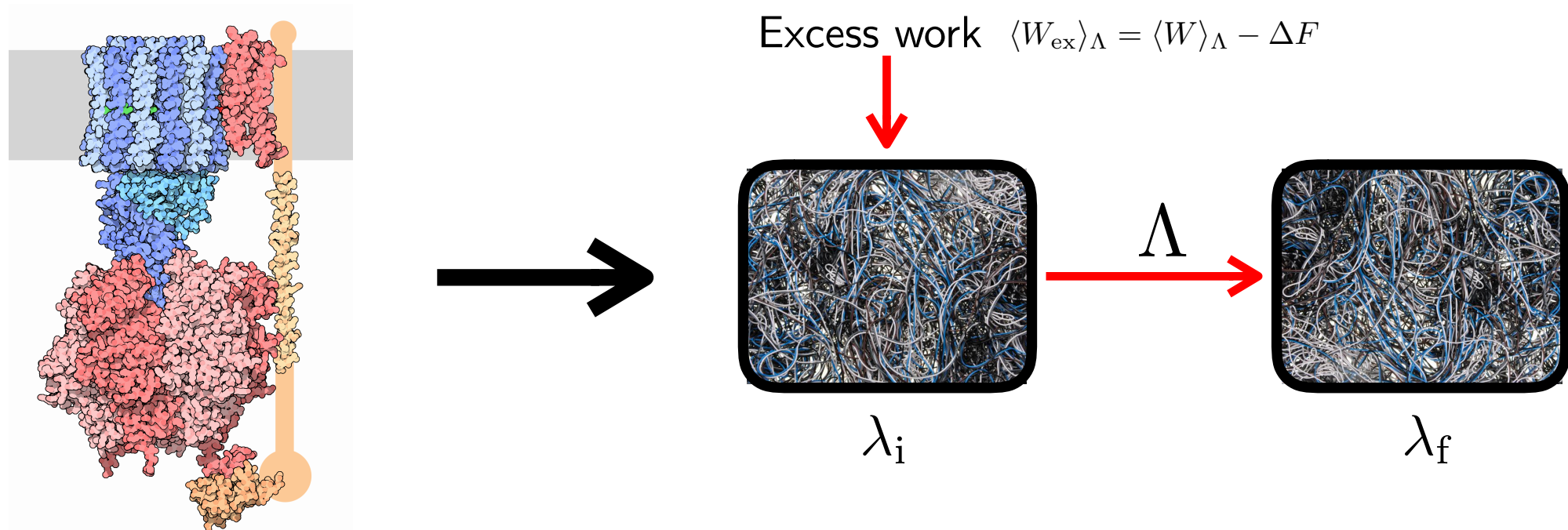
Control protocol velocity

Generalized friction

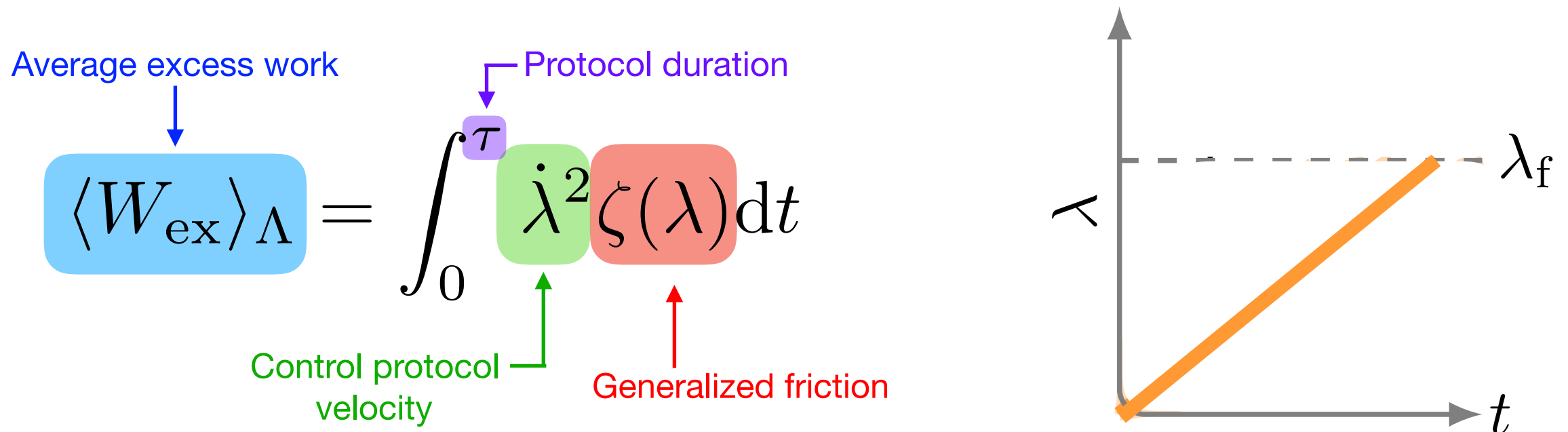
The graph shows λ on the vertical axis and t on the horizontal axis. A dashed horizontal line is at λ_f . An orange curve starts at the origin and rises to meet the dashed line at λ_f .

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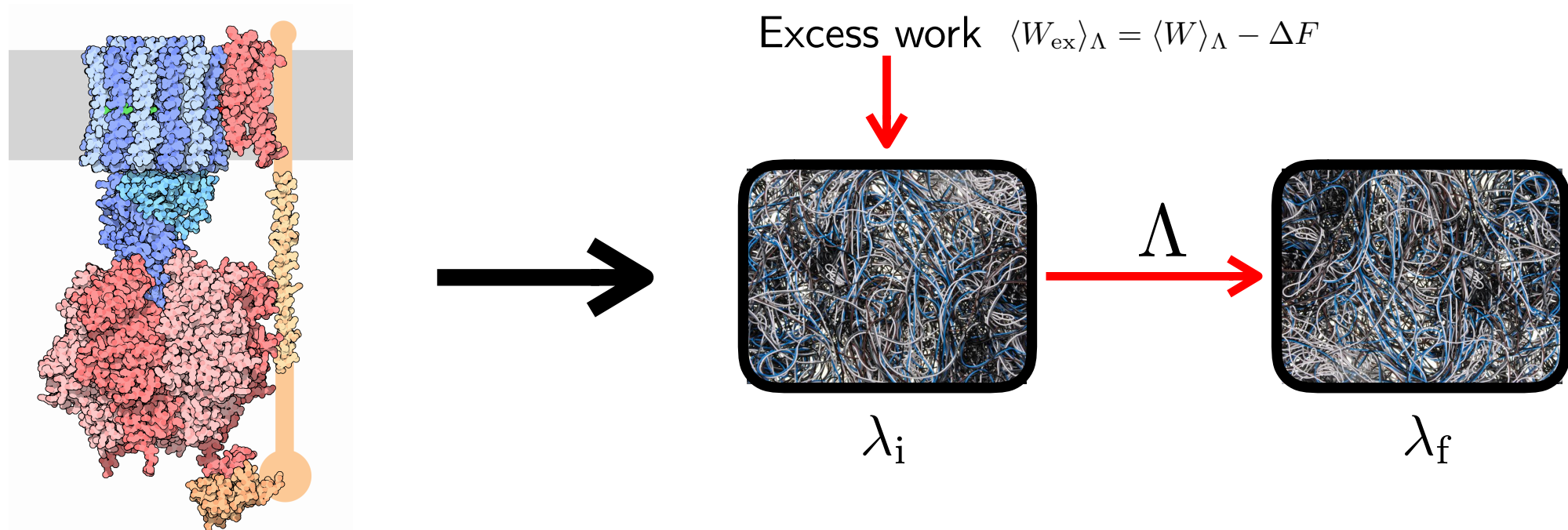


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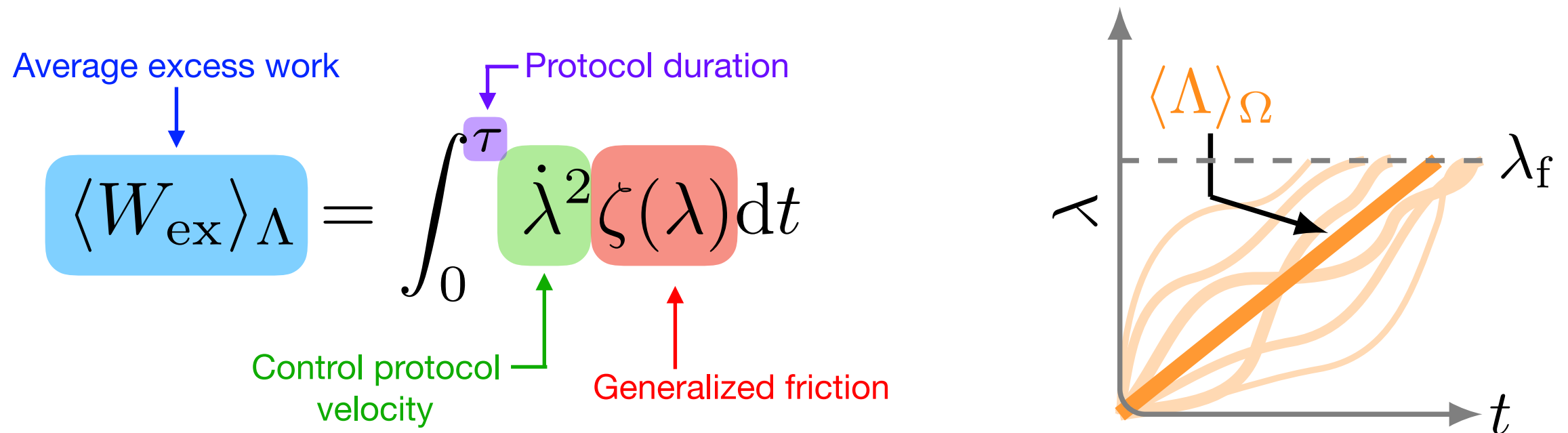


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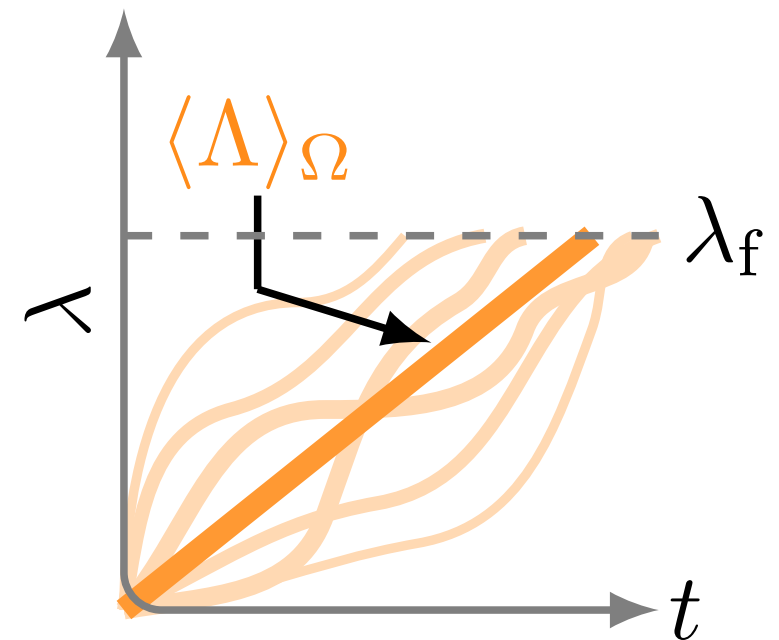
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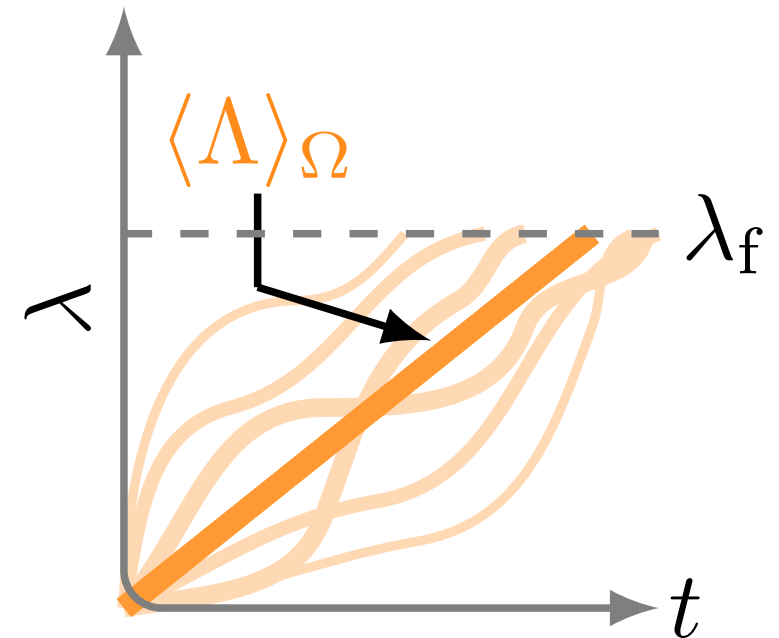
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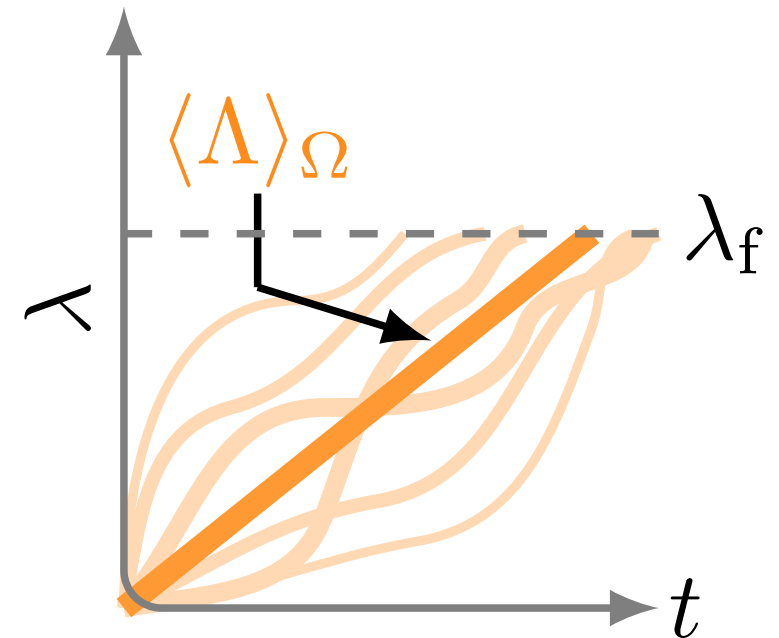
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\uparrow
 Protocol ensemble
 average

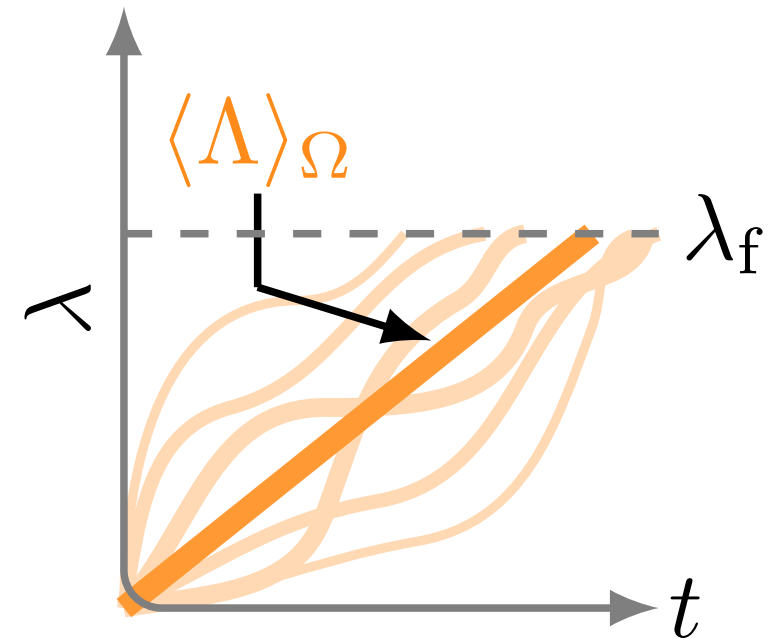


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Excess work of average protocol

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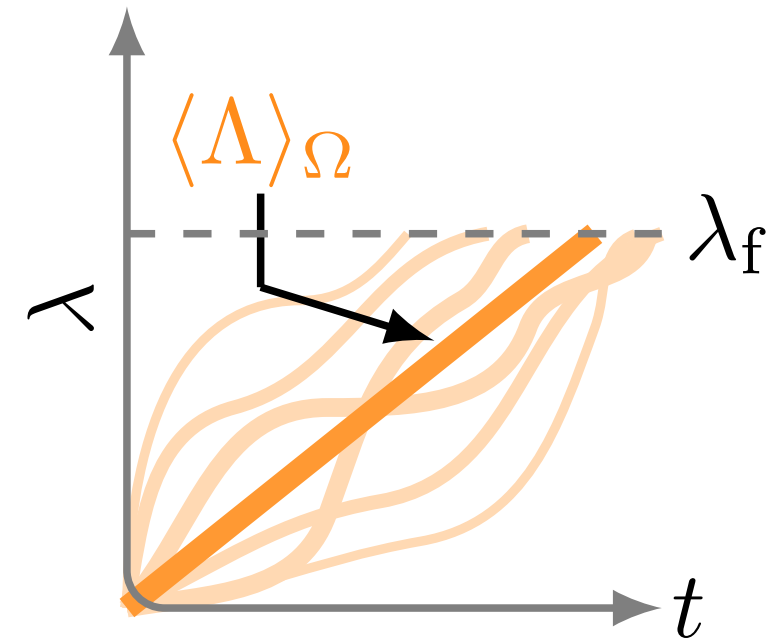
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Correction term



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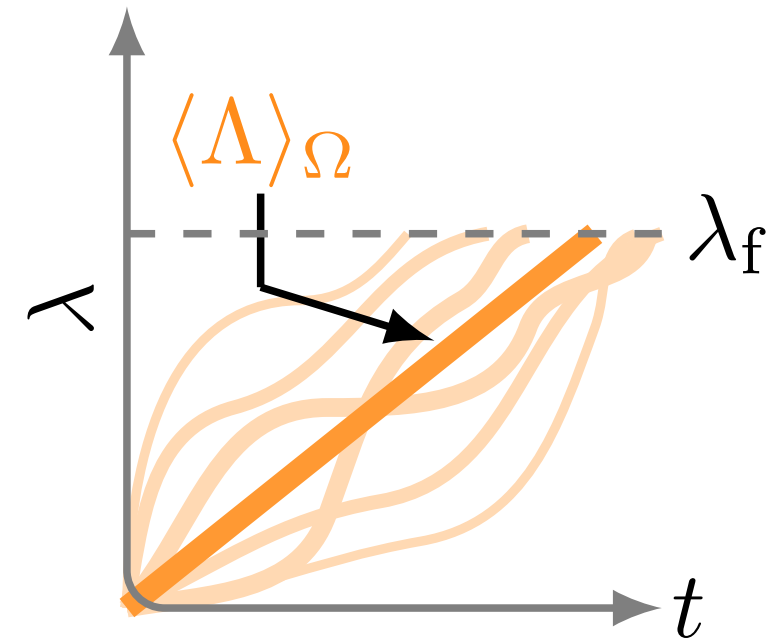
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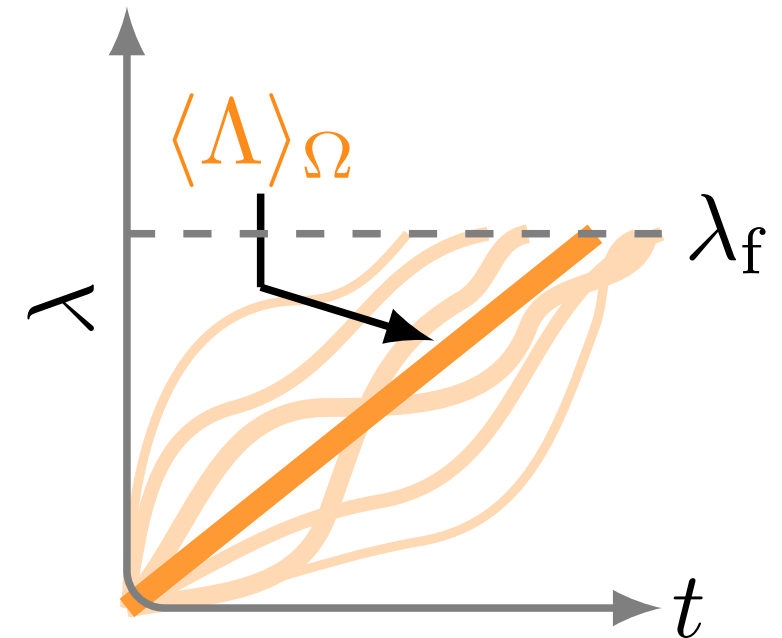
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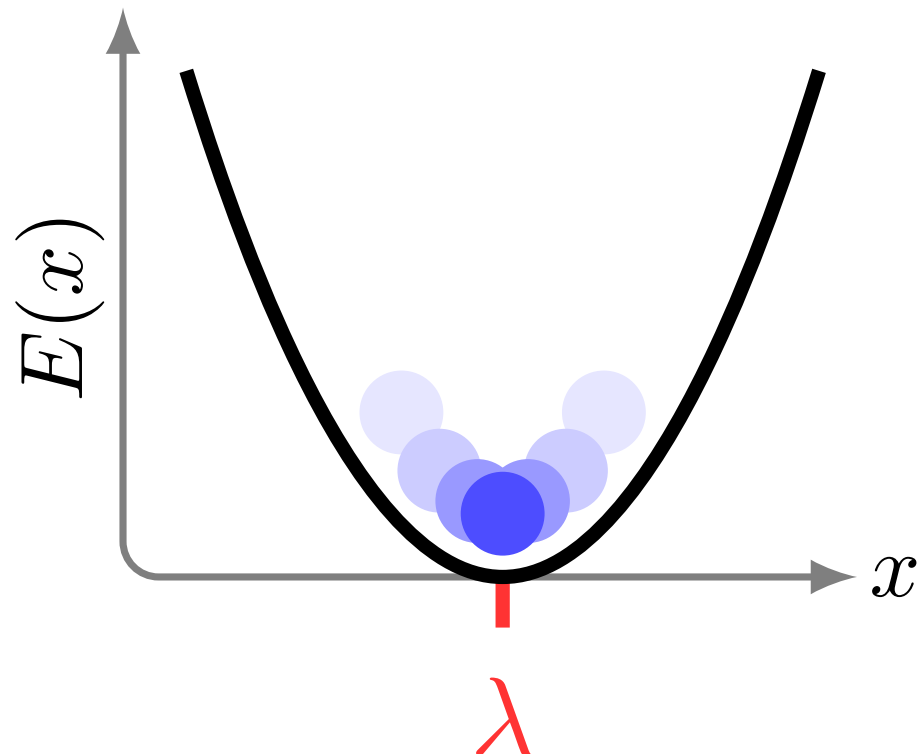
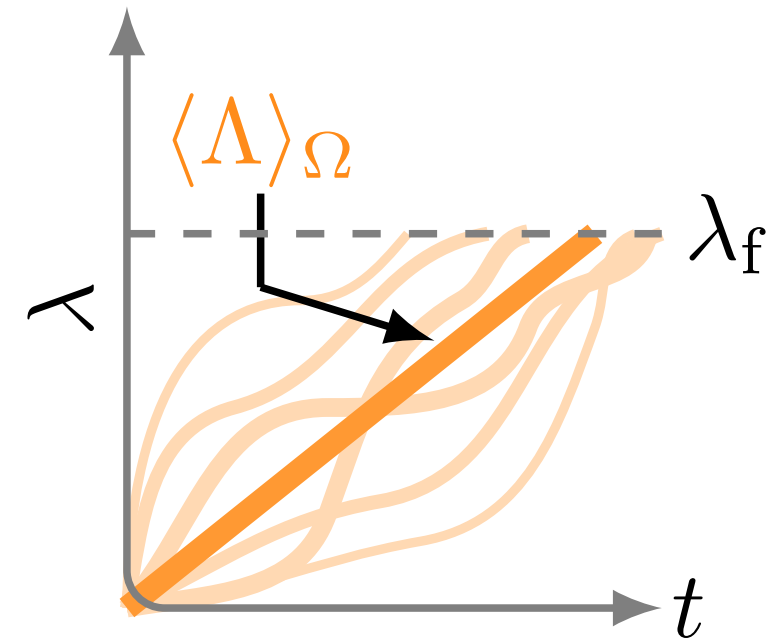
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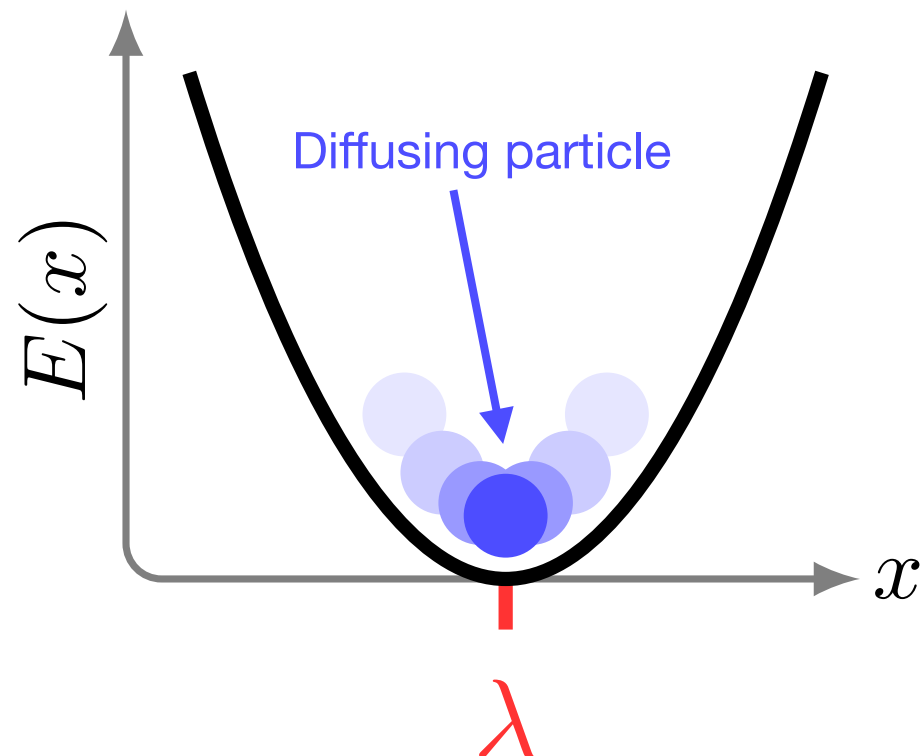
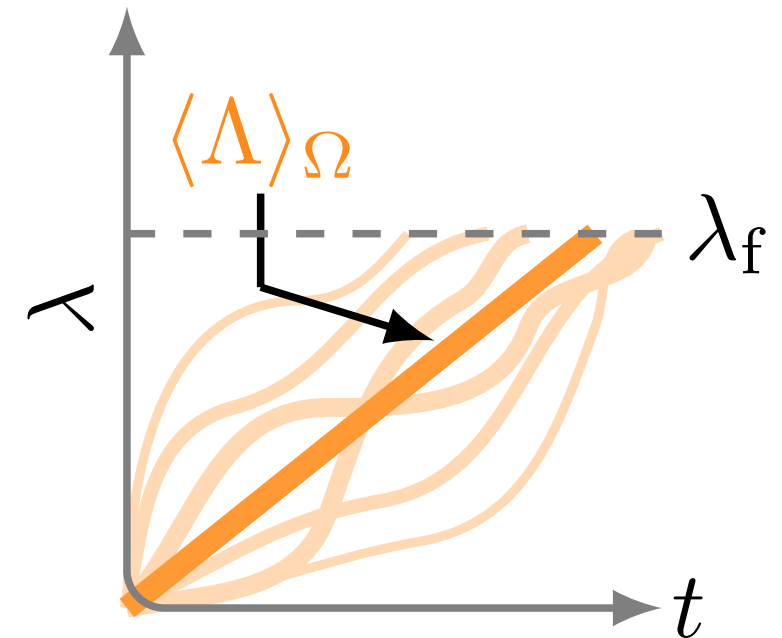
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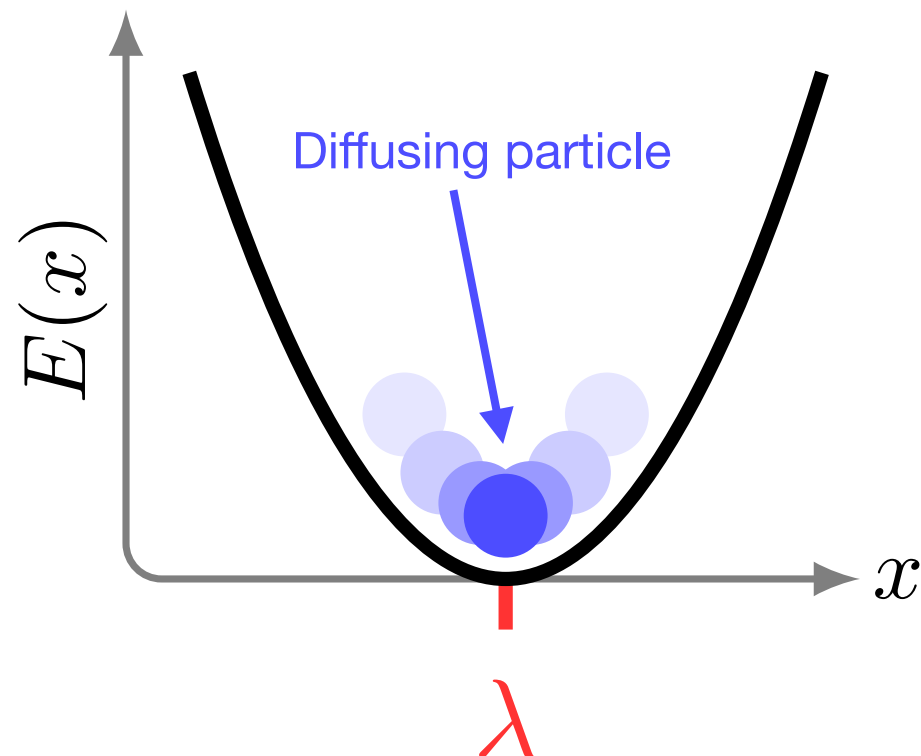
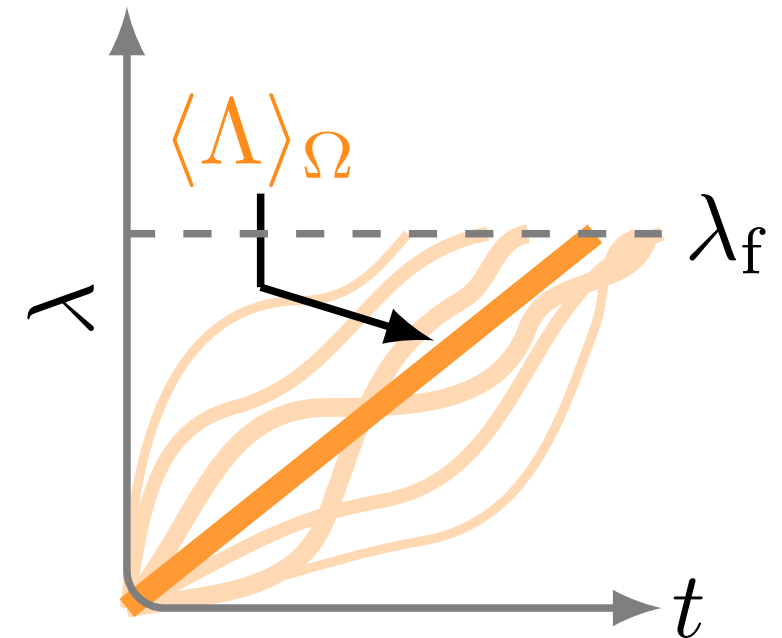
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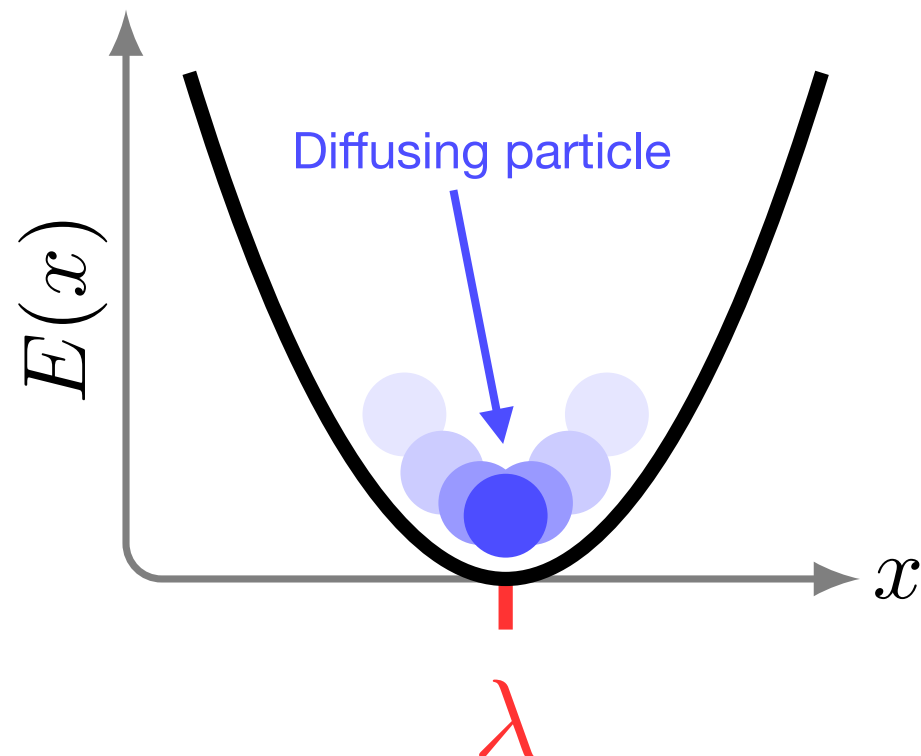
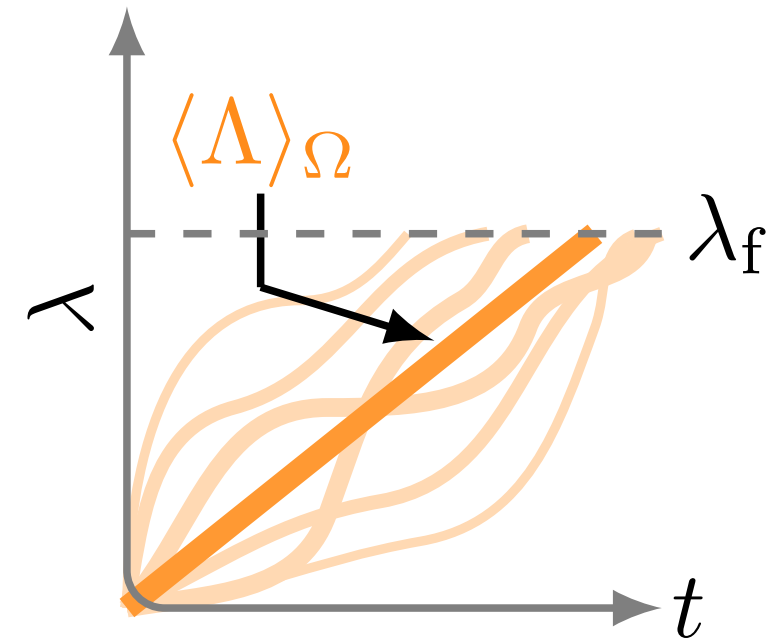
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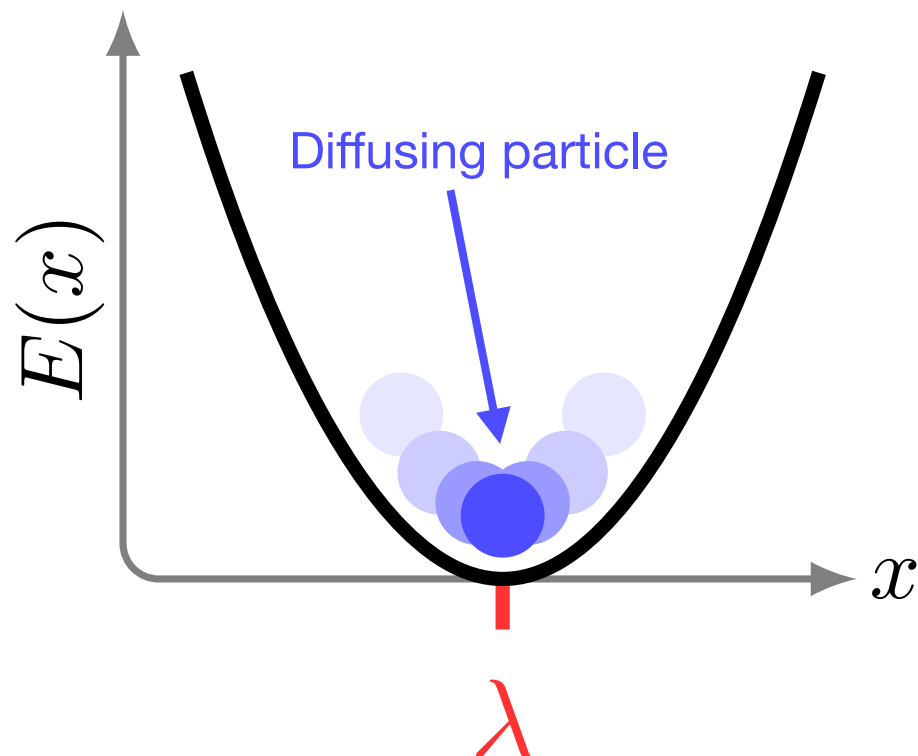
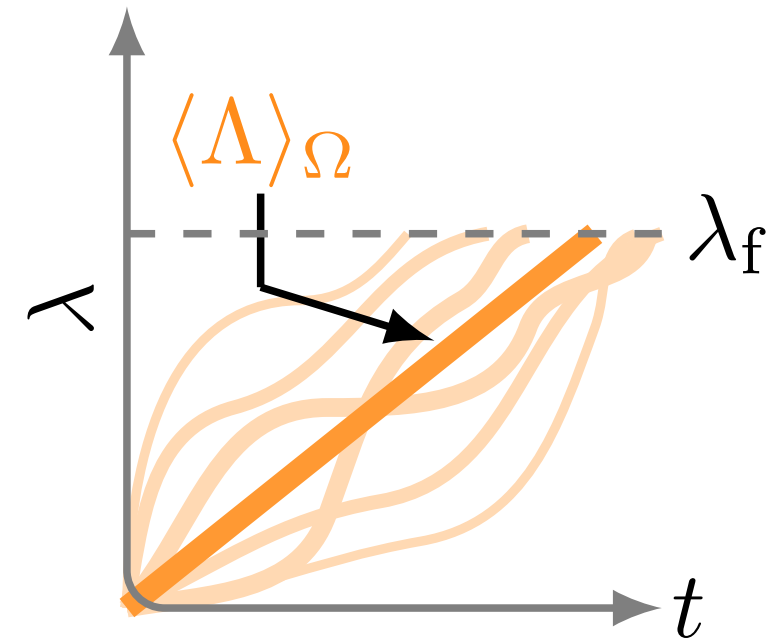
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- Trap minimum evolves under a stochastic dynamics

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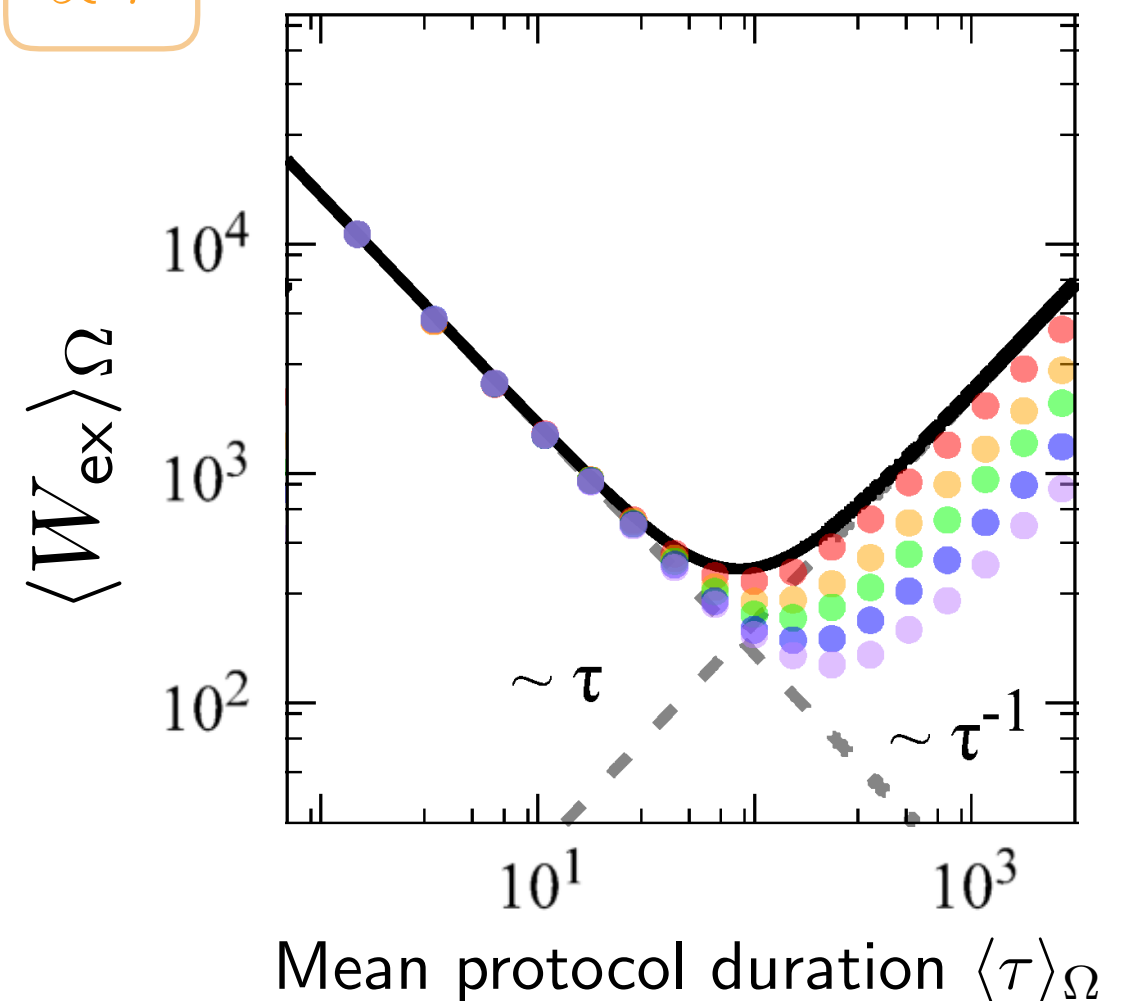
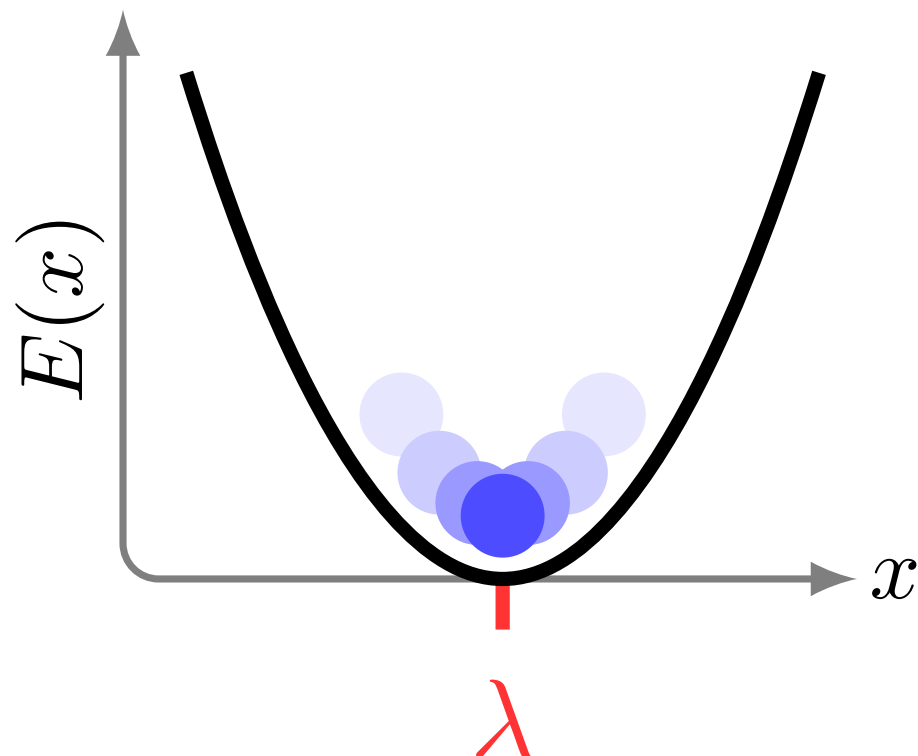
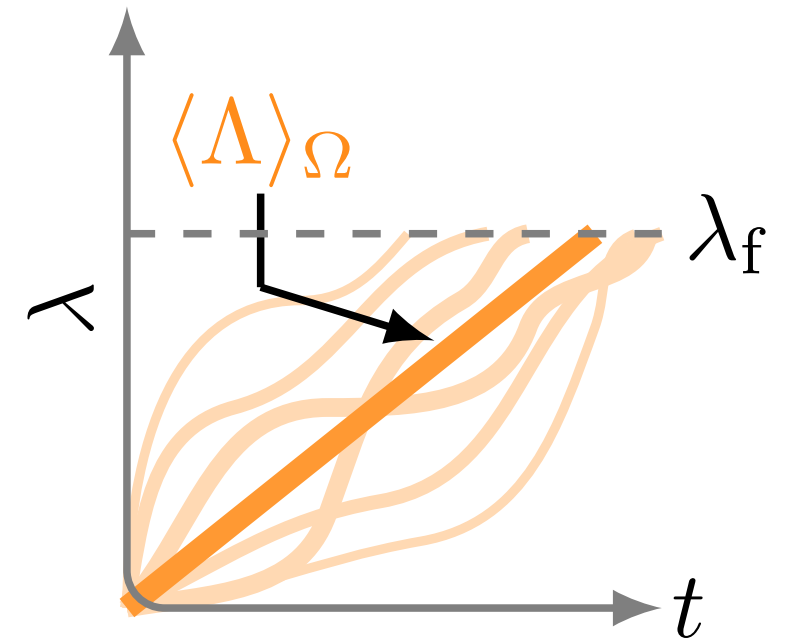
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- For a stochastically driven process, we are interested in the average excess work, over all possible protocols

Excess work of average protocol

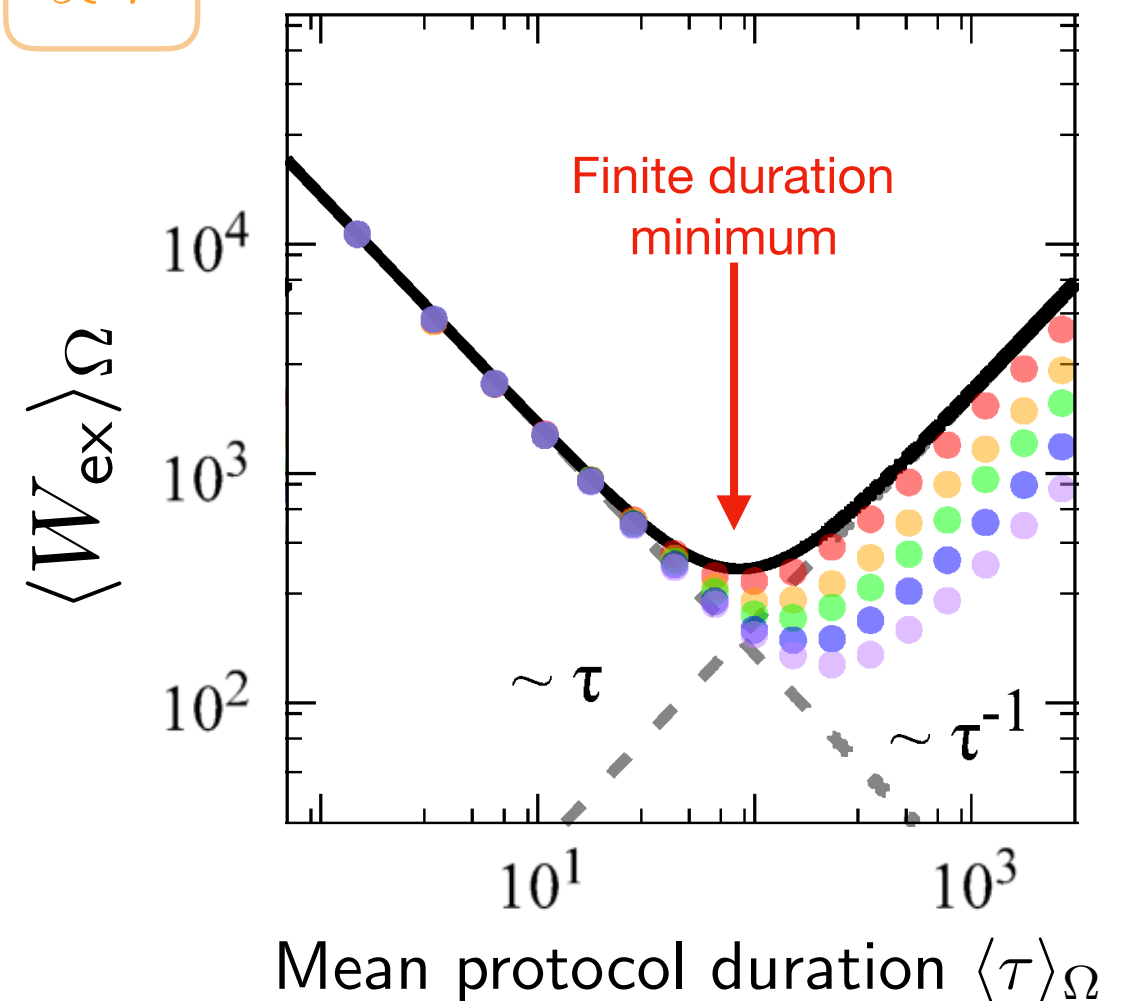
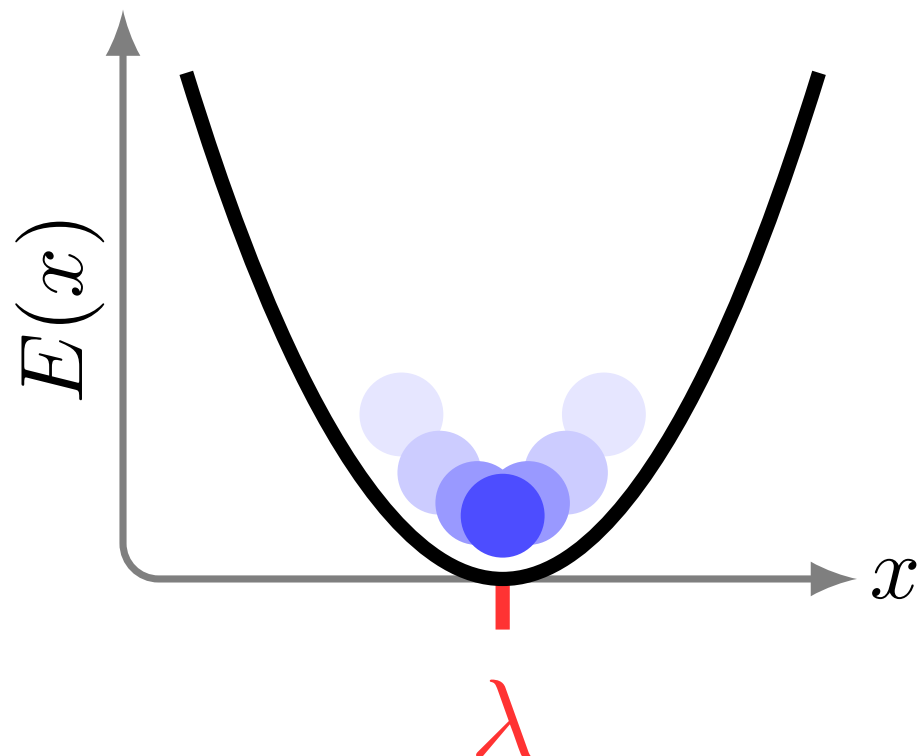
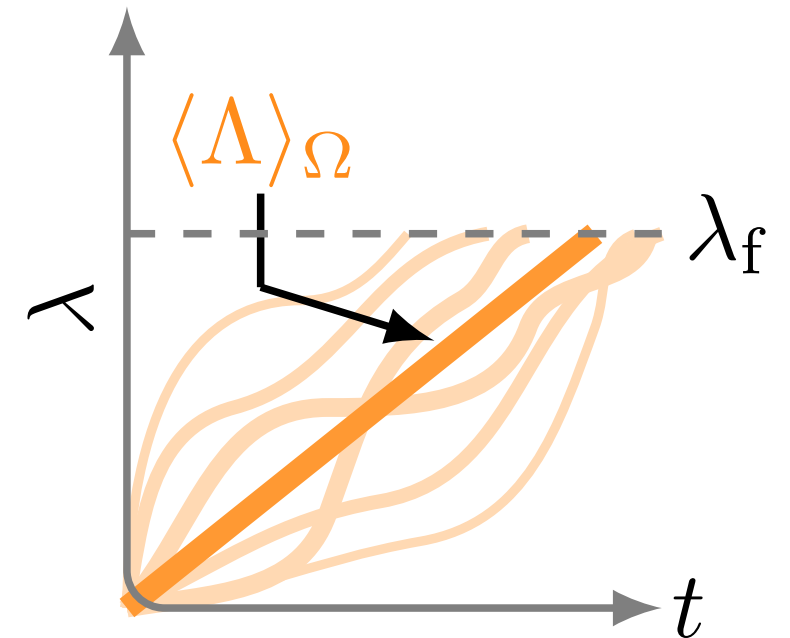
Protocol ensemble average

$$\langle W_{\text{ex}} \rangle_{\Omega} = \int_0^{\tau} \langle \dot{\lambda} \rangle^2 \zeta(\langle \lambda \rangle) dt + \int_0^{\tau} \langle \delta \dot{\lambda}^2 \rangle \zeta(\langle \lambda \rangle) dt$$

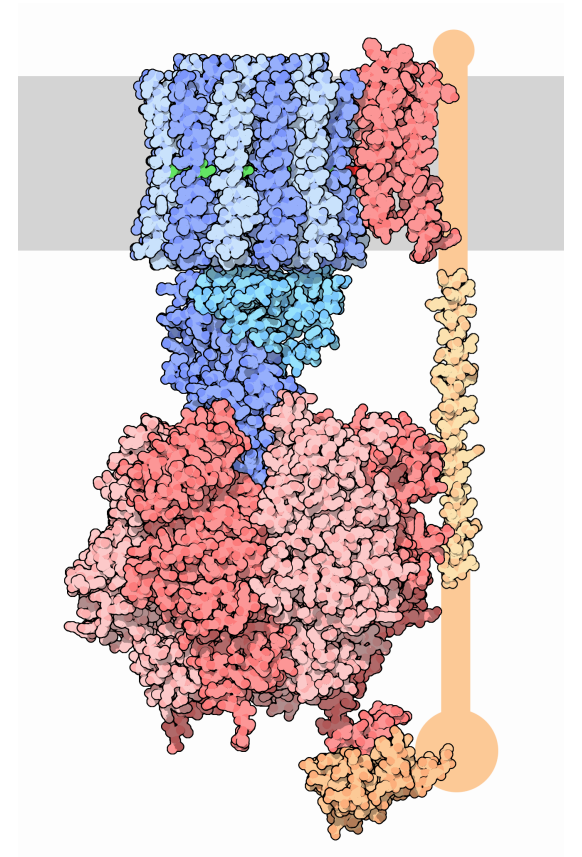
Correction term

$\propto \frac{1}{\tau}$

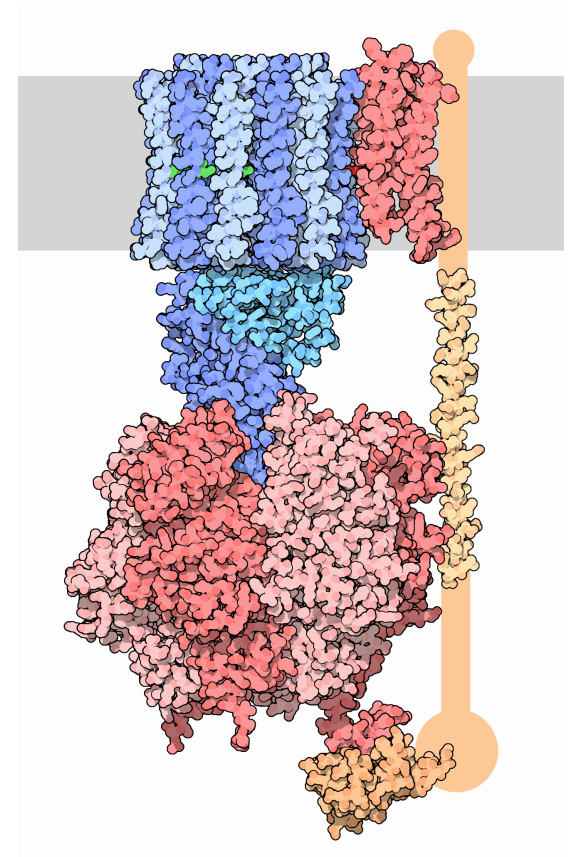
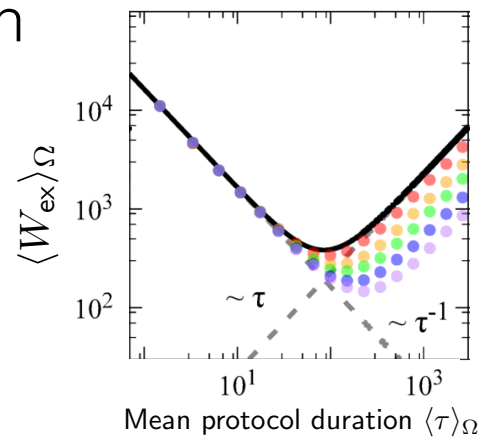
$\propto \tau$



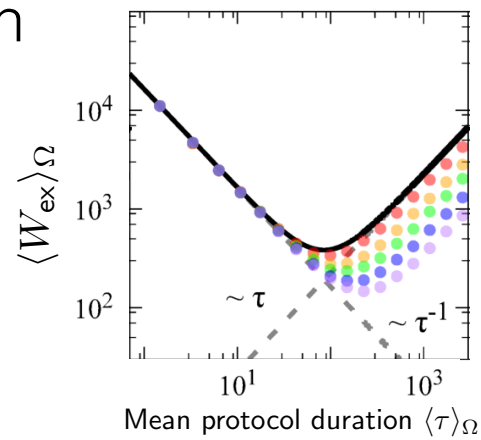
- Fluctuations in control parameter dynamics penalize slow operation



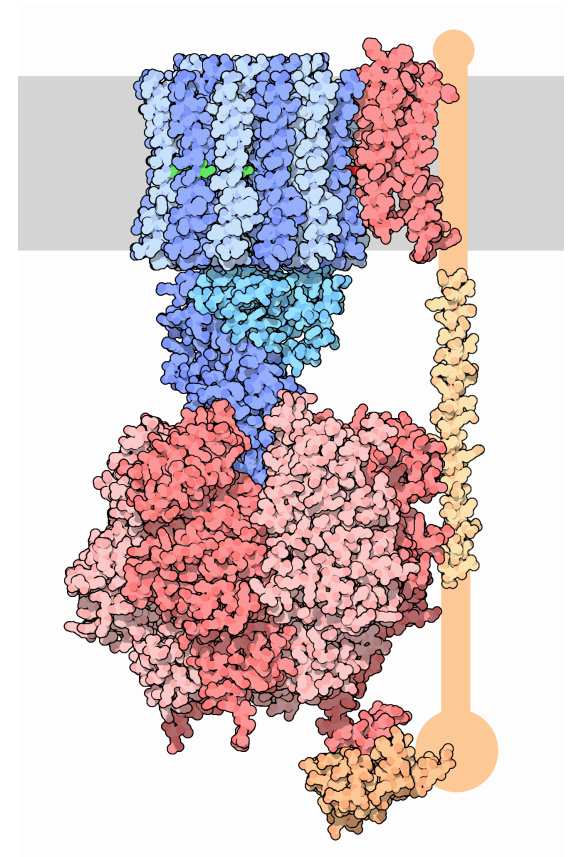
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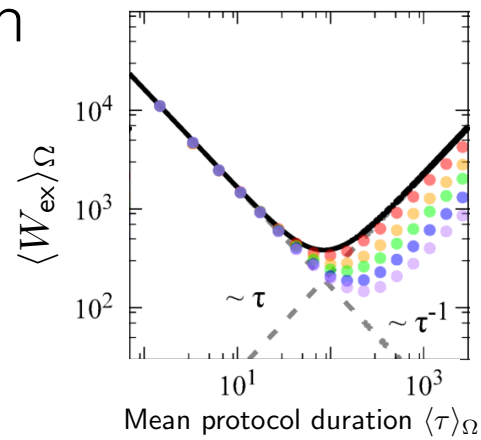
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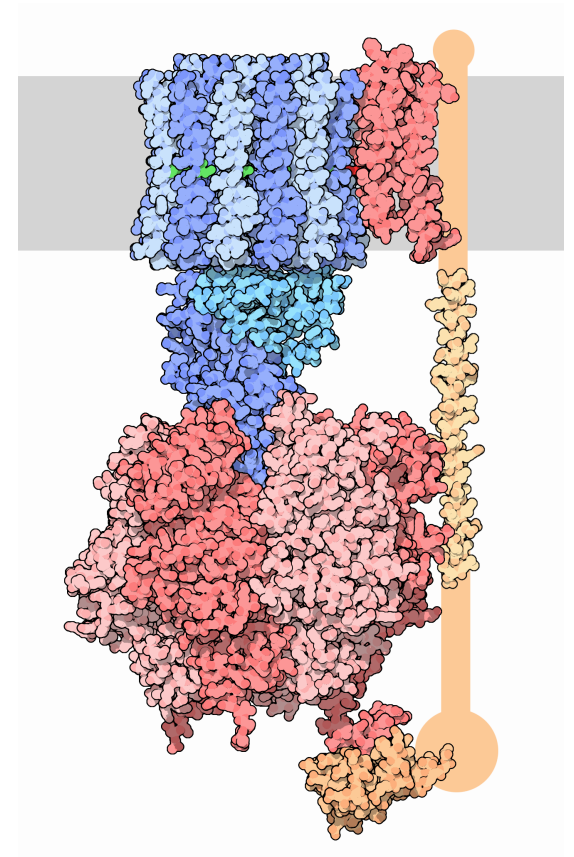
- Finite duration minimum work



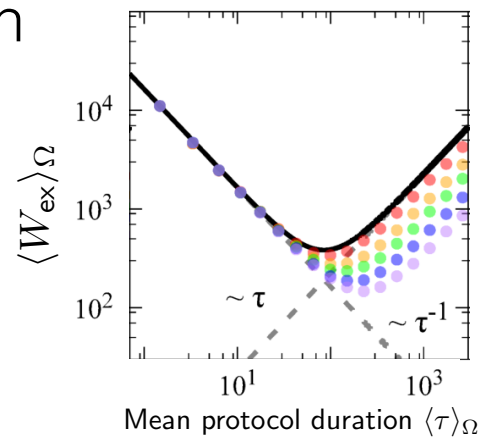
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- Finite duration minimum work
- Thermodynamic justification for rapid operation

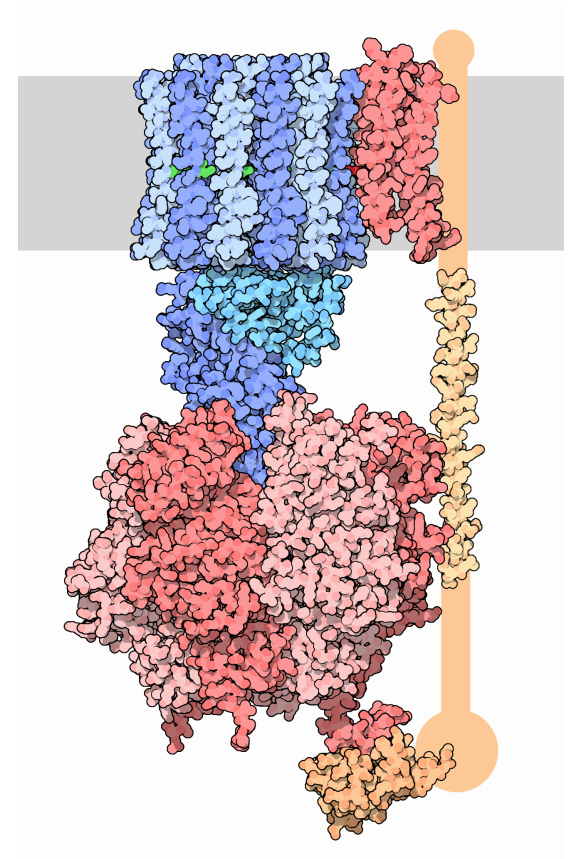


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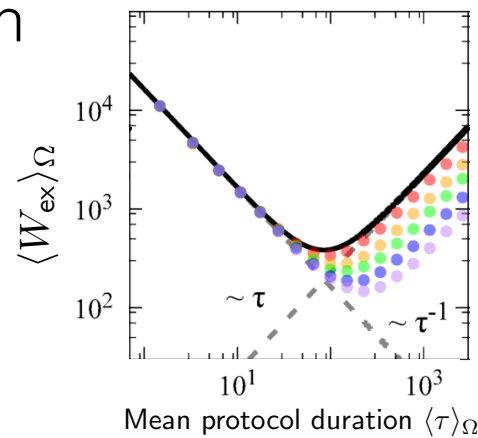


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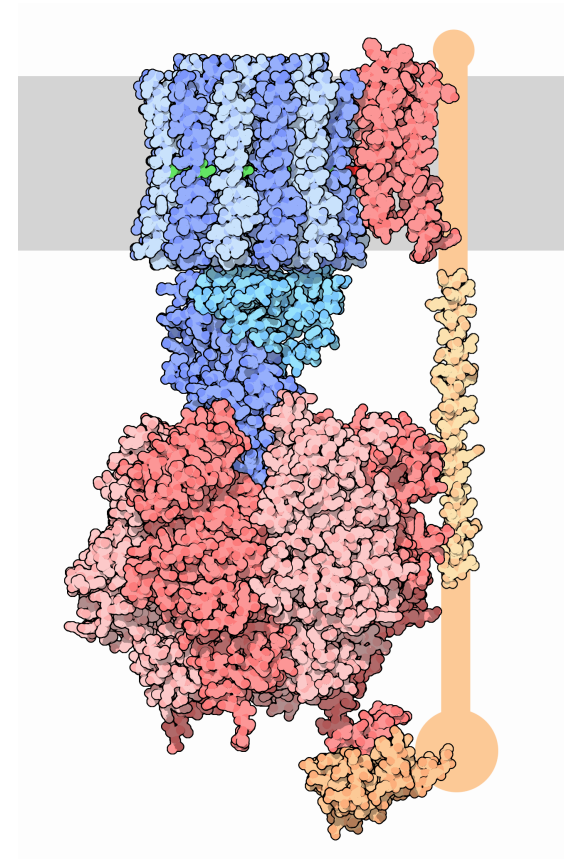
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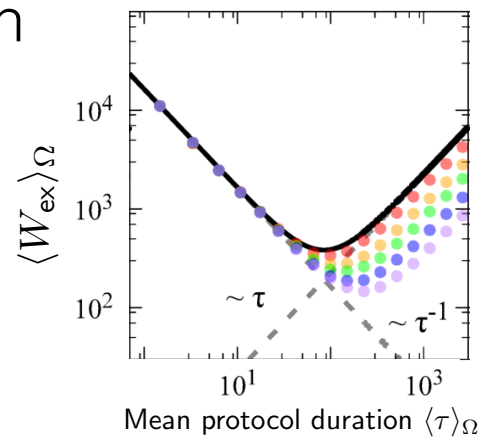
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- Molecular machines are driven by chemical reactions, which are modelled as discrete processes



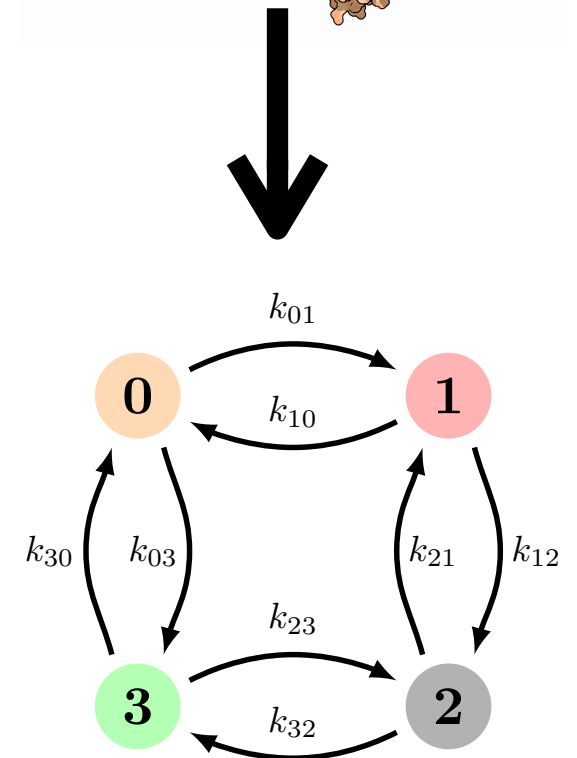
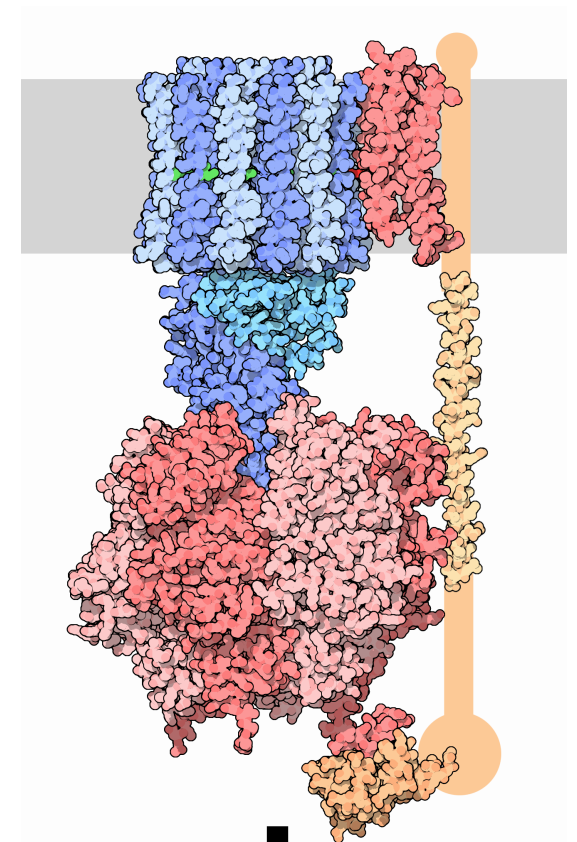
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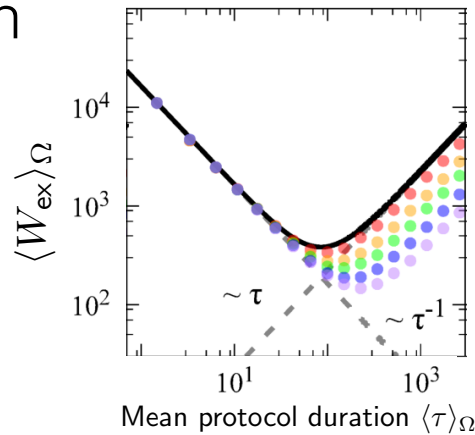
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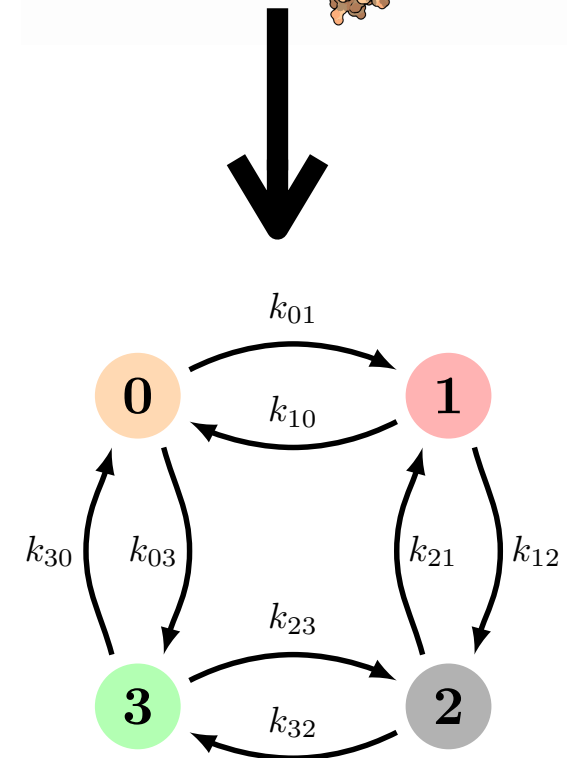
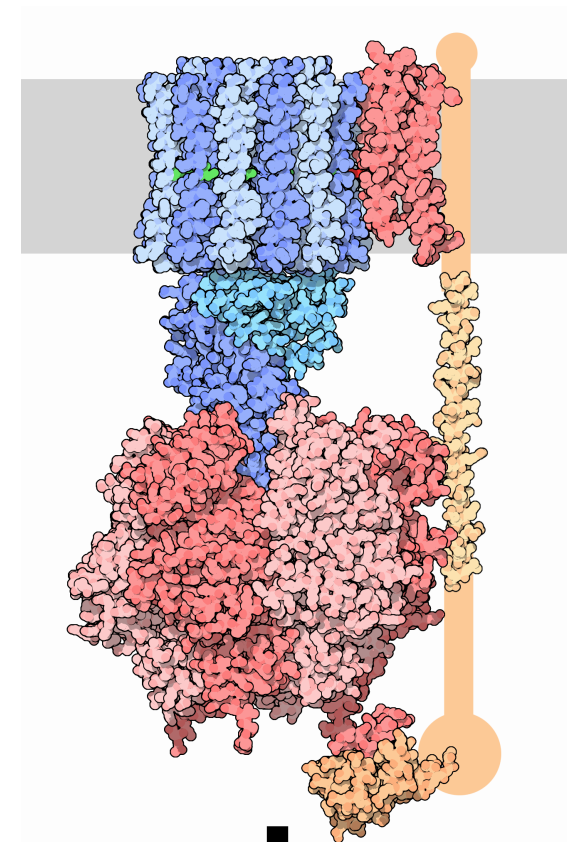
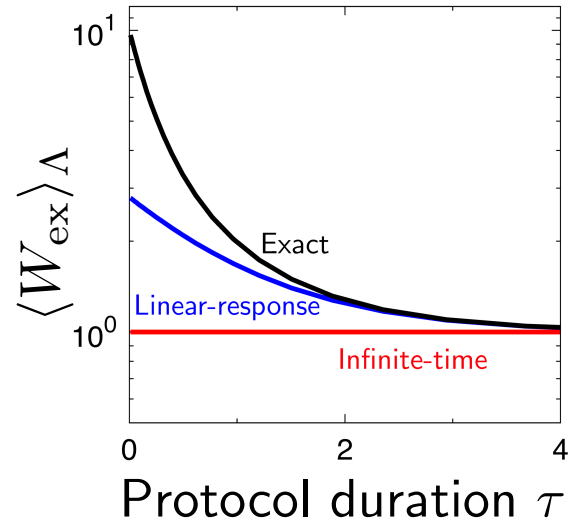
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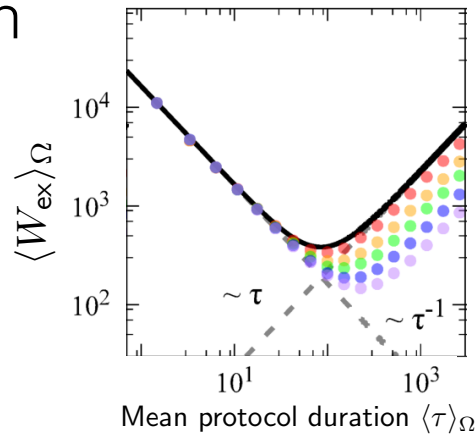
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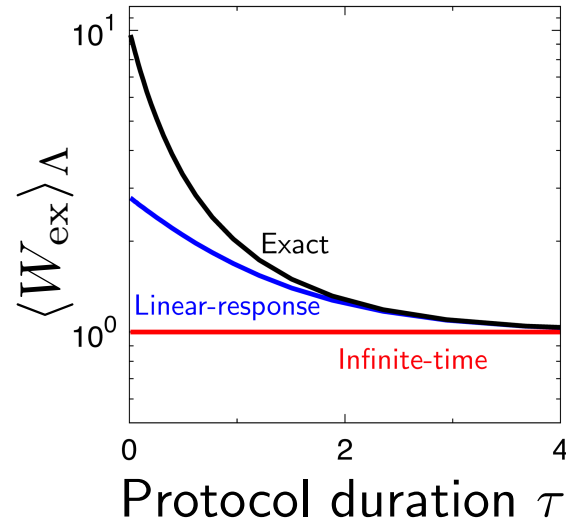
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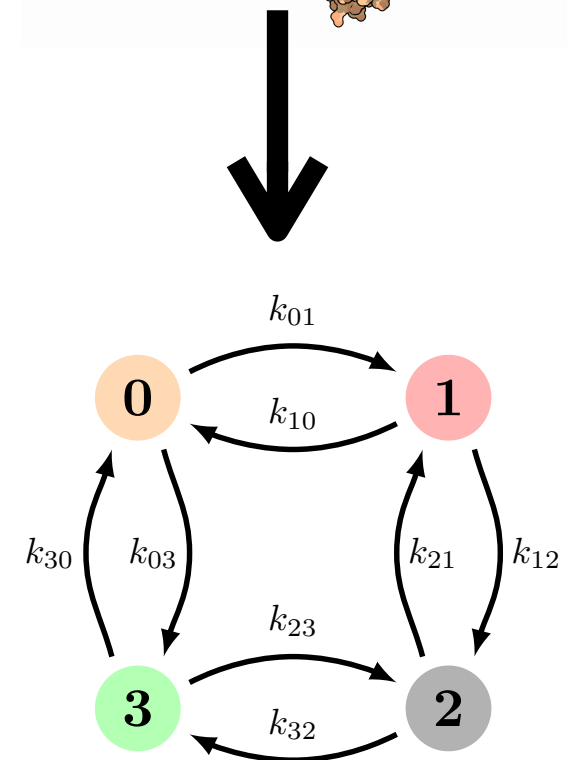
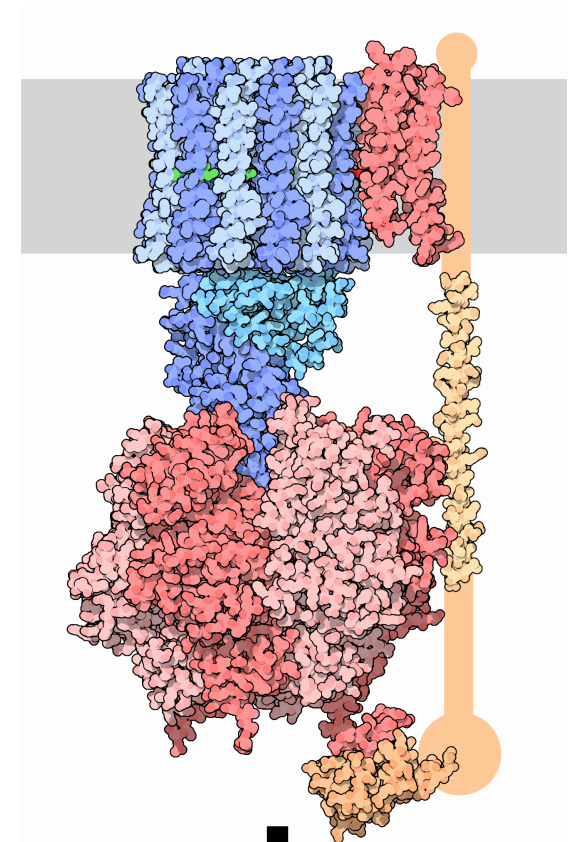
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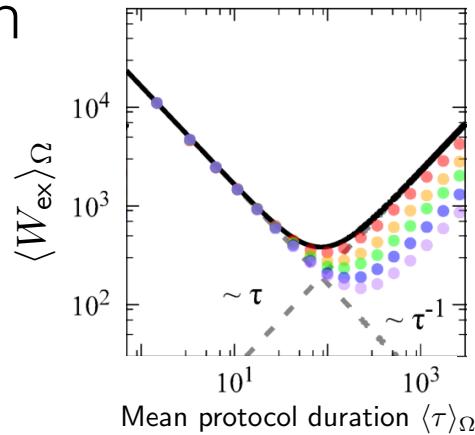
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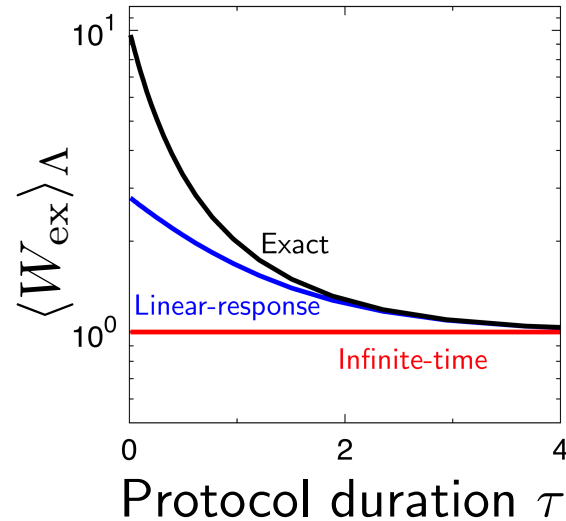
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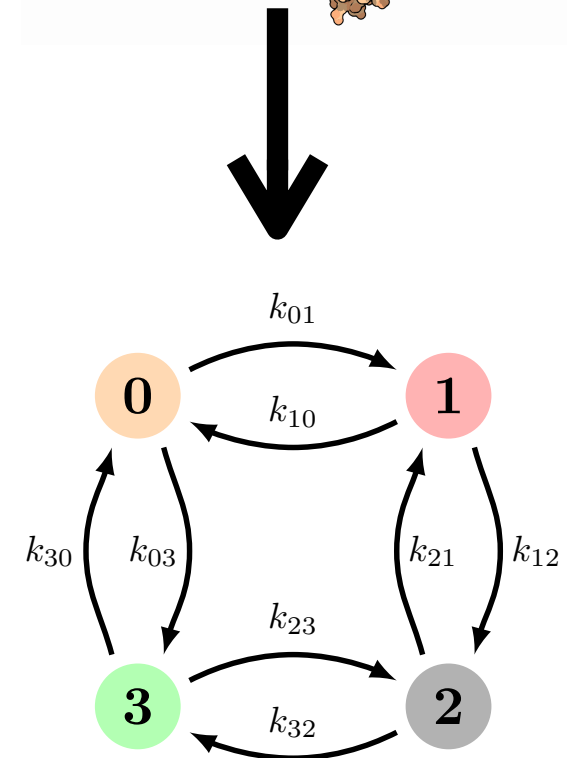
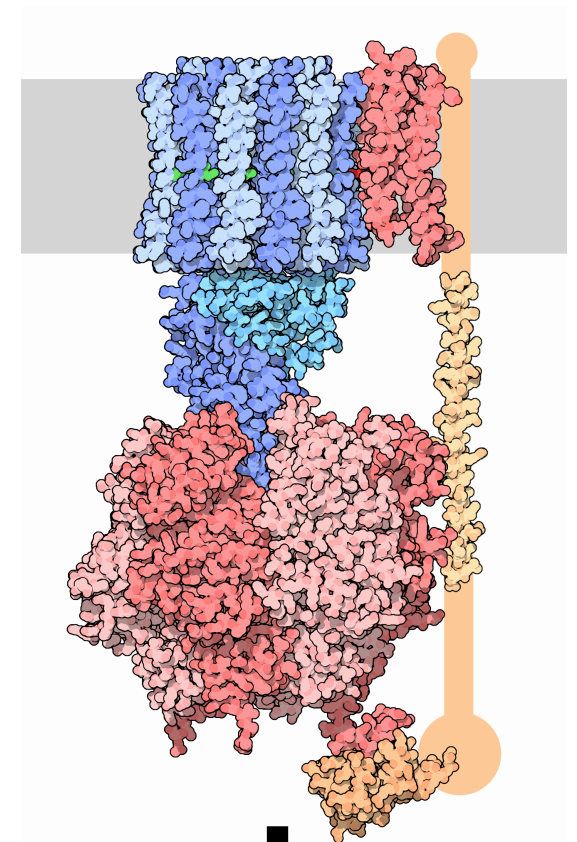
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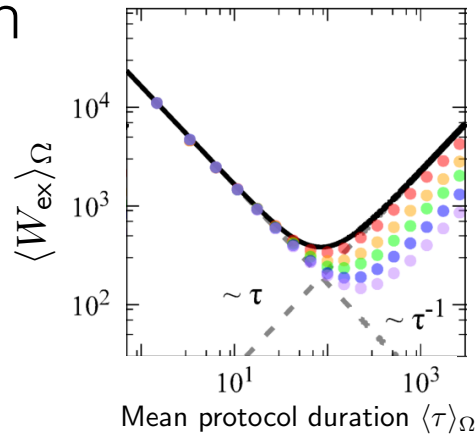
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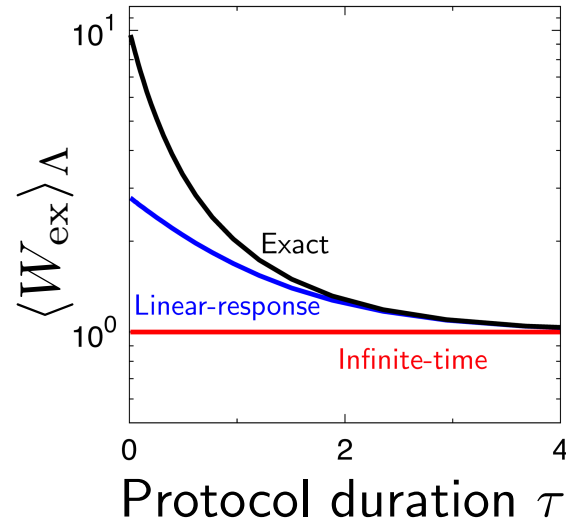
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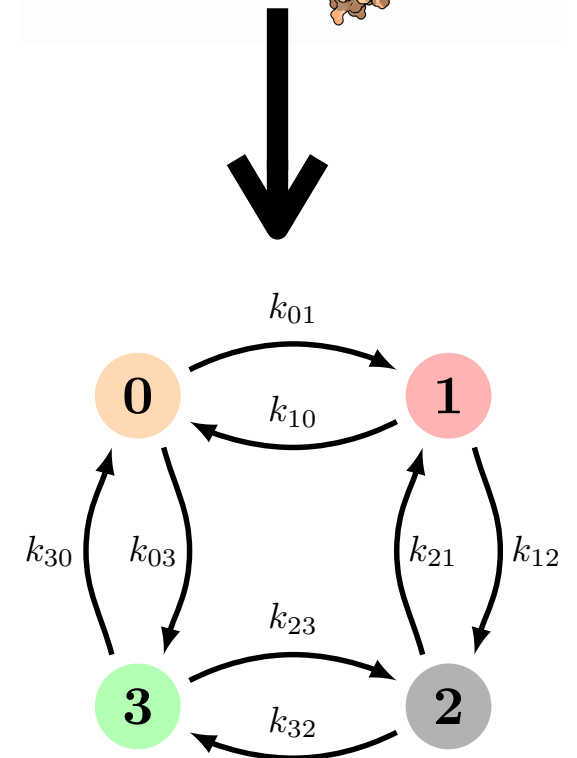
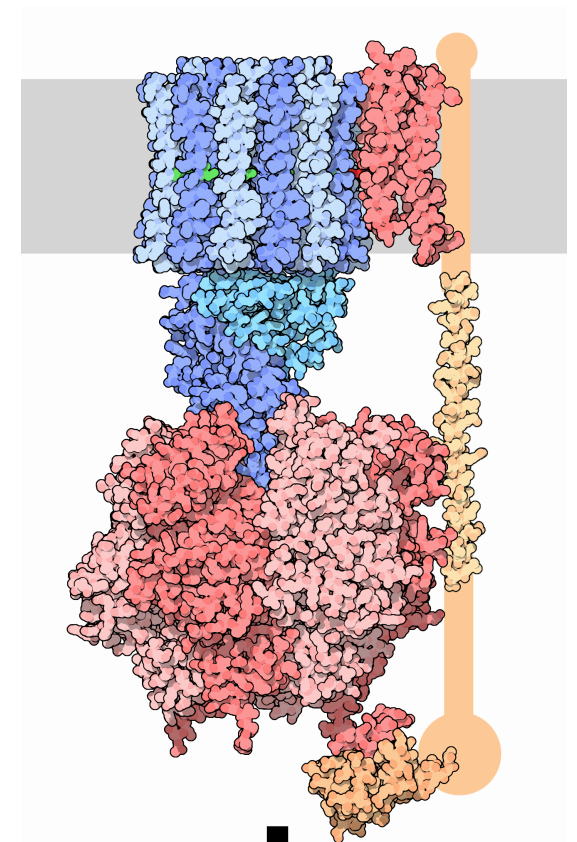
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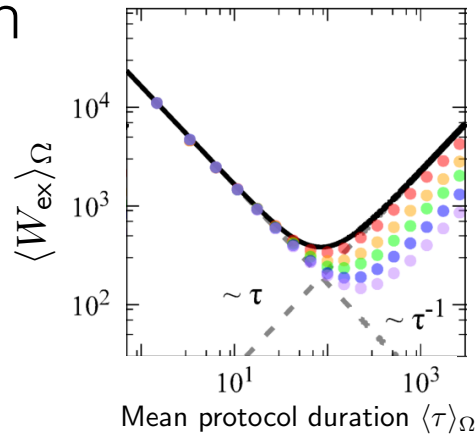


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- No 'quasistatic' limit:



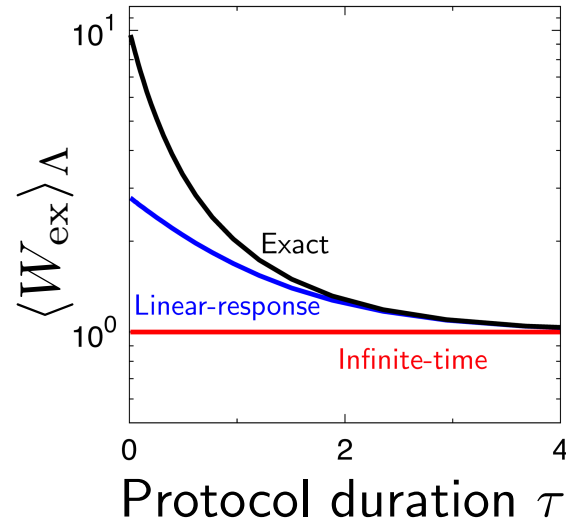
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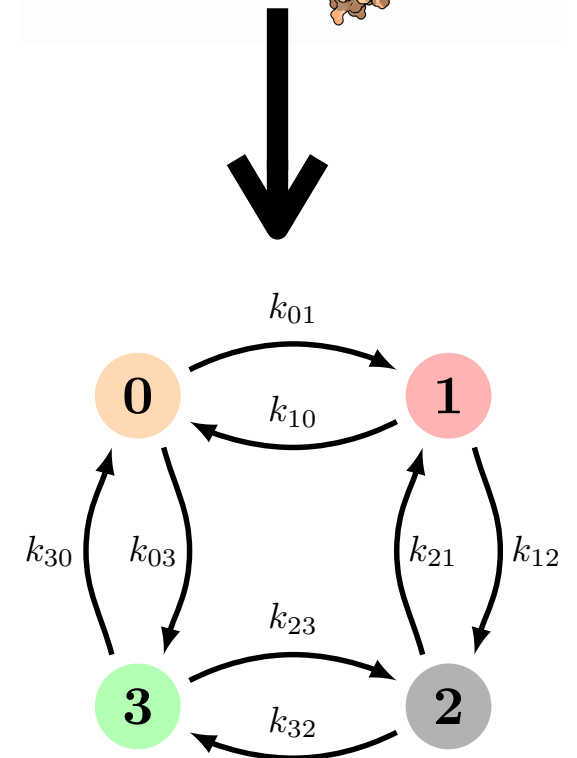
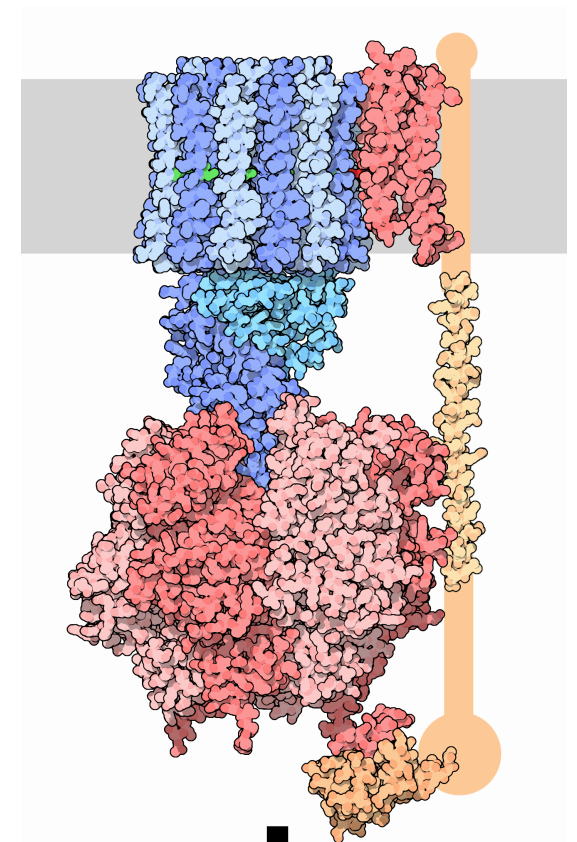
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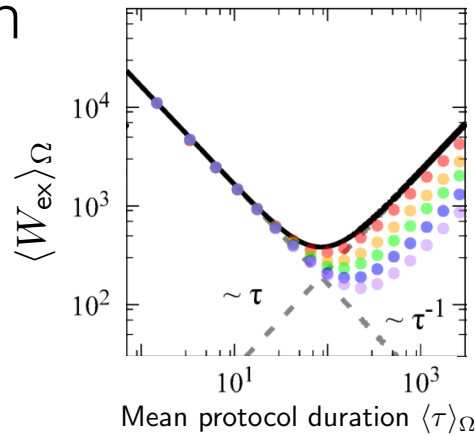


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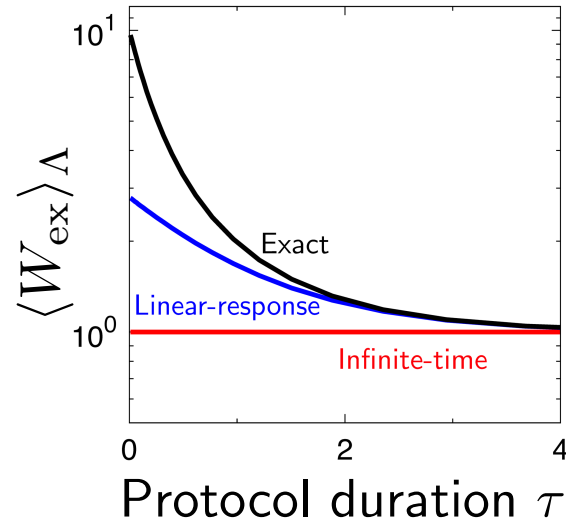
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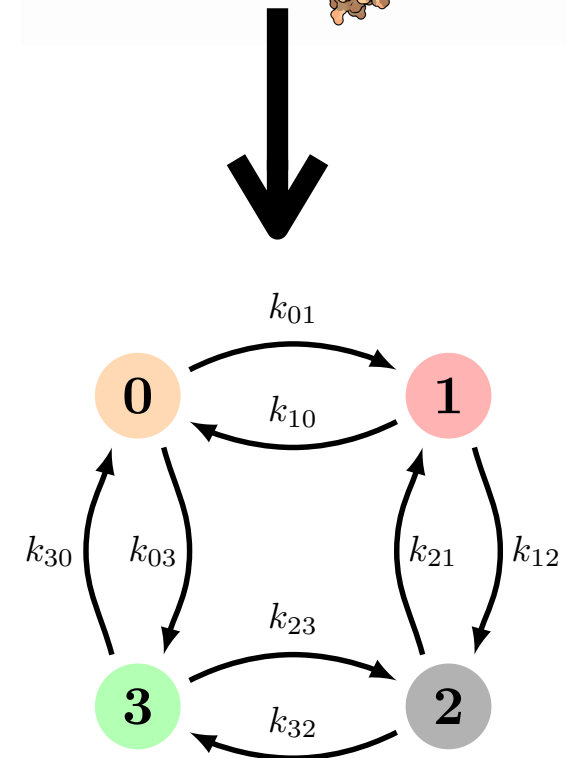
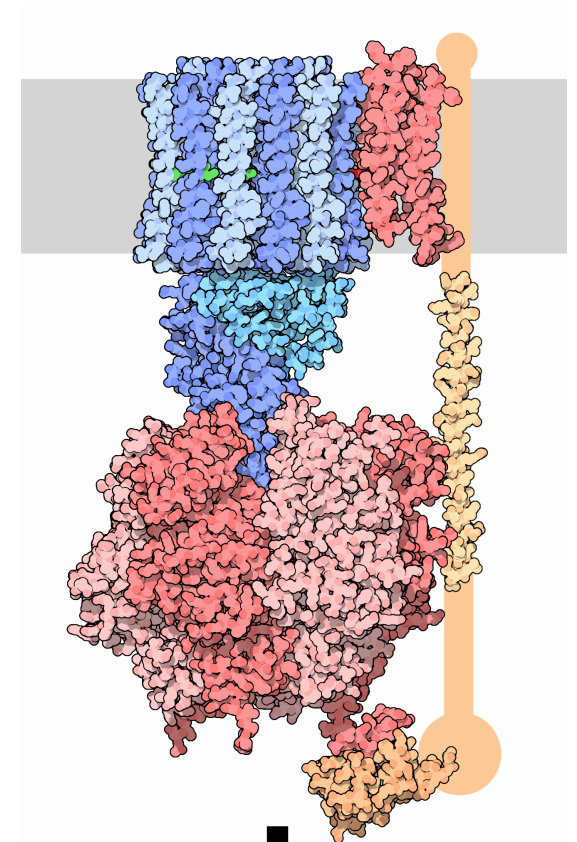
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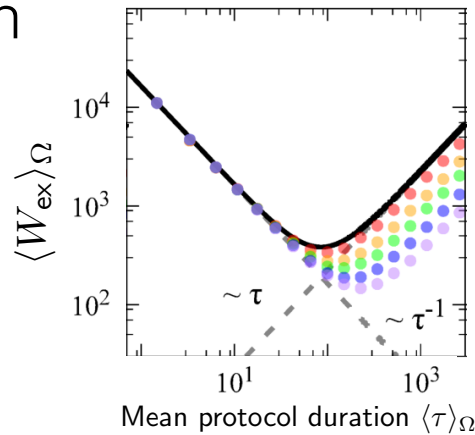


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- Fundamentally different control strategies



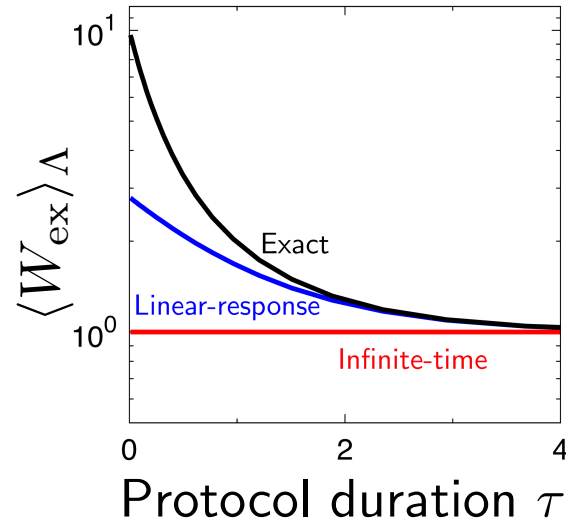
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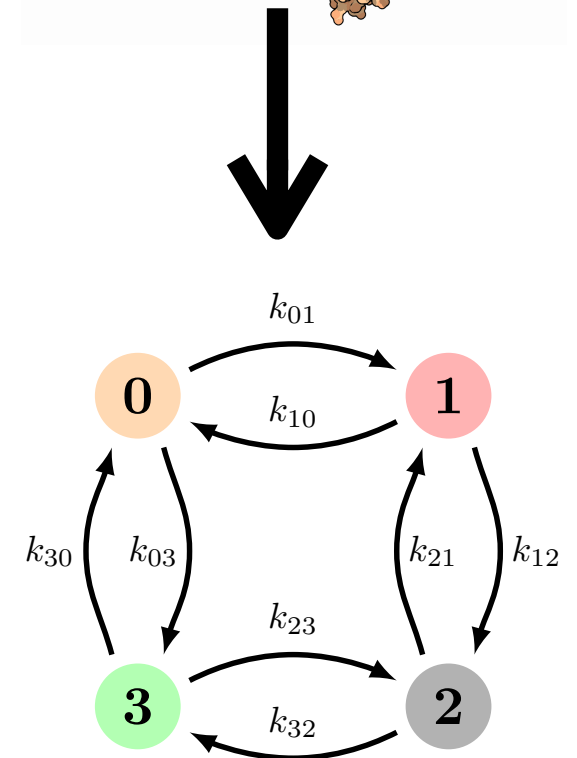
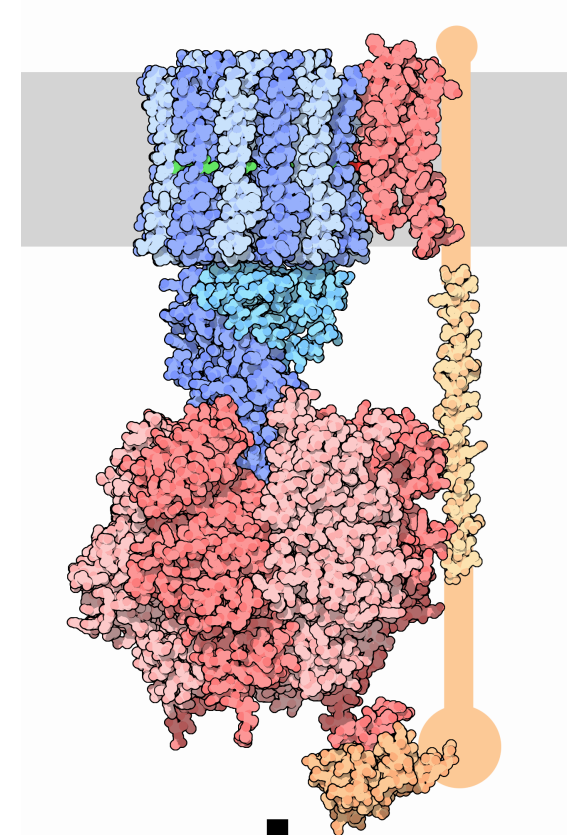
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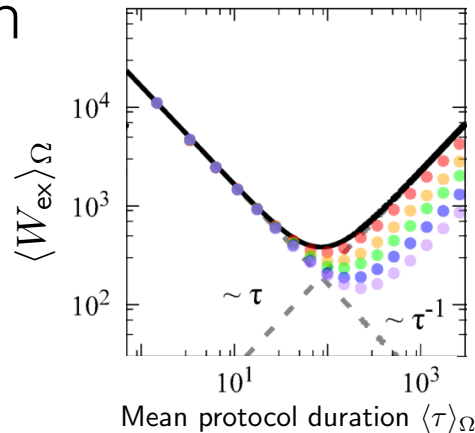
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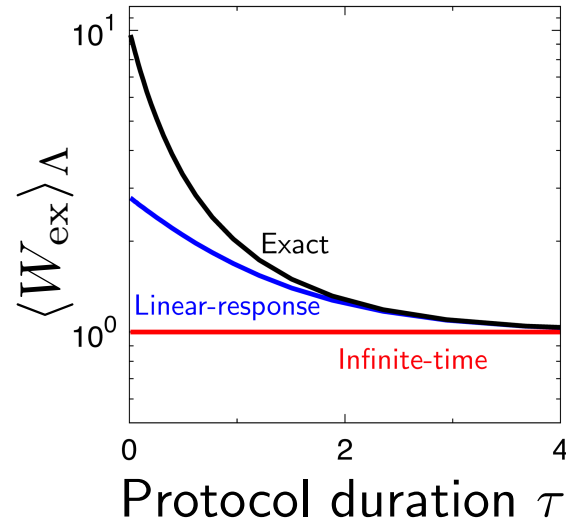
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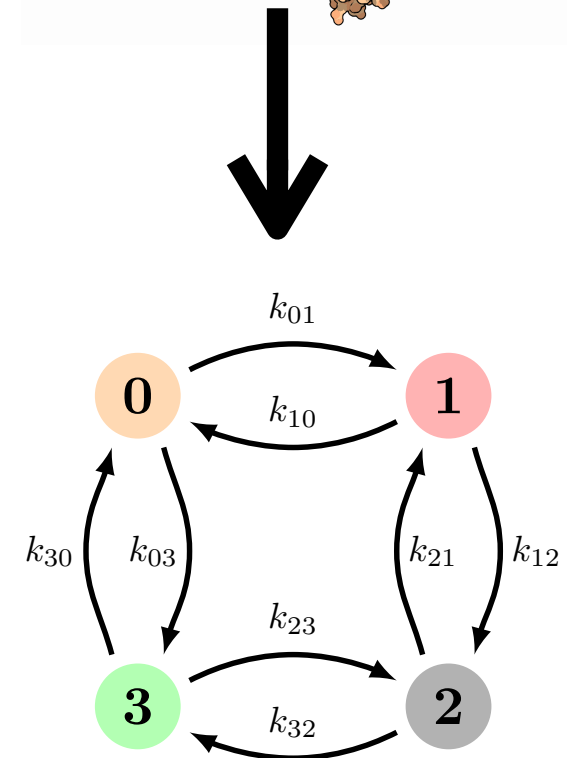
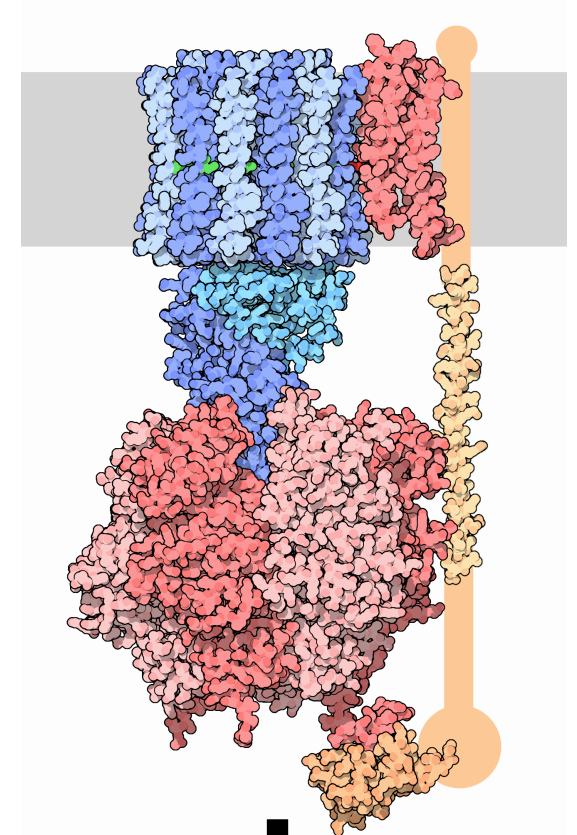


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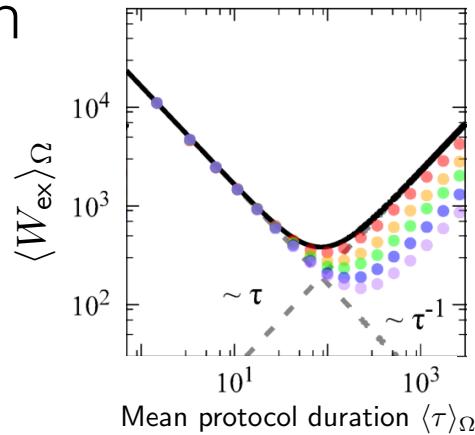
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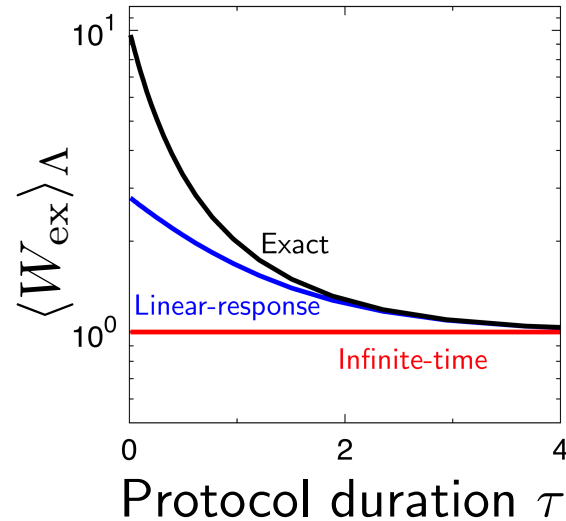
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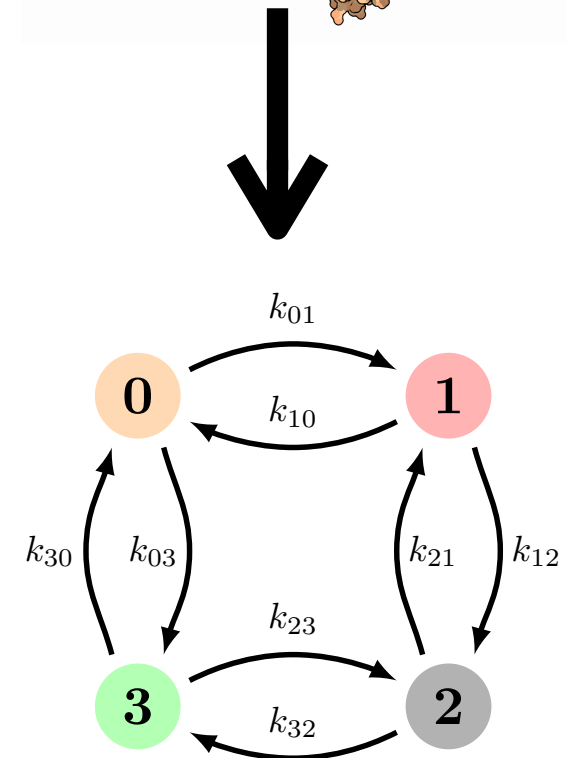
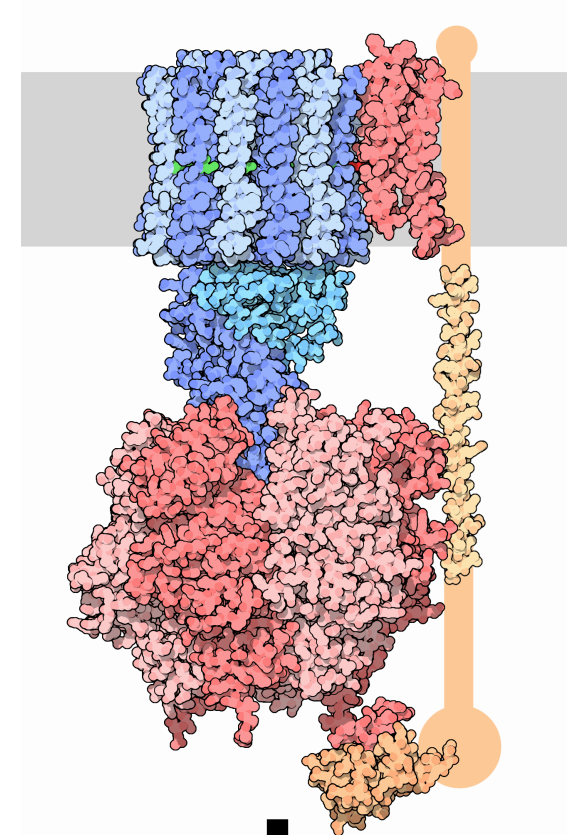
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- How do these theories embed themselves into a broader picture of stochastic thermodynamics?

- What are the implications for molecular machines like ATP-synthase?



Simon Fraser University



Sivak Group

CNRS Researcher



Raphael Chetrite



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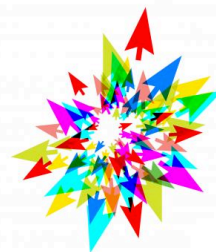
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