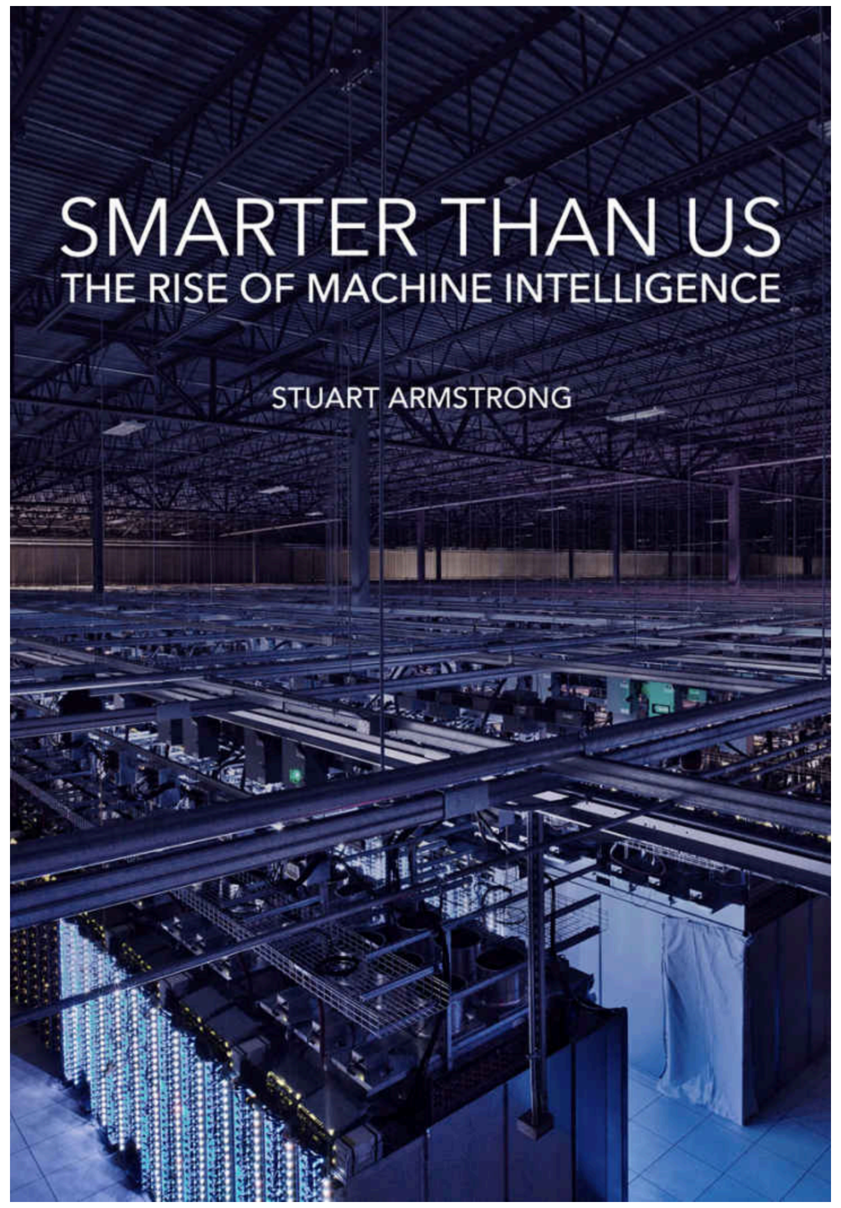
Bayesian Uncertainty Quantification

Part I: Introduction

Petros Koumoutsakos

CSE Laboratory - ETHZ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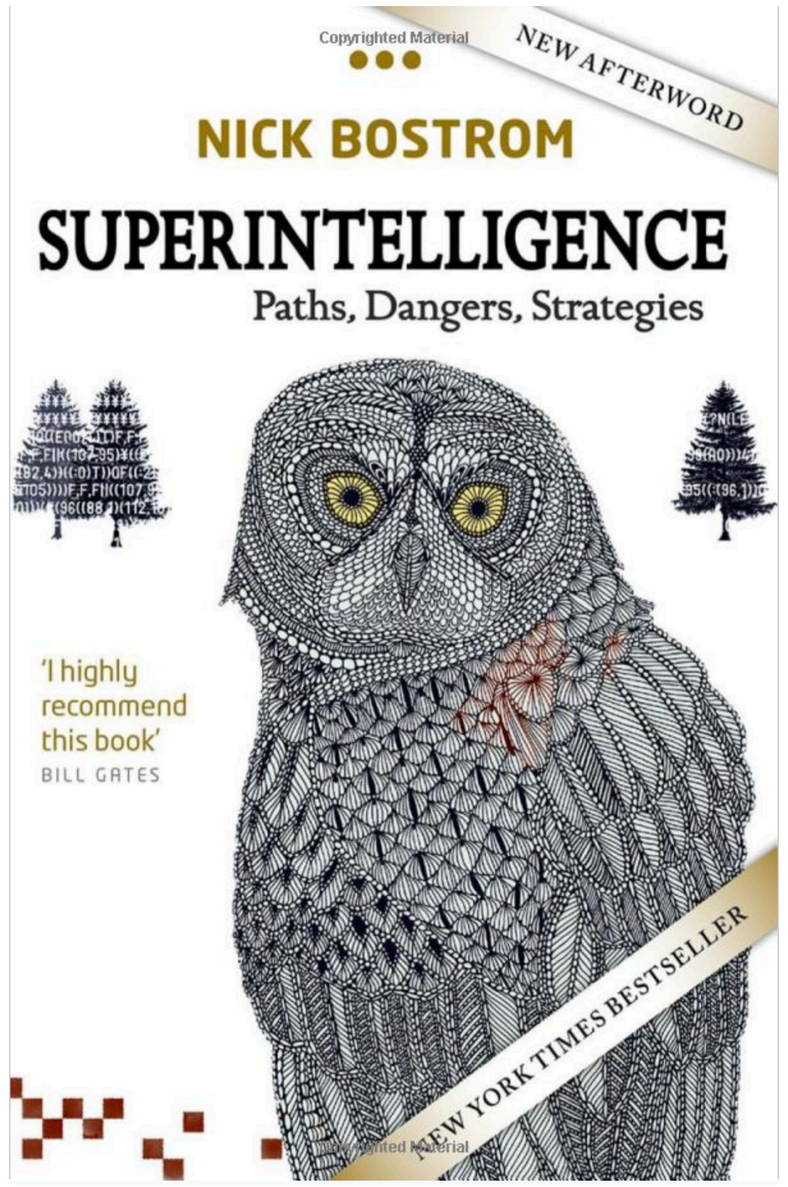
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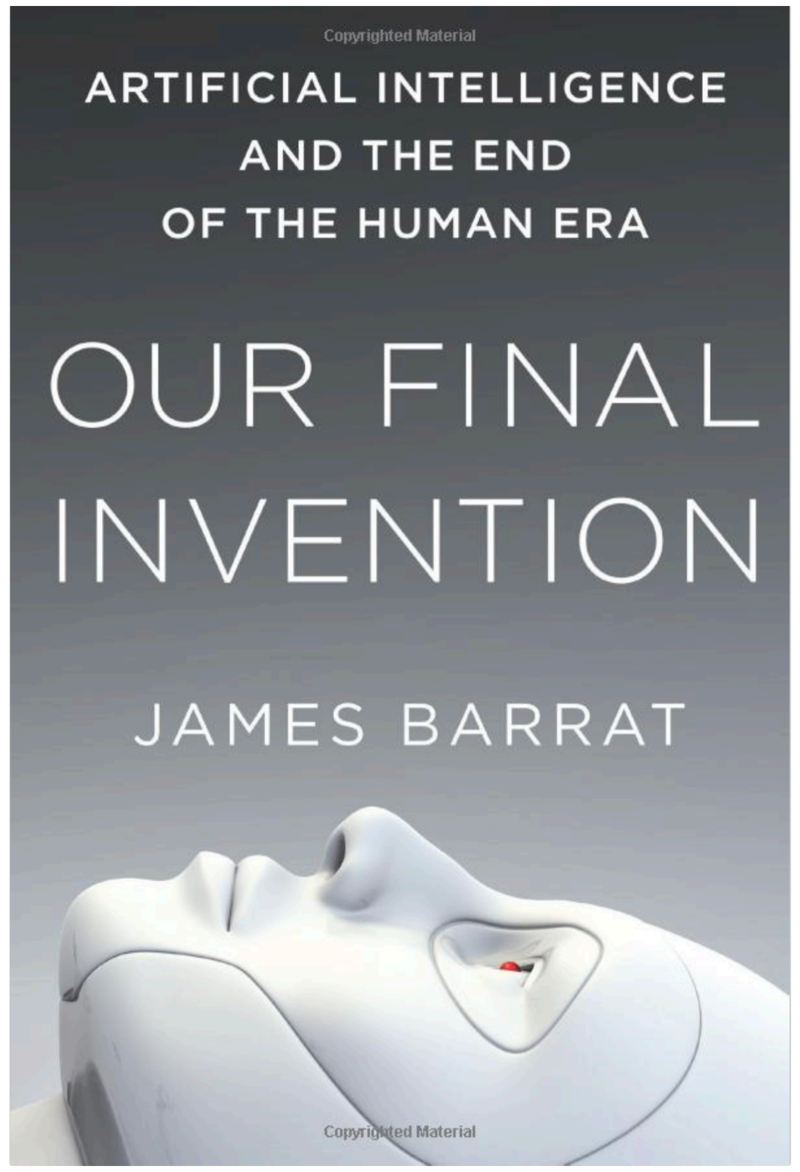
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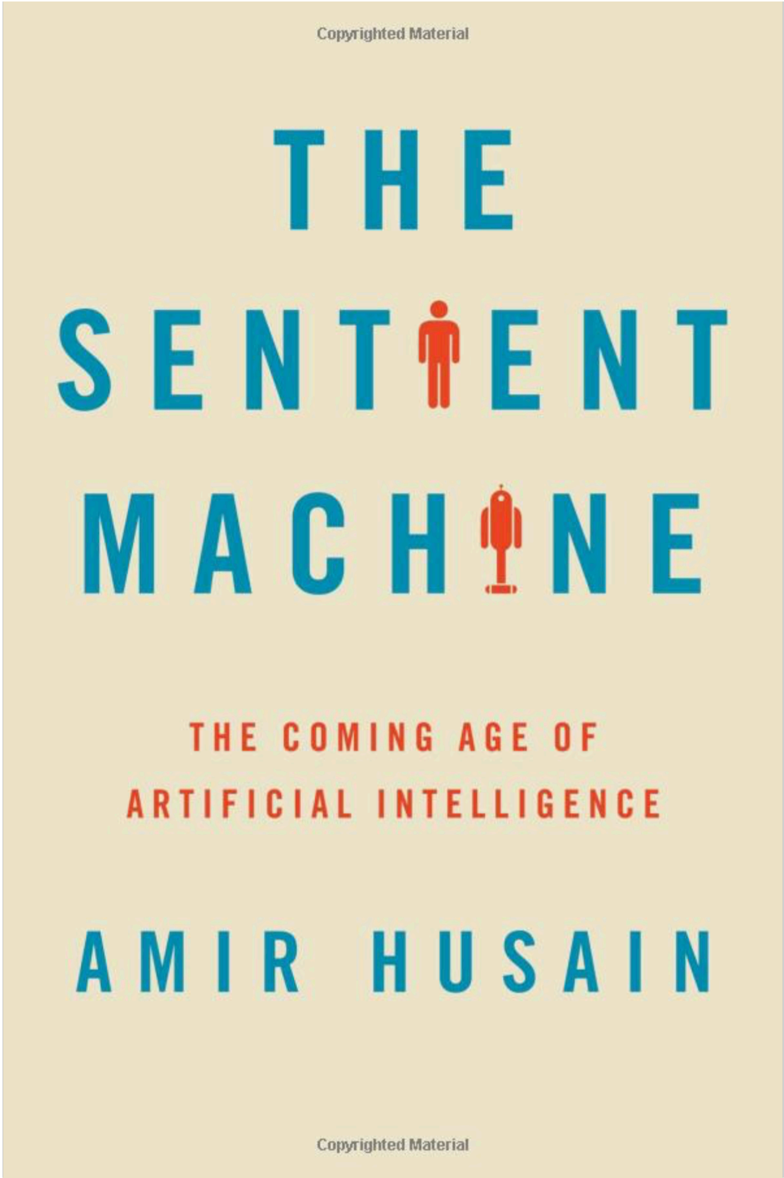
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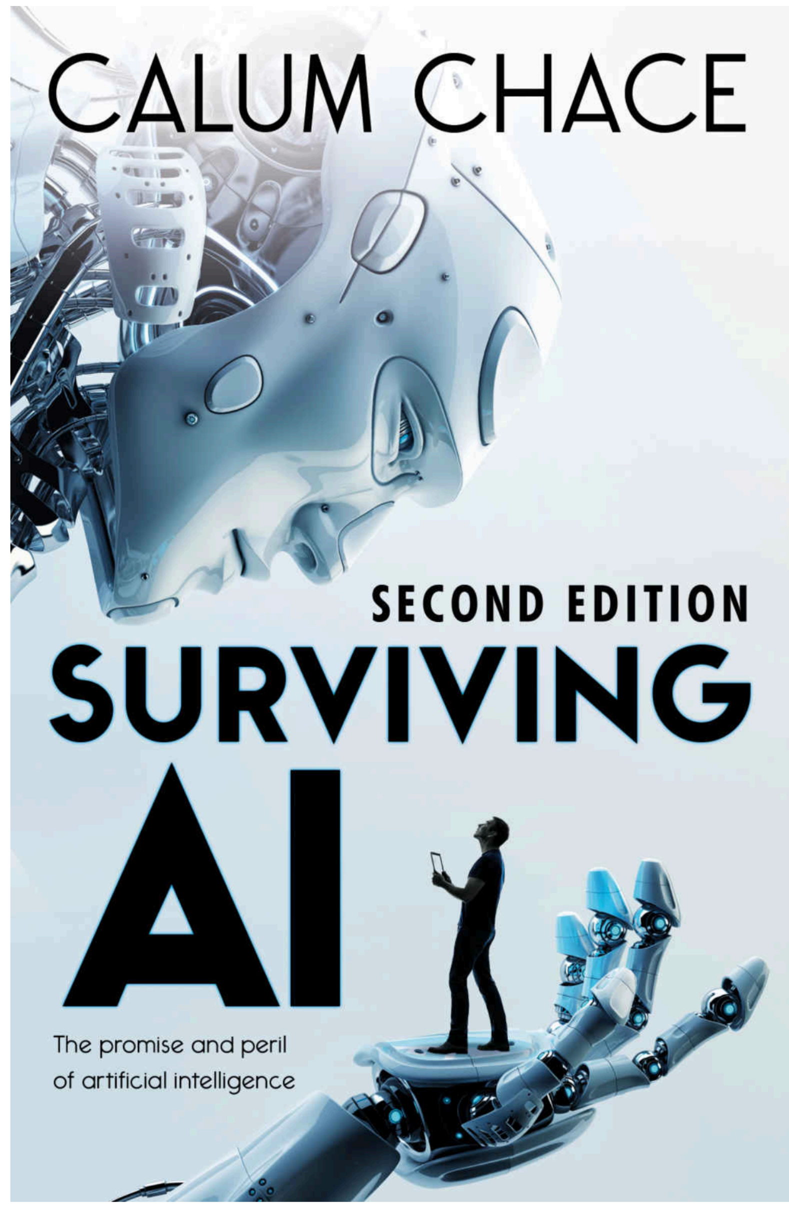
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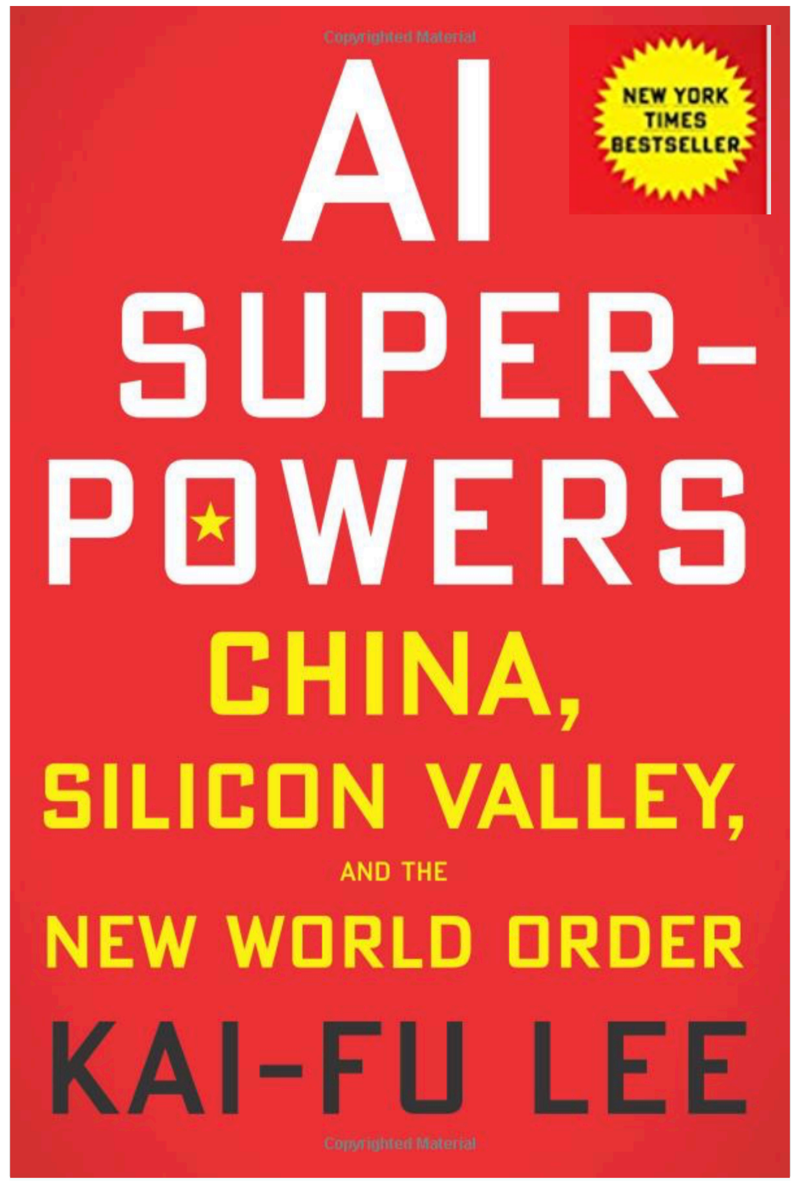
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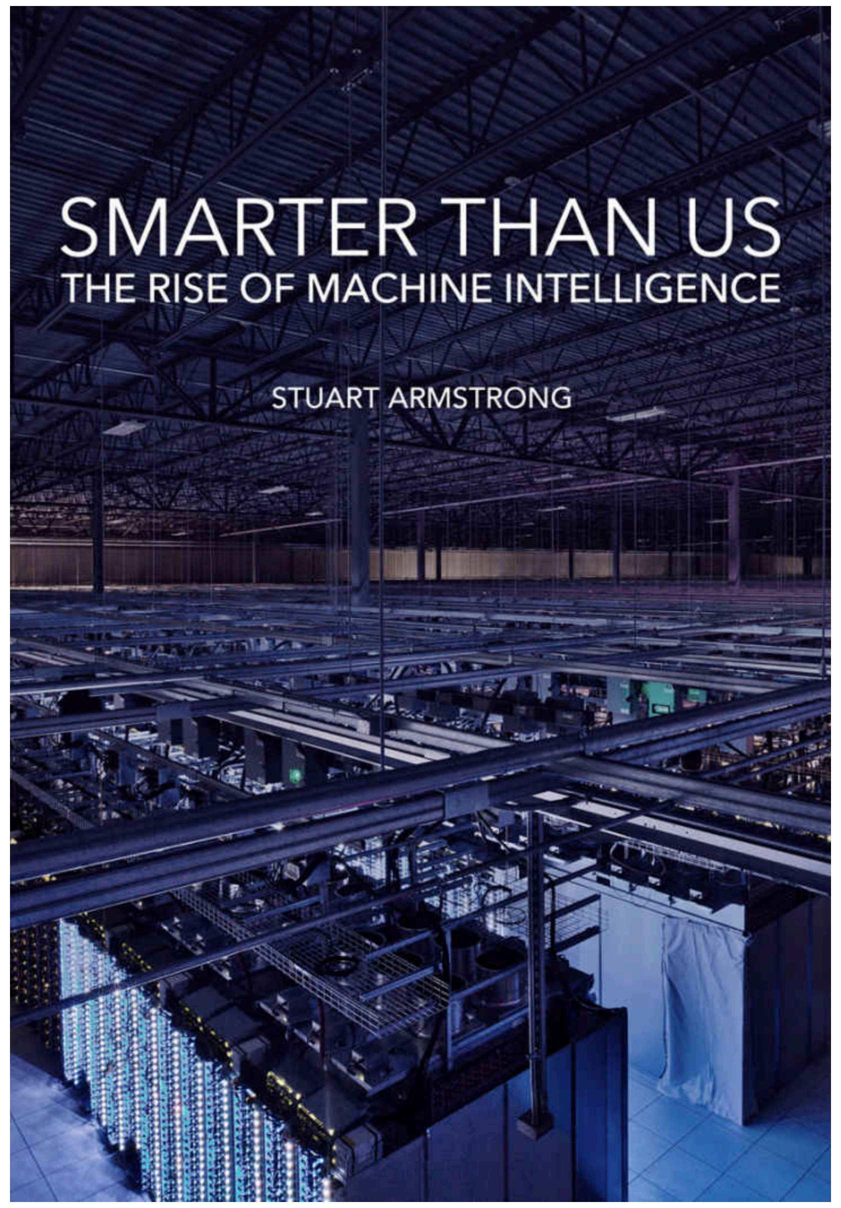
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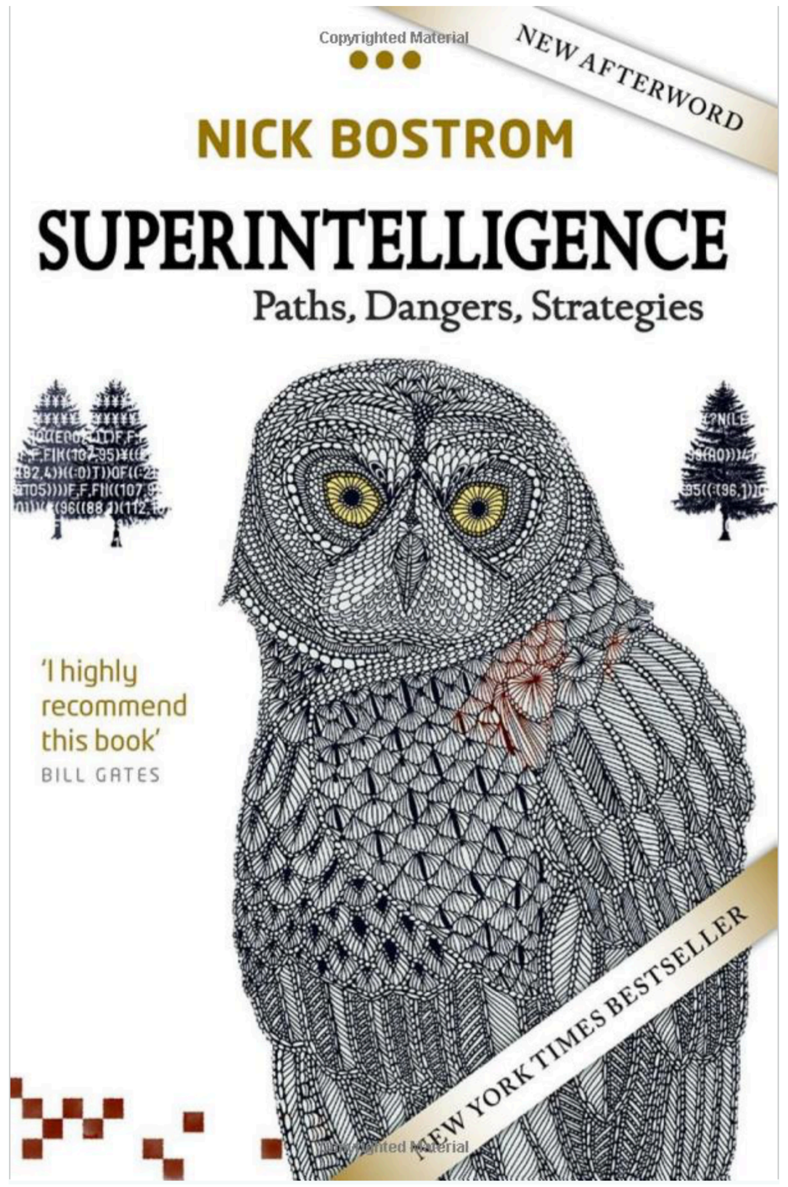
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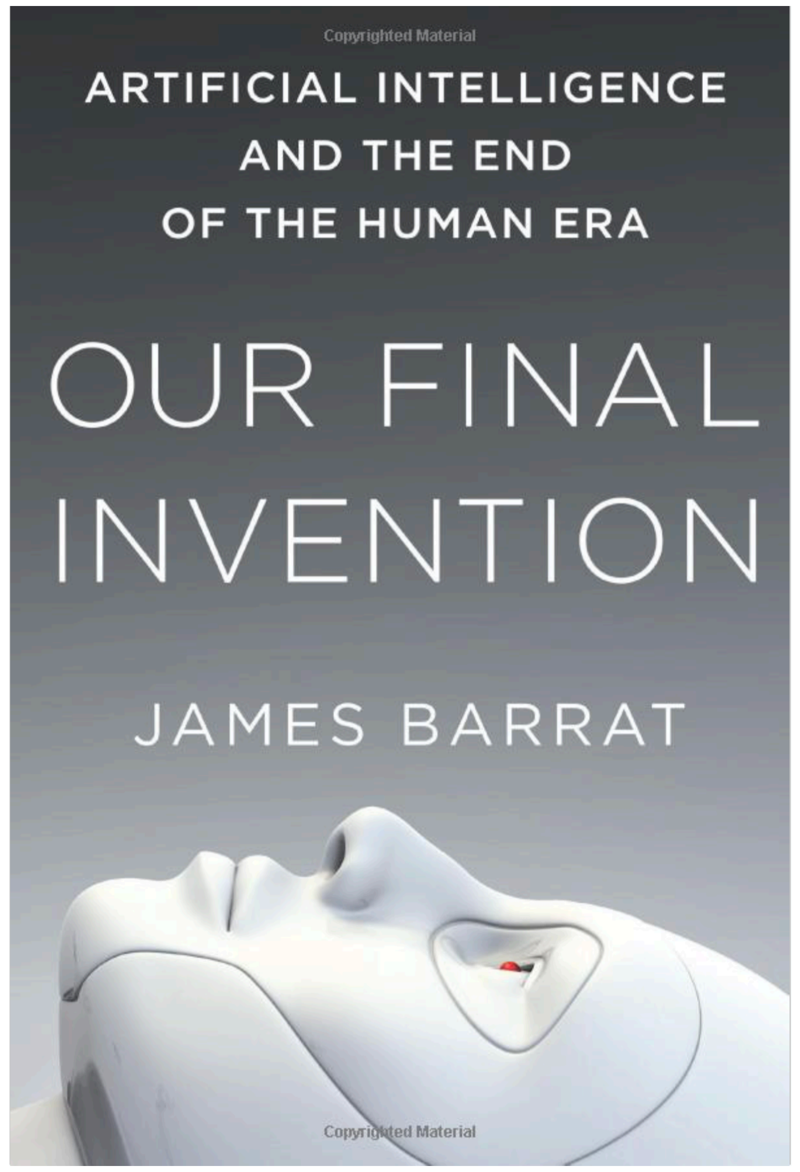
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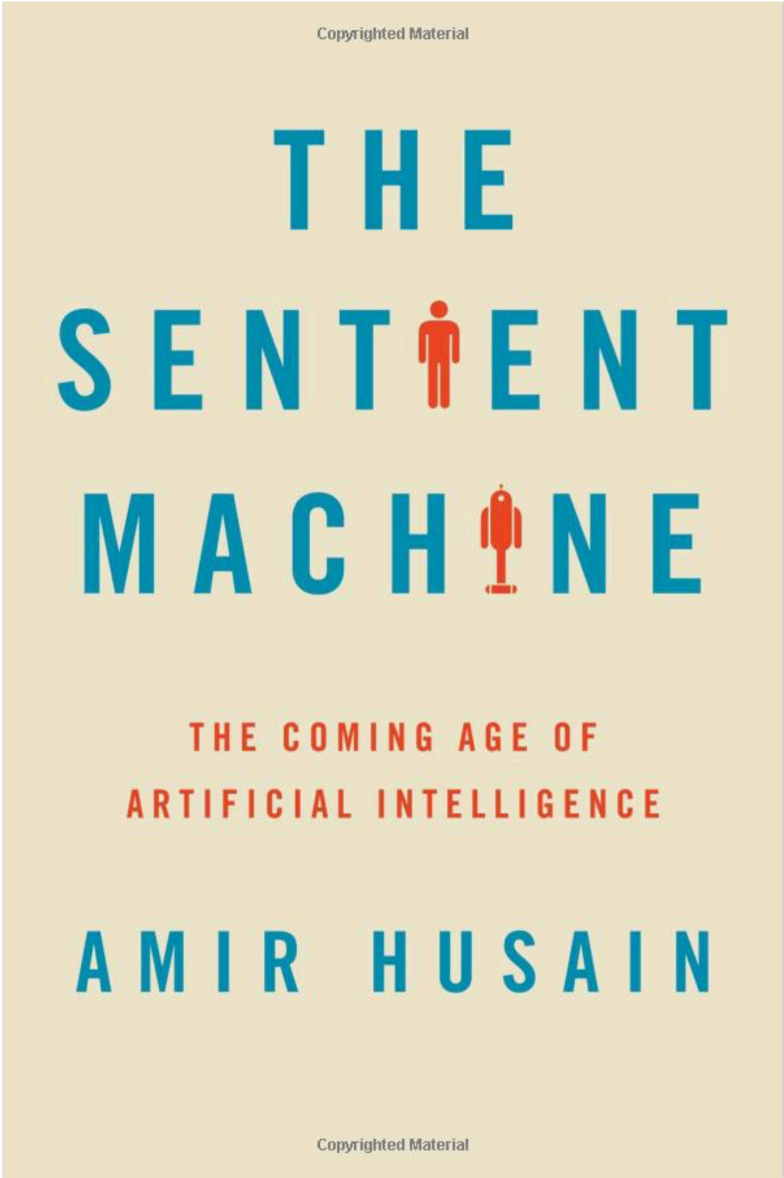
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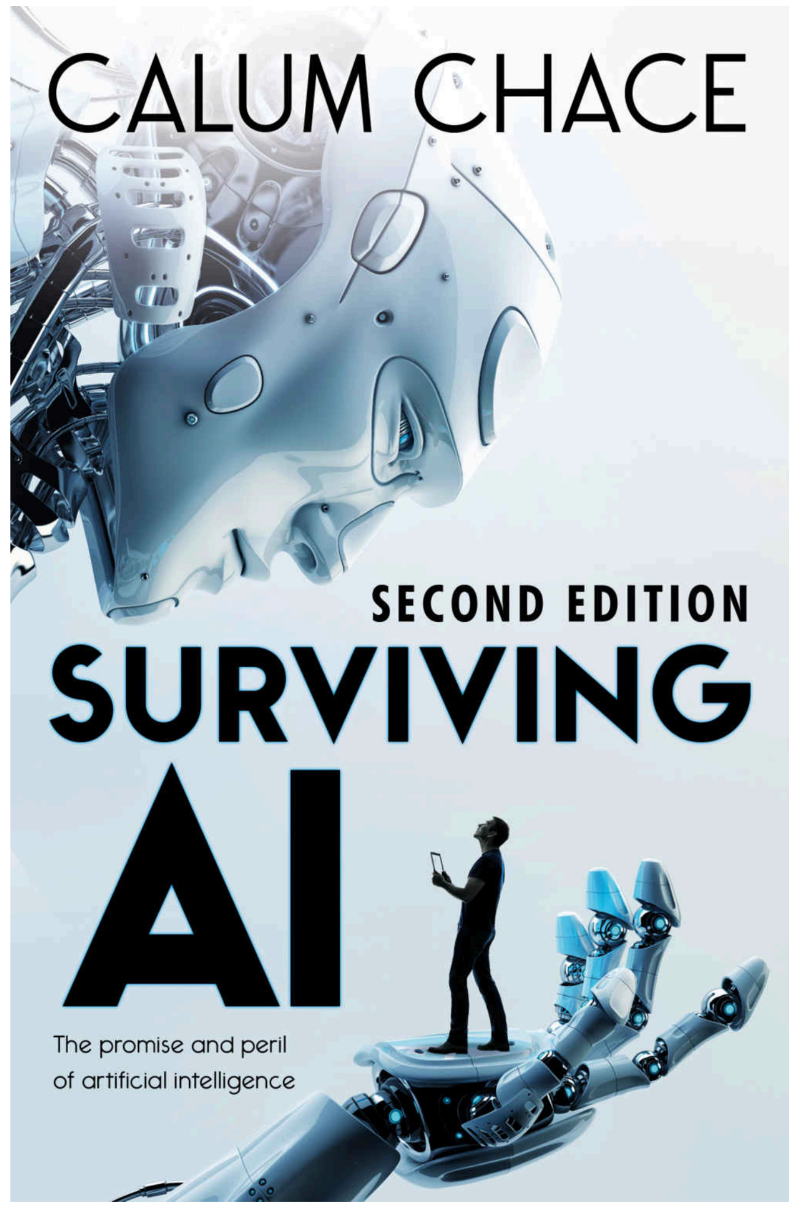
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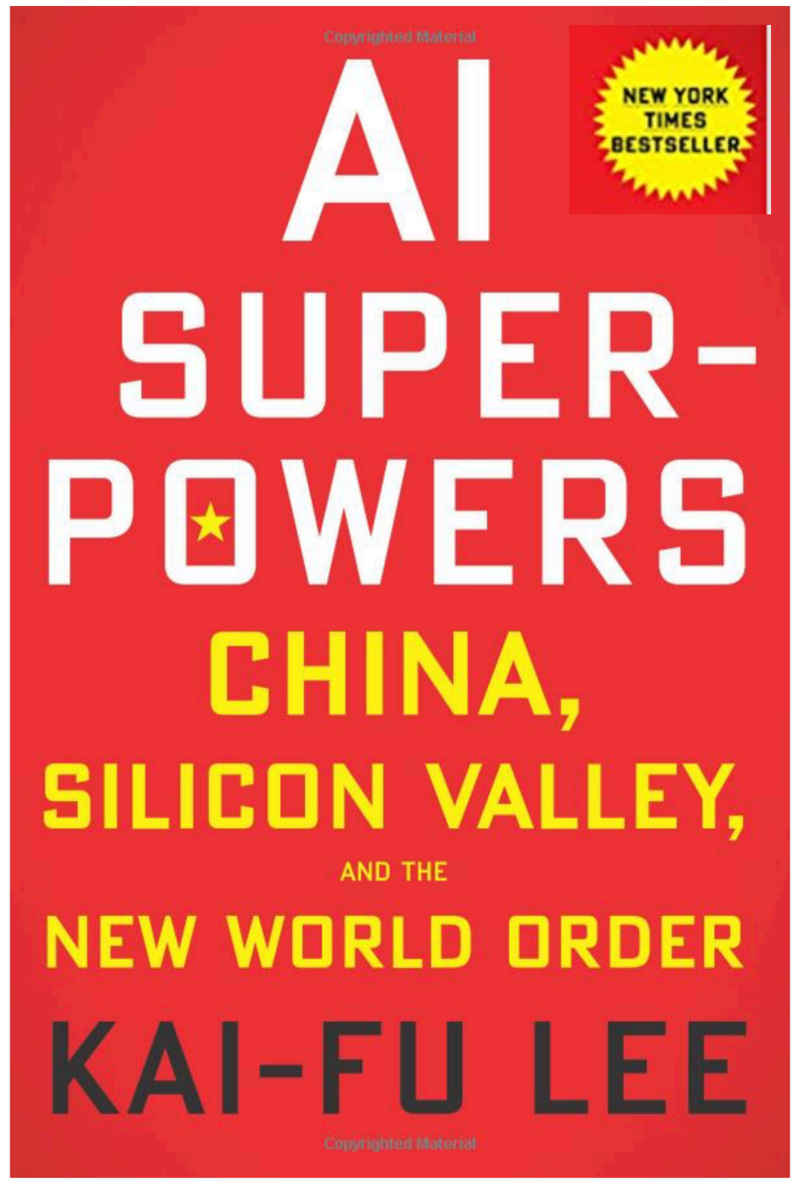
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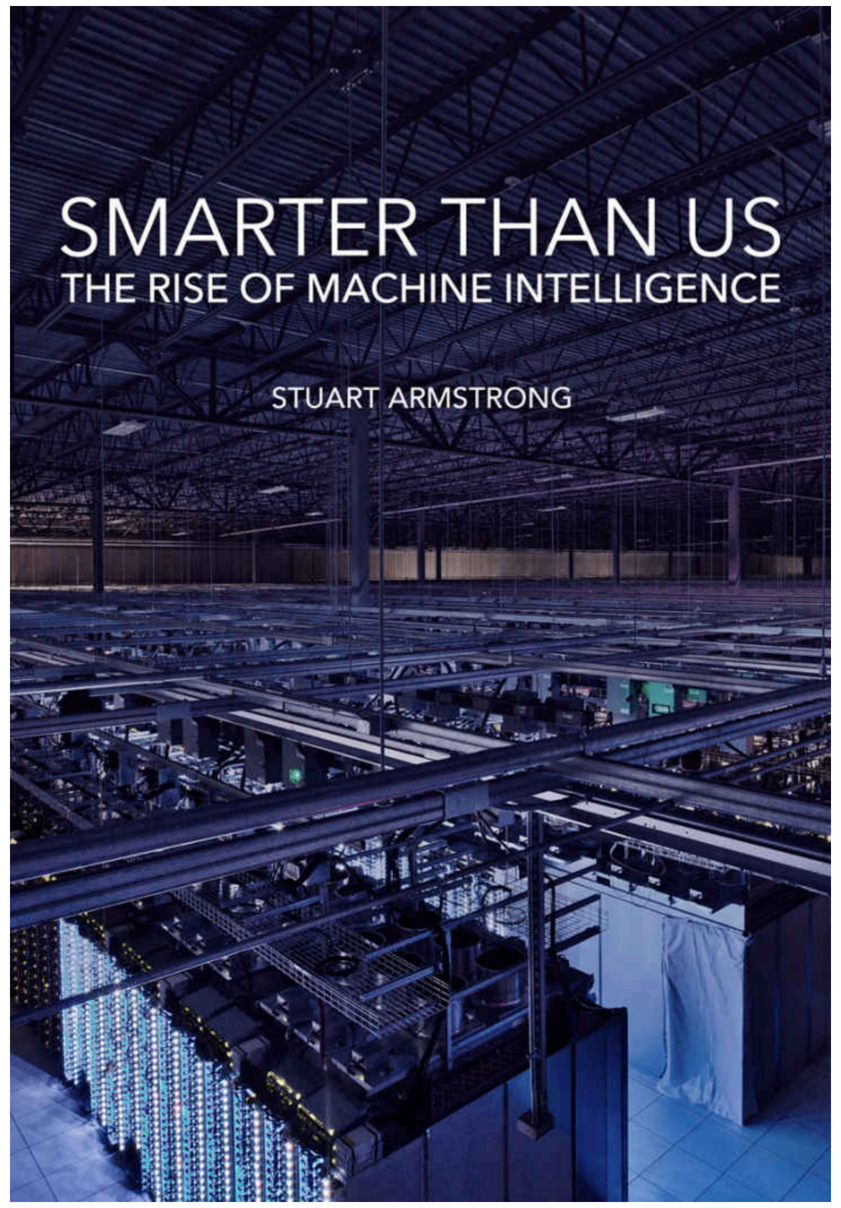
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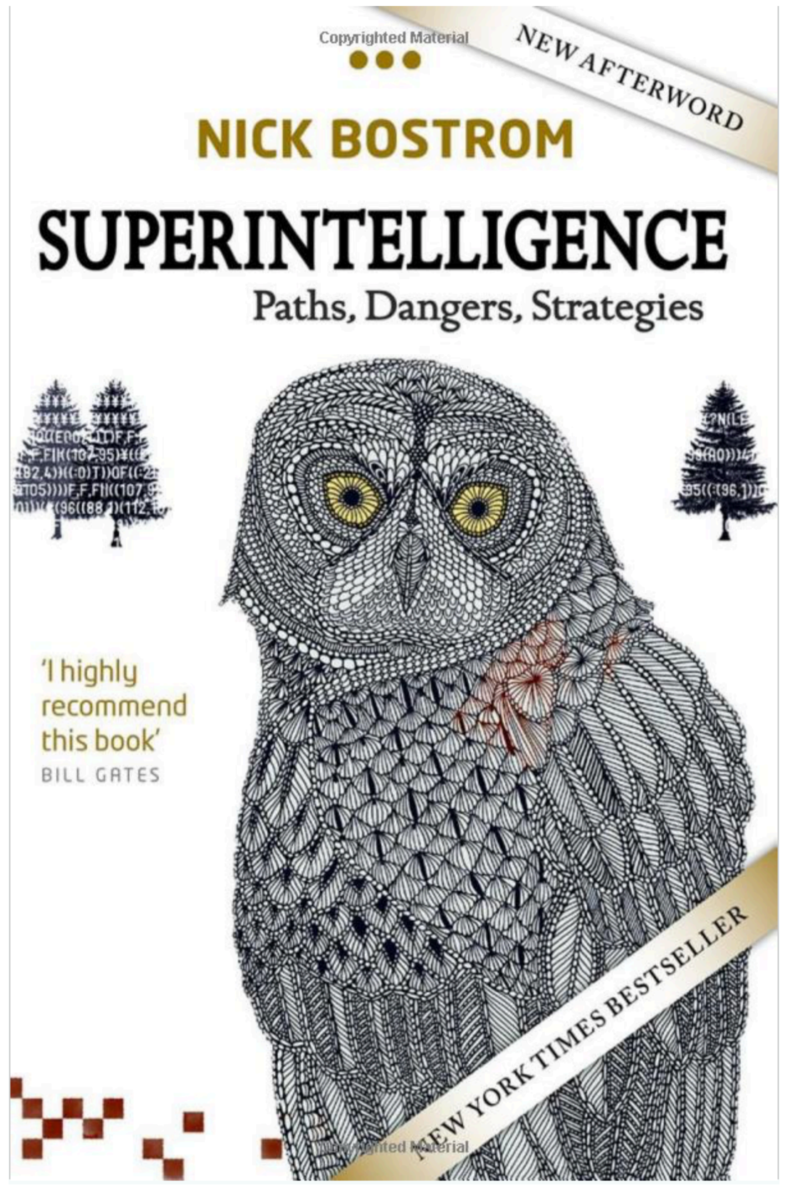
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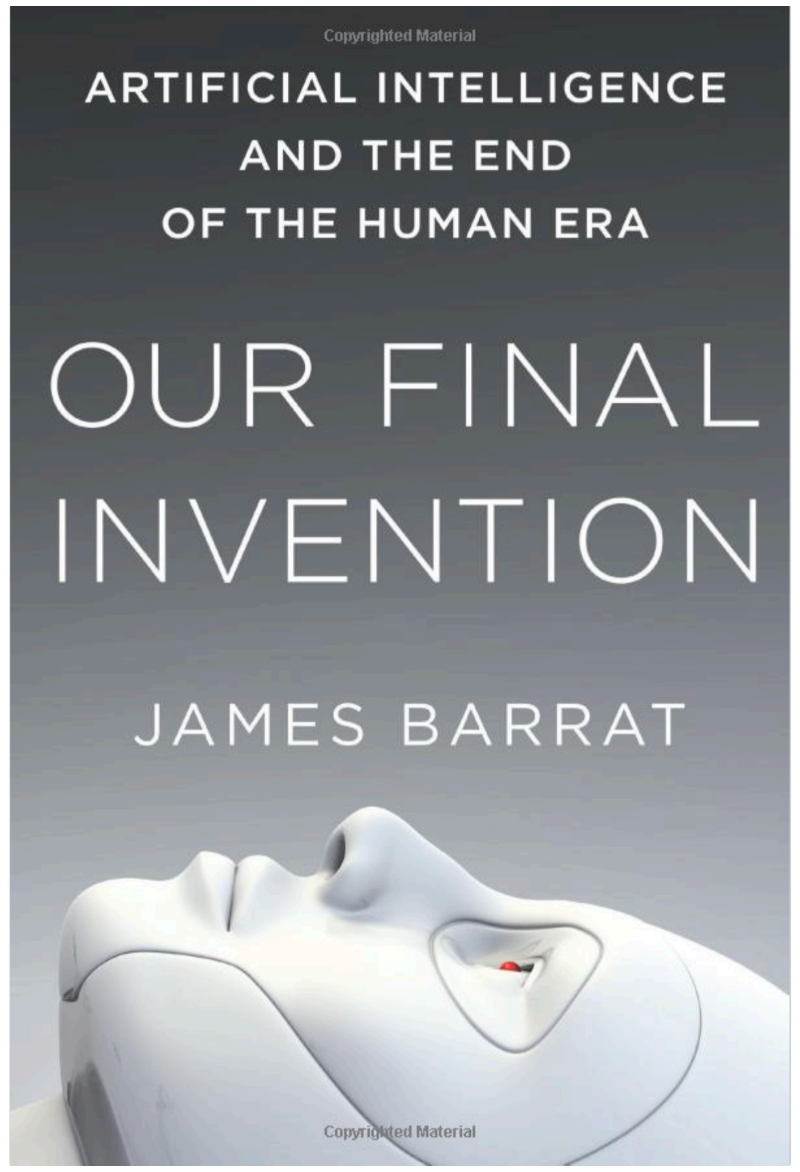
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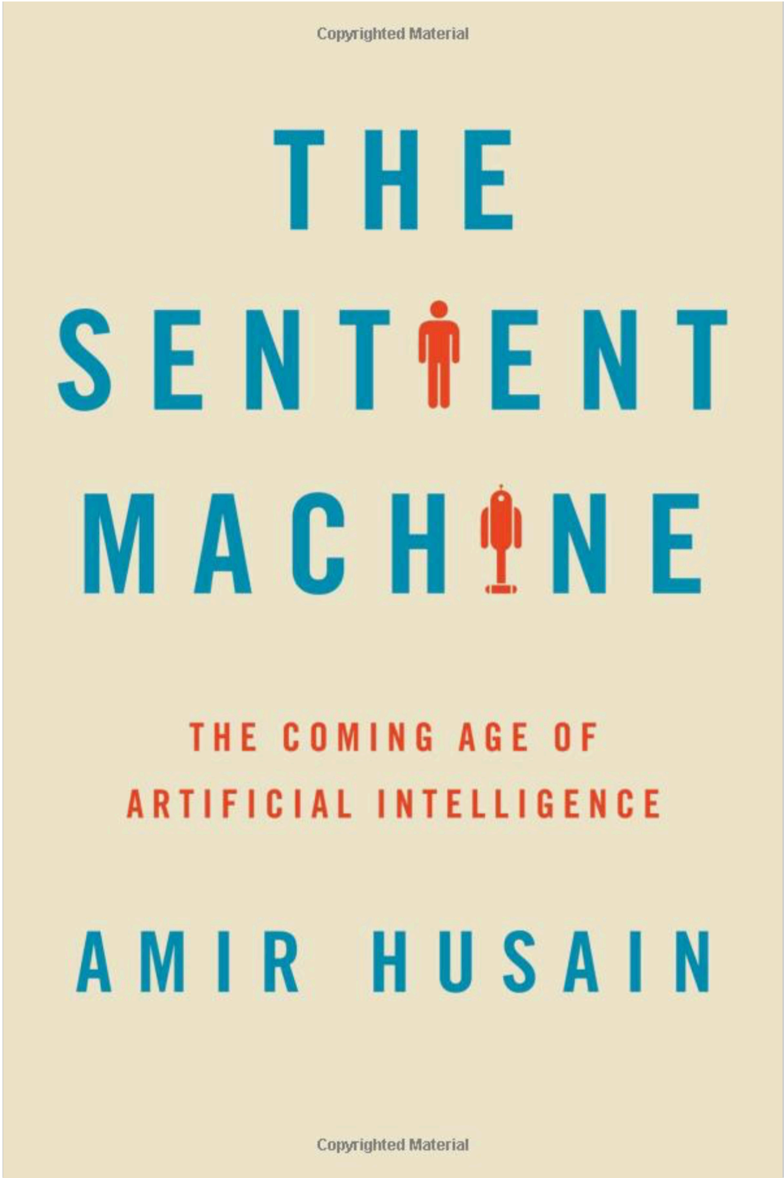
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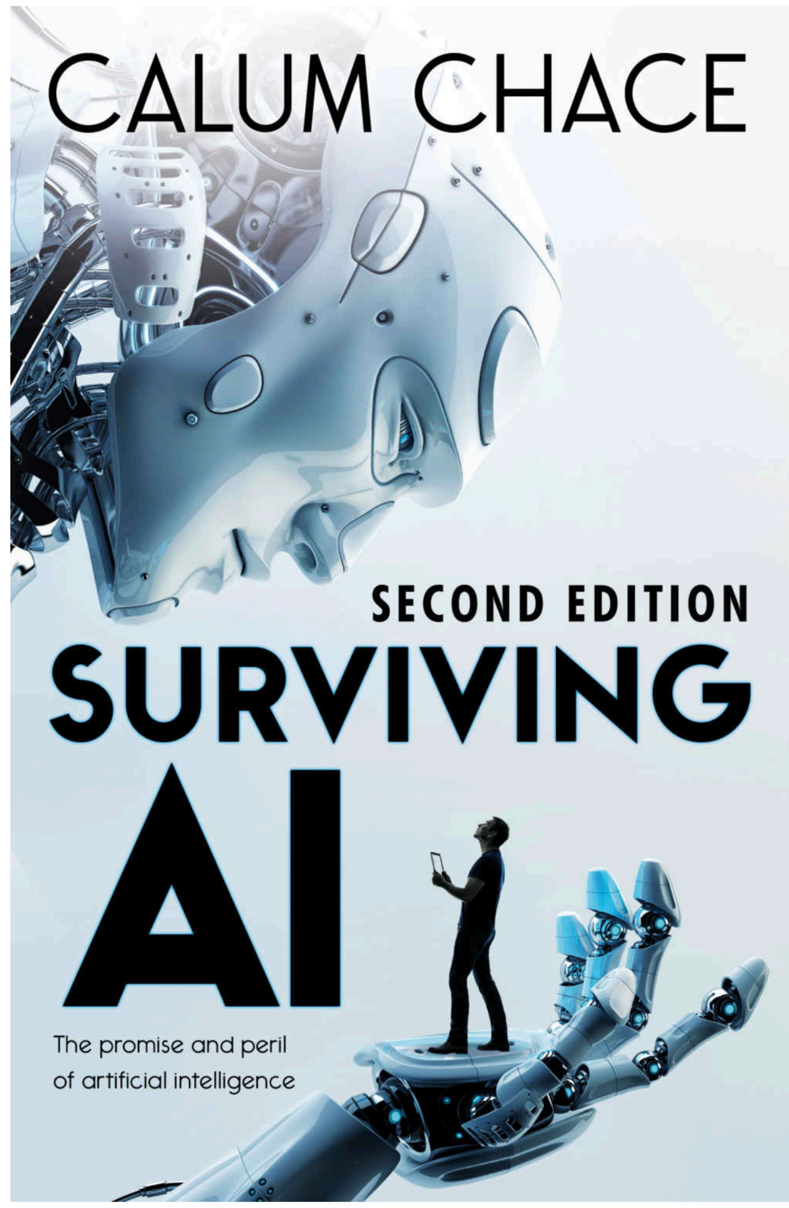
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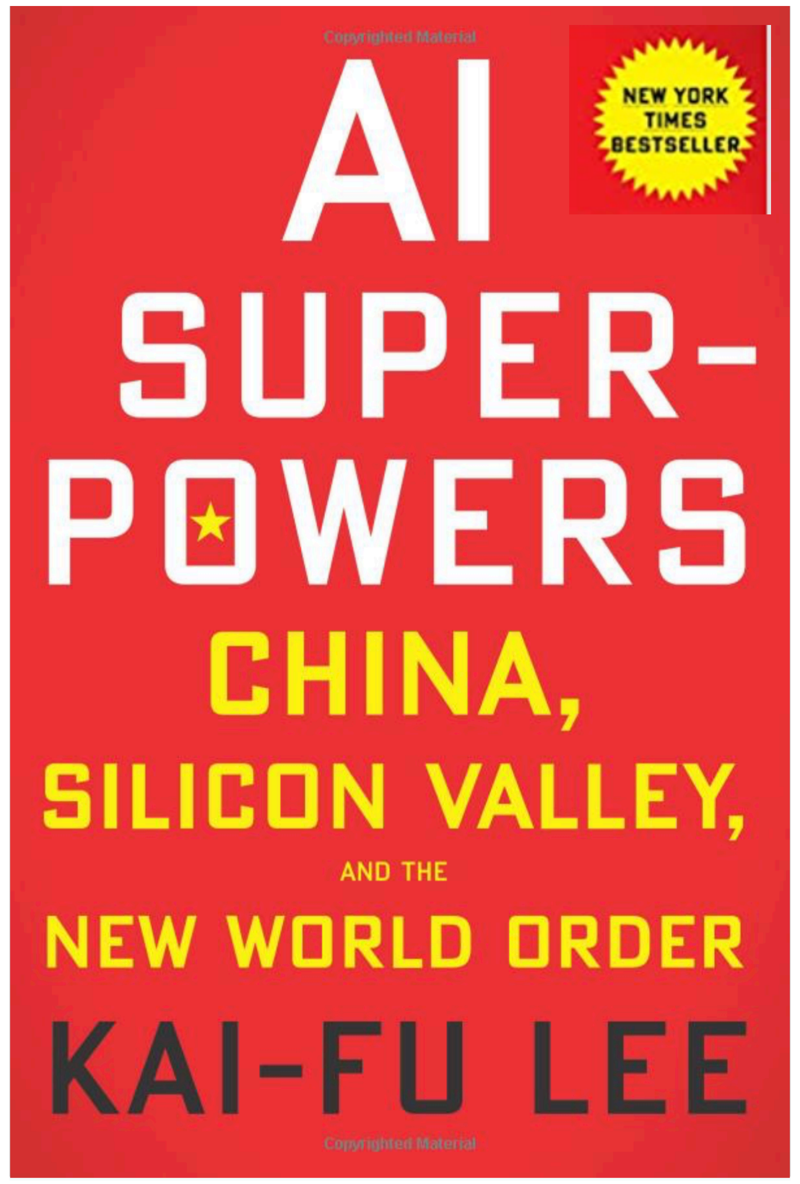
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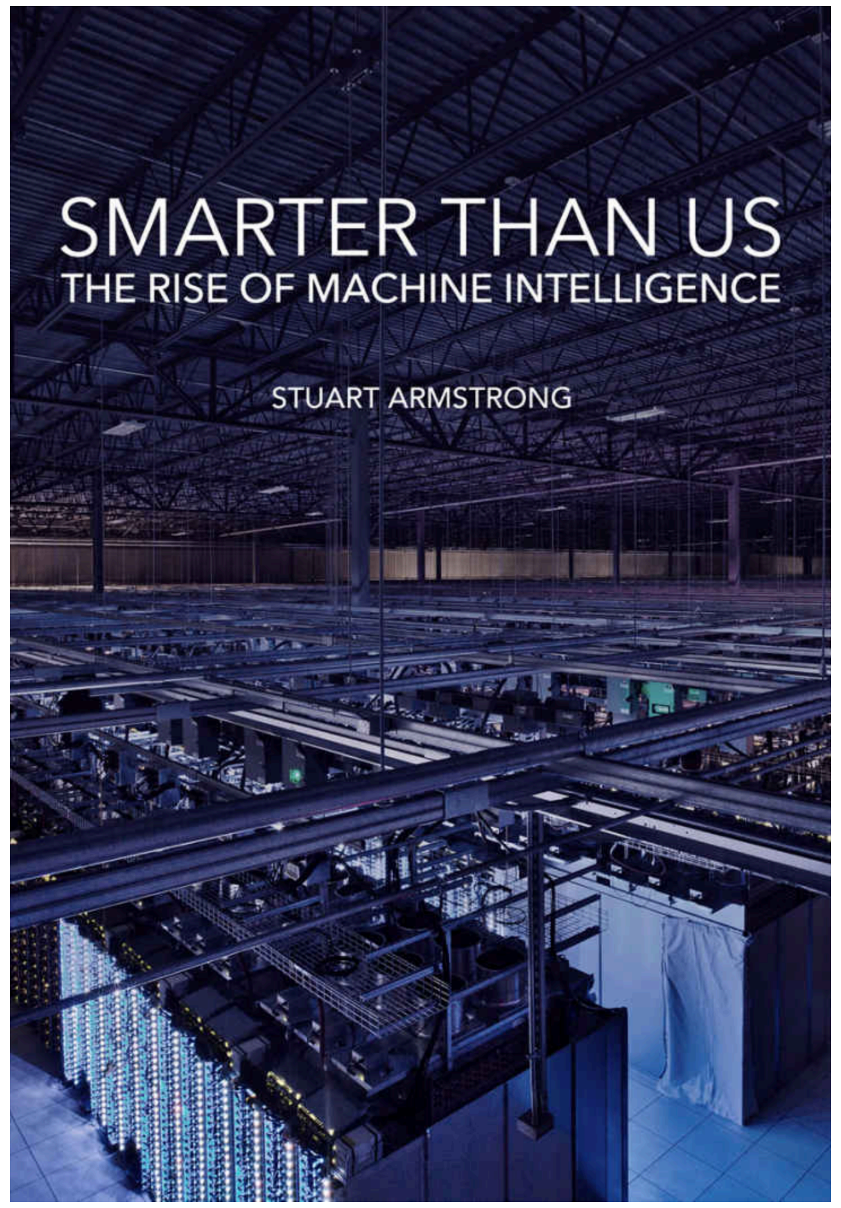
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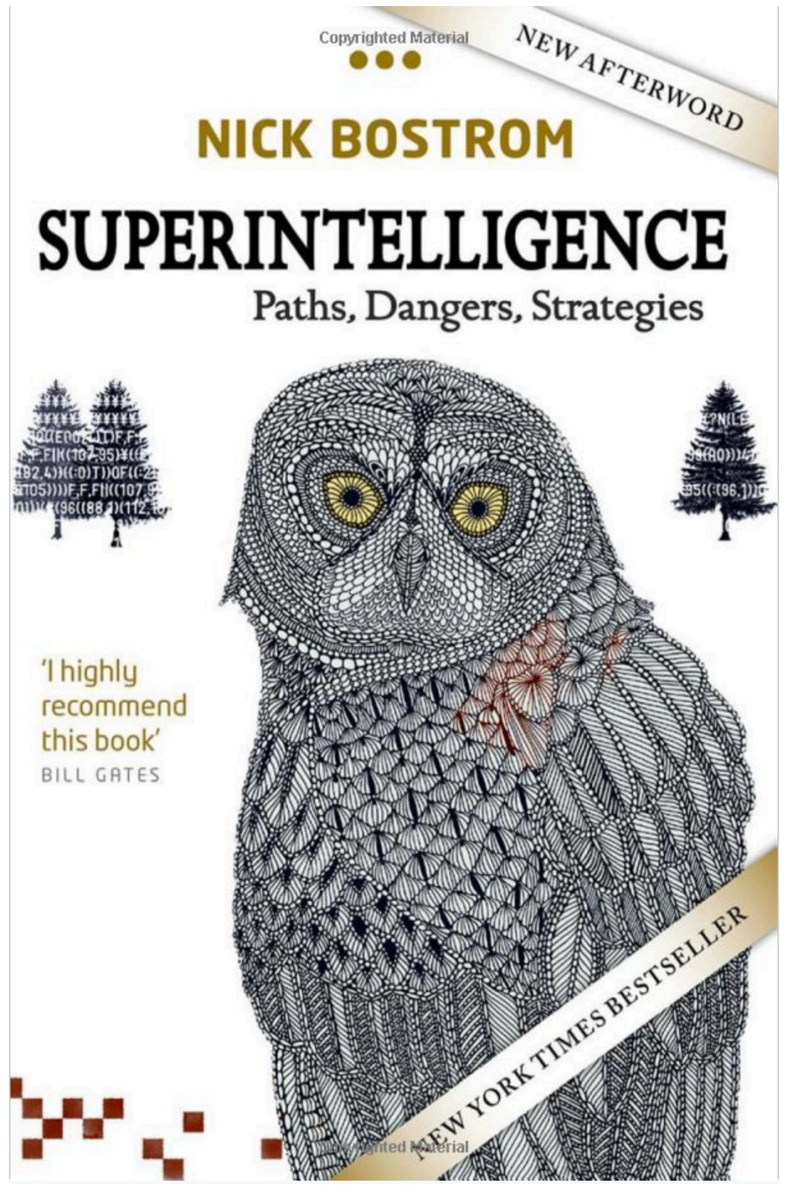
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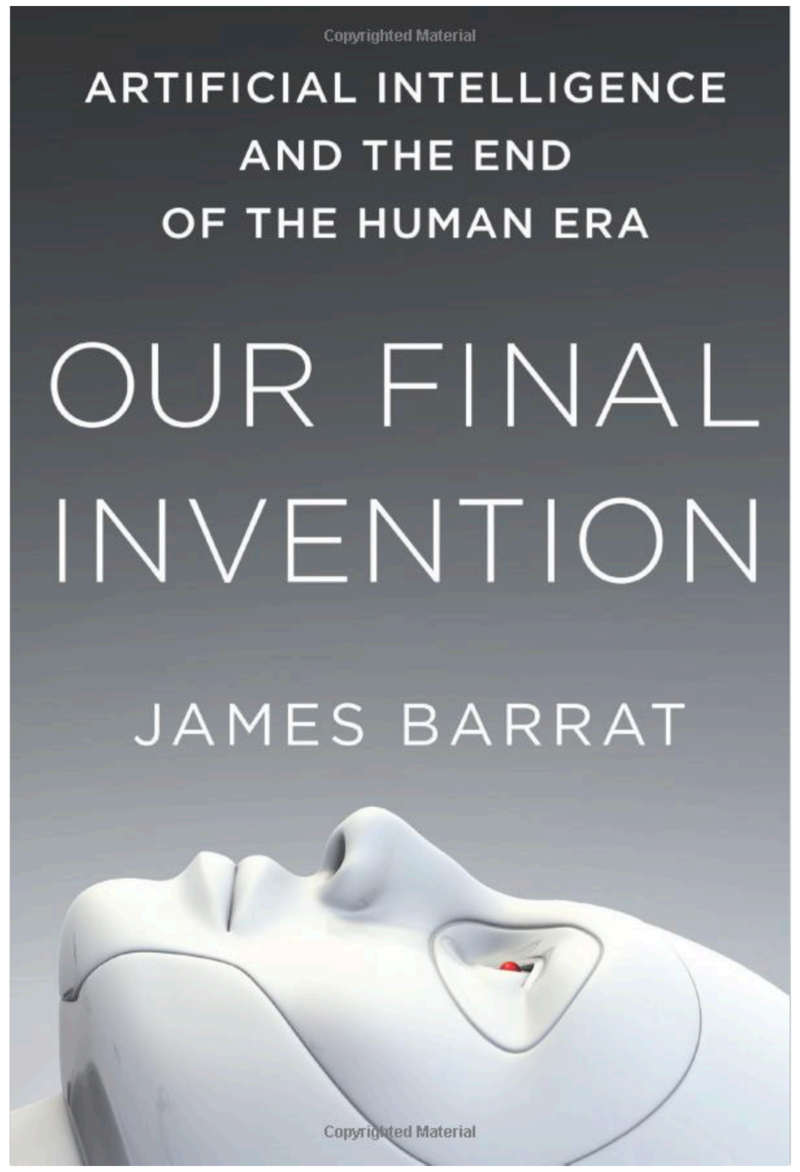
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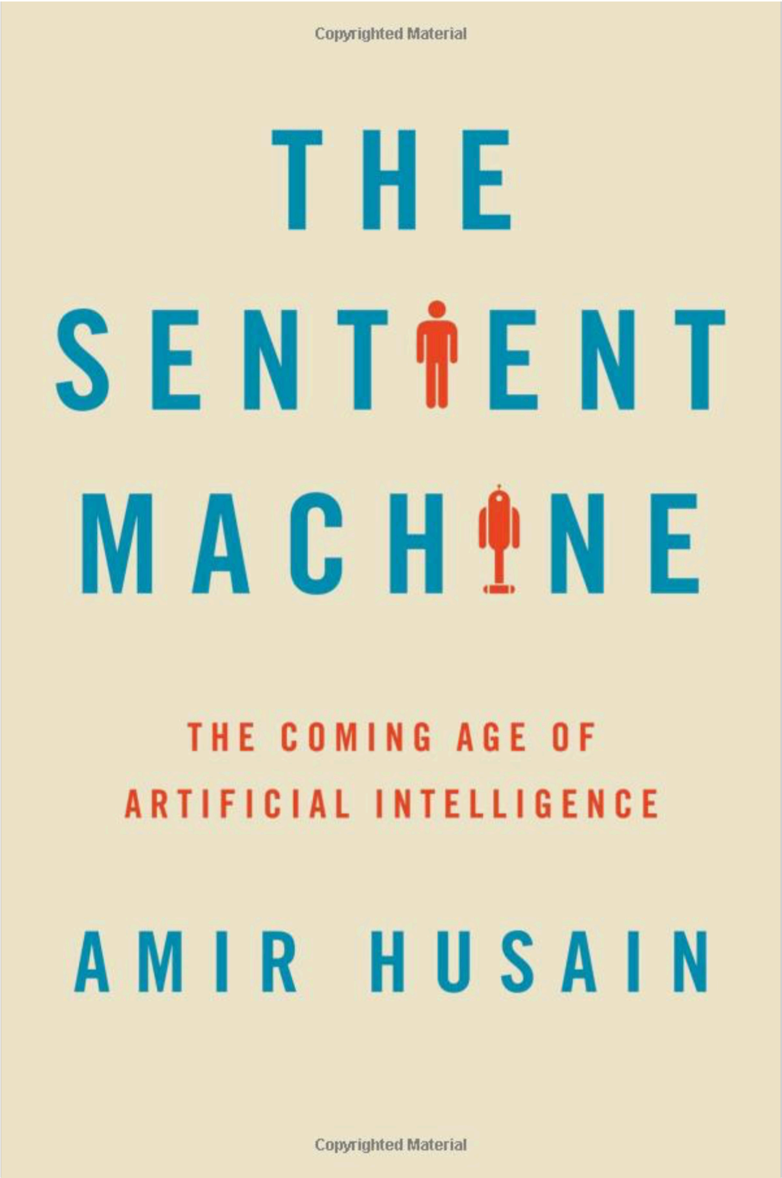
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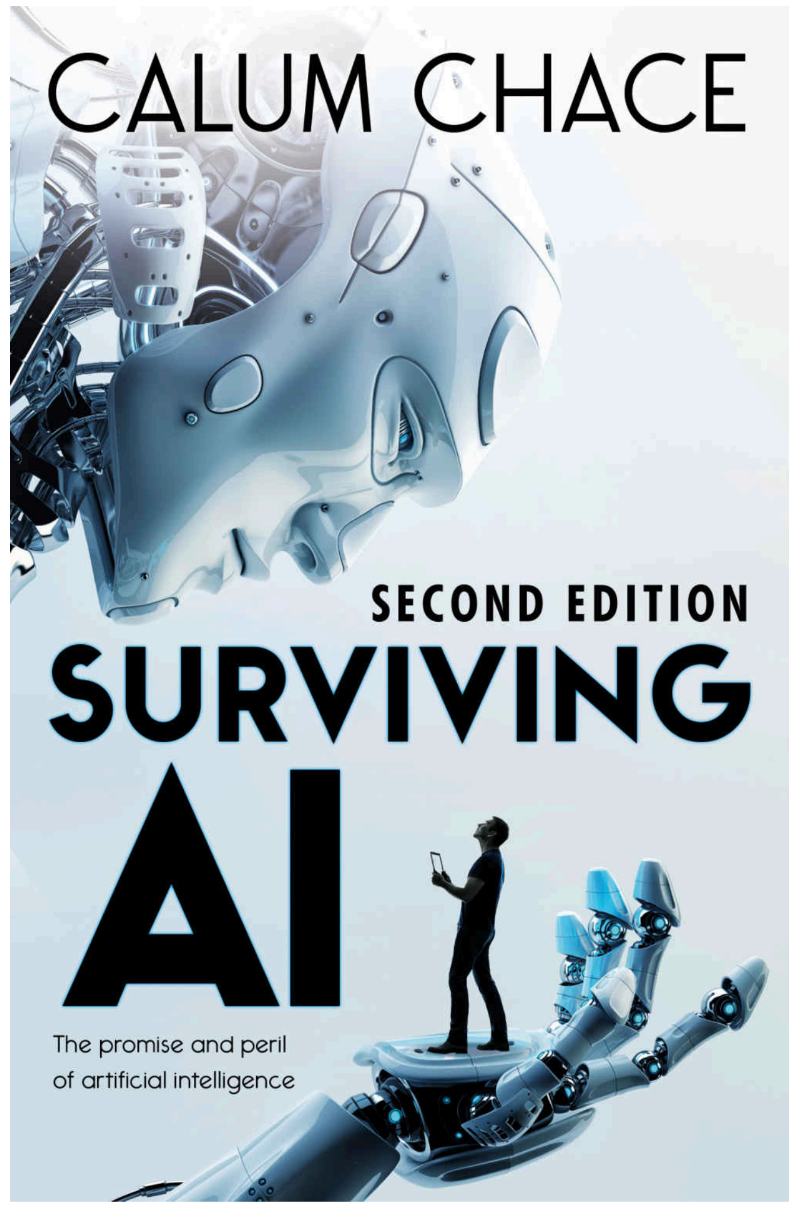
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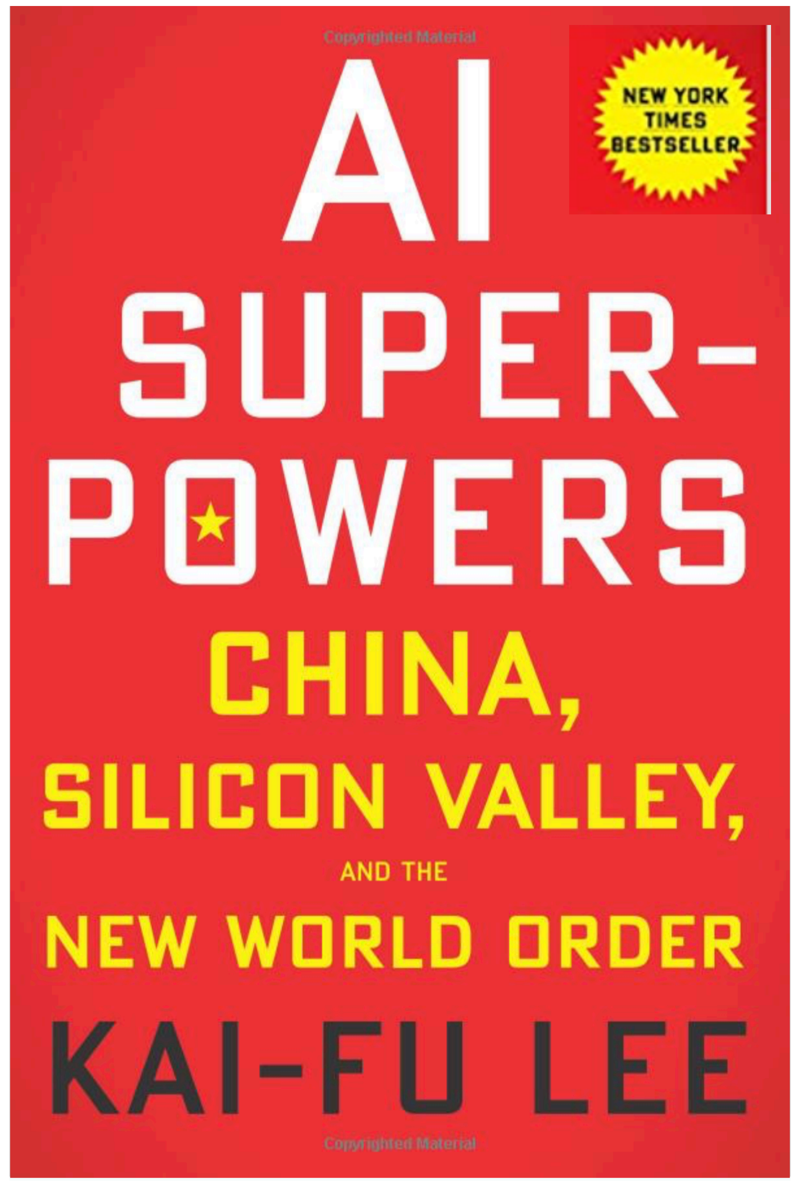
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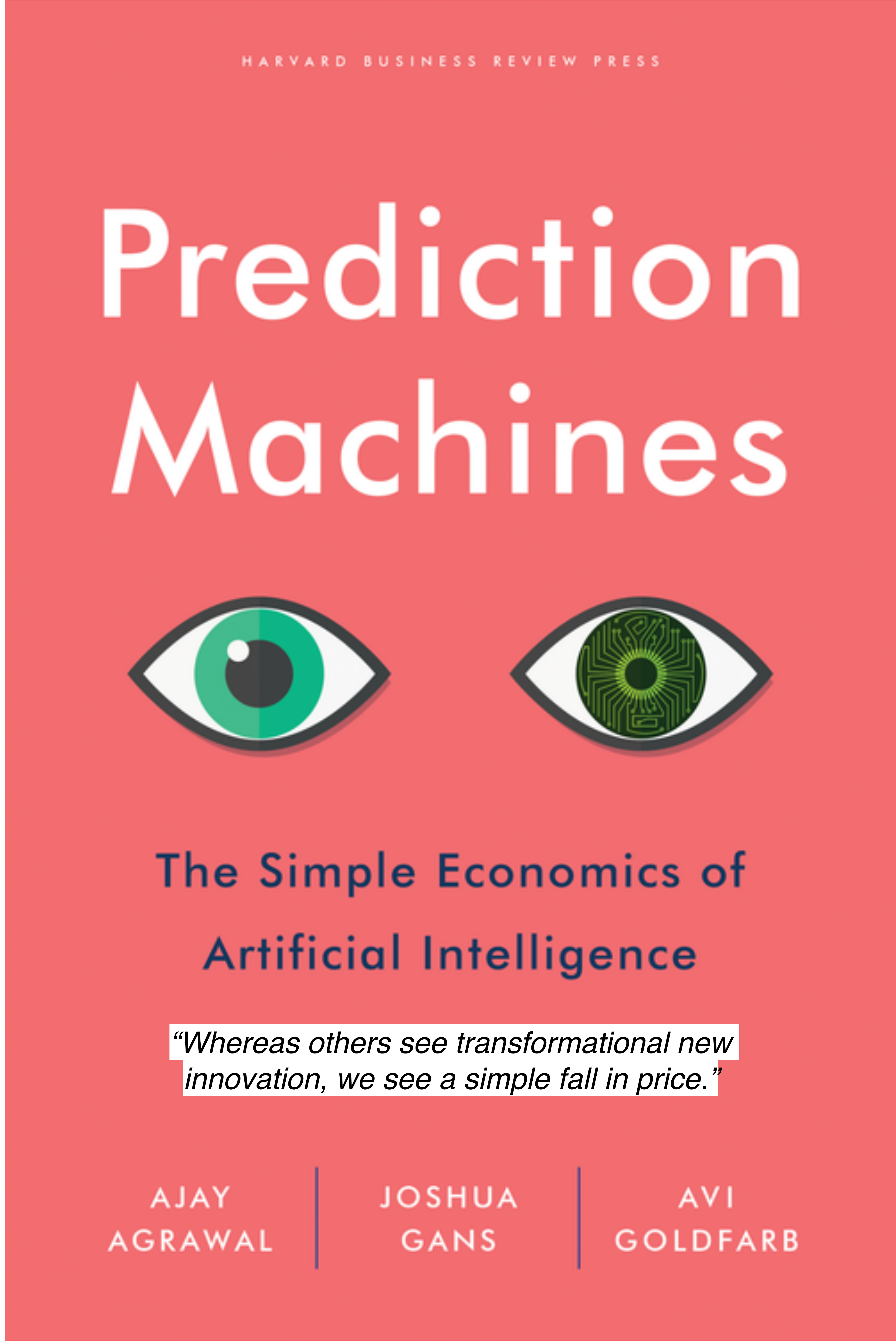

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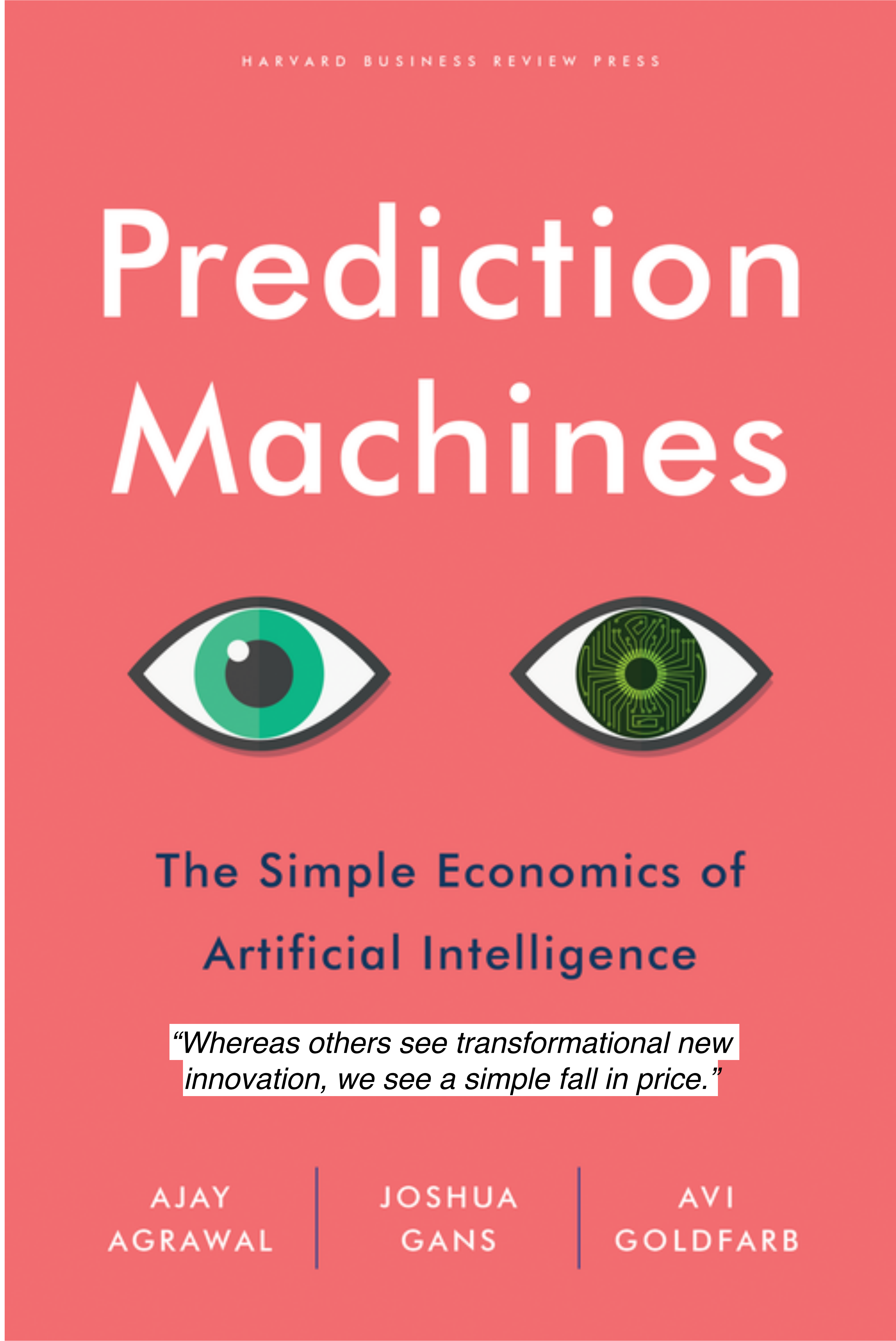

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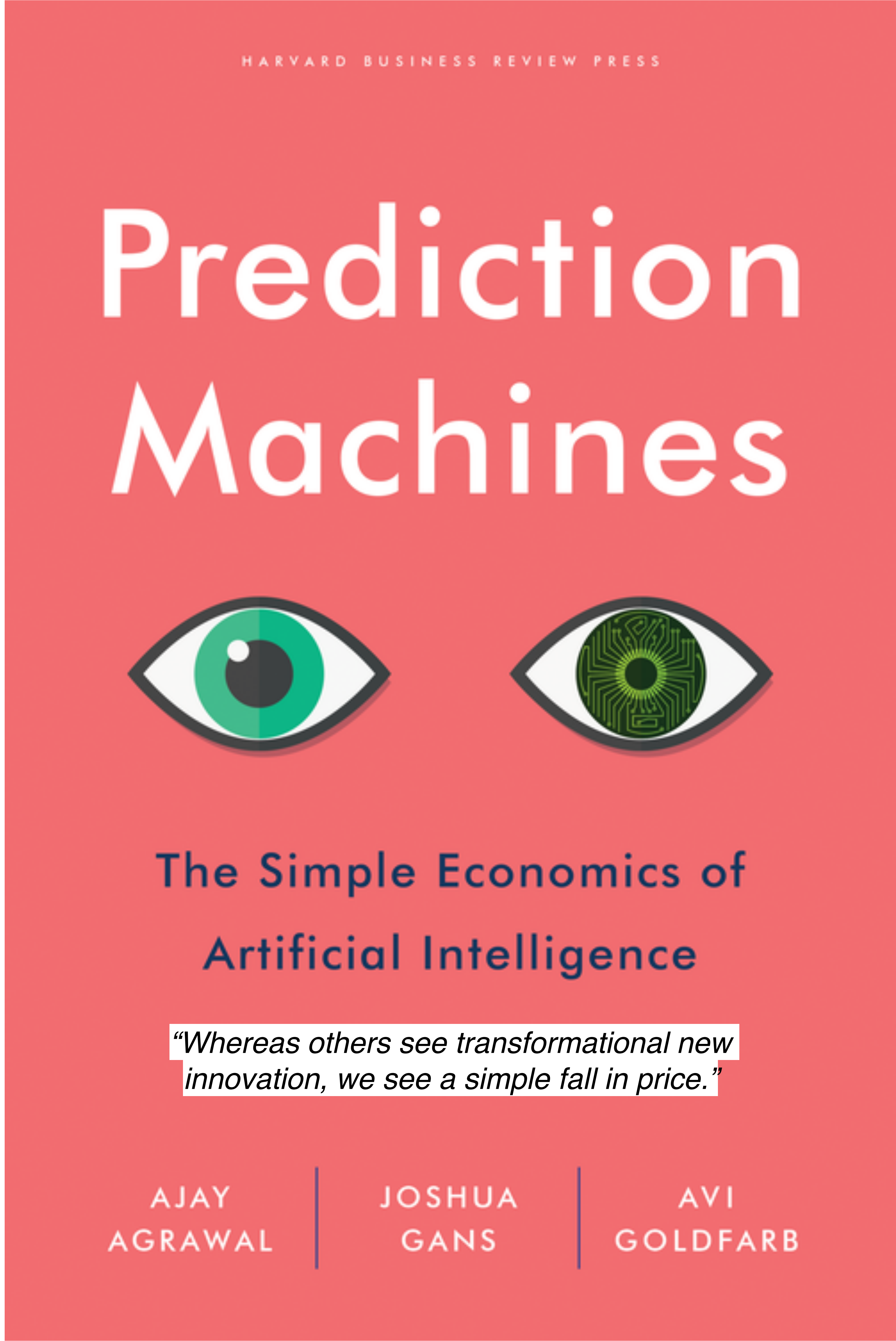

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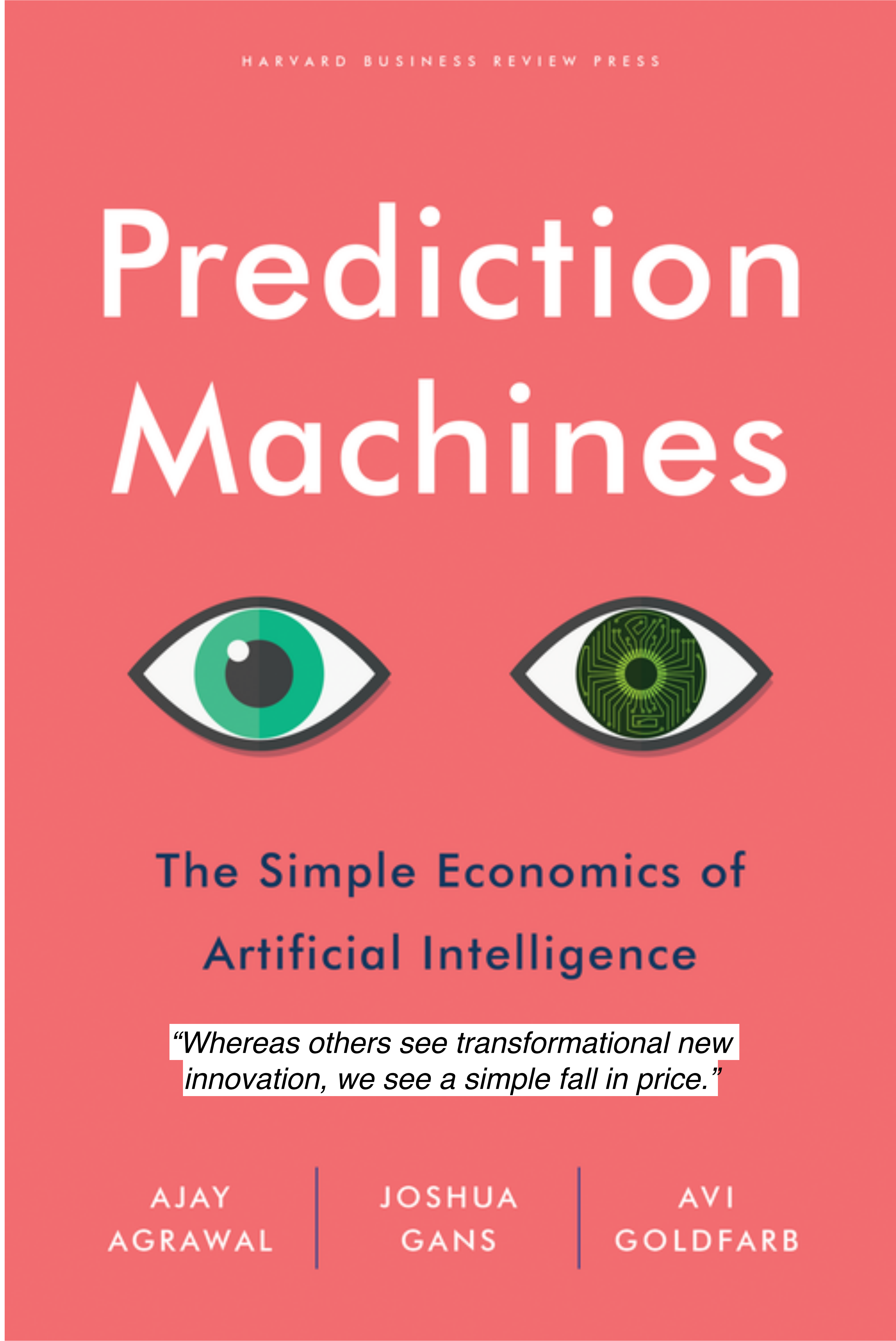

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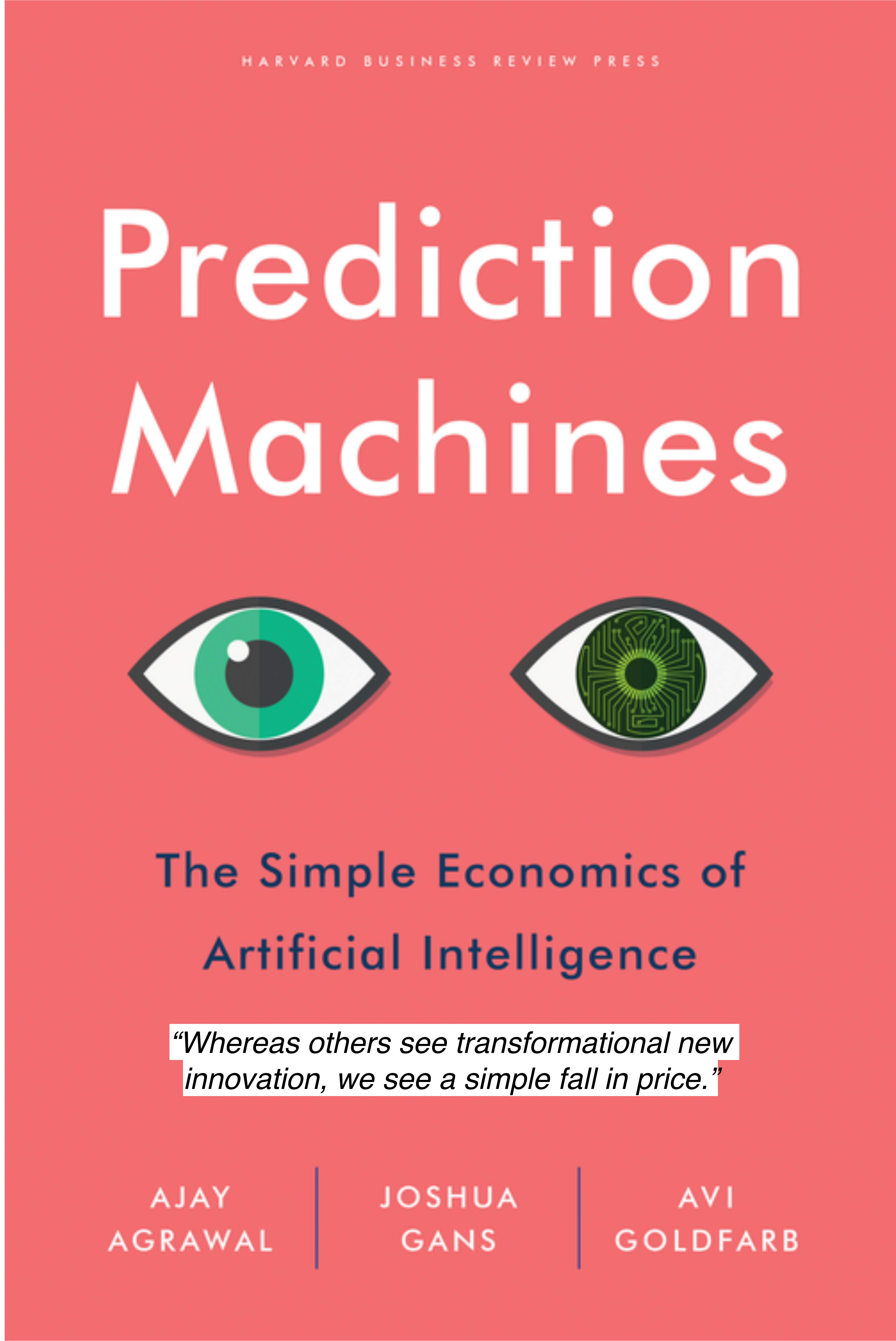

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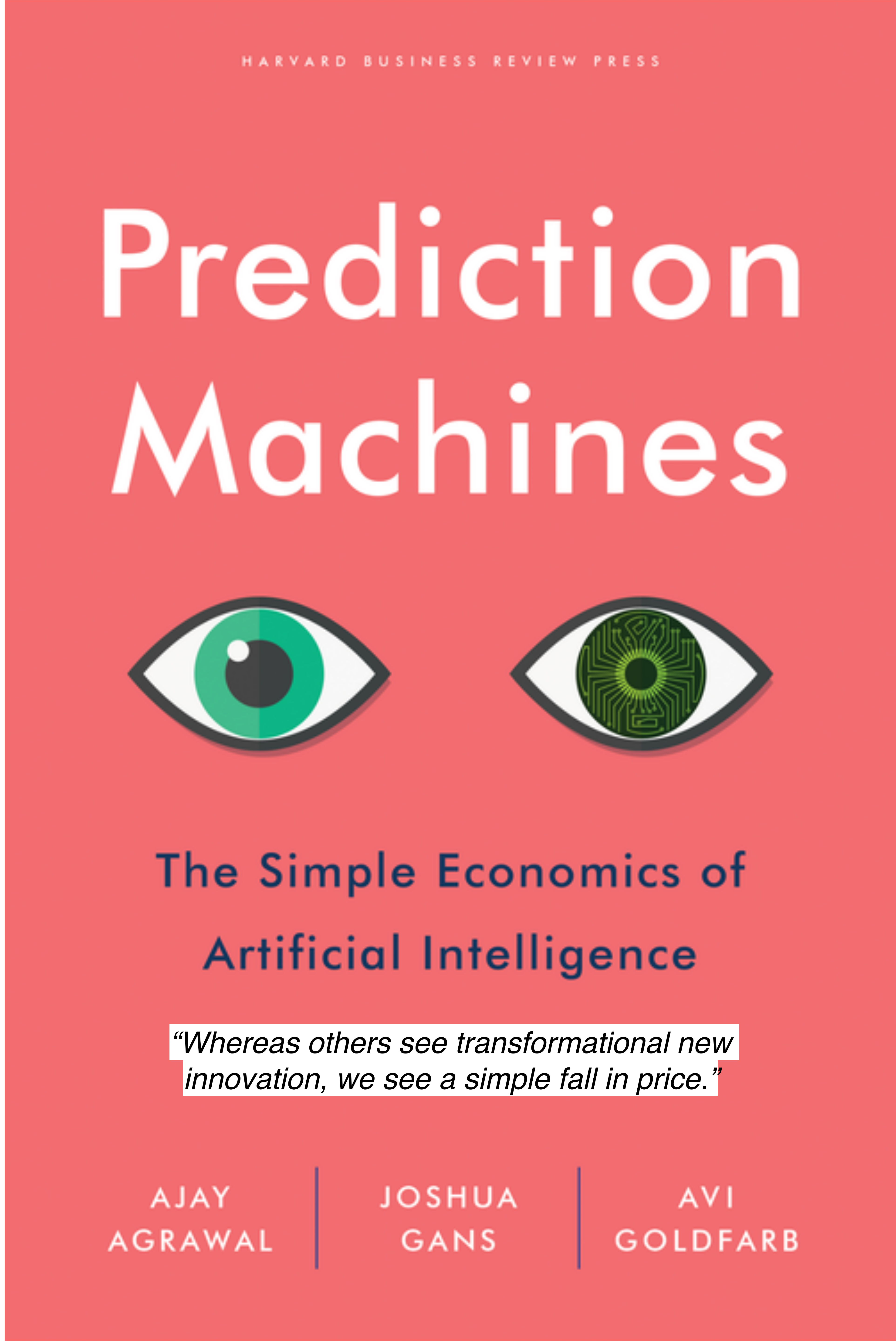
- **Better prediction under uncertainty -> new opportunities for all companies**



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COMPUTERS : A Disruptive Technology

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Posted by: Marco van der Spek **Date:** Oct 2, 2012
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"The automation of activities that we associate with human thinking, activities such as decision-making, problem solving, learning …

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"The study of how to make computers do things at which, at the moment, people are better"

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"The study of the computations that make it possible to perceive, reason, and act"

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ACT **RATIONALLY** - Schalkoff, 1990

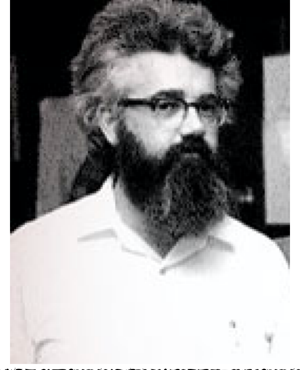
"A field of study that seeks to explain and emulate intelligent behavior in terms of computational processes"

A rationalist approach involves a combination of mathematics and engineering.

Artificial Intelligence, A Modern Approach, S. J. Russell and P. Norvig

People in each group sometimes cast aspersions on work done in the other groups, but the truth is that each direction has yielded valuable insights. Let us look at each in more detail.

What is Intelligence ?



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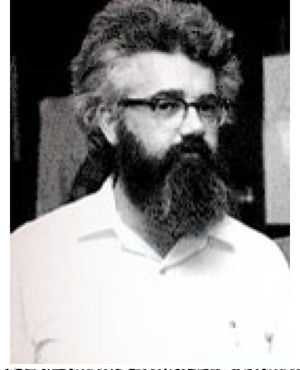

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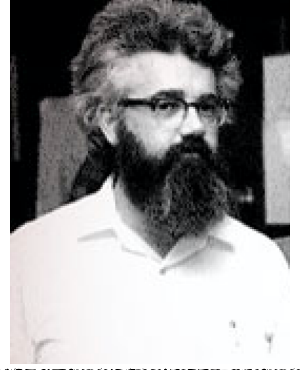

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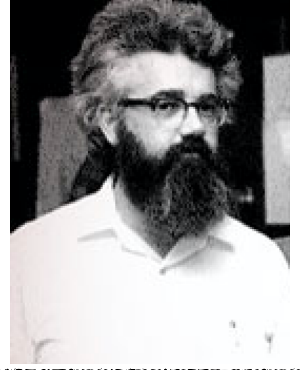

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- The system is most usefully understood/predicted/controlled in terms **of its outcomes rather than its mechanisms.**

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BUT OUR INSTRUCTIONS AND OUR GOALS

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SUBJECT TO UNCERTAINTY IN OUR MODELS

THE IMPERFECT PATHS TO KNOWLEDGE

ADAPTED FROM : R. Moser, T. Oden, O. Ghattas, UT Austin

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KNOWLEDGE:

- true, justified belief *(Plato)*.
- understanding, as opposed to opinion.
- quantifiable relationships between facts/observations and ideas.
    - "He believes it, but it isn't so," vs. "He knows it, but it isn't so." (Wittgenstein)

Immanuel Kant (1724 – 1804)

“Philosophy needs a science to determine the possibility, the principle, and the scope of our whole prior knowledge.”

Our intellect does not draw its laws from nature, but tries – with varying degrees of success – to impose upon nature laws which it freely invents.

Pierre-Simon de Laplace (1749-1827)

"The theory of probabilities is at bottom nothing but common sense reduced to calculus; *it enables us to appreciate with exactness that which accurate minds feel with a sort of instinct for which ofttimes they are unable to account."*

"Life's most important questions are, for the most part, nothing but probability problems."

"What we know is not much. What we do not know is immense."

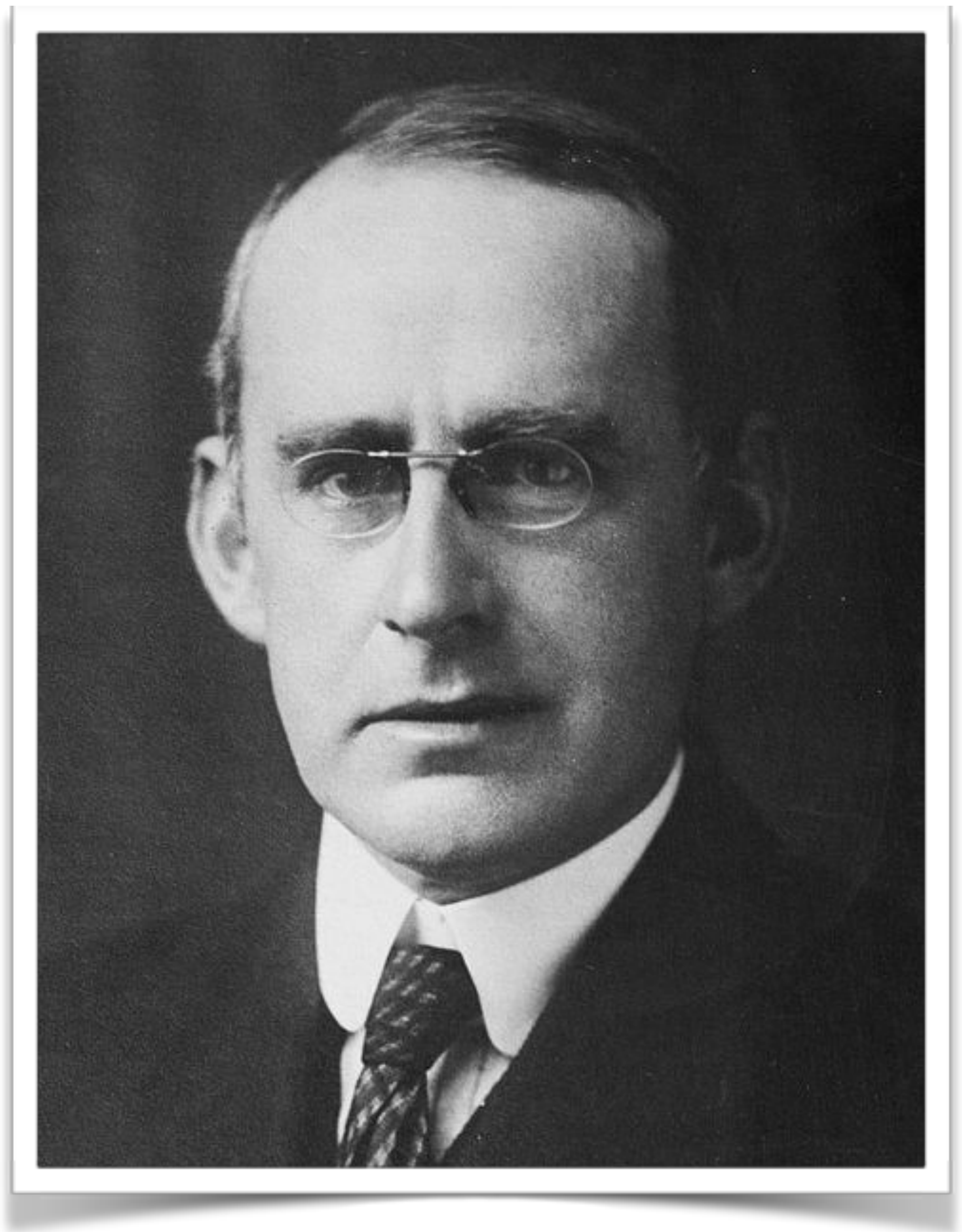
Hans Reichenbach (1891- 1953) The Rise of Scientific Philosophy, 1951.

The Path to Truth . . .

If error is corrected whenever it is
recognized as such,
the path to error is the path of truth.

Sir Arthur Eddington (1882-1944)

"Experimentalists will be surprised to learn that we will not accept any experimental evidence that is not confirmed by theory."



Werner Heissenberg (1901-1976)

"What we observe is not nature itself,
but nature exposed to our method of questioning."

HUMAN QUEST FOR KNOWLEDGE

CREDIT: Vladimir Cherkassky

- Knowledge driven design of a series of experiments :
  - Account for all sources of uncertainty in the experimental campaign
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- Describes well "simple" deterministic systems.
  - "simple" refers to conceptual simplicity, rather than 'technical' system complexity.
  - e.g. a mechanical system with many moving objects interacting with each other; each object is described by simple equations that involve just a few variables.

Classical Approach to Human Knowledge

Classic Knowledge: Describe many facts with few fundamental principles.

- The number of facts (data,observations) used to derive such knowledge is usually **small**.
- The cost of collecting or generating these observations is **high.**
- The principles may **not be “useful”** (i.e. non-predictive).

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Empirical knowledge: useful dependencies (i.e. predictive) estimated from data or derived from experience.

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- has a quantifiable practical utility for a given application (i.e. the “Oracle”)
- **Highly facilitated by the digital processing and acquisition of knowledge**

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MATHEMATICAL MODEL – A collection of laws and mathematical equations introduced to describe the behavior of the actual system (usually based on physical laws or observations). It is based on theory and assumptions often used to construct a model.

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Examples: discretization of PDEs, numerical integration, truncation of infinite sums

STOCHASTIC SYSTEM THEORY

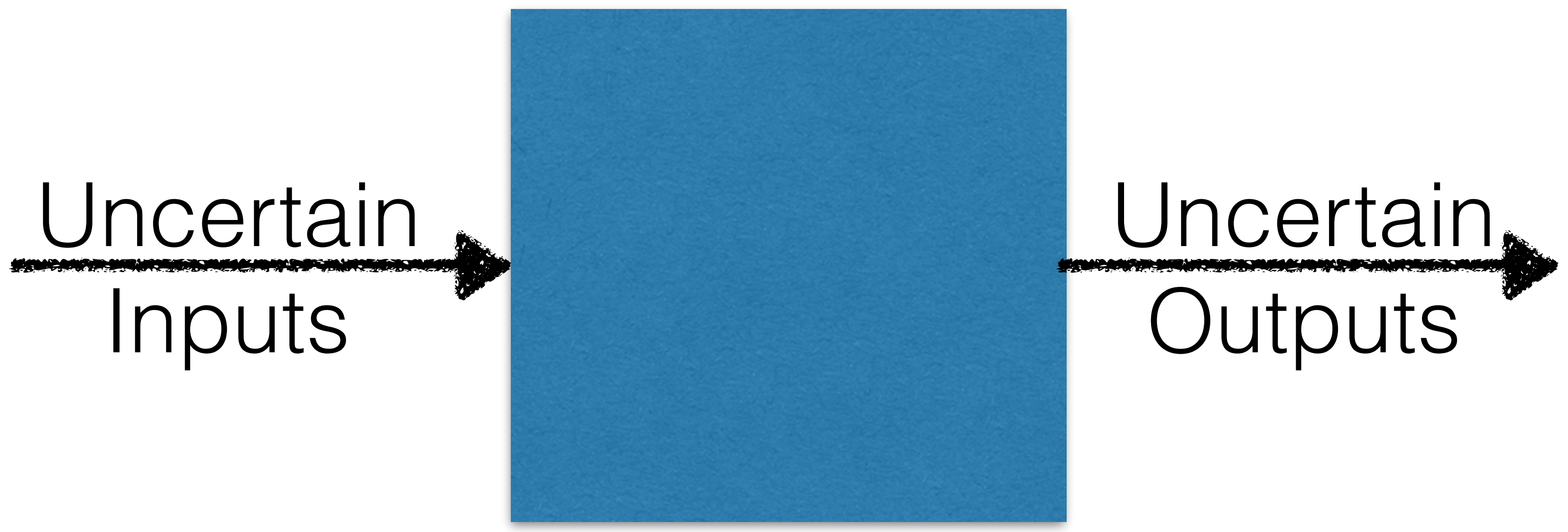
SYSTEM : any part of the world, natural or man-made, that we want to conceptually isolate to study. Inputs and outputs give its connections with the rest of the world
e.g. structural, mechanical, chemical, electrical, biological, economic, and geophysical systems

SYSTEM THEORY : goal is to provide a unified theoretical framework and computational tools to study systems Usually divided: system modeling, system analysis, system identification, system design optimization (including control systems)

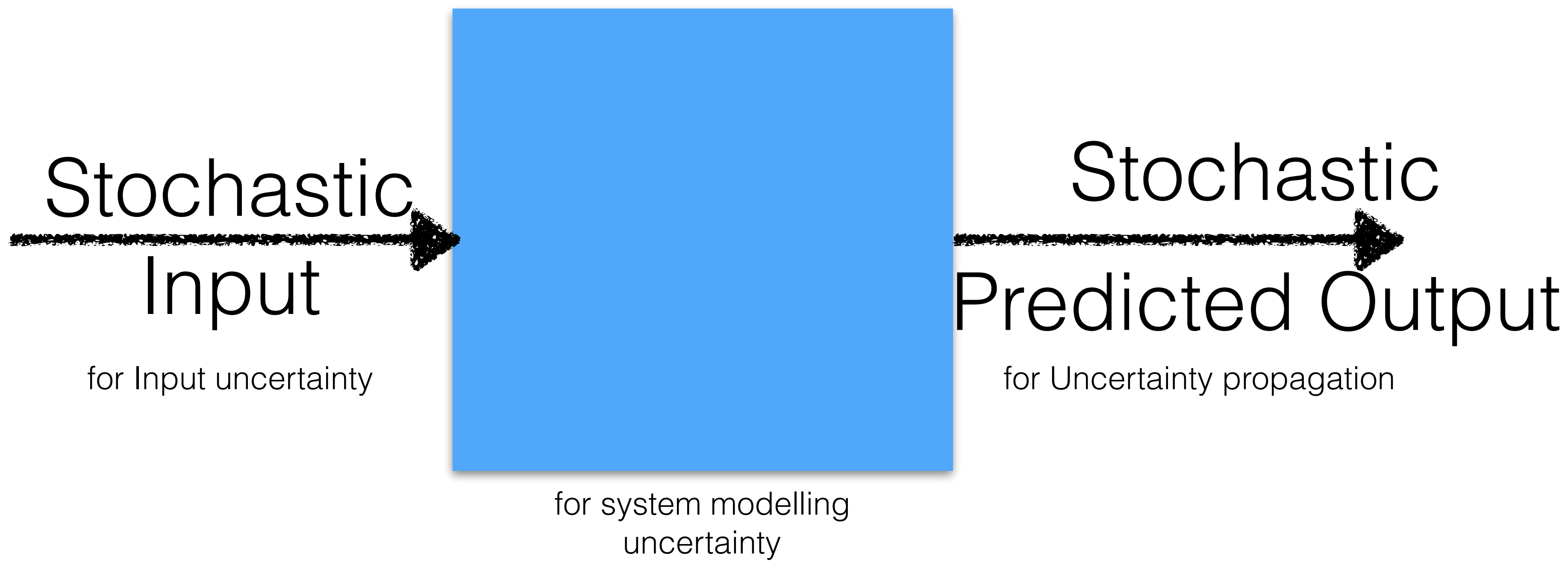
STOCHASTIC SYSTEM THEORY : goal is to quantify the effects of both input and modeling uncertainty using probability, leading to both prior (initial) and posterior (updated using system data) stochastic predictions of the system output and performance. Use "stochastic" and "probabilistic" as synonymous.

REAL WORLD vs MODEL WORLD

REAL WORLD



MODEL WORLD



Sources of Uncertainty I

•Modeling (or Structural) Uncertainty

Arise from assumptions used to build a mathematical model for

A. representing the physical system (the real thing)

B. representing the interactions of the system with the environment

Comes from the lack of knowledge for the underlying true physics, leading to discrepancies (model bias) between the predictions from the model and the observations (measurements). The model inadequacy is always present and the question is how to select the best models over a family of alternative models introduced to model the same physical phenomenon.

•Parametric Uncertainty

Arise from lack of knowledge of the appropriate values of the parameters of a mathematical model.

Examples include the material properties of a continuum such as solid or fluid, the properties involved in constitutive laws, the boundary conditions, etc.

Sources of Uncertainty II

- **Computational (or Algorithmic) Uncertainty**

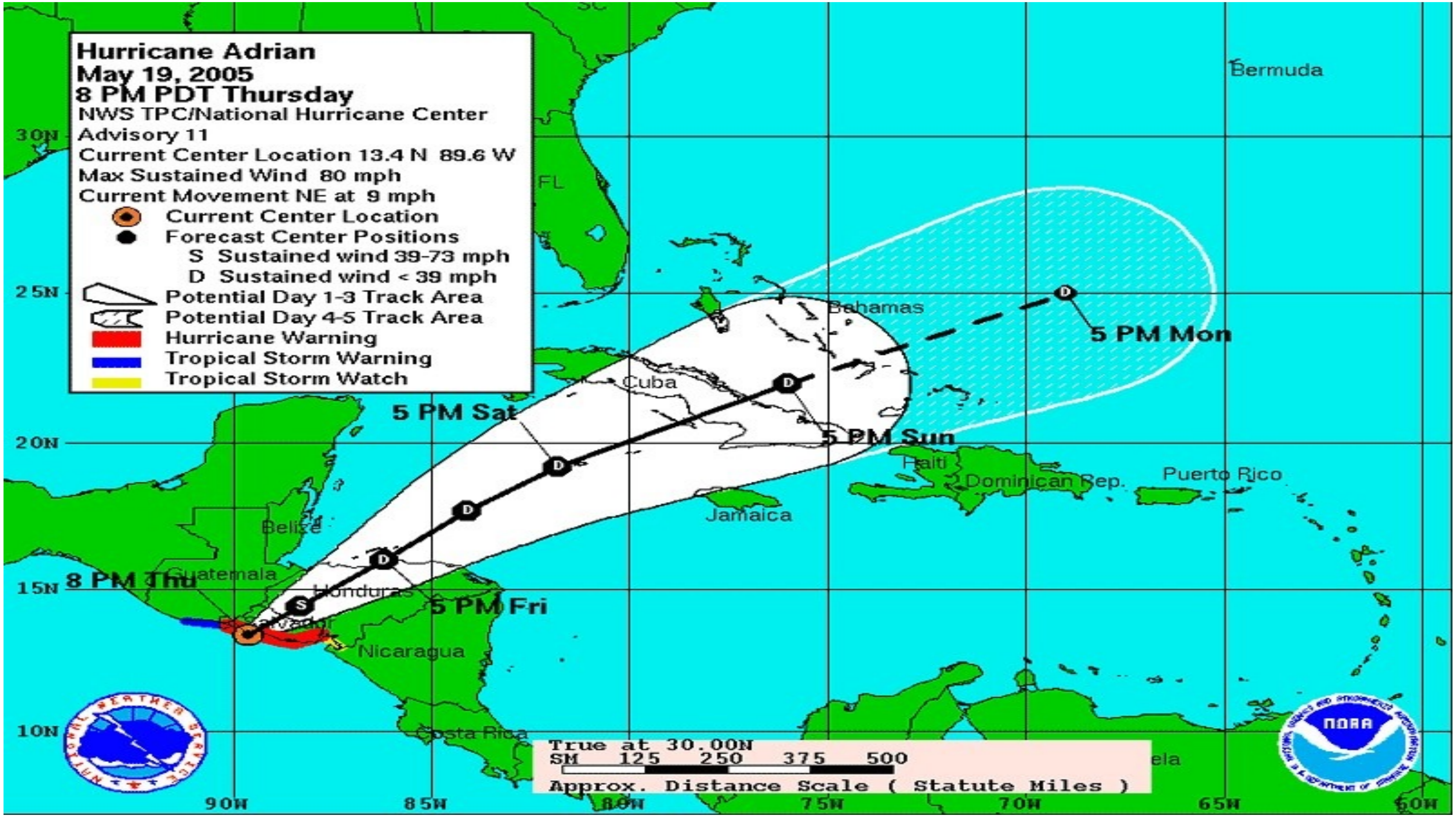
linked to the numerical uncertainty arising from the numerical approximations introduced to implement the analysis in a computer. Examples include spatial and temporal discretization of PDEs using finite element methods, finite difference methods or particle methods.

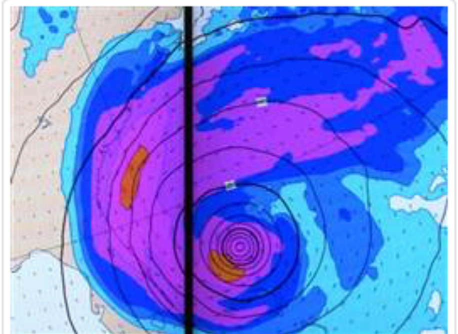
- **Measurement uncertainty**

arises from the variability in the values of the experimental properties due to variability in experimental set up, errors in the measuring equipment, and inaccuracies in the data acquisition system.

Why Uncertainty Quantification (UQ)? UQ for Decision Making

- Example: hurricane forecasting





Nightly News | March 08, 2013

European weather forecasts superior to US models

The predictions from European computer models, which have 10 times the computing ability of the National Weather Service, have increasingly become more accurate than our models with the starkest example being Hurricane Sandy. NBC's Al Roker reports.


Boston
NYC

Why UQ ?

UQ for Validation

Example: measurements of the speed of light (1870-1960)

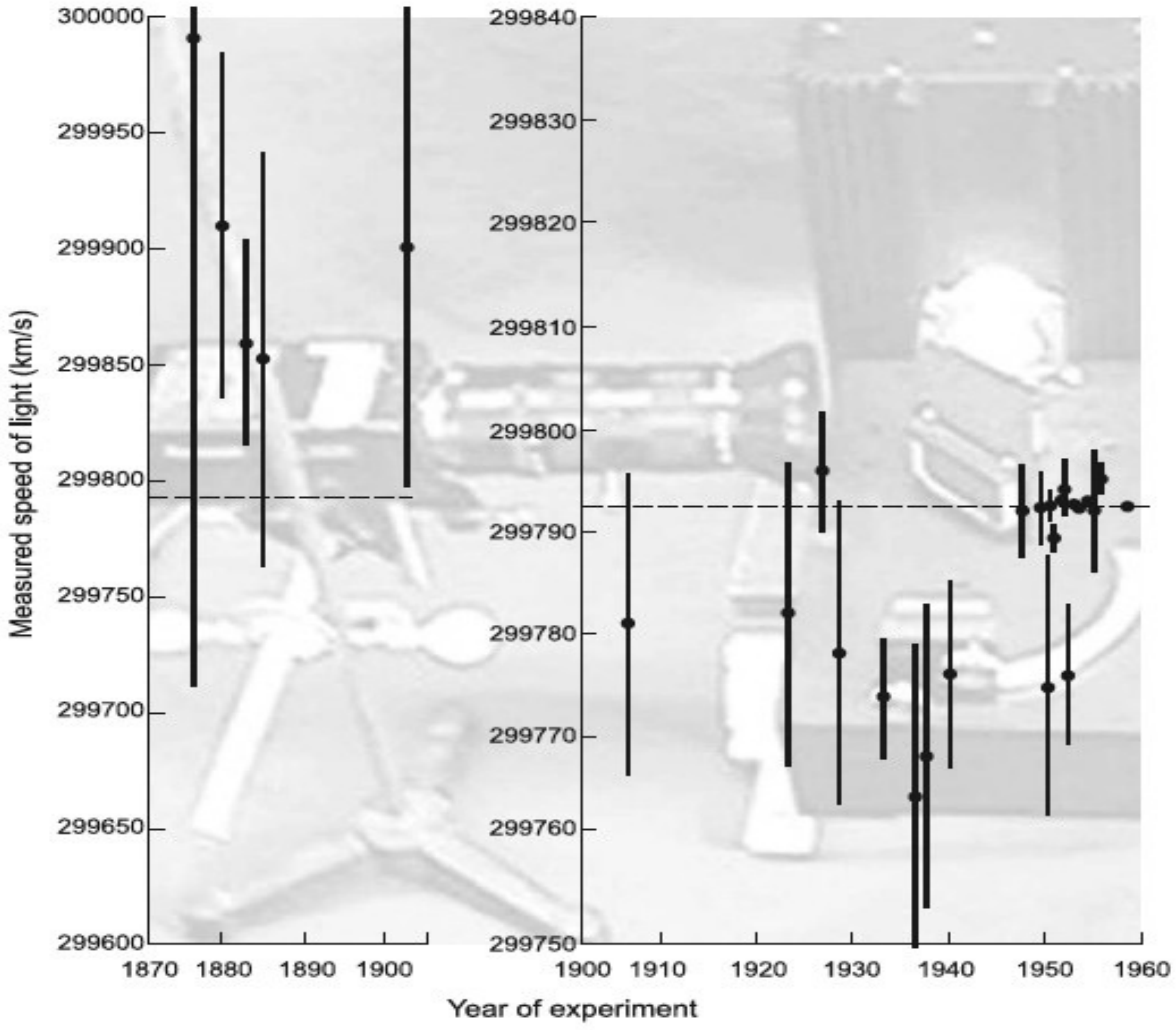


Image from Christie et al., Los Alamos Science, #29, 2005

Why UQ ?

UQ for Design/Optimization -

<u>Example</u>: transonic wing shape optimization

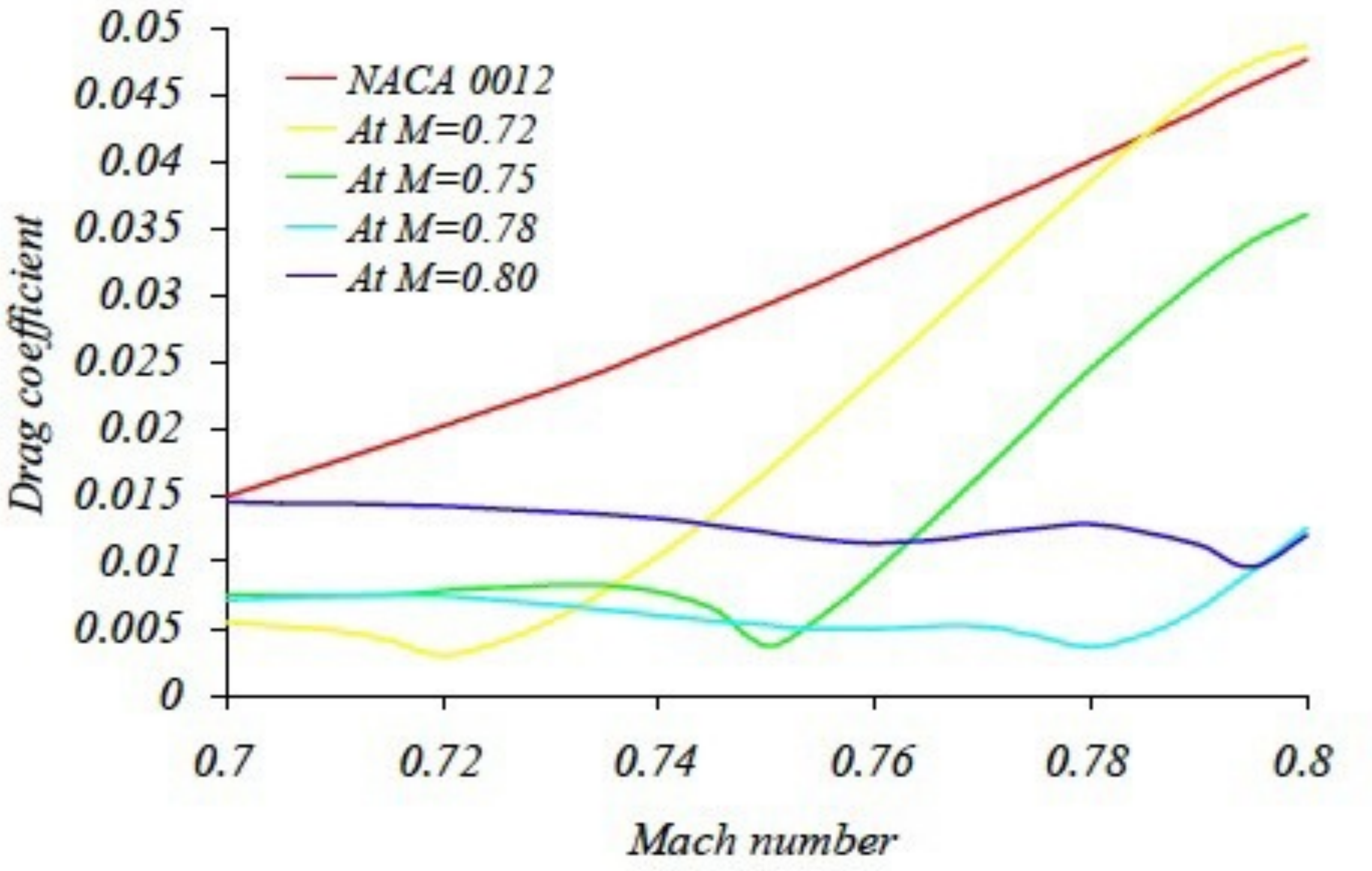


Image from T. Zang, 2003

- Choice of design conditions can dramatically affect performance
- Impact of flight conditions uncertainties can lead to unknown/unexpected consequences

Example: Solid Mechanics/Structural Dynamics

- **Modeling (or Structural) Uncertainty**
  - Selection of linear or nonlinear constitute laws to represent the material behavior (e.g. stress-strain relationship)
  - Selection of boundary conditions
- **Parametric Uncertainty**
  - Values of the constant parameters involved in the constitutive laws are not completely known (modulus of elasticity, Poisson ratio, etc)
  - The values of the stiffness in isolated parts of the structure are unknown
  - stiffness and damping values of isolation devices are uncertain (dampers, etc)
  - For contact problems, friction, restitution coefficients are not completely known
- **Computational (or Algorithmic) Uncertainty**
  - Spatial discretization of the PDEs using finite element methods
  - Temporal discretization of the resulting ODEs
- **Measurement uncertainty**
  - Uncertainties in measuring the acceleration, strains, etc, in various locations of the structure due to errors in the measuring equipment, and inaccuracies in the data acquisition system.

Example: Fluid Dynamics

- **Modeling (or Structural) Uncertainty**
  - Selection of flow model (Filtered Navier Stokes equations + Turbulence model)
  - Selection of boundary conditions
- **Parametric Uncertainty**
  - The values of the constant parameters involved in the Turbulence model
  - The values of the model are not suitable near boundaries
  - For some problems (flow in hydrophobic surfaces) the parameters of the boundary conditions are not known.
- **Computational (or Algorithmic) Uncertainty**
  - Spatial discretization of the PDEs using numerical methods (grids, particles, etc.)
  - Temporal discretization of the resulting ODEs
- **Measurement uncertainty**
  - Uncertainties in measuring flow quantities such as flow fields and drag coefficients due to errors in the measuring equipment, and inaccuracies in the data acquisition system.

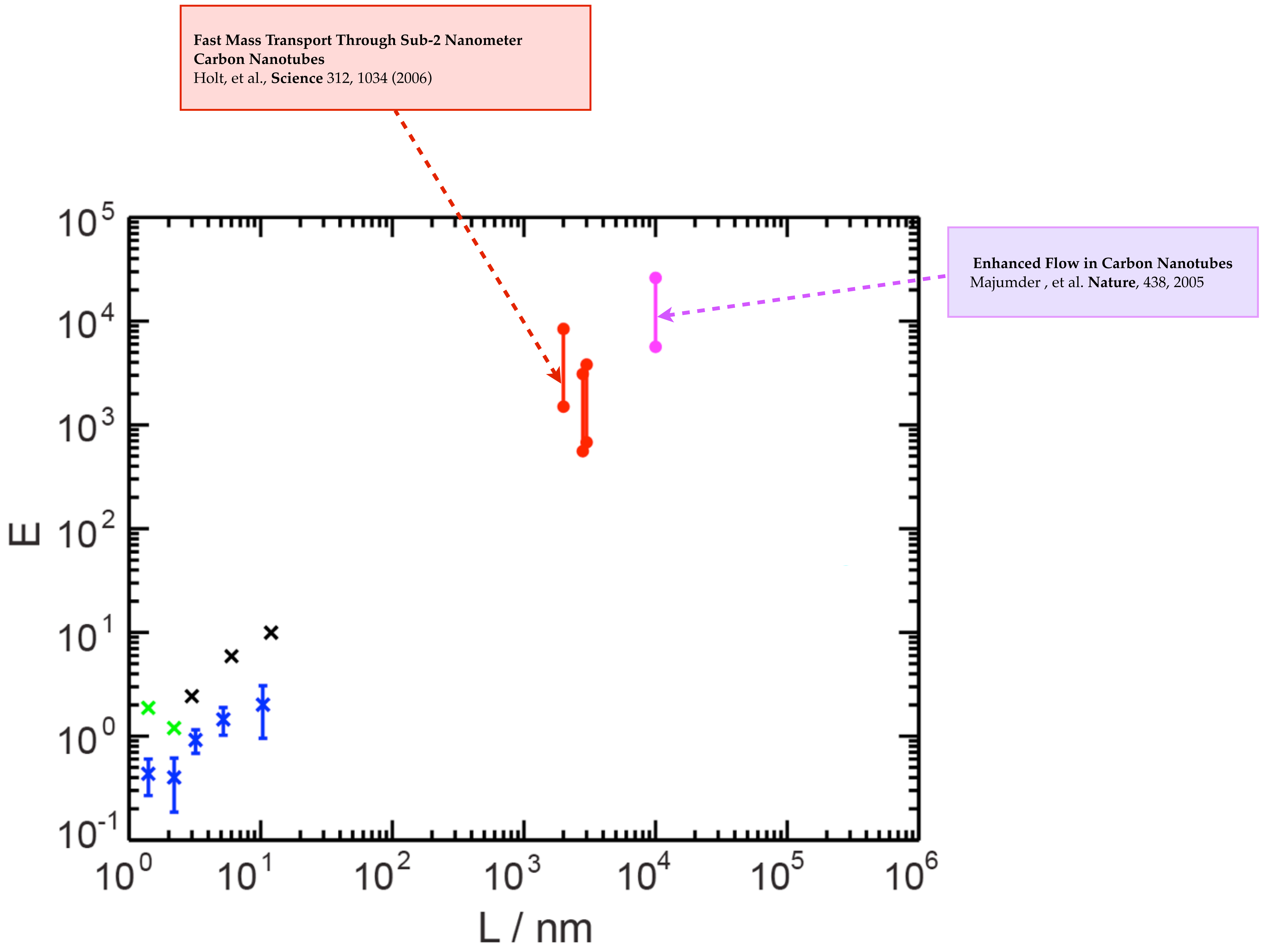
Large Scale MD Simulations of Water Transport in CNTs

L = 2μm & R ~ 2nm

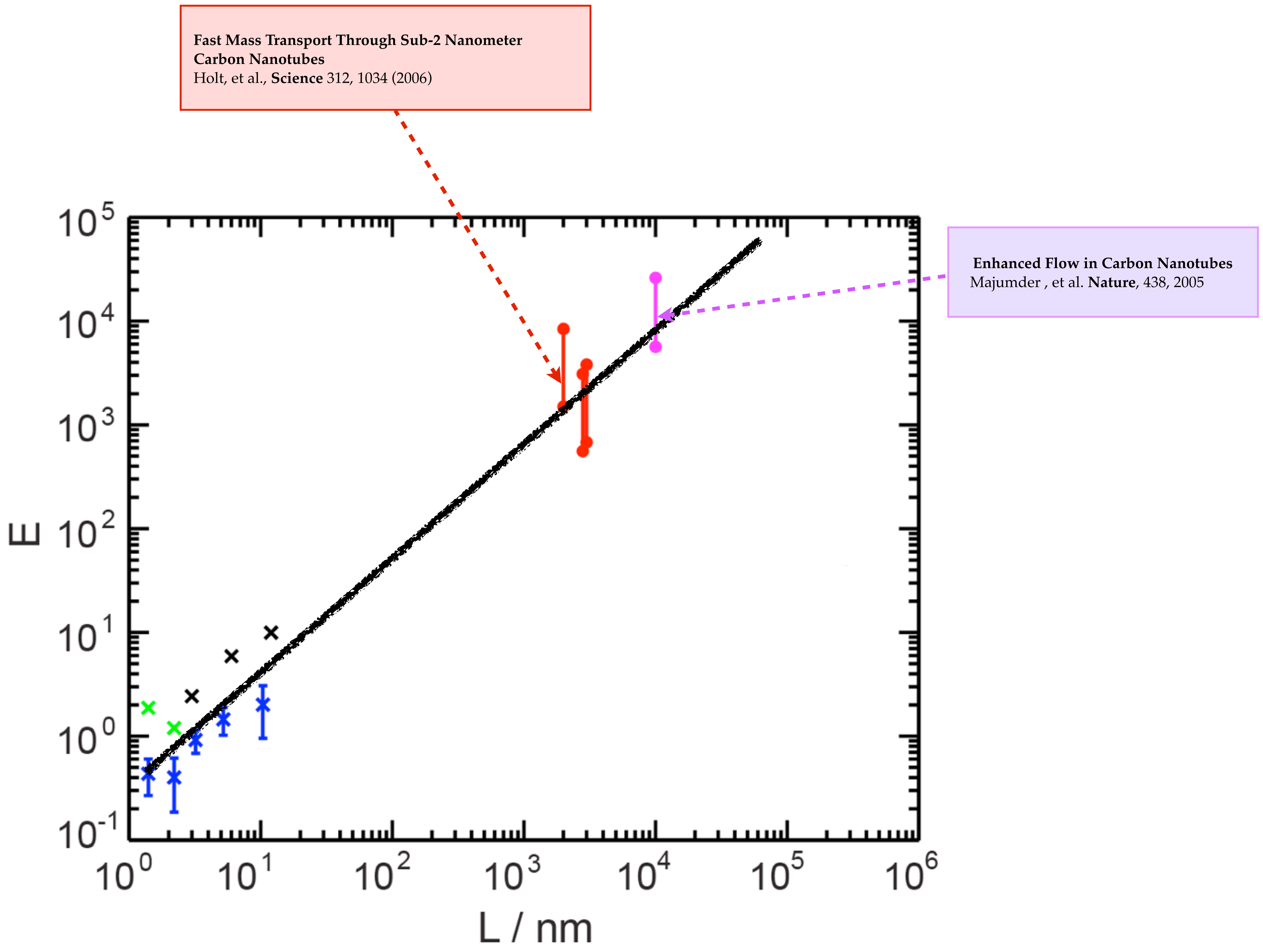
$$Q_{HP} = \frac{\pi R^2}{8\mu}\frac{\Delta P}{L}$$

$$E = \frac{Q}{Q_{HP}}$$

Walther JH, Ritos K, Cruz-Chu E, Megaridis CM, Koumoutsakos P. , Barriers to Superfast Water Transport in Carbon Nanotube Membranes. **Nano Letters**, 2013, 13 (5)



Fast Mass Transport Through Sub-2 Nanometer Carbon Nanotubes
Holt, et al., Science 312, 1034 (2006)
Enhanced Flow in Carbon Nanotubes
Majumder , et al. Nature, 438, 2005
E
L / nm



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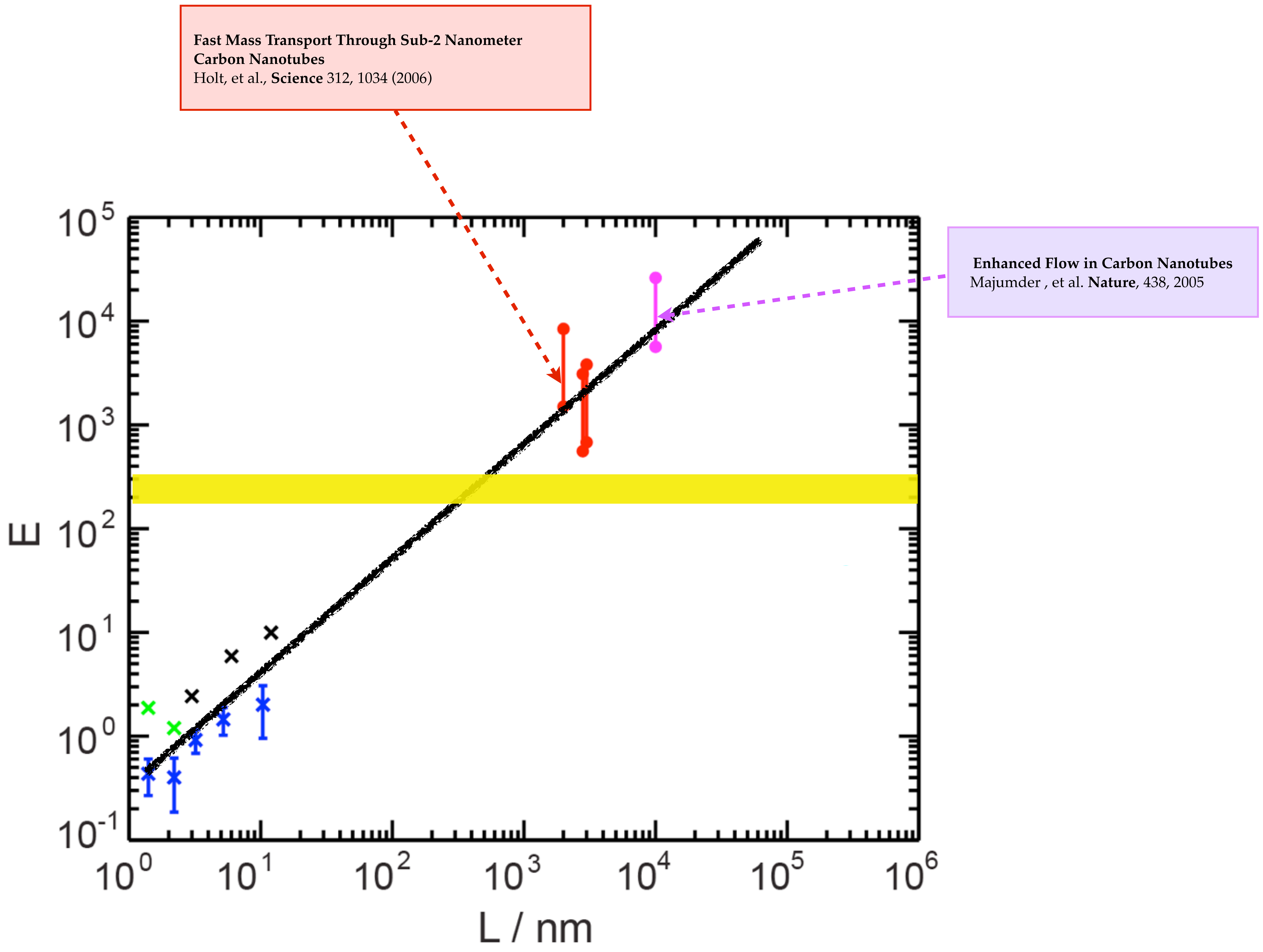

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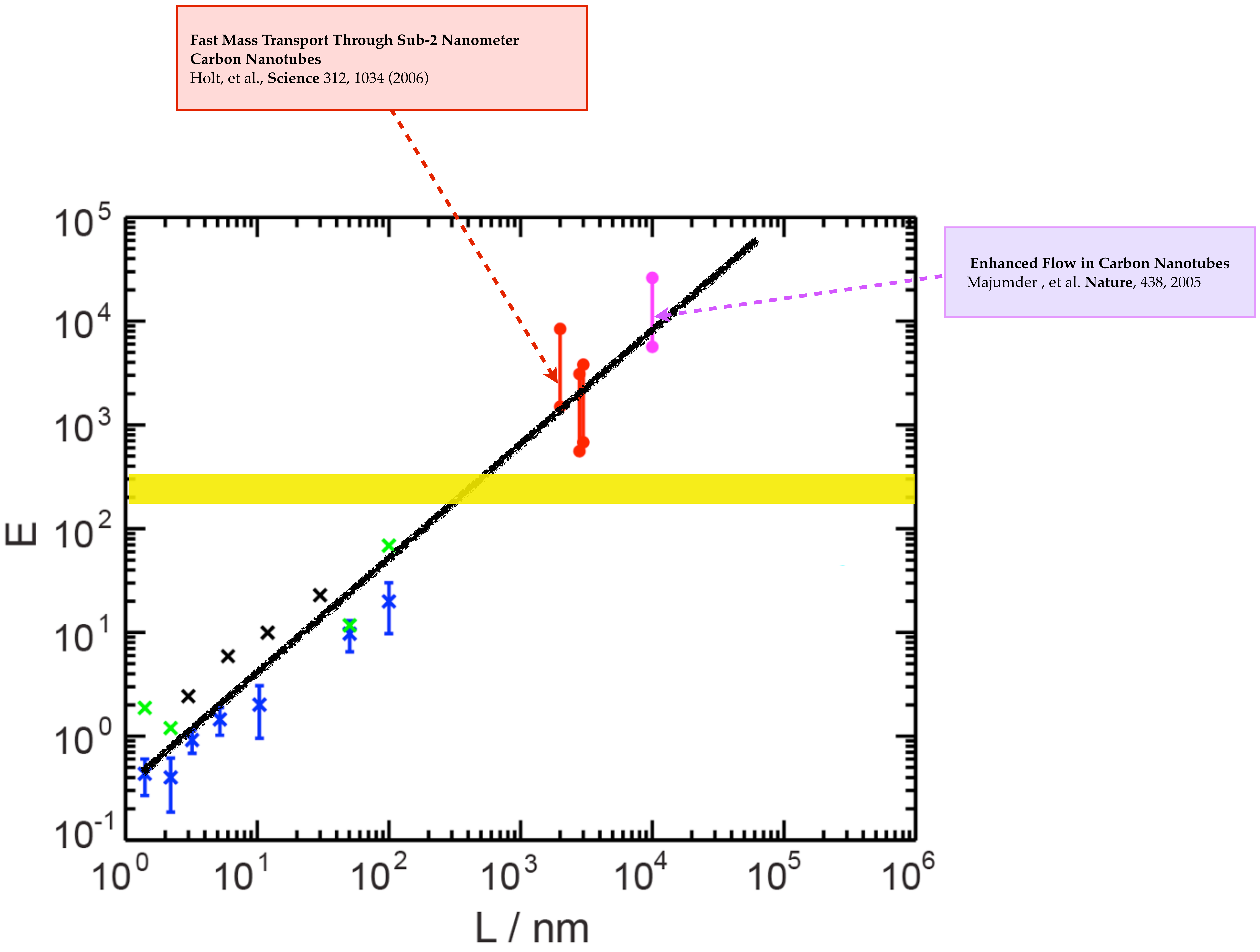
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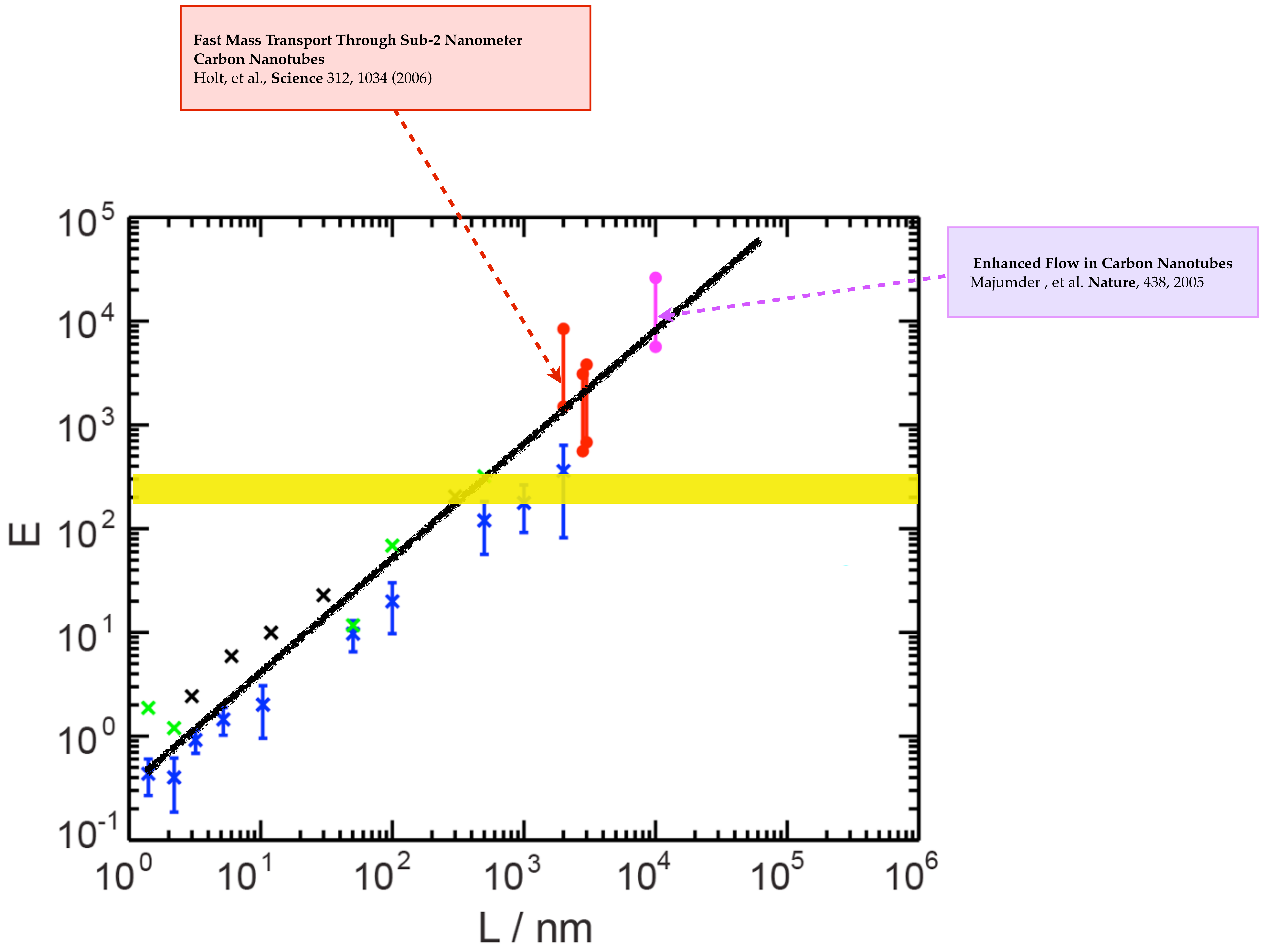

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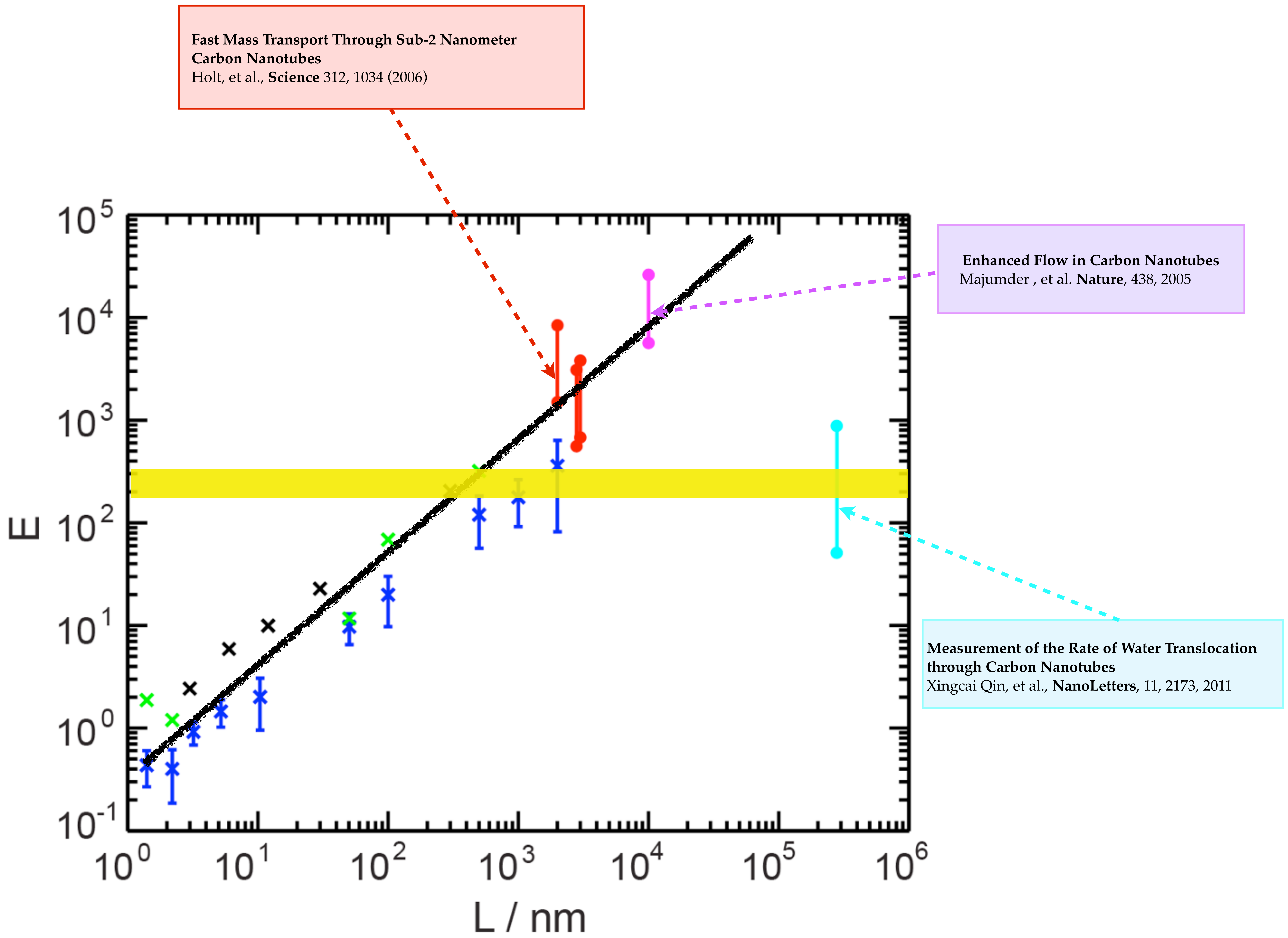
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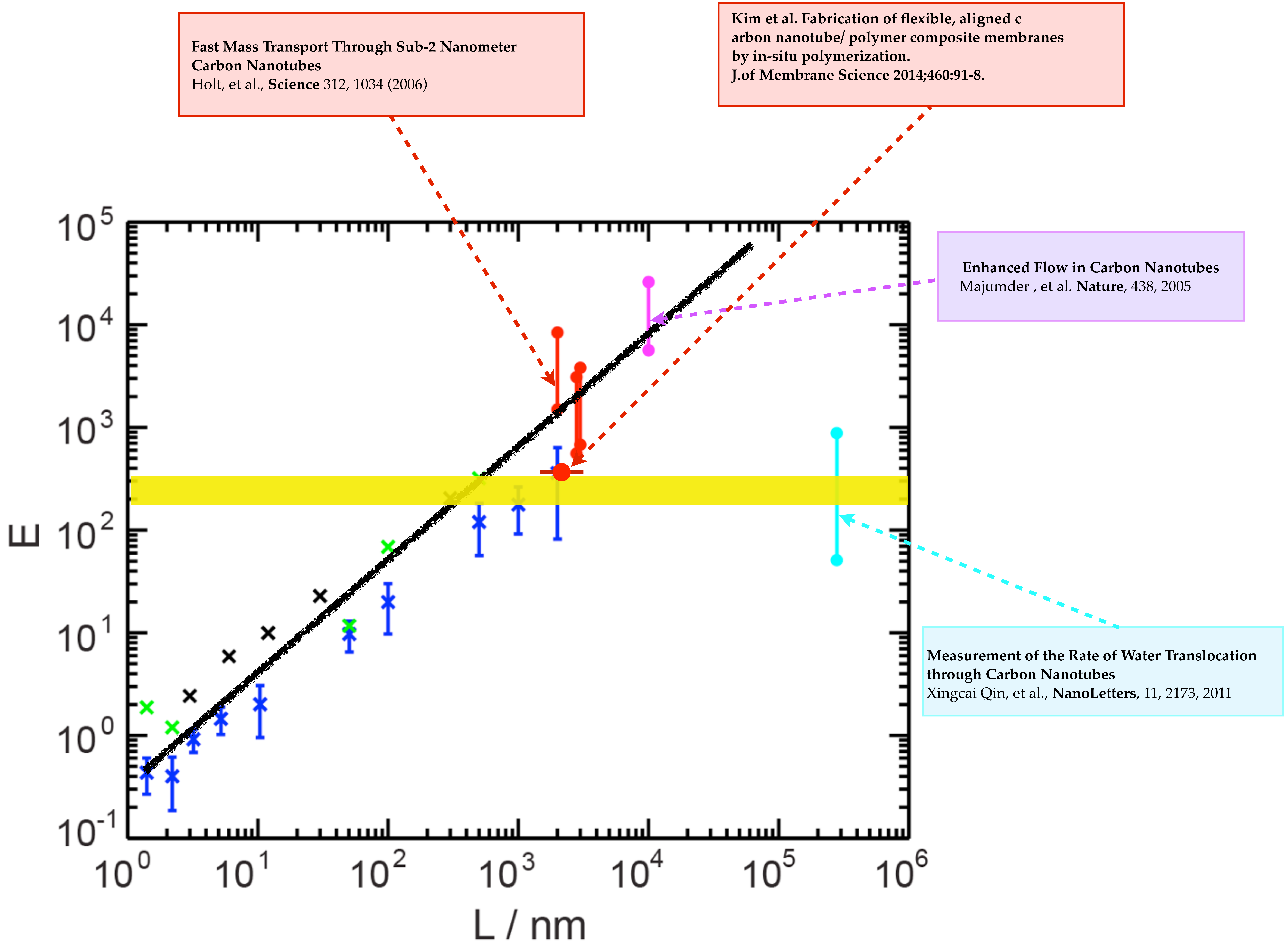
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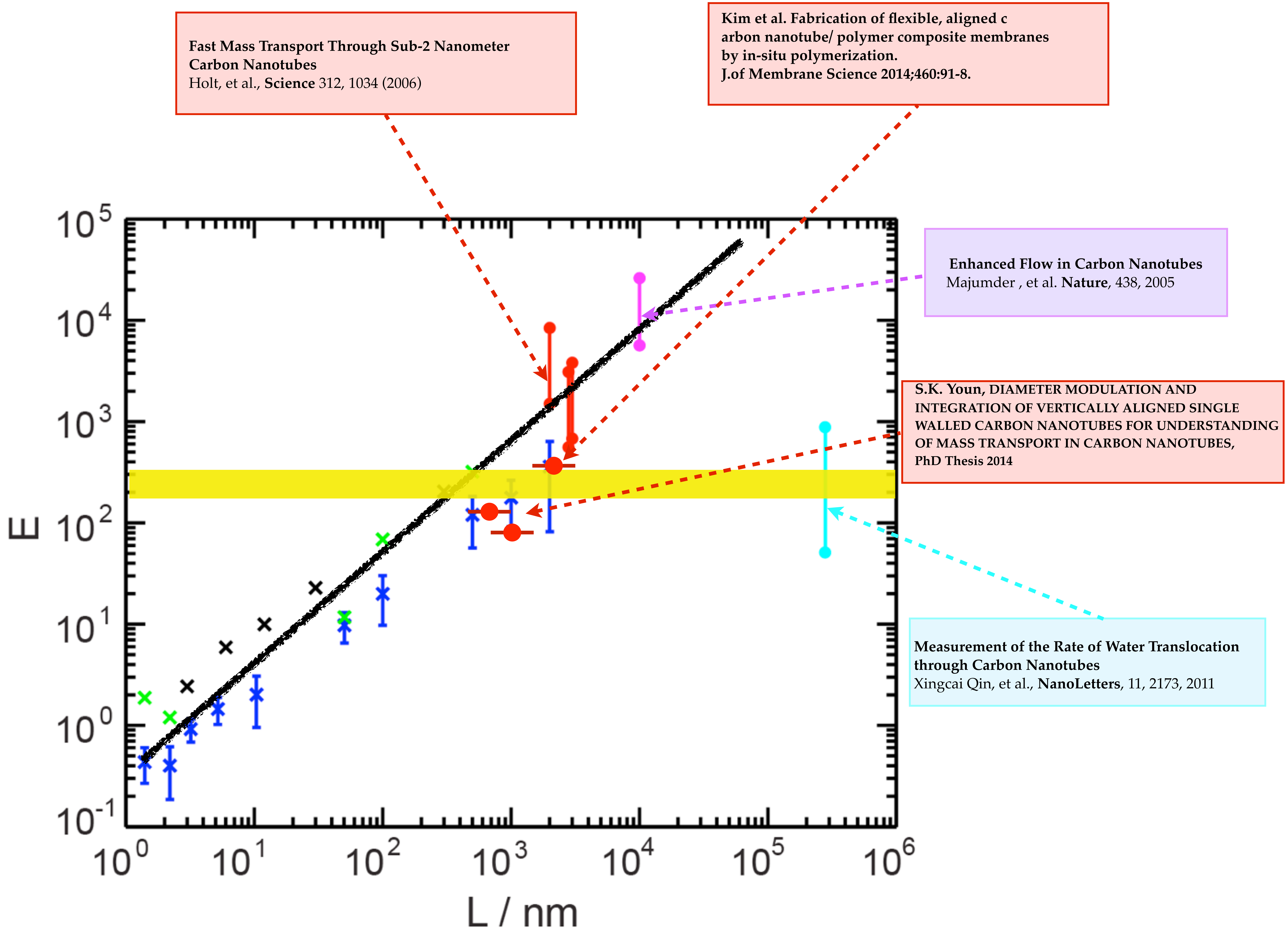
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Sources of Uncertainty in Water-Graphite Systems

MODELLING PARAMETRIC COMPUTATIONAL MEASUREMENT

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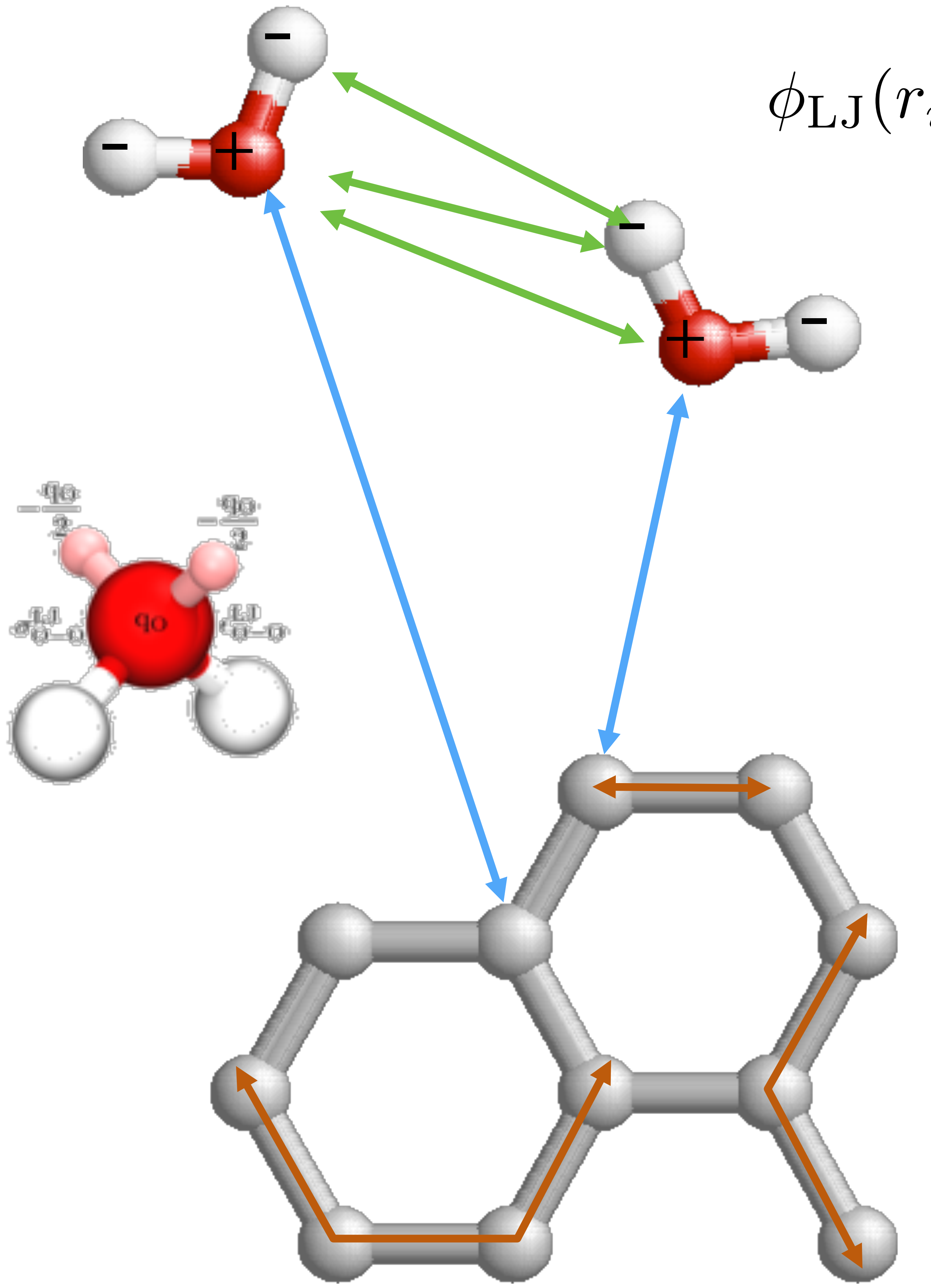

$$\phi_{\mathrm{LJ}}(r_{ij}) = 4\epsilon_{\mathrm{LJ}}\left[\left(\frac{\sigma_{\mathrm{LJ}}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{\mathrm{LJ}}}{r_{ij}}\right)^{6}\right]$$

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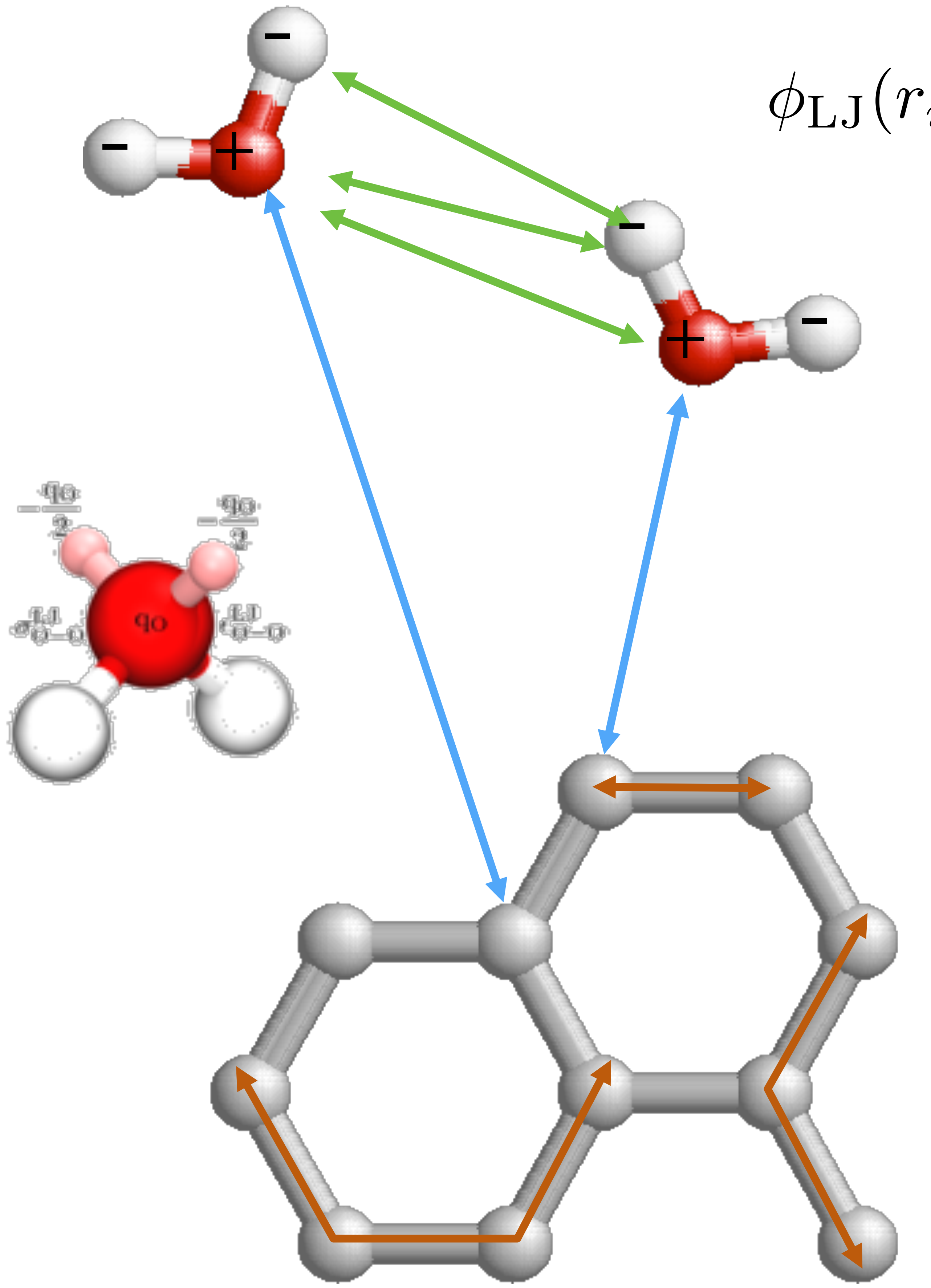

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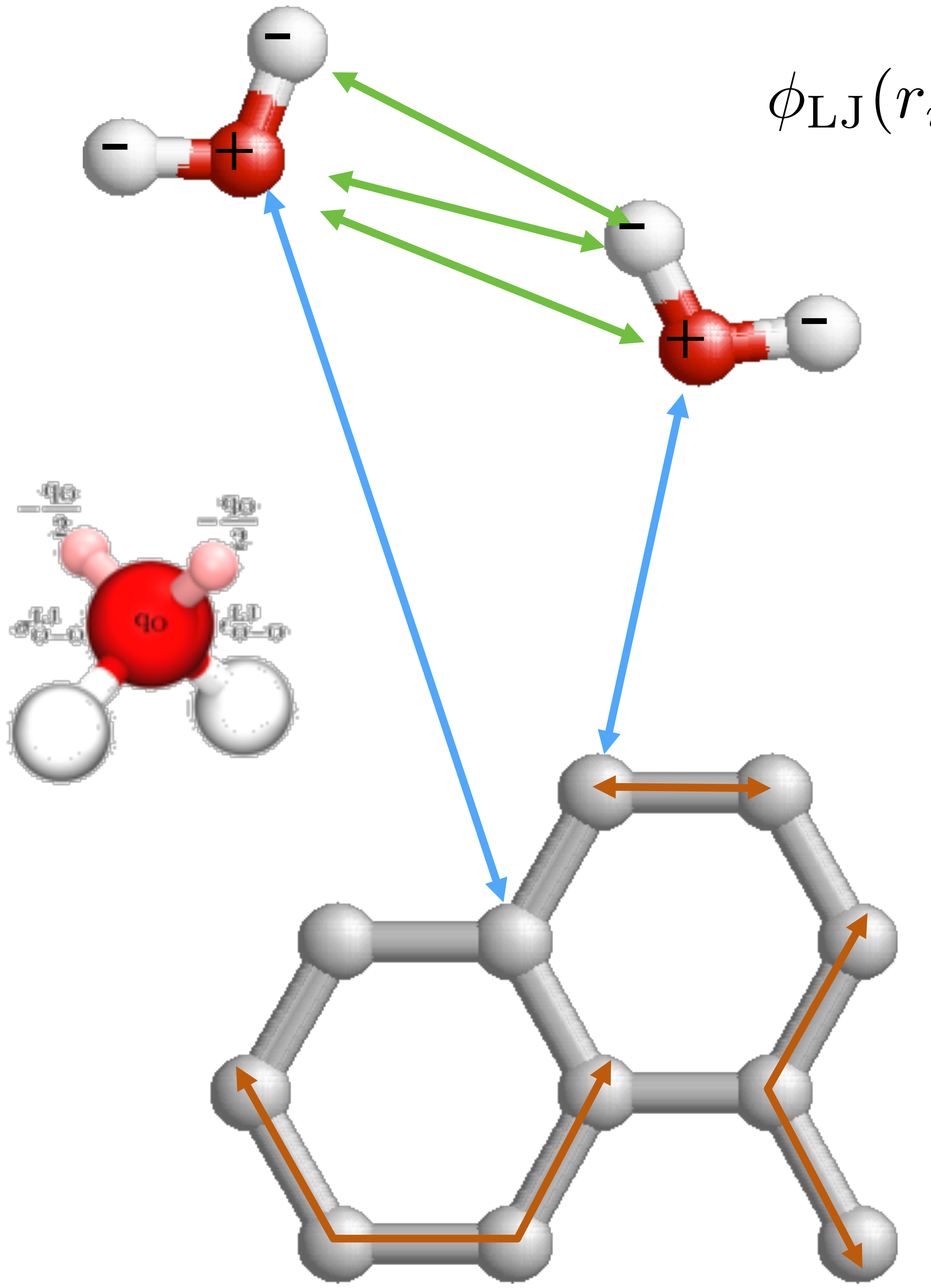
MODELLING PARAMETRIC **COMPUTATIONAL** MEASUREMENT



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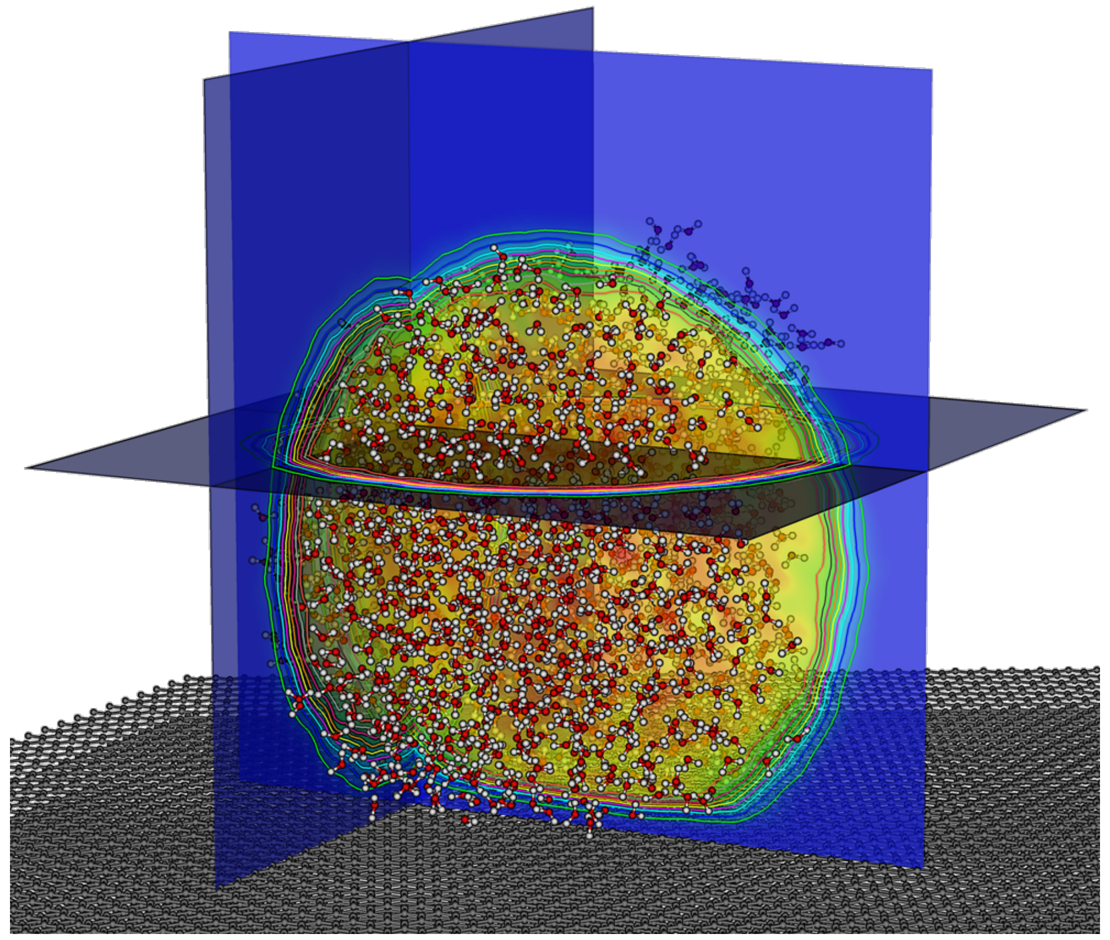
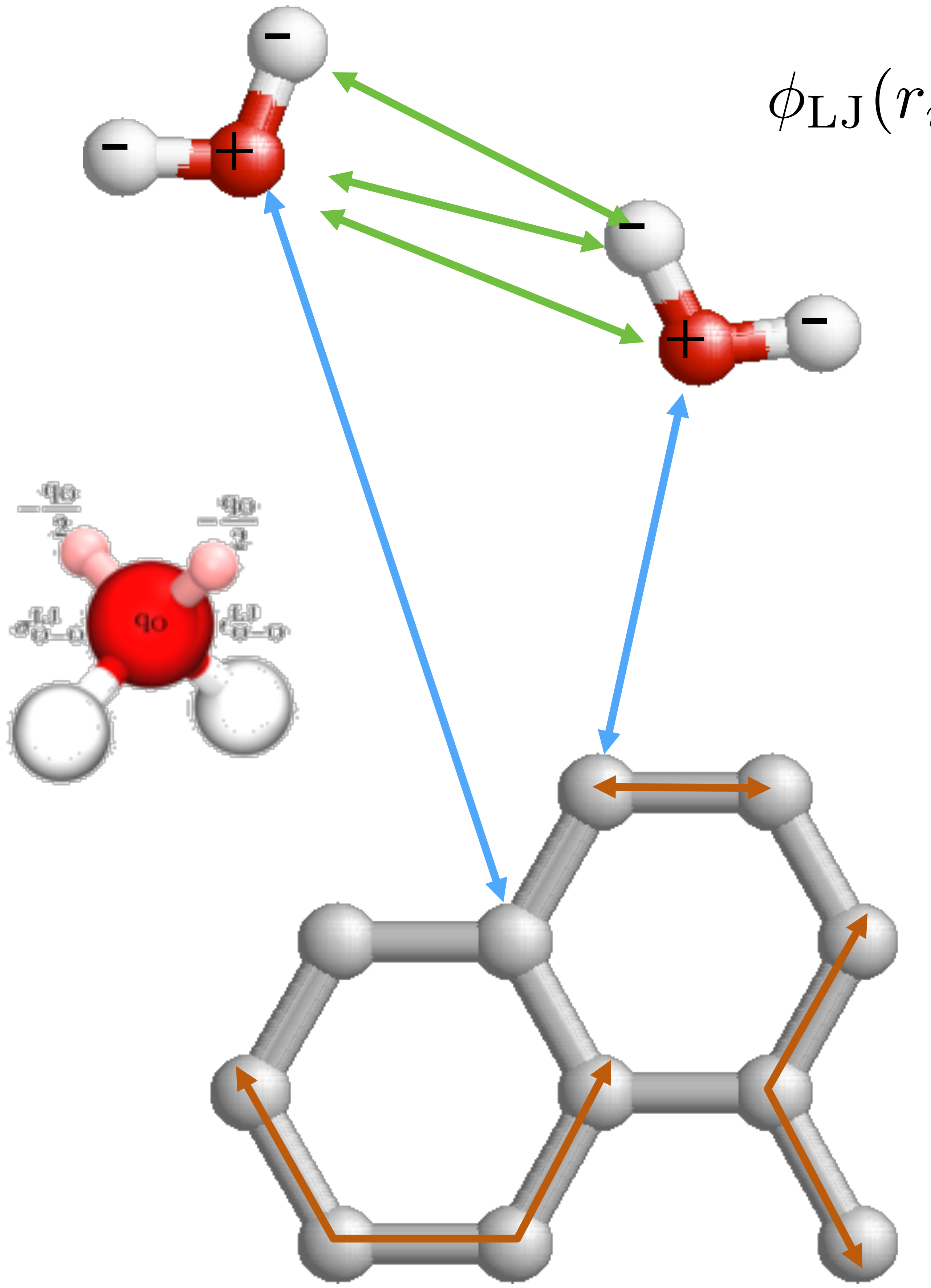


Sources of Uncertainty in Water-Graphite Systems

MODELLING   PARAMETRIC   COMPUTATIONAL   **MEASUREMENT**



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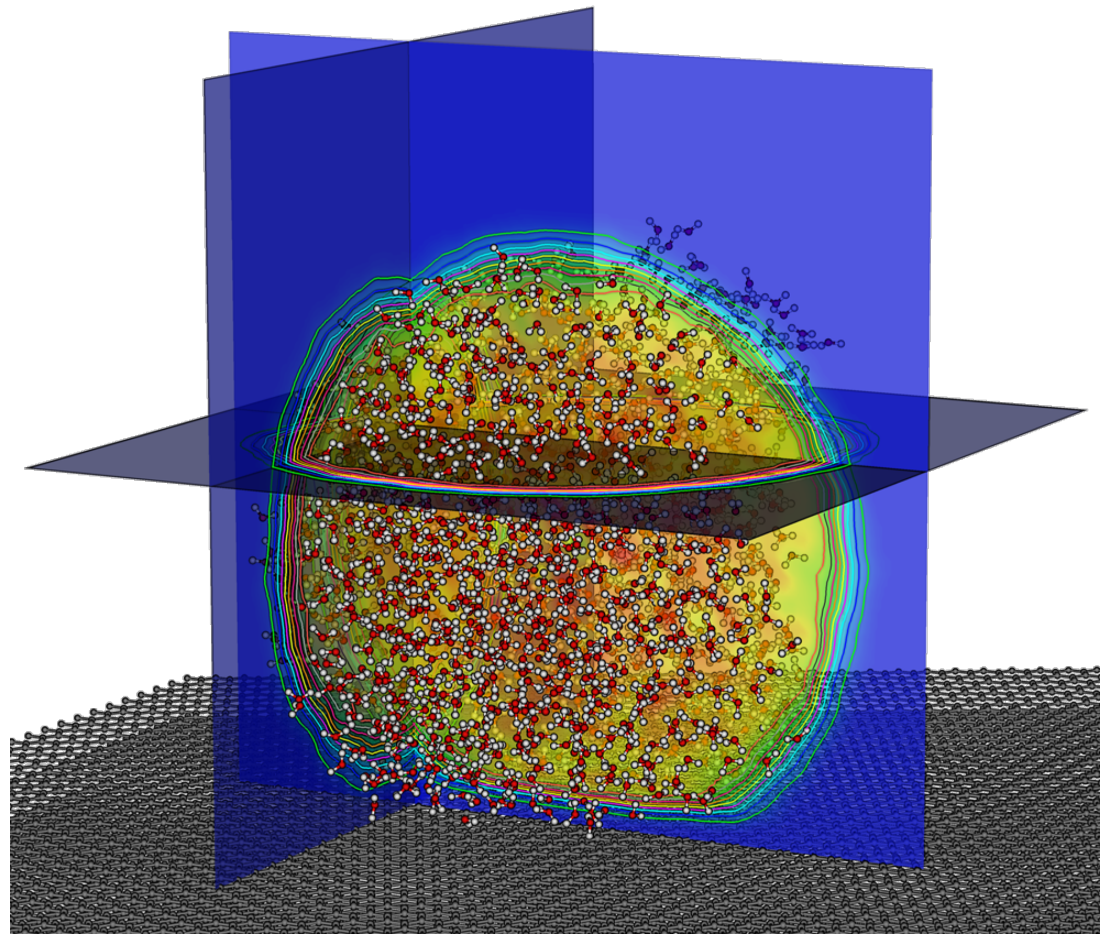
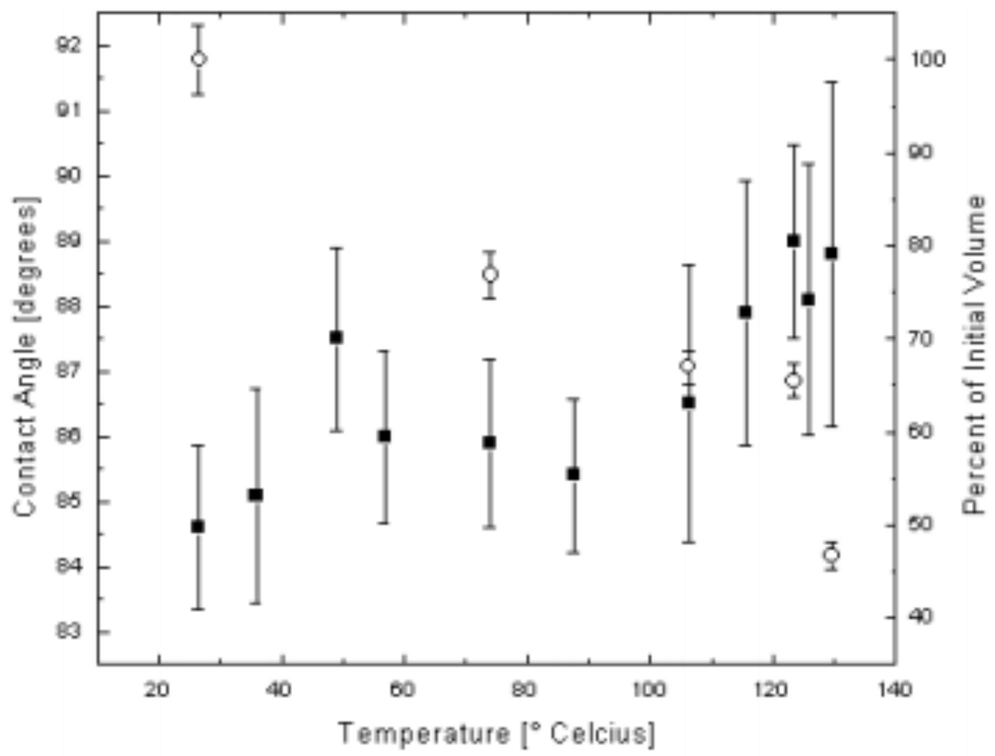
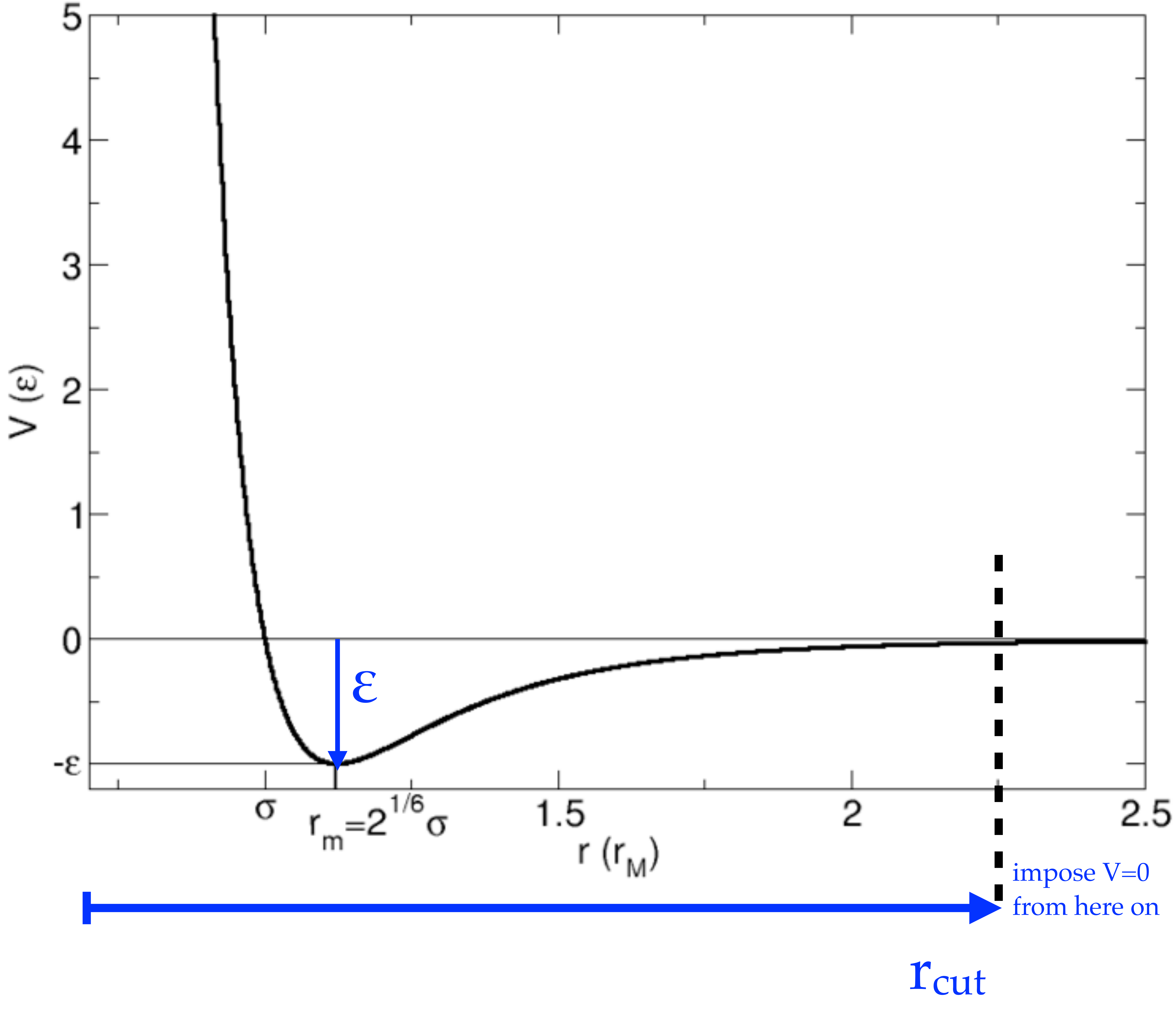




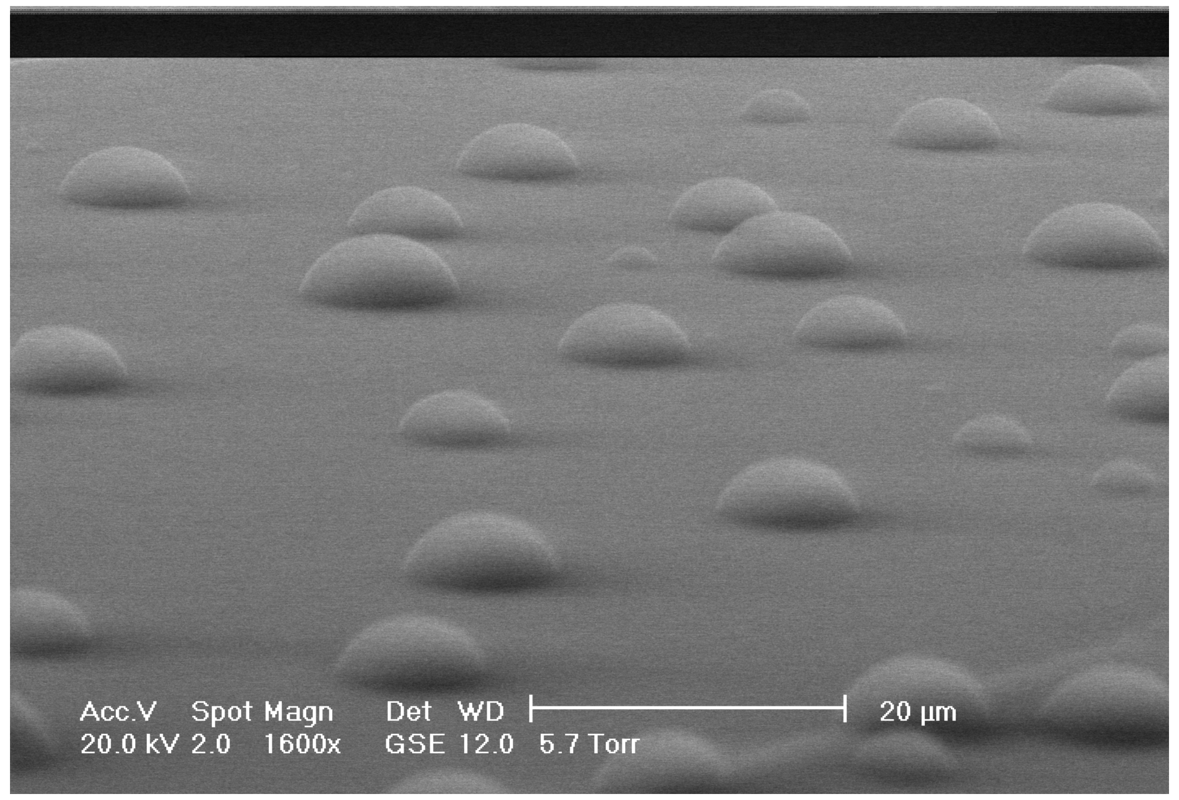
K. Osborne III (2009)

ennard-Jones potential : well depth and cut-off

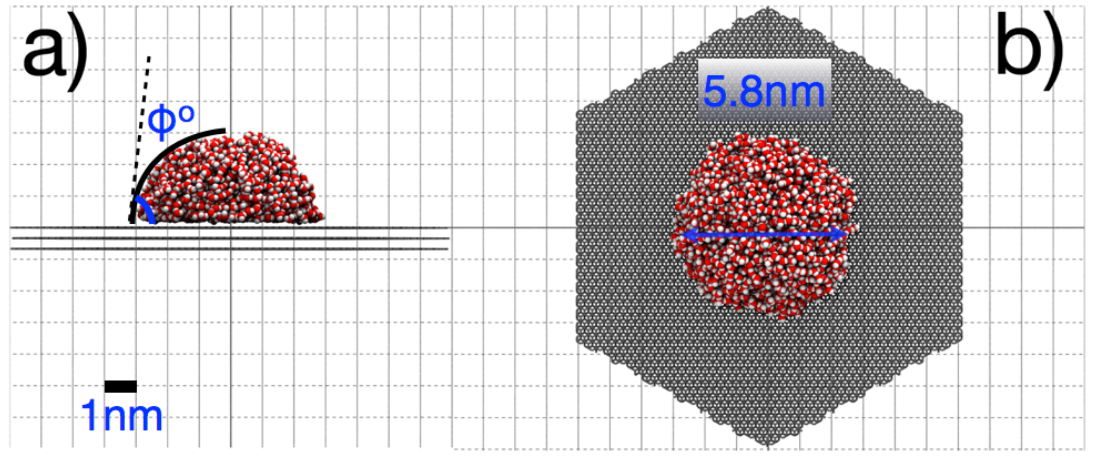


BAYESIAN UNCERTAINTY FOR NANOSCALE FLOWS

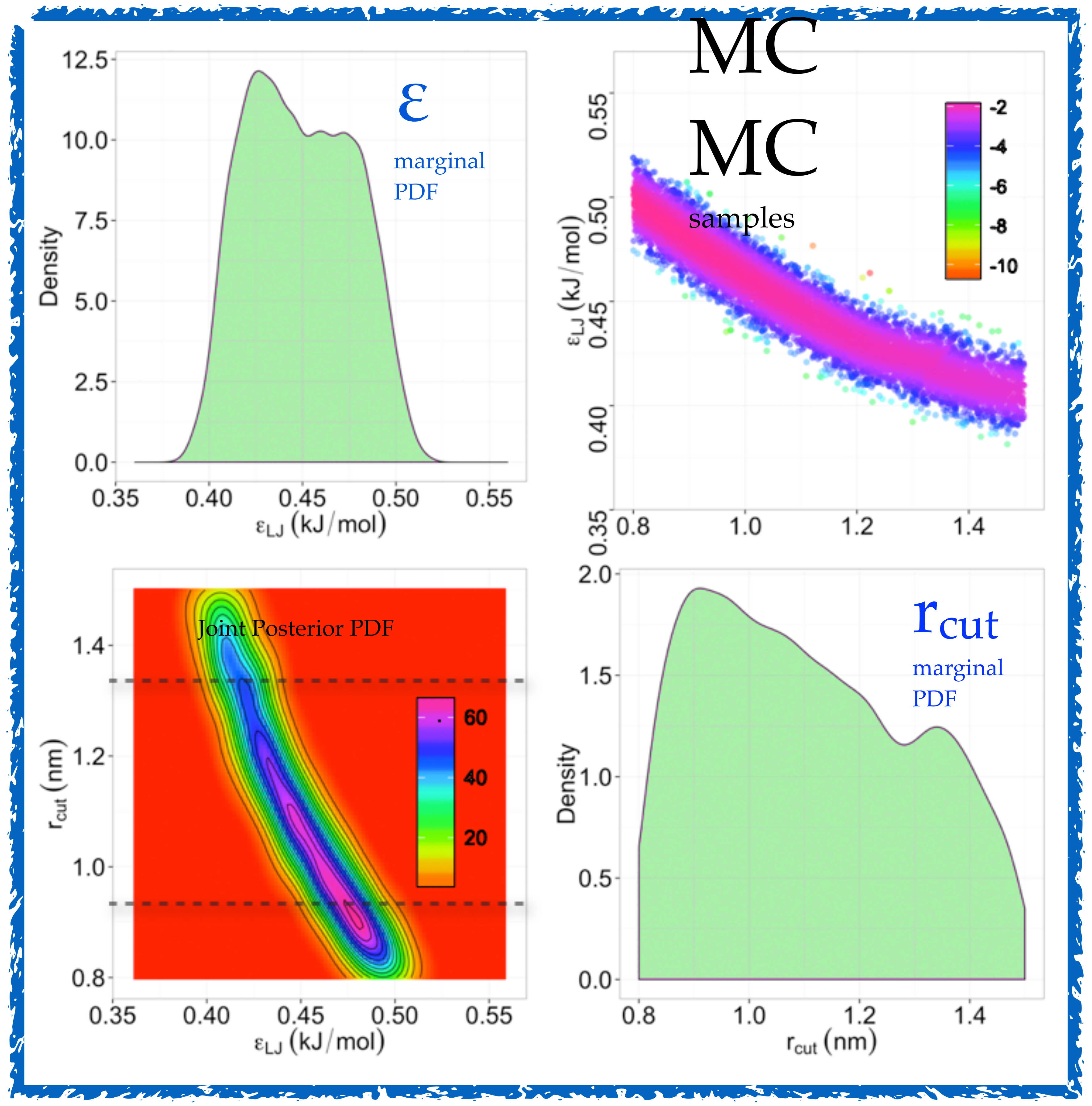
MODEL CALIBRATION



Water Contact Angle



Parameters: ε, r_{cut}



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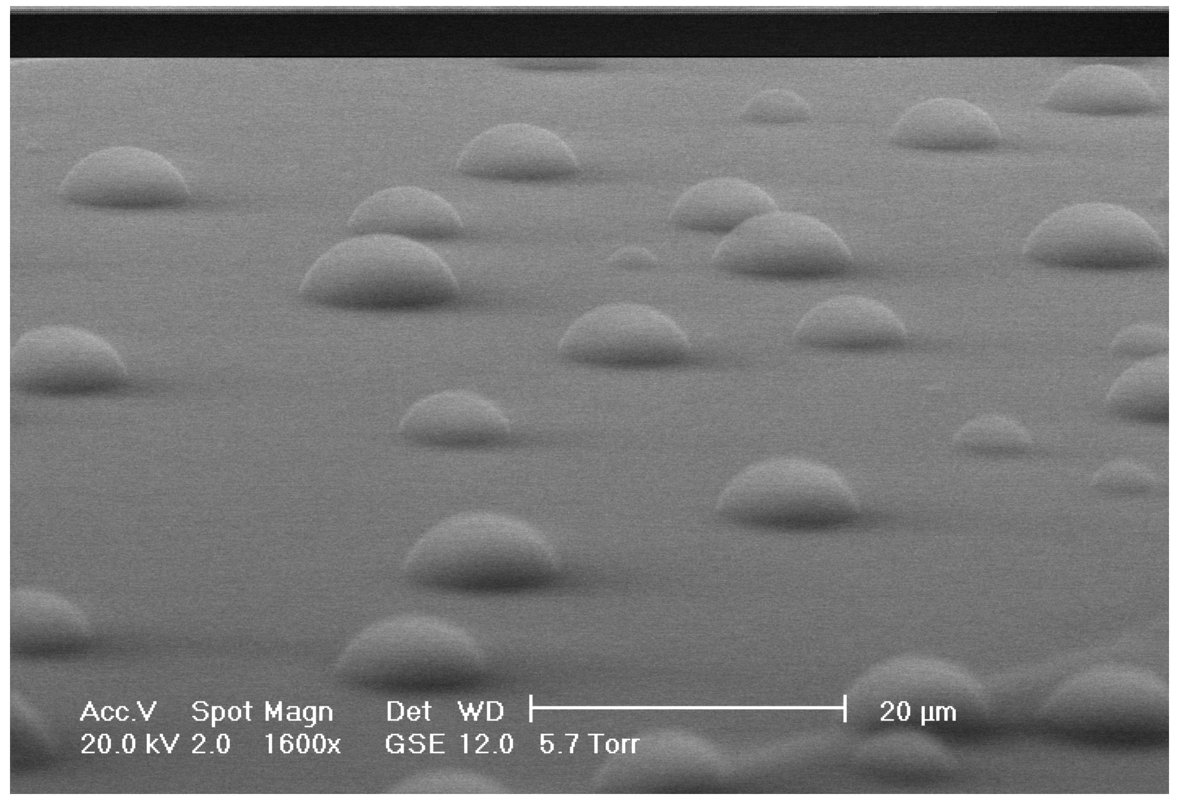

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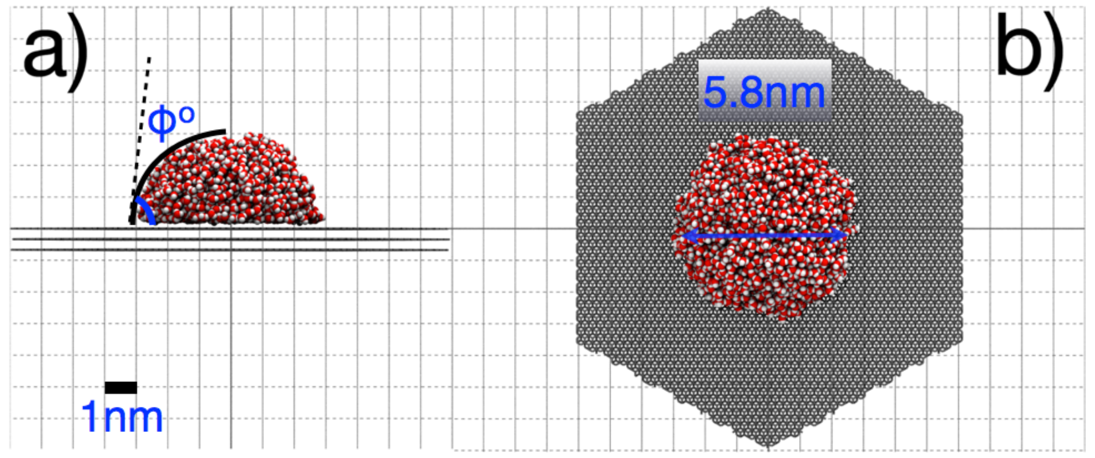

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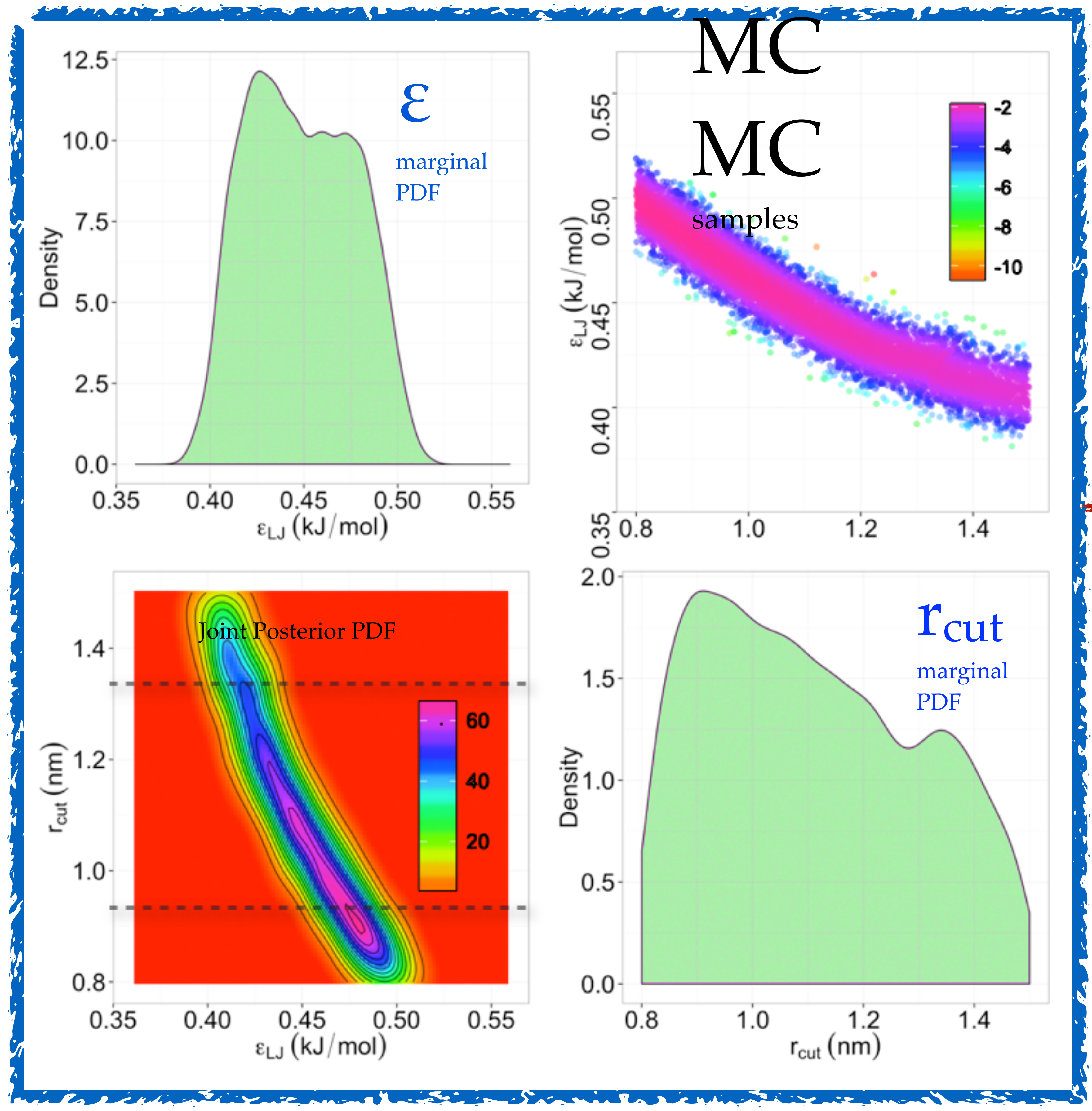
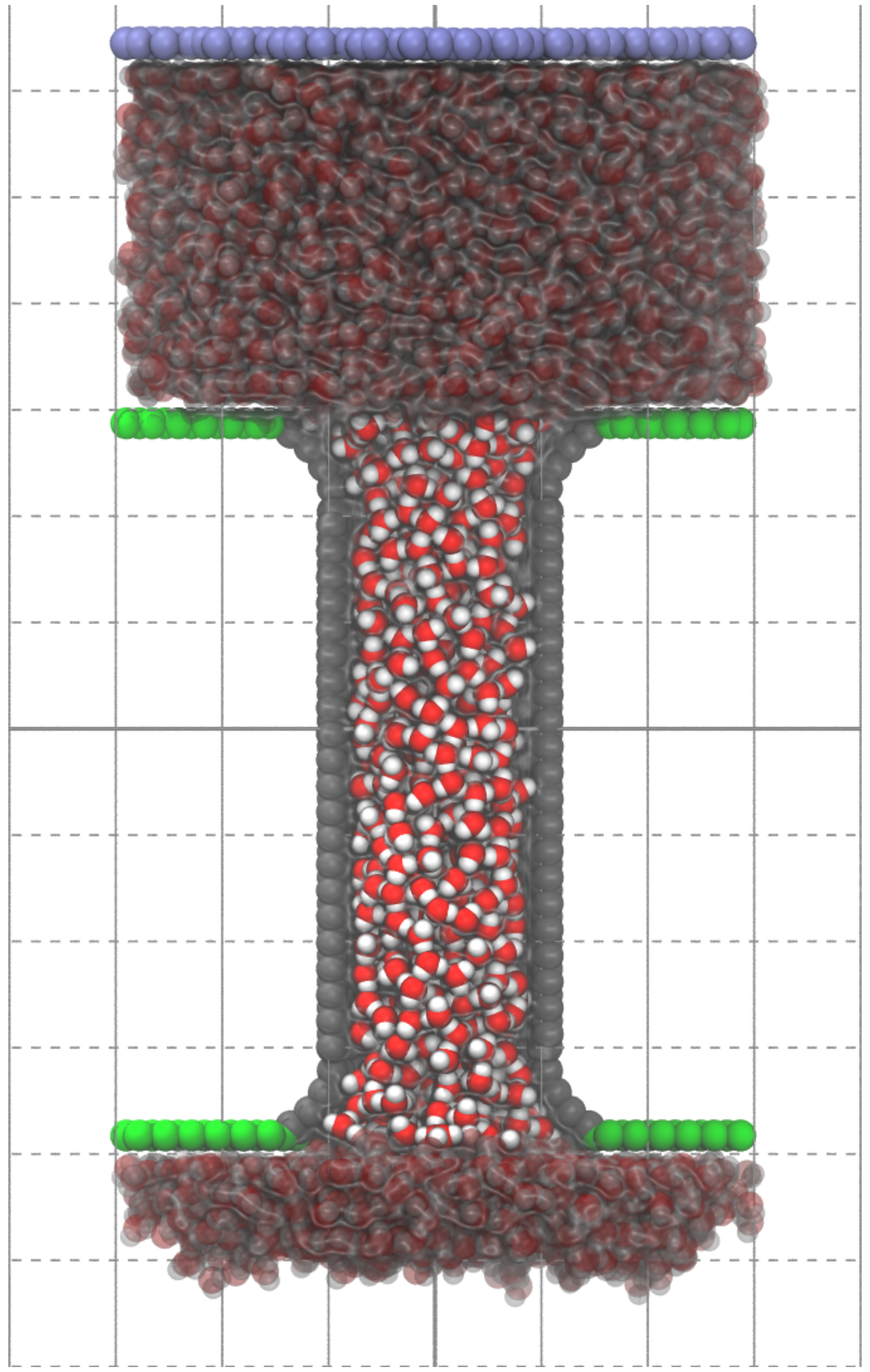


Water Transport in CNTs

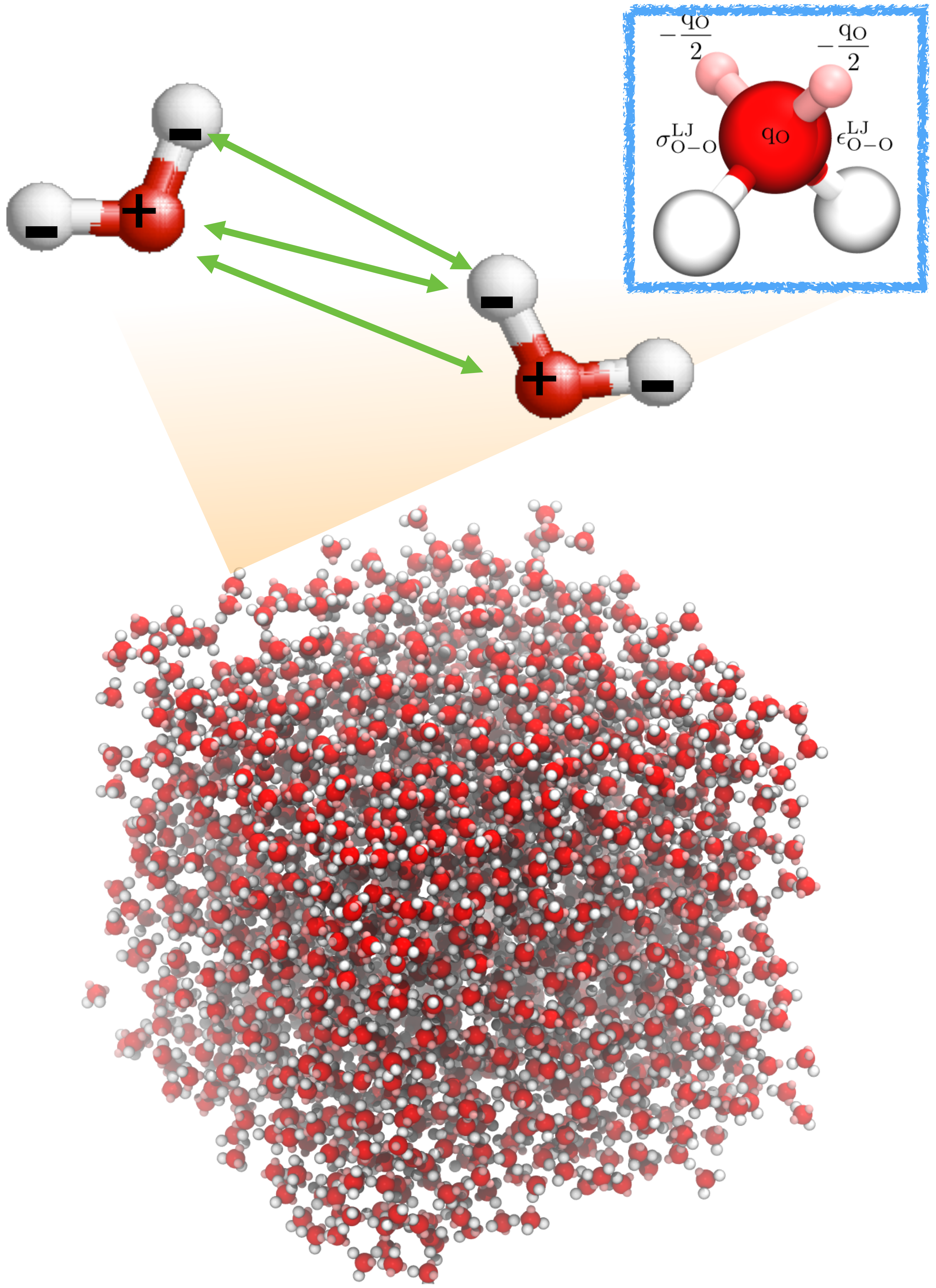


Friction coefficient and slip length of water inside CNTs

Example 2: Calibrating MD simulation for water

- **HETEROGENEOUS DATA**
  - *Diffusion coefficient*
  - *Density*
  - *Radial Distribution Function (RDF)*

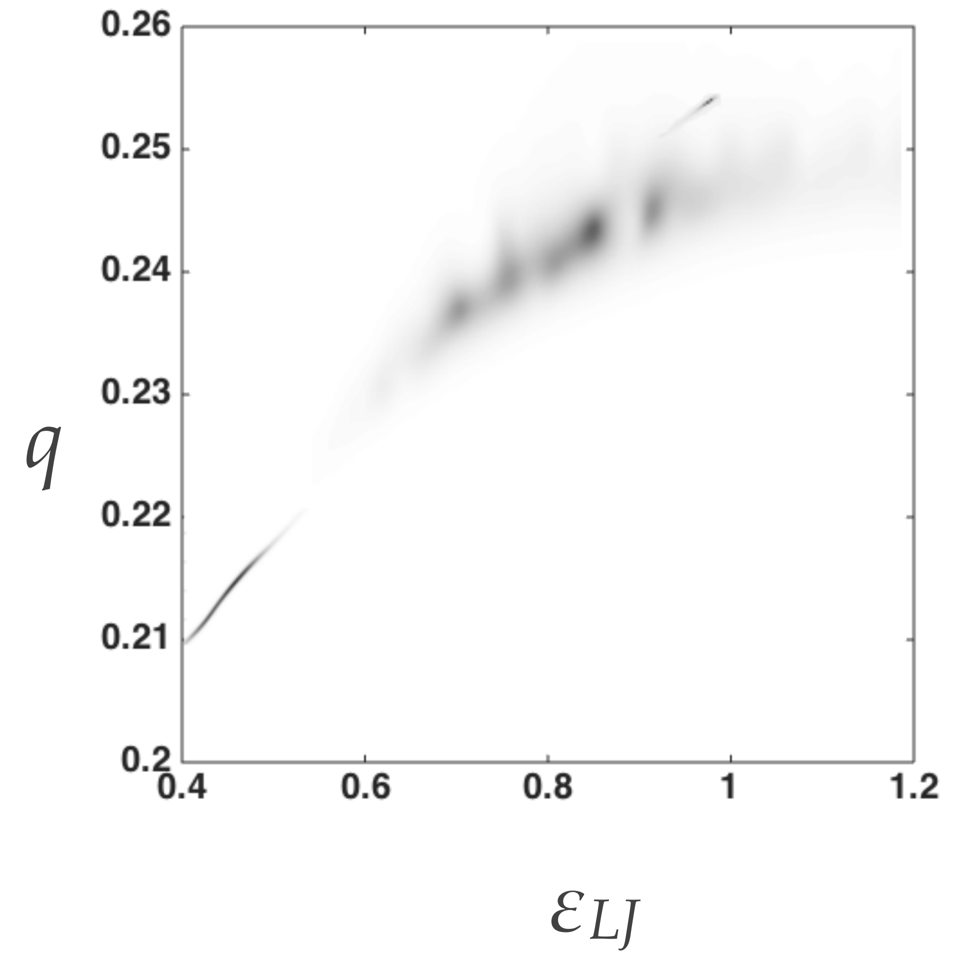
Data sources: Holz et al. 2000; Jones & Harris 1992; Soper 2013



Bayesian Inference using Individual Data Set

Calibrate for each data set individually…

Likelihood values



* Calibrate q and ε_{LJ} only, σ_{LJ} highly correlated with ε_{LJ}

Bayesian Inference using Individual Data Set

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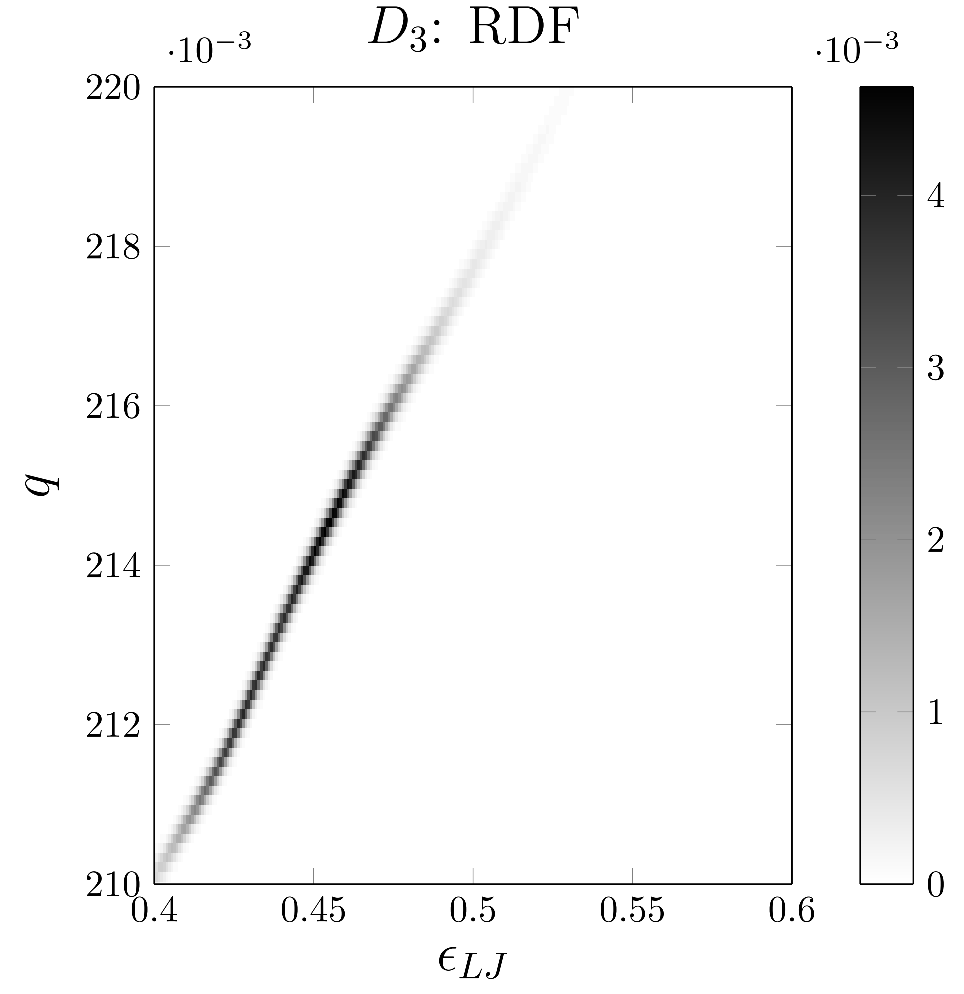
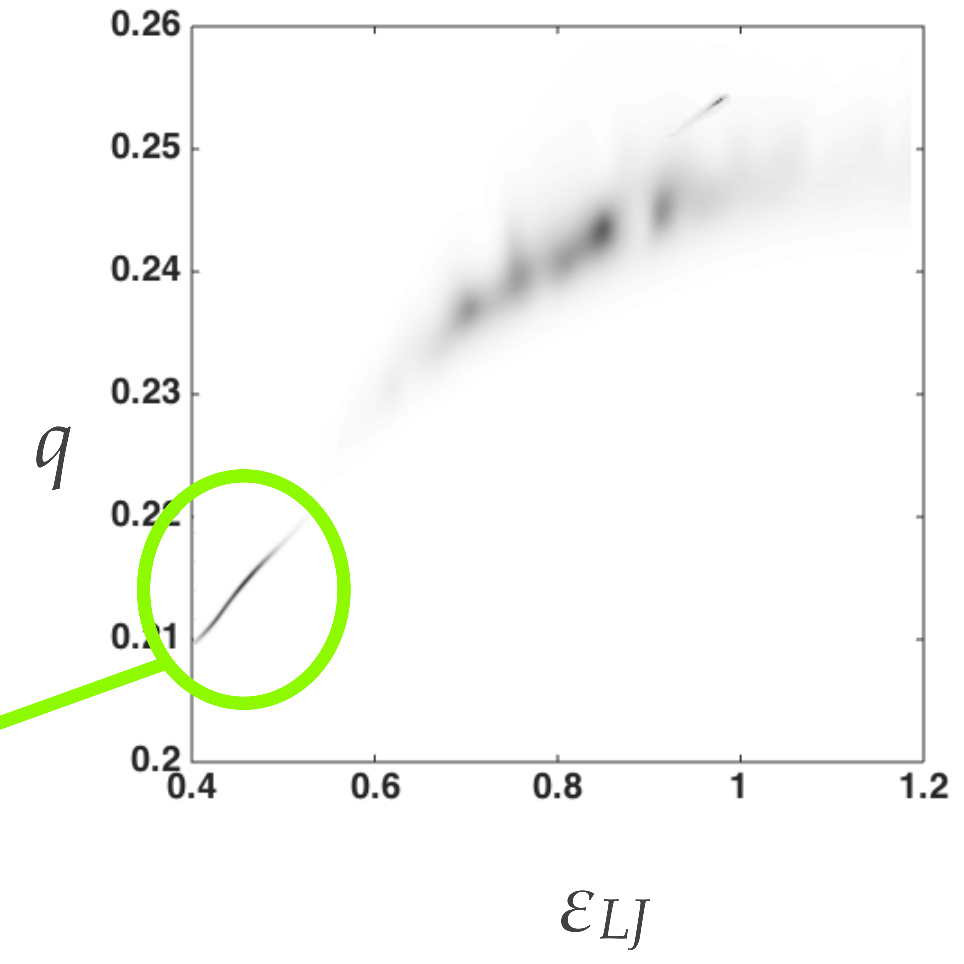


Likelihood values



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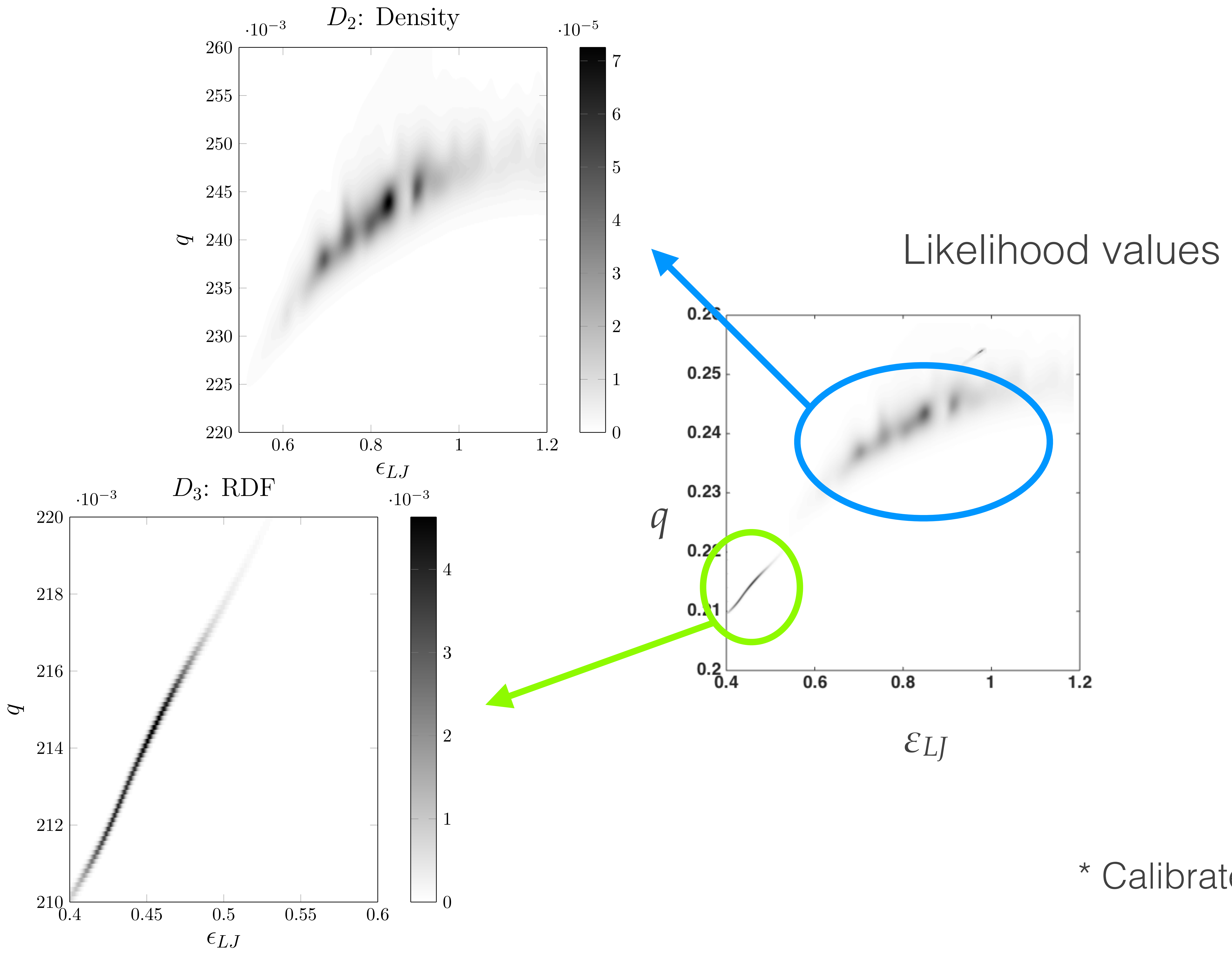

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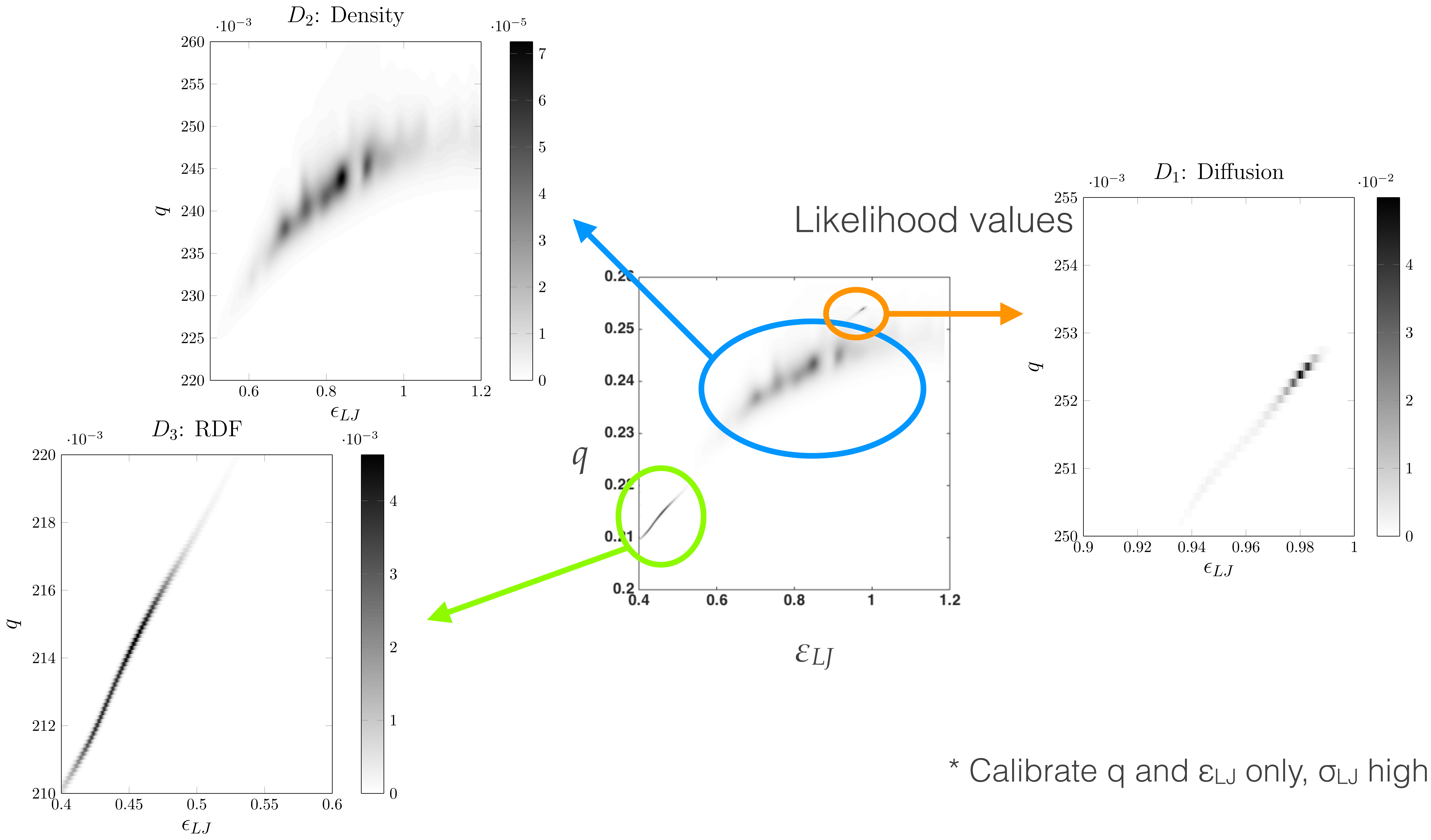

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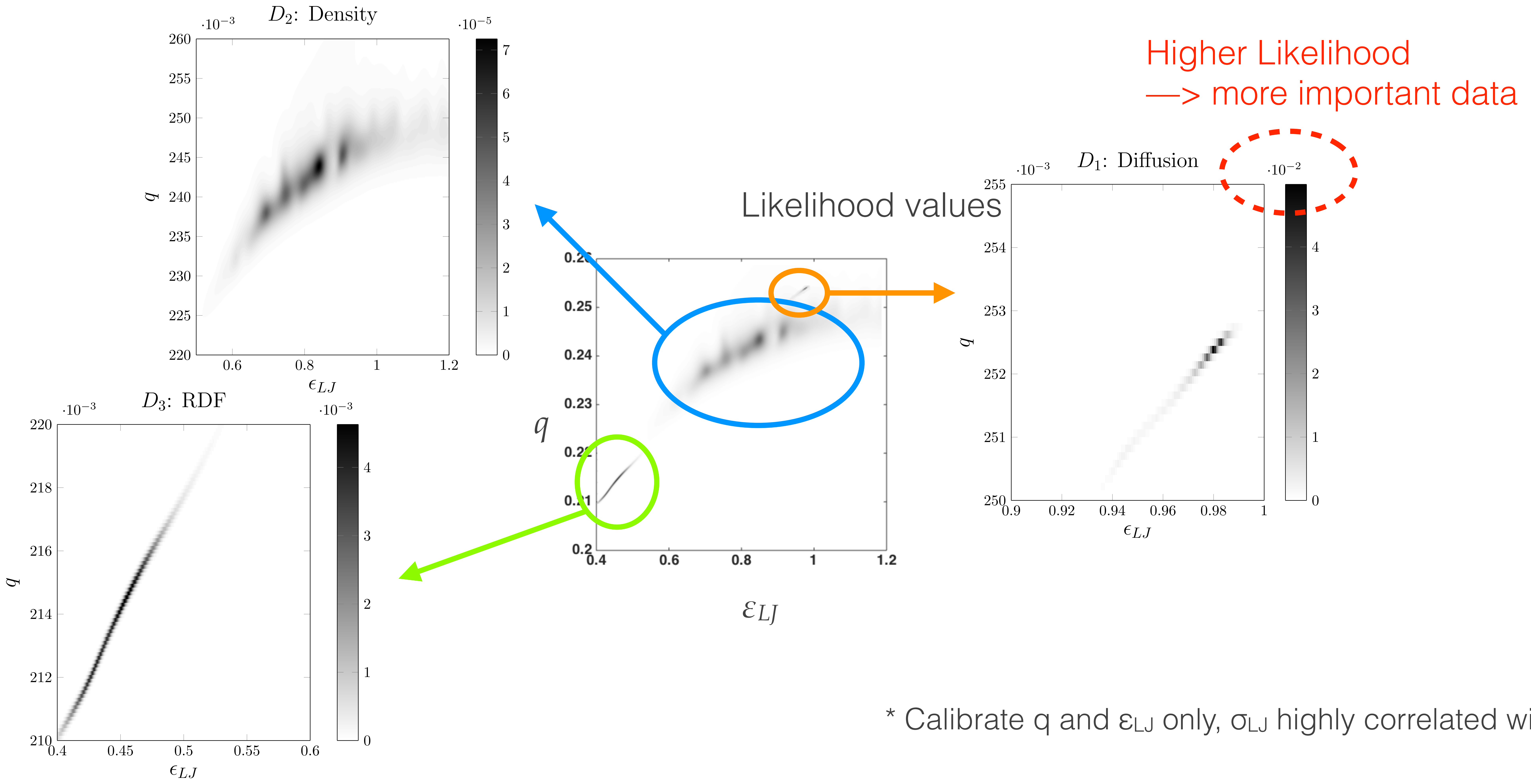

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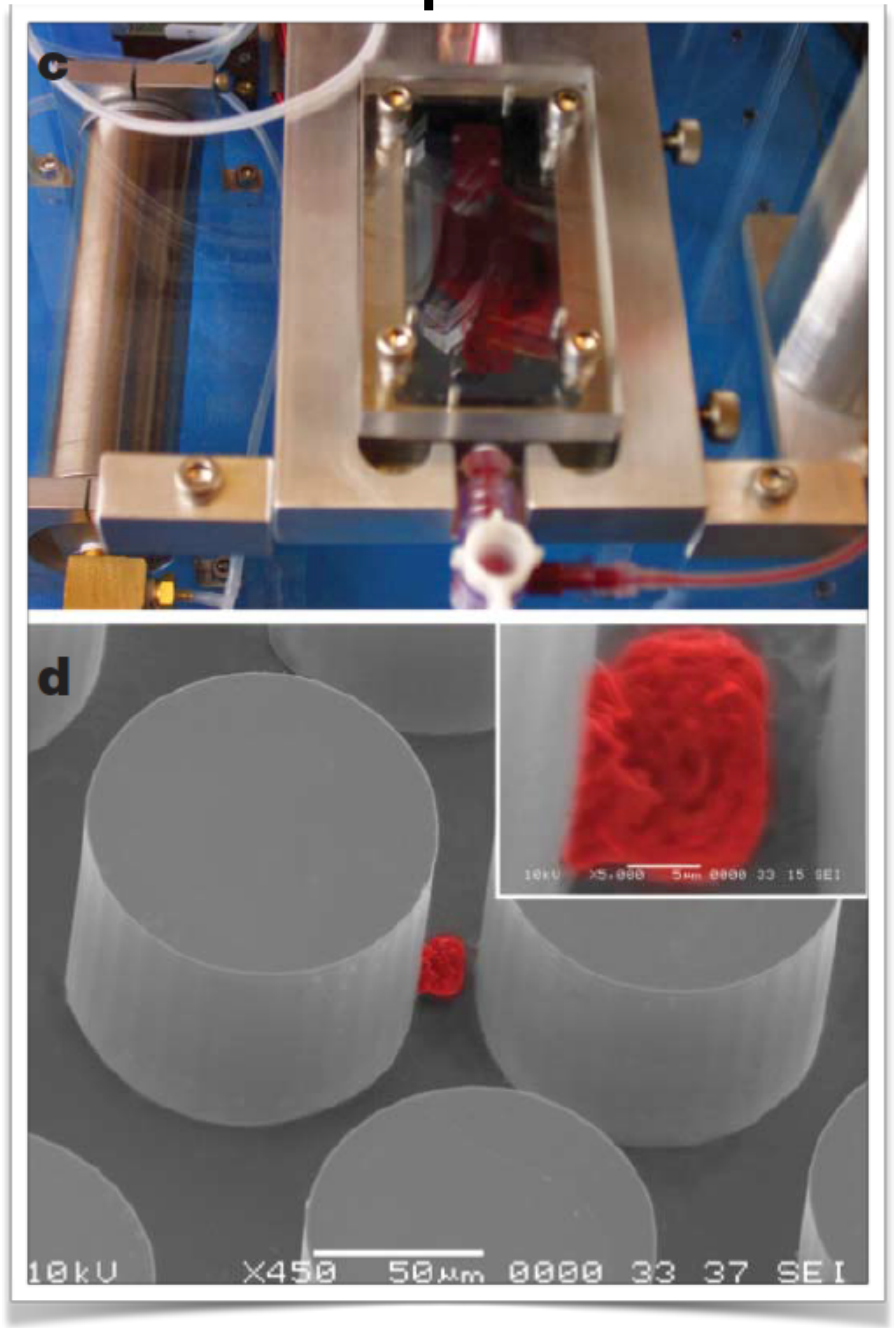
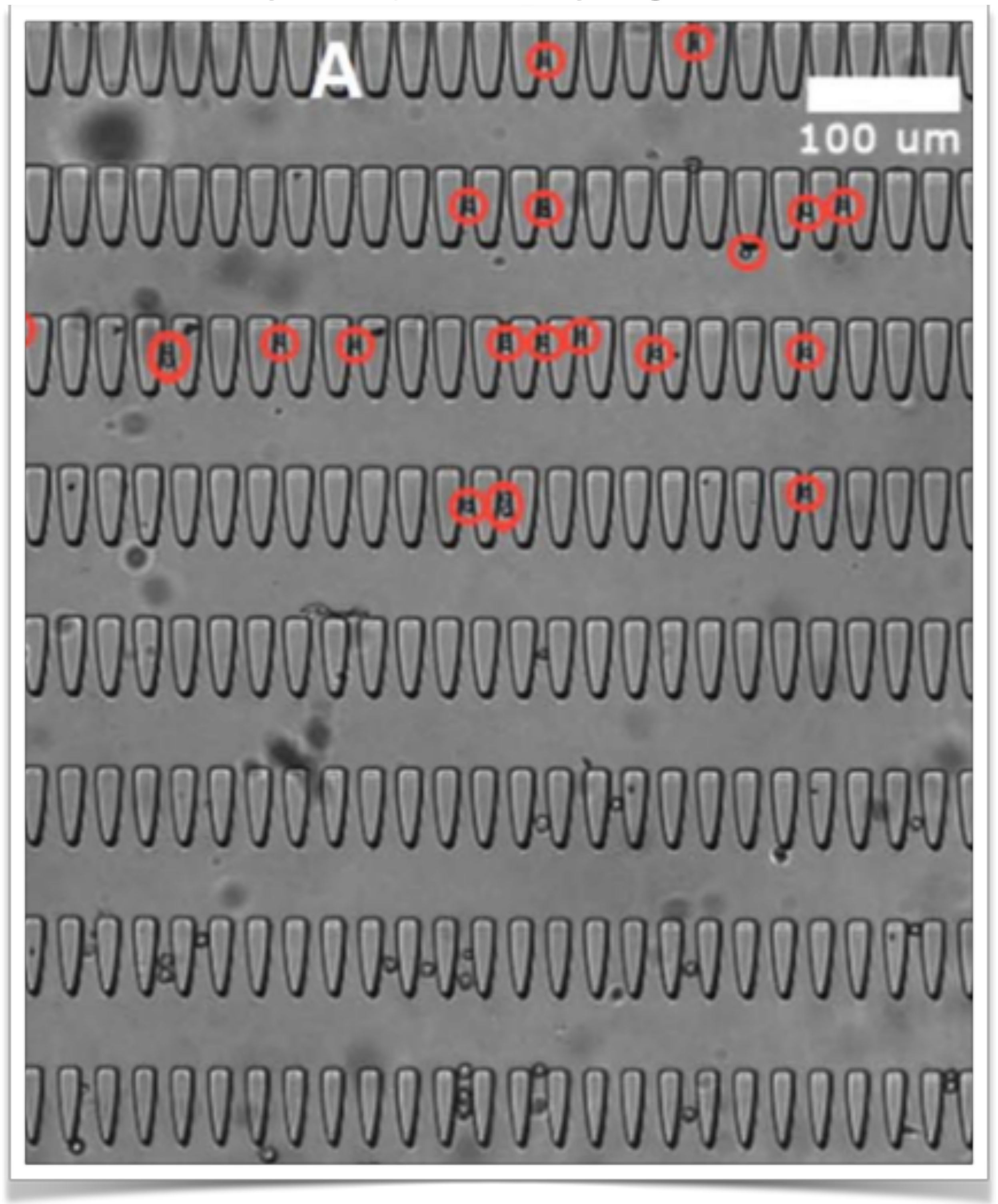
Why interested in blood?

CTC-chip



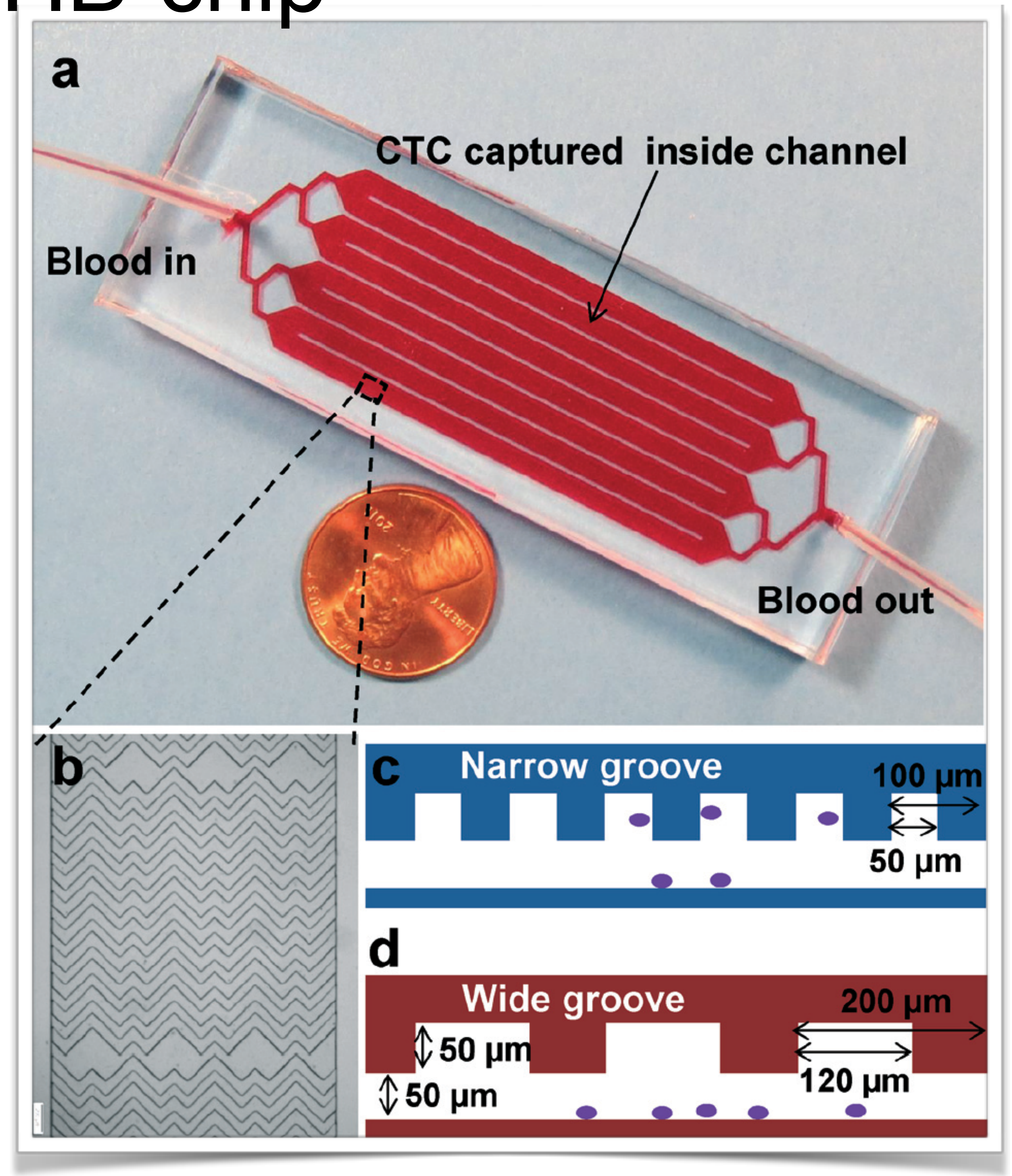
Isolation of rare circulating tumour cells in cancer patients by microchip technology, Nagrath et al., Nature, 2007

Funnel ratchets



Cell separation based on size and deformability using microfluidic funnel ratchets, McFaul et al., Lab on a Chip, 2012

HB-chip

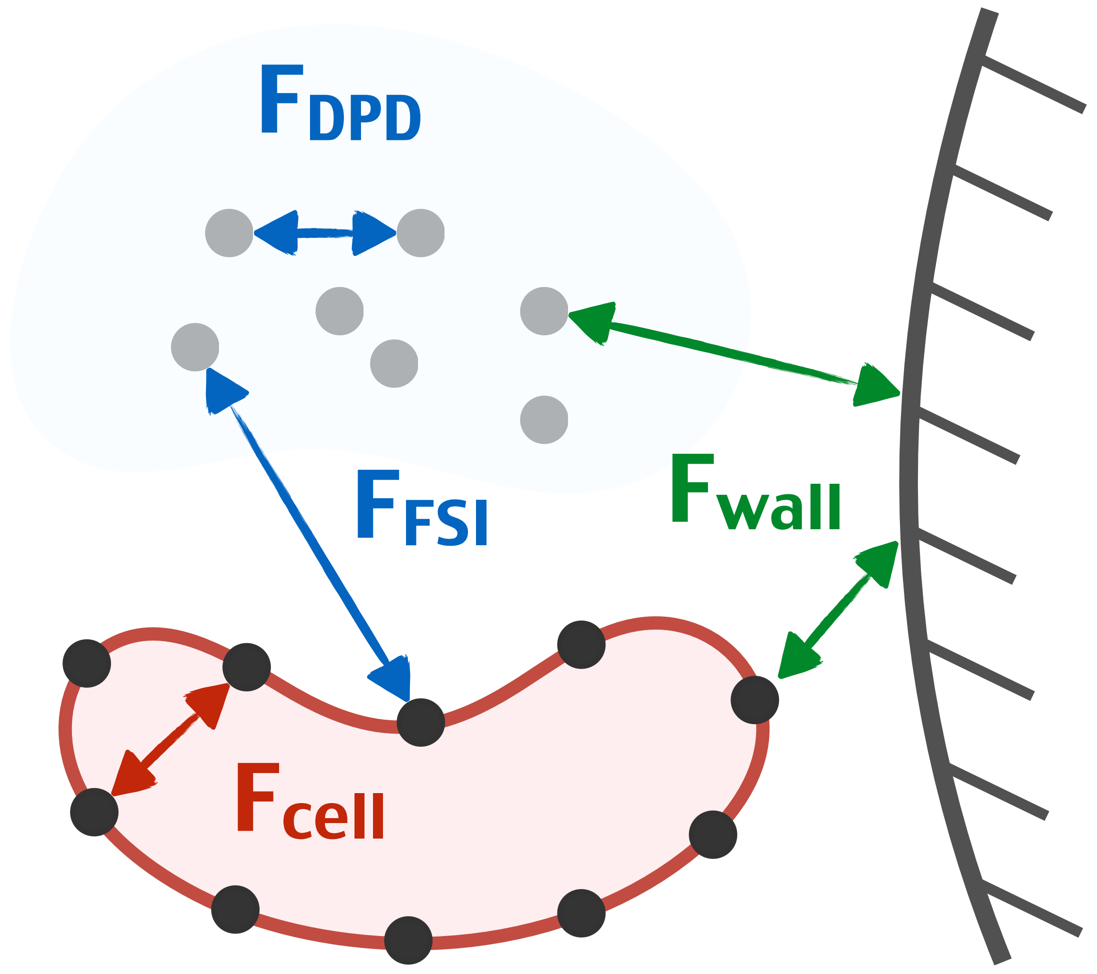


Isolation of circulating tumor cells using a microvortex generating herringbone-chip, Scott et al.,Proc. Nat. Acad. Sci., 2014

CTC detection → High throughput - mL Samples

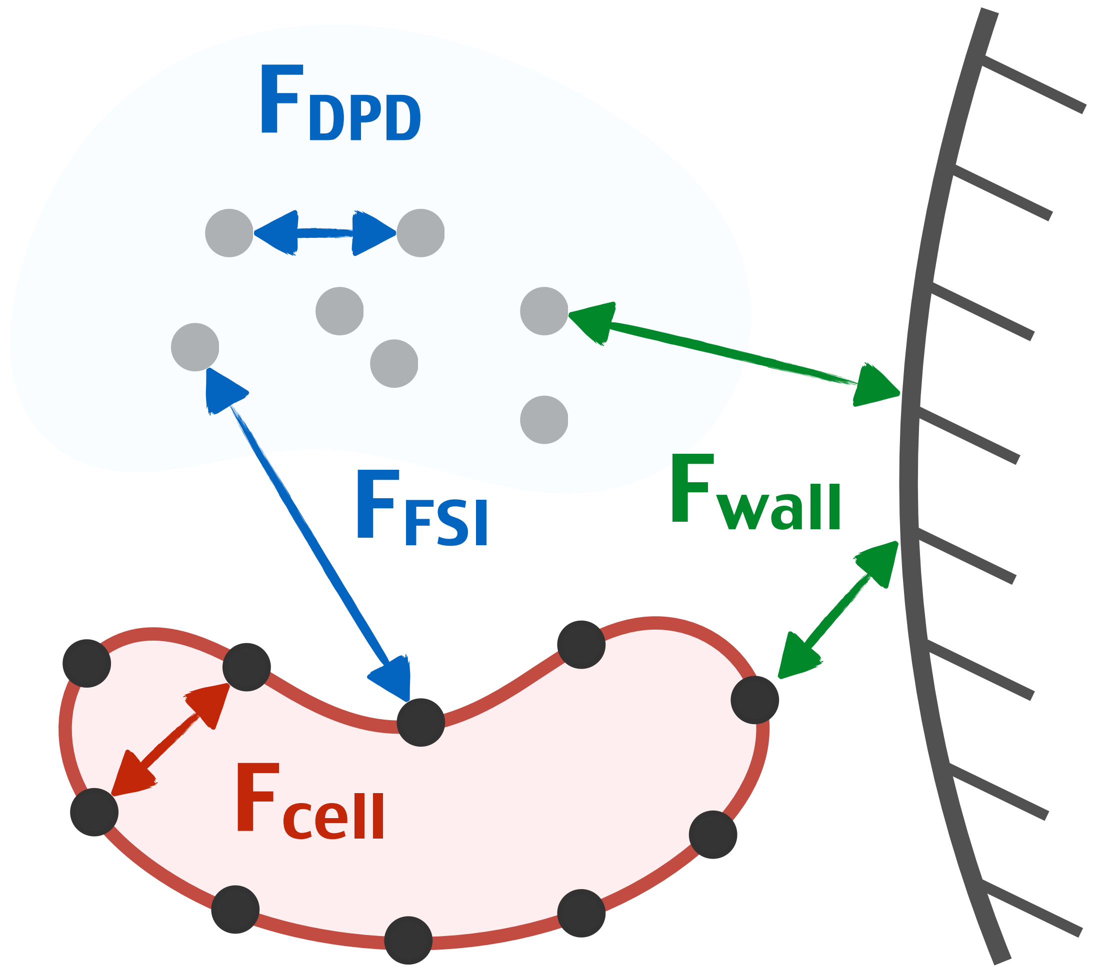
DPD FORCES : N-body Interactions + Stochastics

$$\mathbf{F}_i = \sum_{n=1,n\neq i}^{N} \mathbf{F}_{i,n}^{C,\mathrm{DPD}} + \mathbf{F}_{i,n}^{D,\mathrm{DPD}} + \mathbf{F}_{i,n}^{R,\mathrm{DPD}}$$
$$+ \sum_{k=1,k\neq i}^{K} \mathbf{F}_{i,k}^{C,\mathrm{FSI}} + \mathbf{F}_{i,k}^{D,\mathrm{FSI}} + \mathbf{F}_{i,k}^{R,\mathrm{FSI}}$$
$$+ \sum_{m=1,m\neq i}^{M} \mathbf{F}_{i,m}^{C,\mathrm{wall}} + \mathbf{F}_{i,m}^{D,\mathrm{wall}} + \mathbf{F}_{i,m}^{R,\mathrm{wall}}$$



DPD FORCES : N-body Interactions + Stochastics

$$\mathbf{F}_i = \sum_{n=1,n\neq i}^{N} \mathbf{F}_{i,n}^{C,\mathrm{DPD}} + \mathbf{F}_{i,n}^{D,\mathrm{DPD}} + \mathbf{F}_{i,n}^{R,\mathrm{DPD}}$$
$$+ \sum_{k=1,k\neq i}^{K} \mathbf{F}_{i,k}^{C,\mathrm{FSI}} + \mathbf{F}_{i,k}^{D,\mathrm{FSI}} + \mathbf{F}_{i,k}^{R,\mathrm{FSI}}$$
$$+ \sum_{m=1,m\neq i}^{M} \mathbf{F}_{i,m}^{C,\mathrm{wall}} + \mathbf{F}_{i,m}^{D,\mathrm{wall}} + \mathbf{F}_{i,m}^{R,\mathrm{wall}}$$



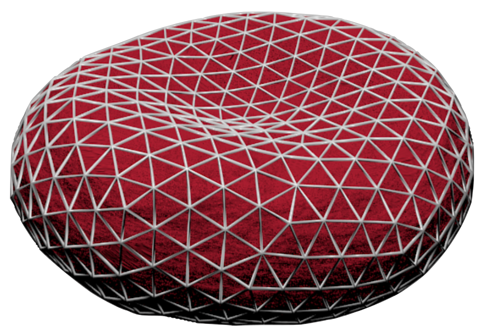
$$\mathbf{F}_{ij}^{C} = \begin{cases} a_{ij}(1-r_{ij})\mathbf{e}_{ij}, & \text{if } r_{ij} < 1 \\ 0, & \text{if } r_{ij} \geq 1 \end{cases}$$
$$\mathbf{F}_{ij}^{D} = -\gamma w^{D}(r_{ij})(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\mathbf{e}_{ij}$$
$$\mathbf{F}_{ij}^{R} = \sigma w^{R}(r_{ij})\theta_{ij}\mathbf{e}_{ij}$$

$$\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$$
$$r_{ij} = ||\mathbf{r}_{ij}||$$
$$\mathbf{e}_{ij} = \mathbf{r}_{ij}/||\mathbf{r}_{ij}||$$
$$\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$$

$$w^{D}(r) = (w^{R}(r))^2$$
$$\sigma^2 = 2\gamma k_B T$$

The Red Blood Cell (RBC) model

$$V(\{\mathbf{x}_i\}) = V_{in-plane} + V_{bending} + V_{area} + V_{volume}$$

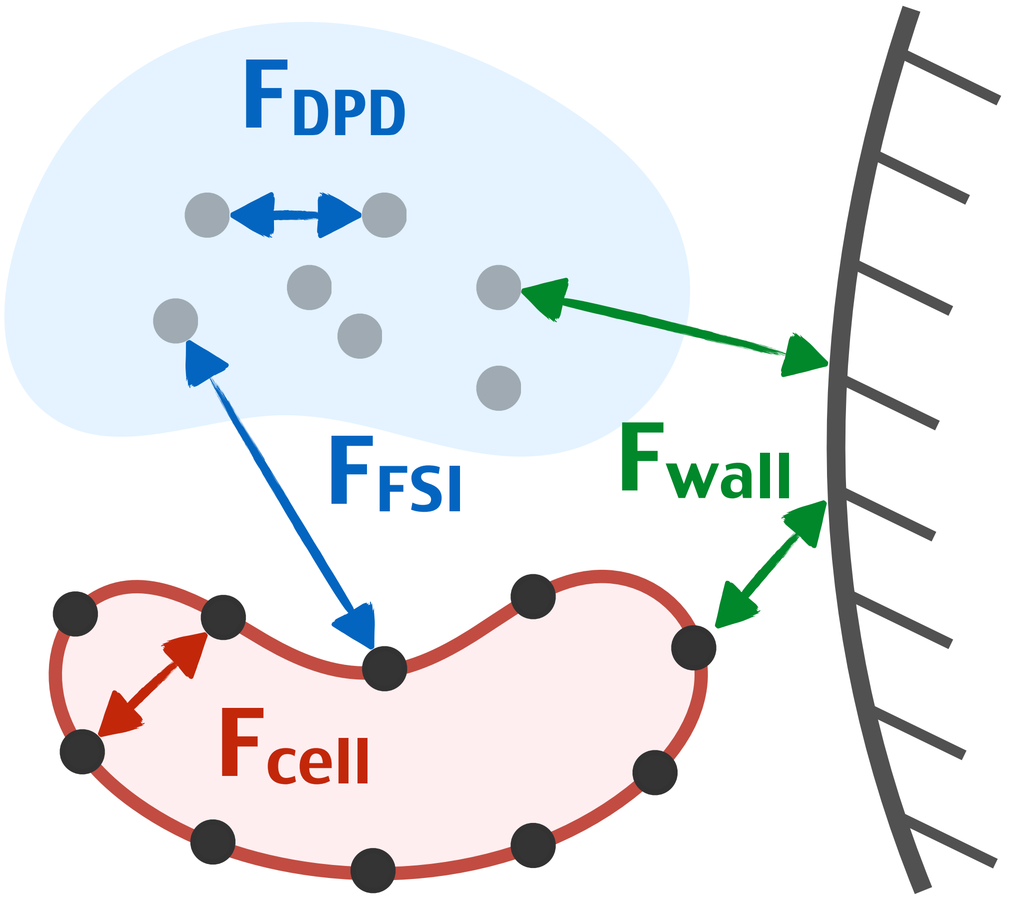


$$V_{in-plane} = \sum_{j \in 1 \ldots N_s} \left[\frac{k_B T l_{max} \left(3x_j^2 - 2x_j^3\right)}{4p(1-x_j)} + \frac{k_p}{(n-1) l_j^{n-1}} \right]$$

$$V_{bending} = \sum_{j \in 1 \ldots N_s} k_b \left[1 - cos(\theta_j - \theta_0)\right]$$

$$V_{area} = \frac{k_a (A^{tot} - A_0^{tot})^2}{2A_0^{tot}} + \sum_{j \in 1 \ldots N_t} \frac{k_d (A_j - A_0)^2}{2A_0}$$

$$V_{volume} = \frac{k_v (V^{tot} - V_0^{tot})^2}{2V_0^{tot}}$$



Mechanical Properties

membrane shear modulus

$$\mu_0 = \frac{\sqrt{3} k_B T}{4 p l_{max} x_0} \left(\frac{x_0}{2(1-x_0)^3} - \frac{1}{4(1-x_0)^2} + \frac{1}{4} \right) + \frac{\sqrt{3} k_p (n+1)}{4 l_0^{n+1}}$$

where: $x_0 = \frac{l_0}{l_{max}}$

area compression modulus

$$K = 2\mu_0 + k_a + k_d$$

membrane bending rigidity

$$k_b = \frac{2k_c}{\sqrt{3}}$$

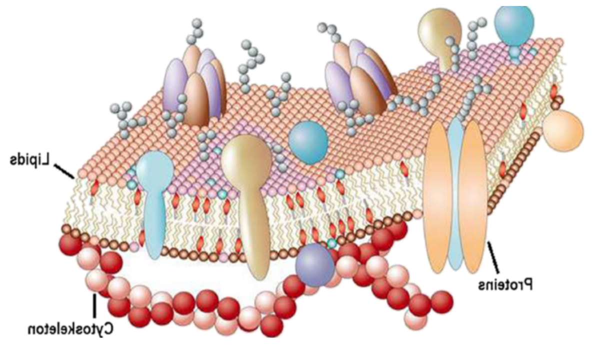
Young's modulus

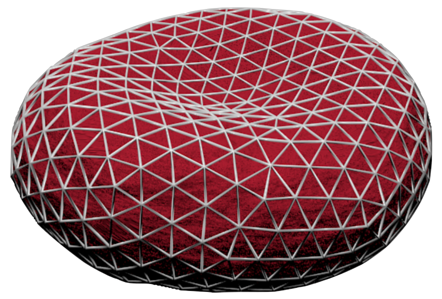
$$Y = \frac{4K\mu_0}{K + \mu_0}$$

membrane shear viscosity

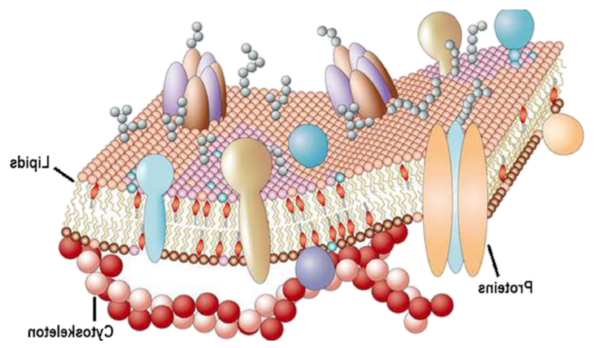
$$\eta_m = \sqrt{3}\gamma^T + \frac{\sqrt{3}\gamma^C}{4}$$

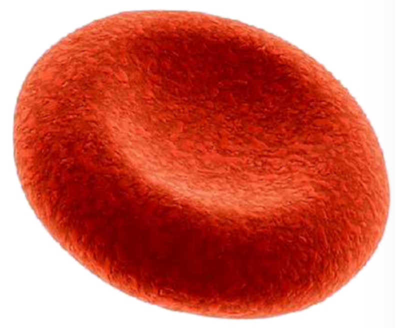
DPD FORCES: Red Blood Cells

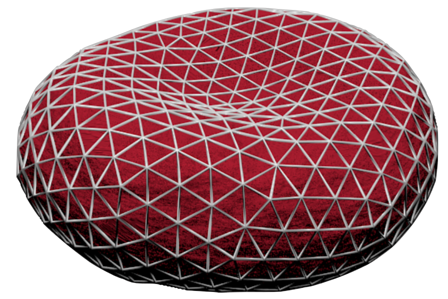




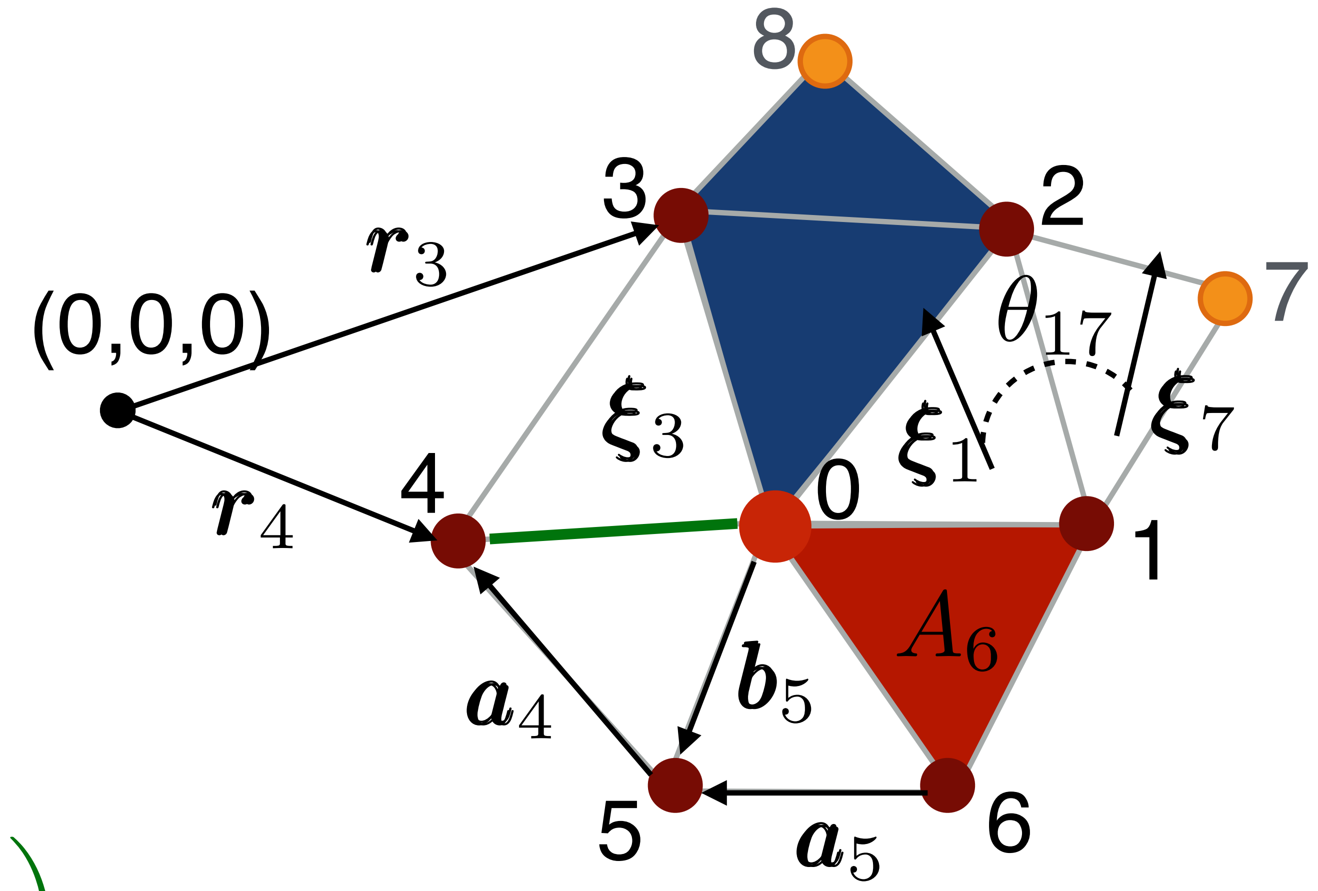
DPD FORCES: Red Blood Cells







$$
\begin{aligned}
\mathbf{F}^{\text{cell}} &= \sum_{n=1}^{N} \boldsymbol{F}^{\text{dihedral},1}_{0,n-1,n,n+1} + \boldsymbol{F}^{\text{dihedral},2}_{0,n,N+n,n+1} + \boldsymbol{F}^{\text{triangle}}_{0,n,n+1} + \boldsymbol{F}^{\text{bond}}_{0,n} \\
&= \sum_{n=1}^{N} \beta^b_{n,n+1} \left[\frac{\boldsymbol{\xi}_n \times \boldsymbol{a}_{n+1} + \boldsymbol{\xi}_{n+1} \times \boldsymbol{a}_n}{\xi_n \xi_{n+1}} - \cos\theta_{n,n+1} \left(\frac{\boldsymbol{\xi}_n \times \boldsymbol{a}_n}{\xi_n^2} + \frac{\boldsymbol{\xi}_{n+1} \times \boldsymbol{a}_{n+1}}{\xi_{n+1}^2} \right) \right] \\
&+ \beta^b_{n,N+n} \left[\frac{\boldsymbol{\xi}_{N+n} \times \boldsymbol{a}_n}{\xi_n \xi_{N+n}} - \cos\theta_{n,N+n} \frac{\boldsymbol{\xi}_n \times \boldsymbol{a}_n}{\xi_n^2} \right] \\
&+ \left(\frac{qC_q}{A_n^{q+1}} - k_a \frac{A - A_0^{tot}}{A_0^{tot}} \right) \frac{\boldsymbol{\xi}_n \times \boldsymbol{a}_n}{4A_n} \\
&- \frac{k_v}{18} \frac{V - V_0^{tot}}{V_0^{tot}} (\boldsymbol{\xi}_n + (\boldsymbol{r}_0 + \boldsymbol{r}_n + \boldsymbol{r}_{n+1}) \times \boldsymbol{a}_n) \\
&- \frac{k_B T}{p} \left(\frac{1}{4(1 - b_n/l_m)^2} - \frac{1}{4} + \frac{b_n}{l_m} \right) \frac{\boldsymbol{b}_n}{b_n} \\
&+ \sqrt{2k_B T} \left(\sqrt{2\gamma^T} d\overline{\boldsymbol{W}^S_{ij}} + \sqrt{3\gamma^C - \gamma^T} \frac{tr[d\boldsymbol{W}_{ij}]}{3} \boldsymbol{I} \right)
\end{aligned}
$$



$$x_0 = l_0/l_m$$

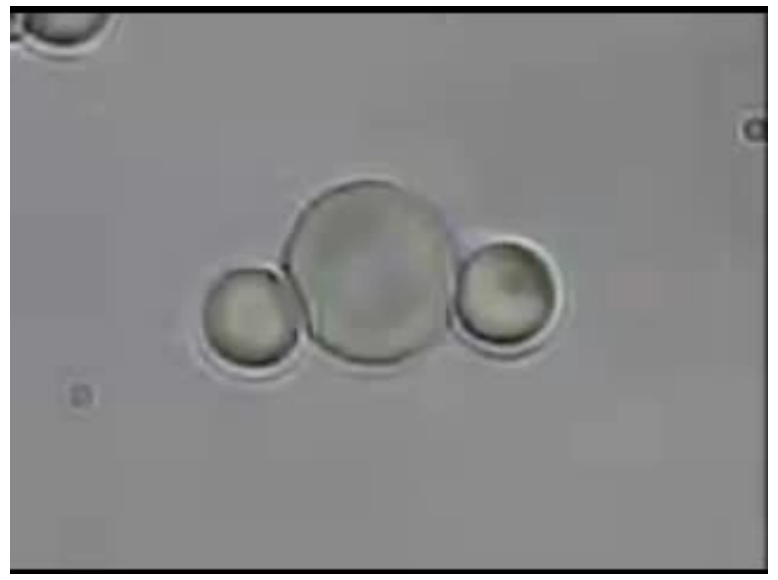
$$A_0 = \sqrt{3} l_0^2/4$$

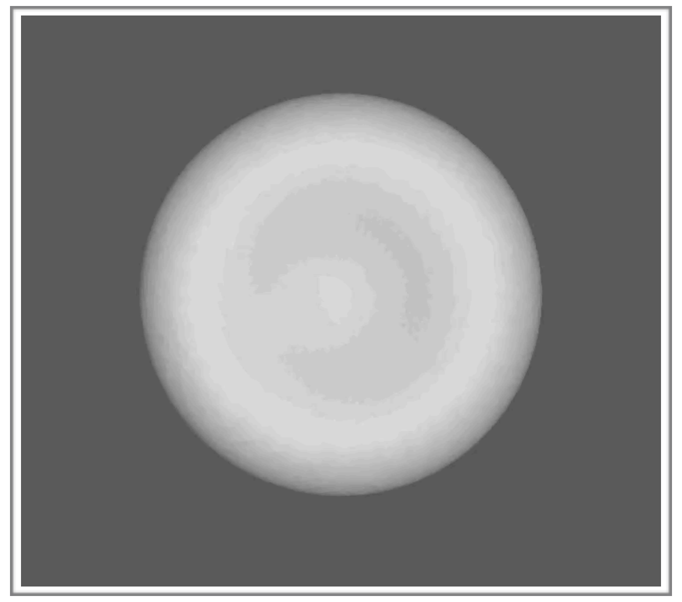
$$C_q = \frac{\sqrt{3} A_0^{q+1} k_B T (4x_0^2 - 9x_0 + 6)}{4pql_m(1 - x_0)^2}$$

$$\beta^b_{ij} = k_b \frac{\sin\theta_{ij}\cos\theta_0 - \cos\theta_{ij}\sin\theta_0}{\sqrt{1 - \cos^2\theta_{ij}}}$$

$$d\overline{\boldsymbol{W}^S_{ij}} = d\boldsymbol{W}^S_{ij} - tr[d\boldsymbol{W}^S_{ij}]\mathbf{1}/3$$

VALIDATION





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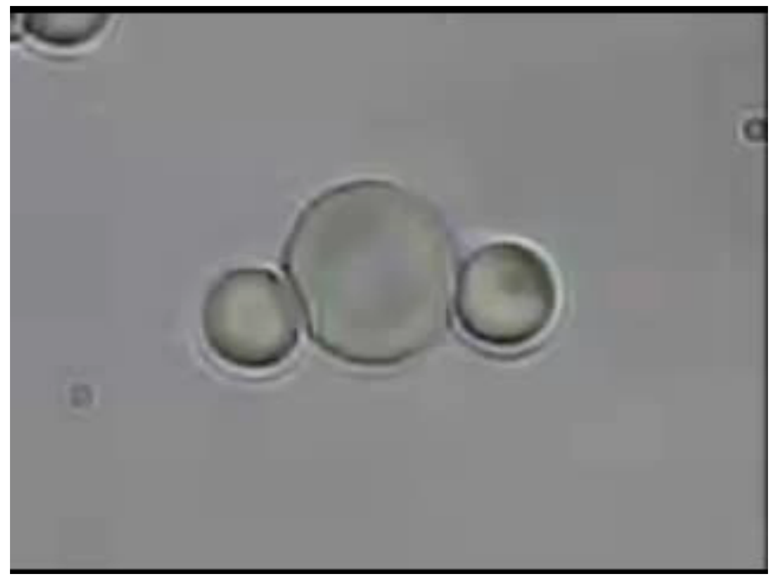

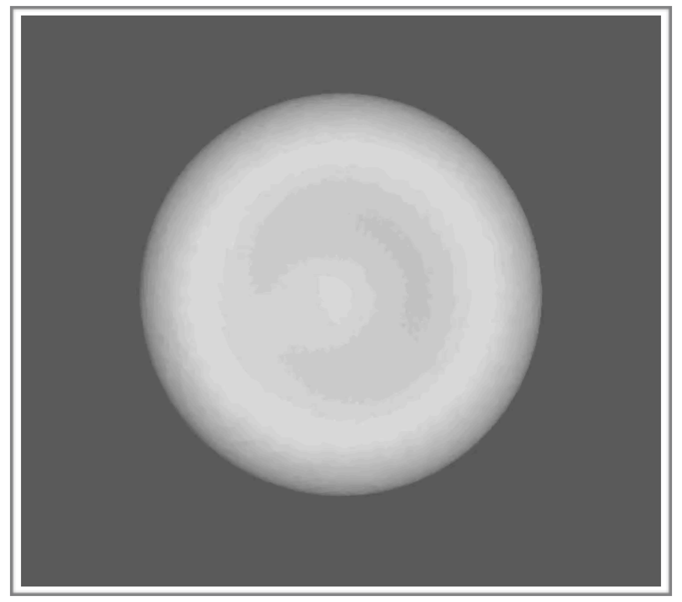

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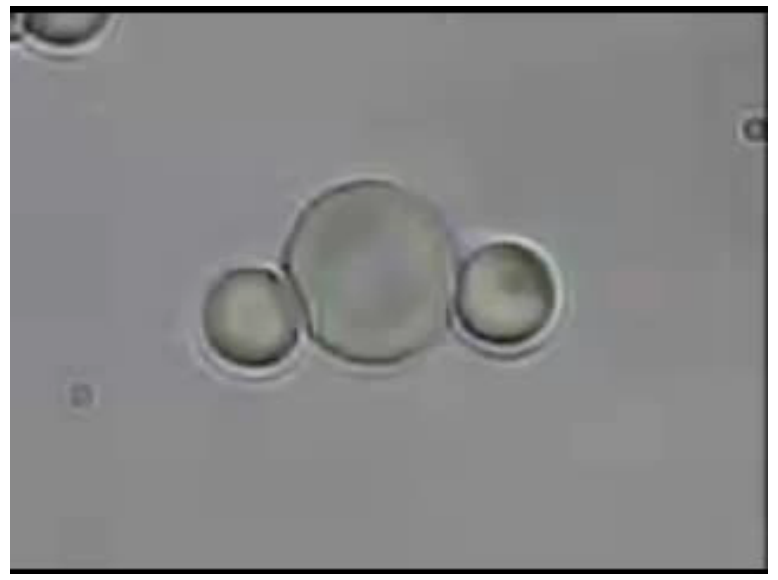

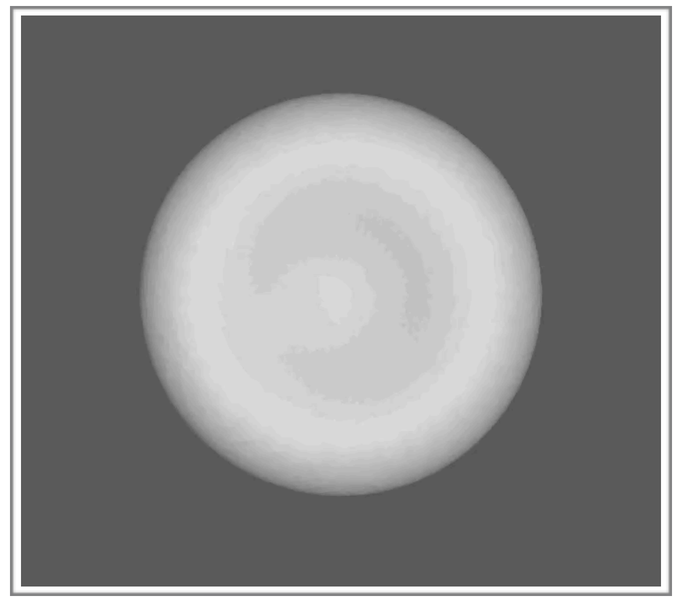

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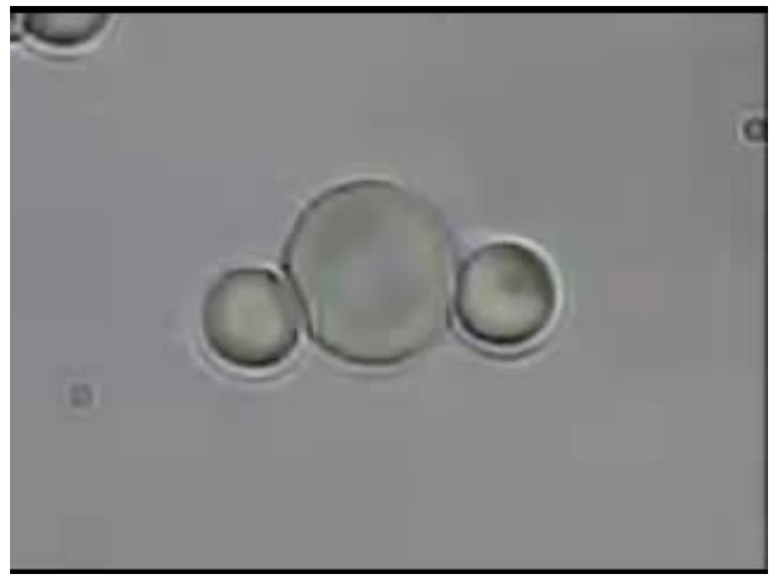

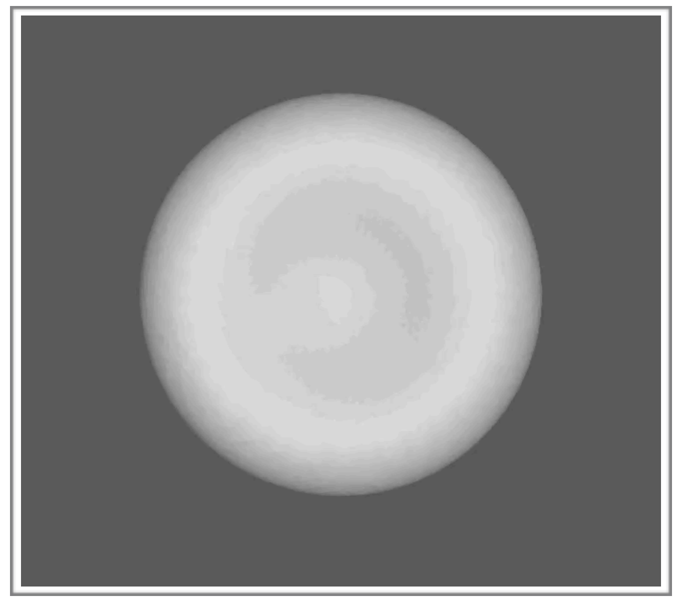

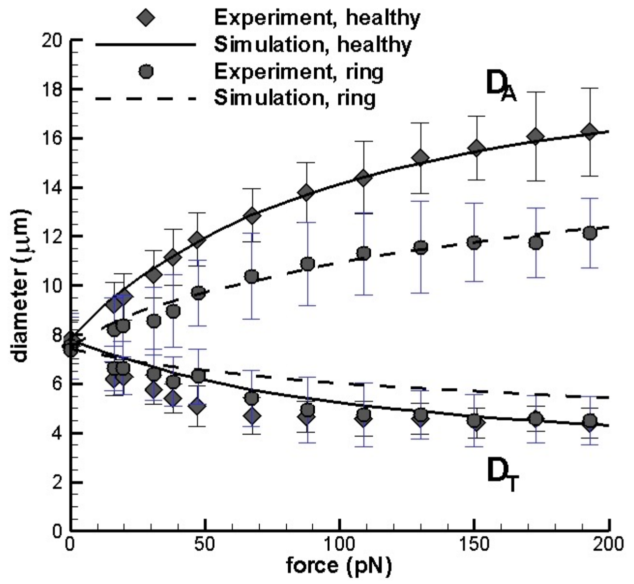

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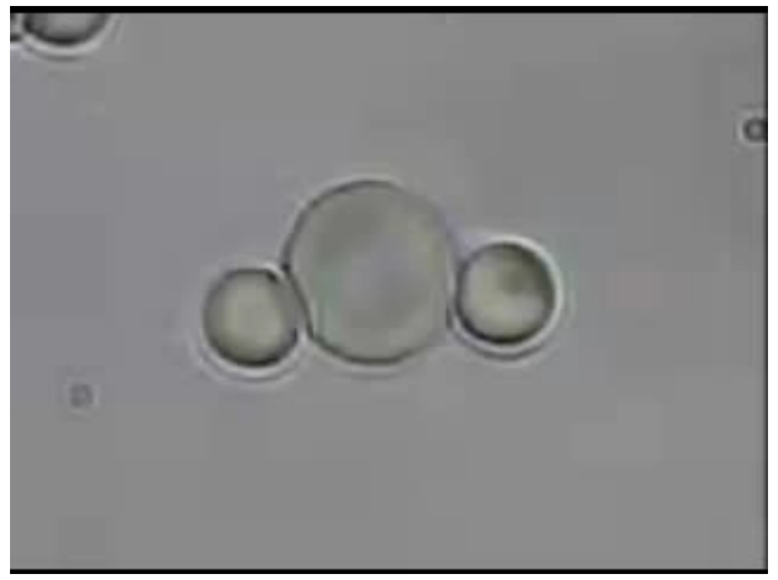

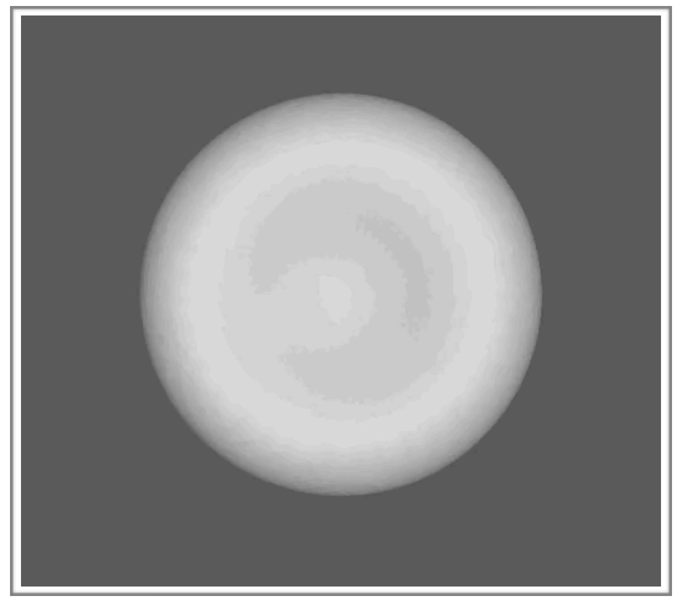

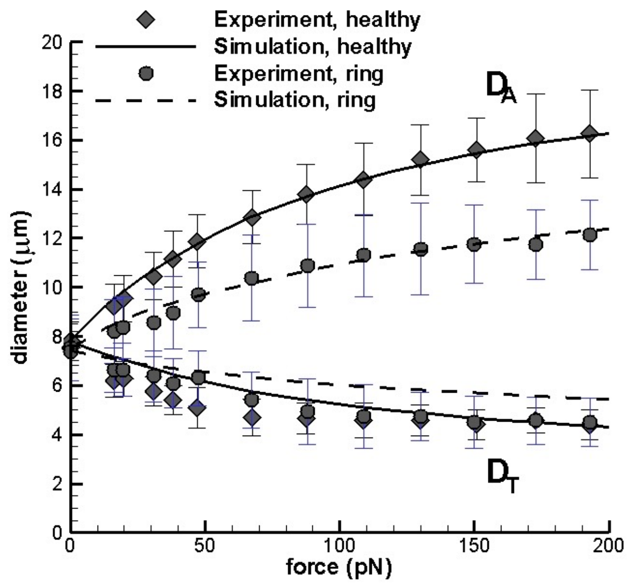

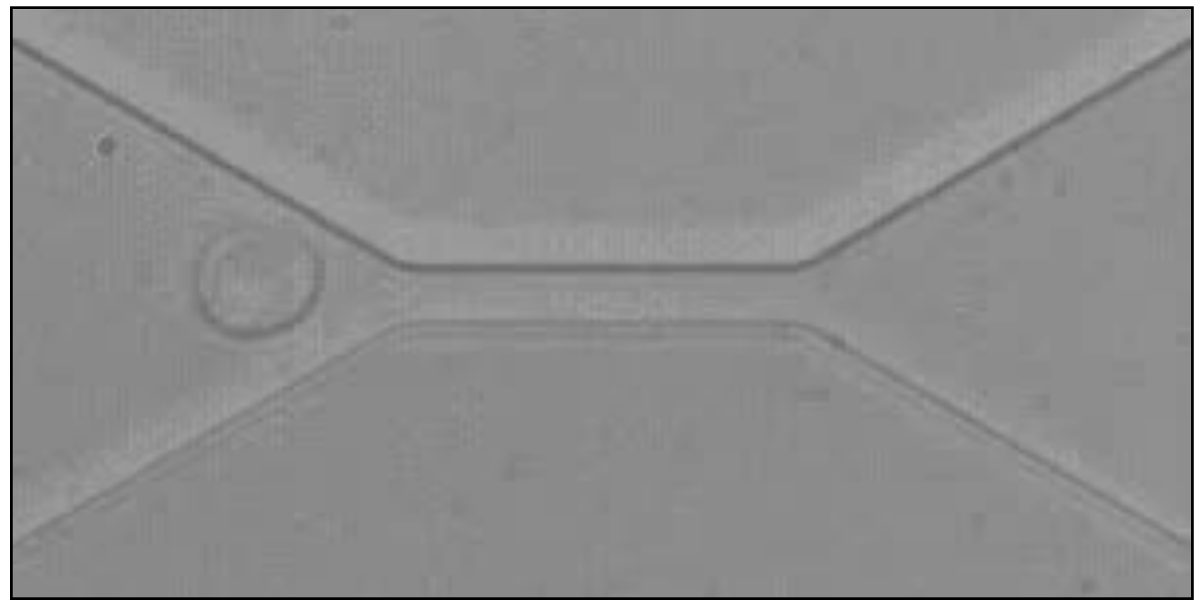

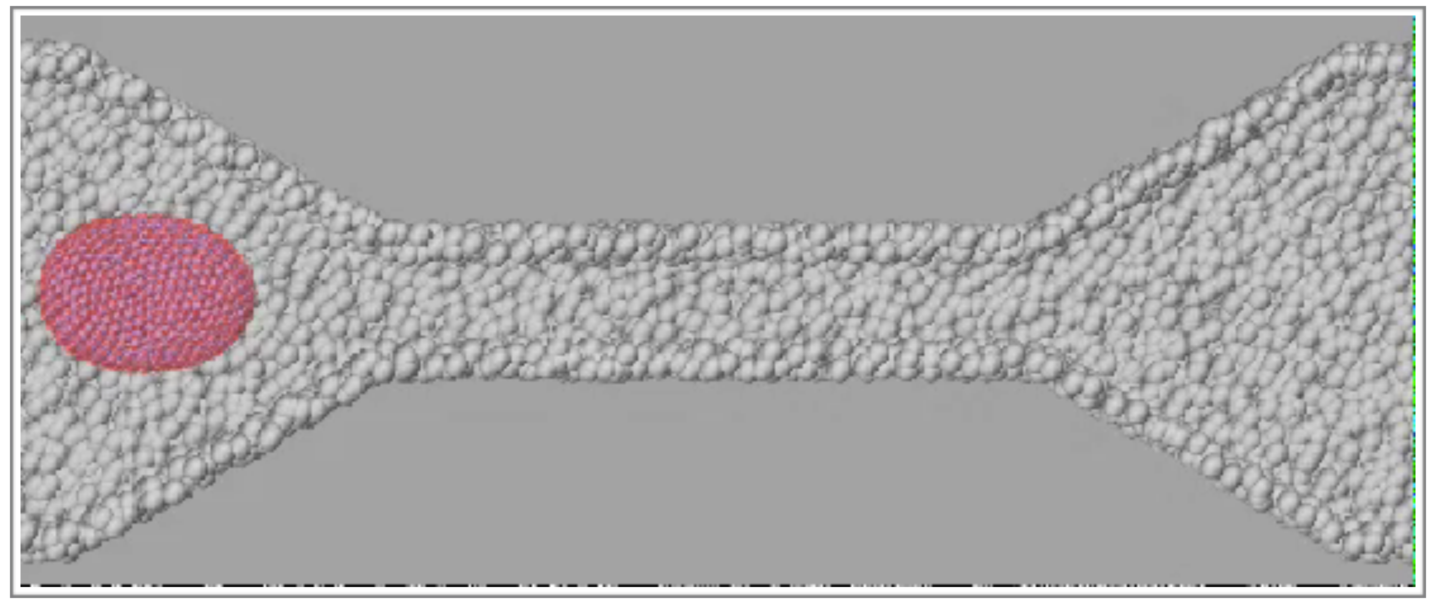

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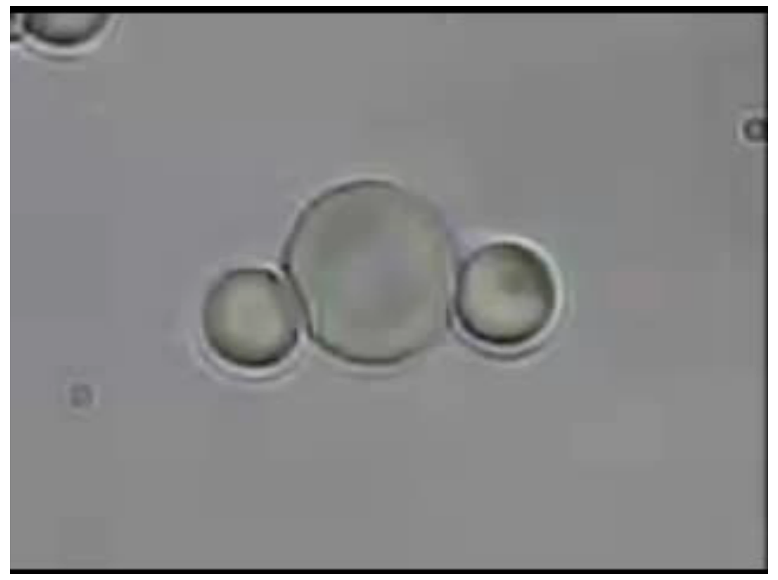

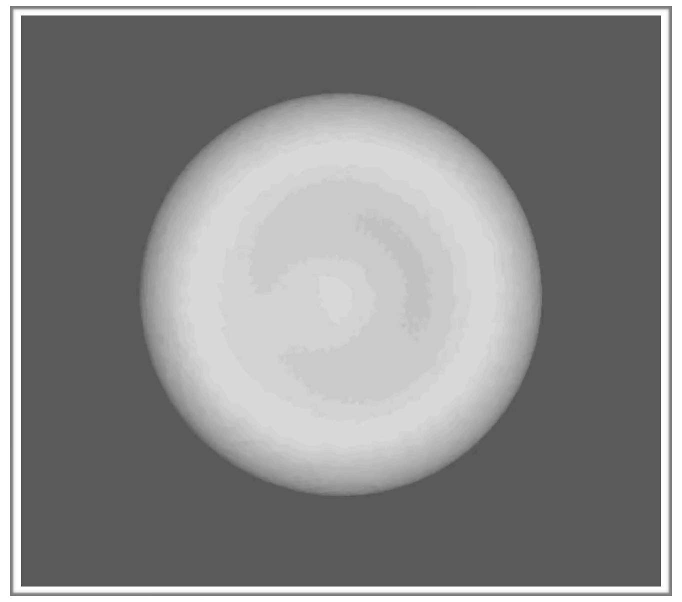

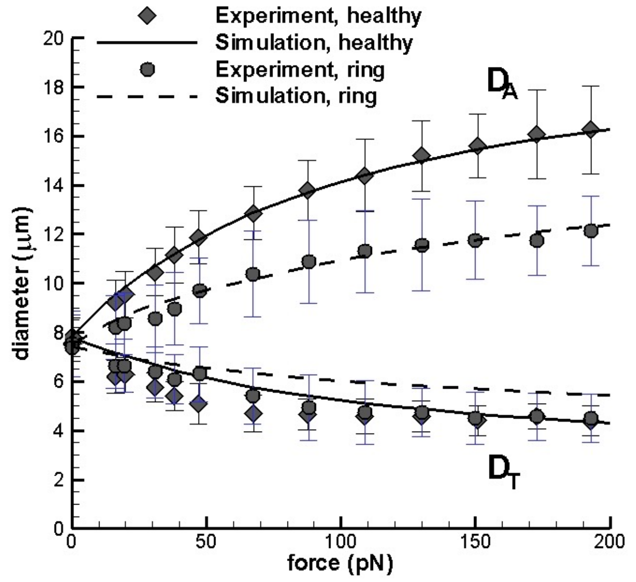

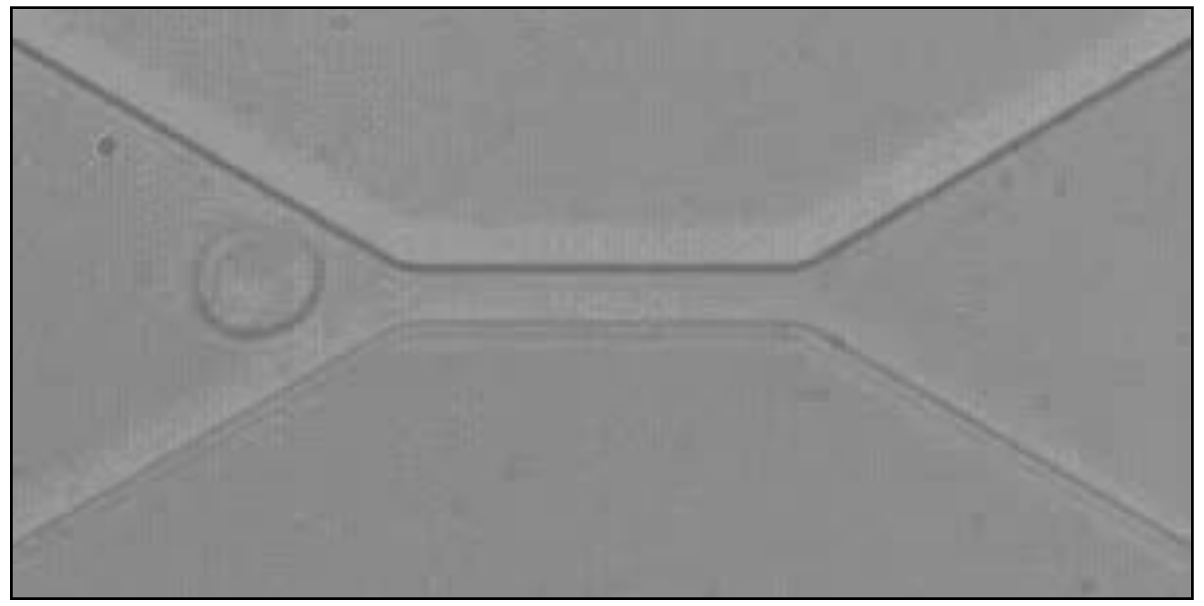

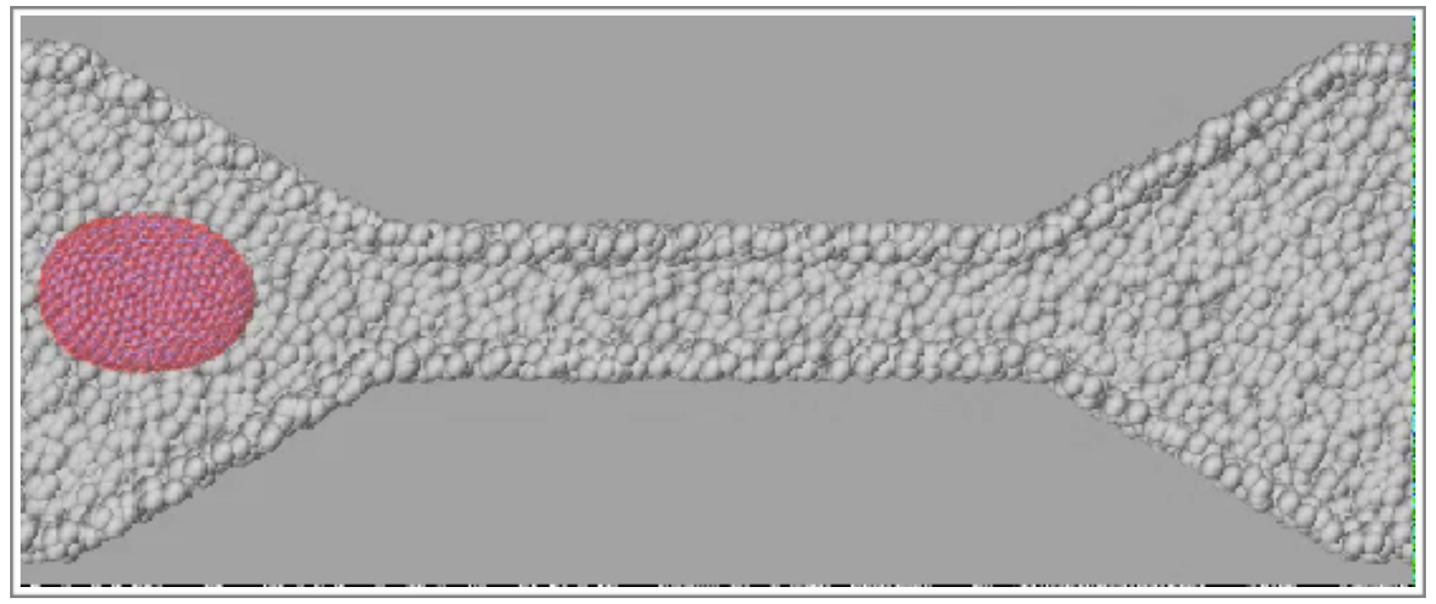

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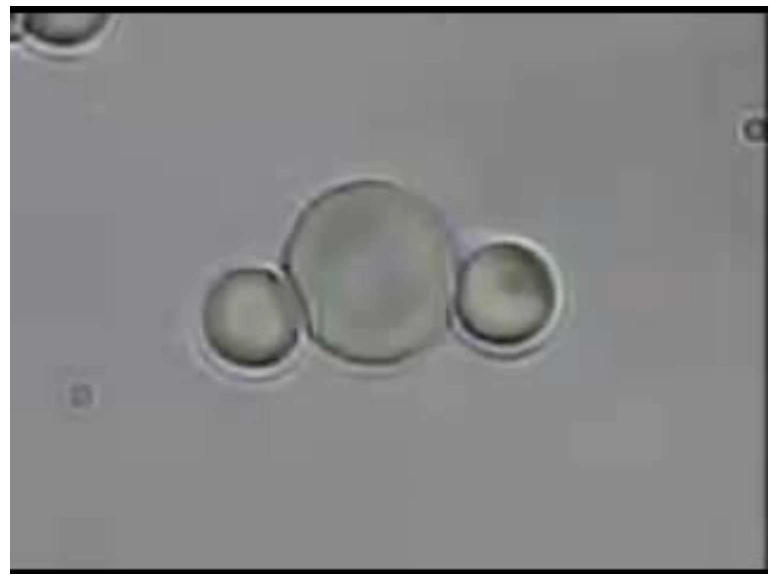

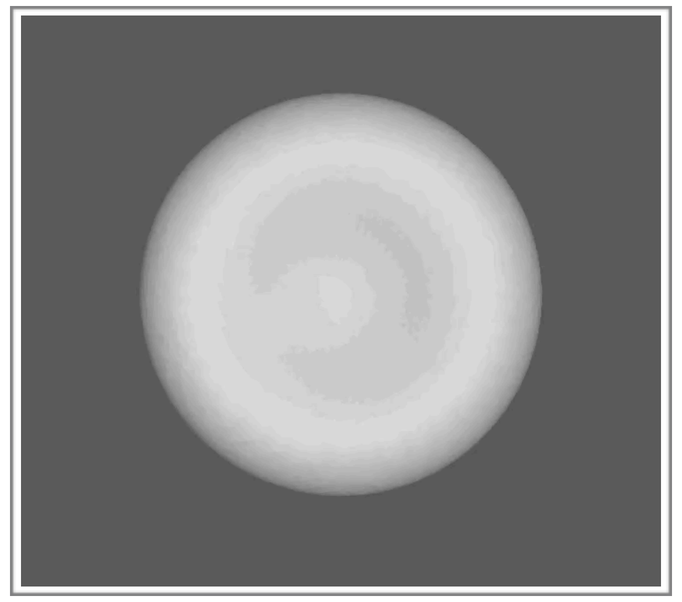

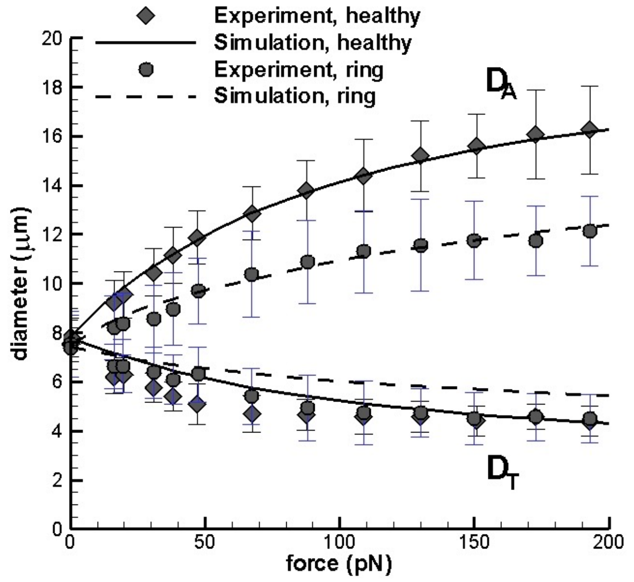

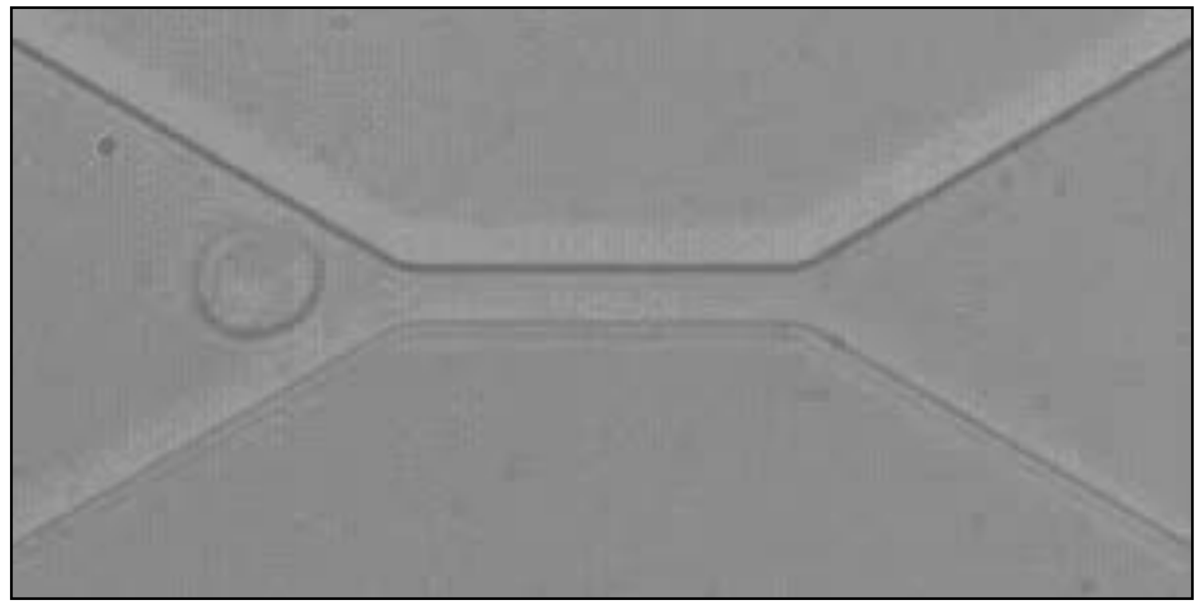

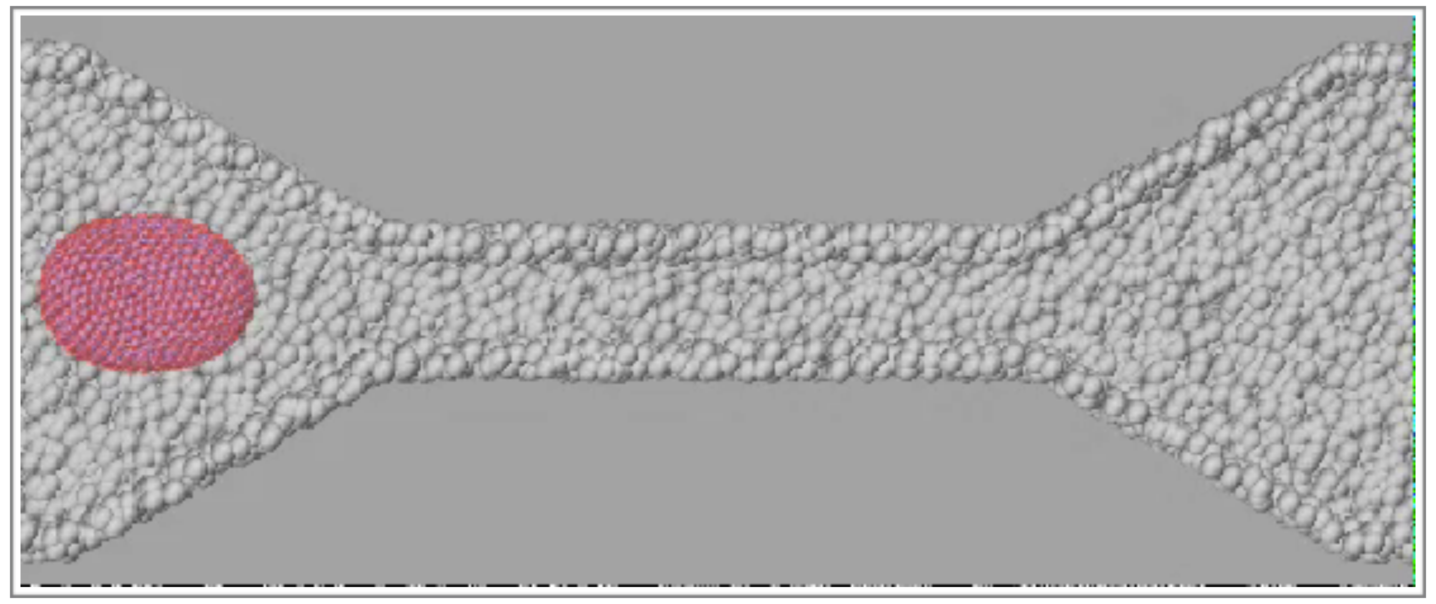

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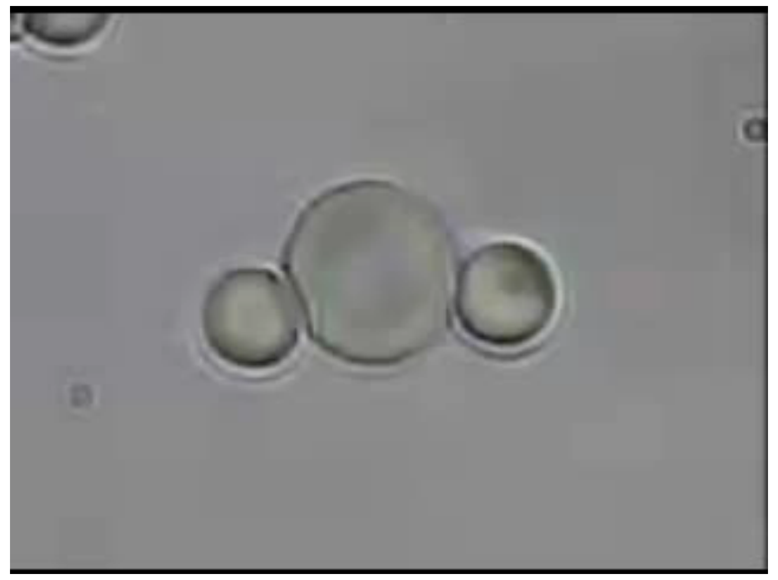

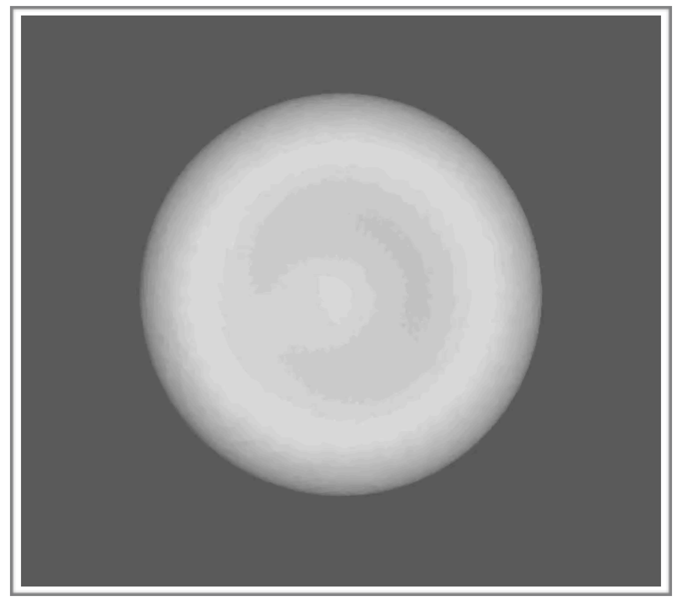

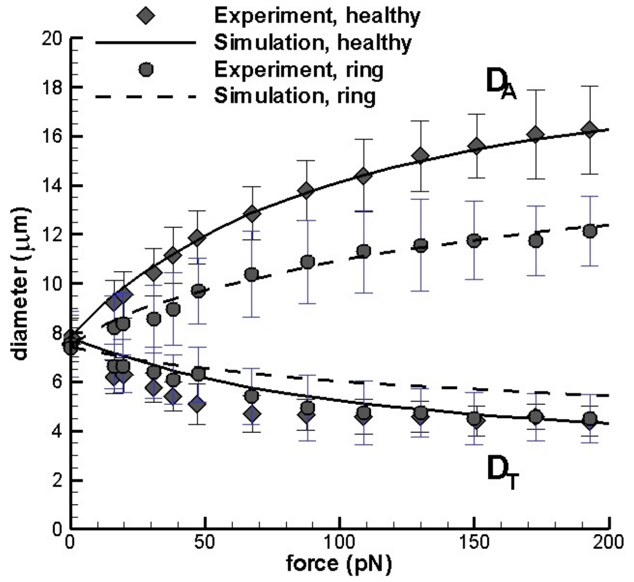

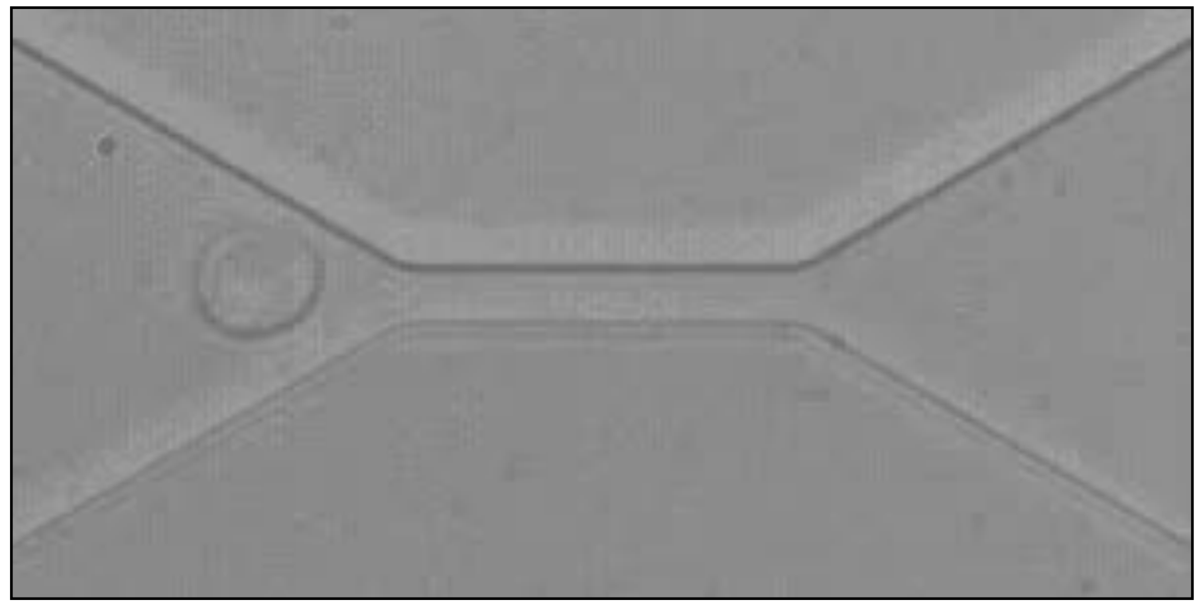

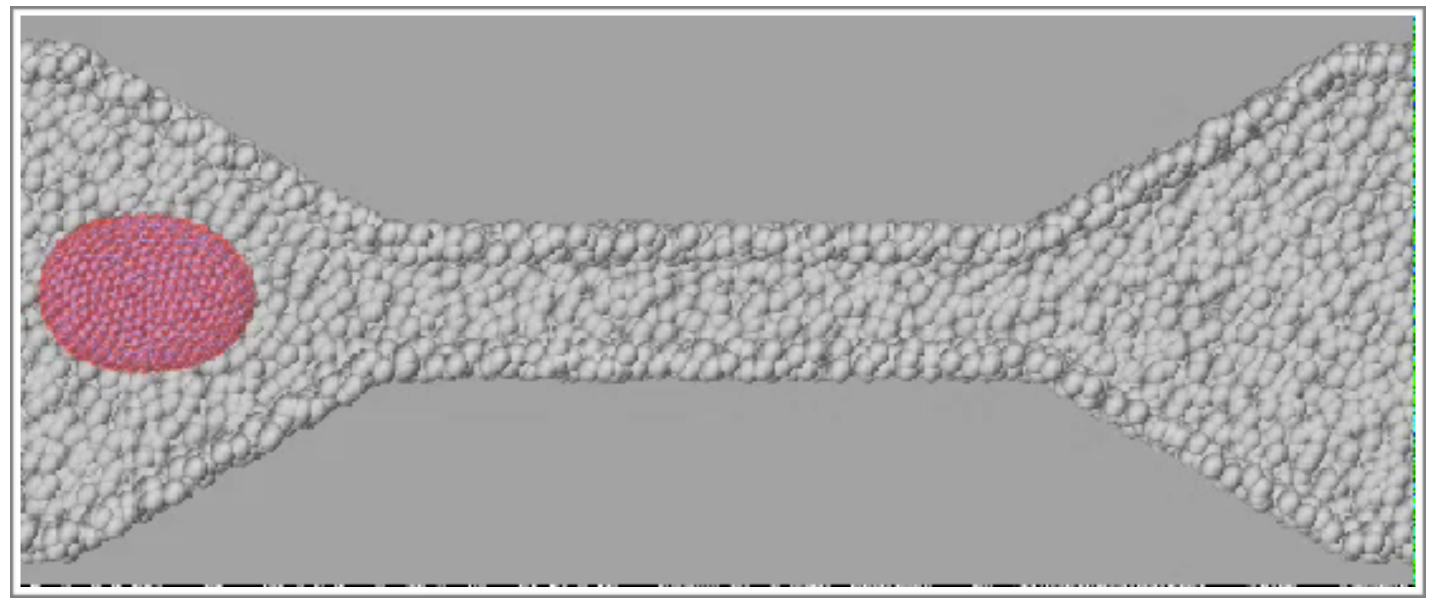

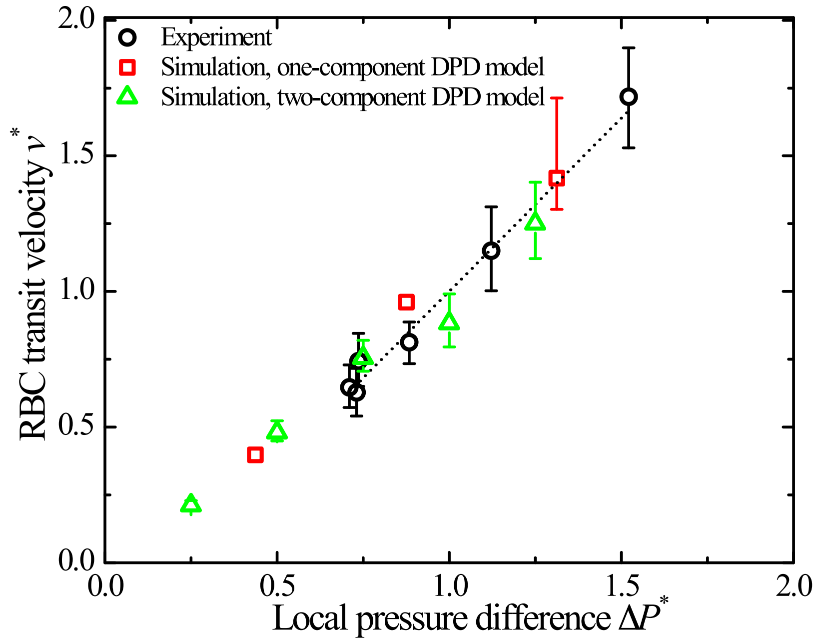

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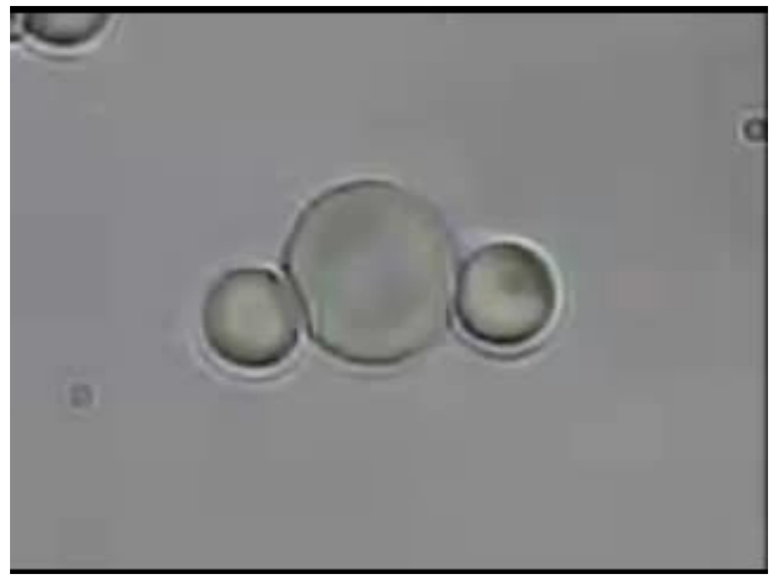

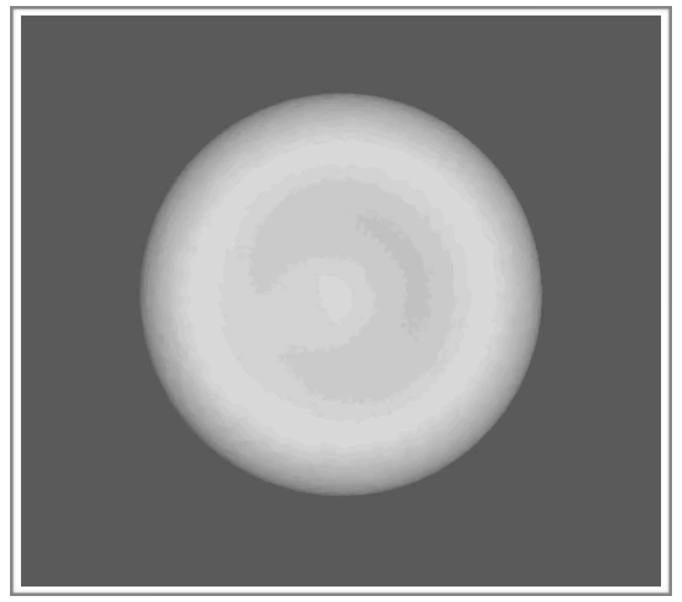

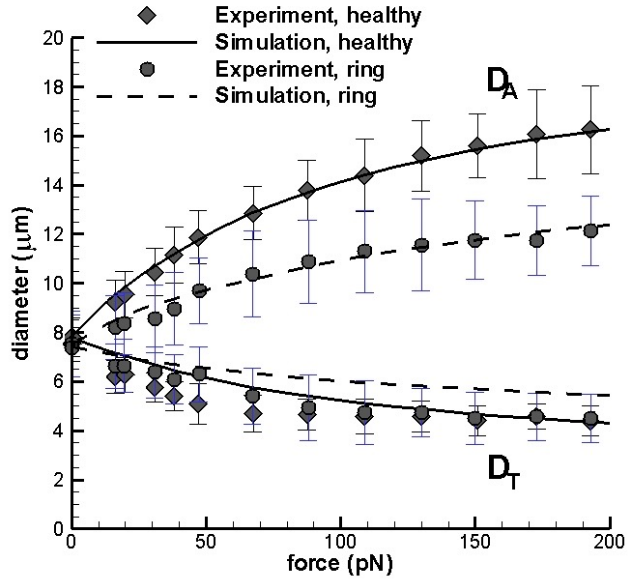

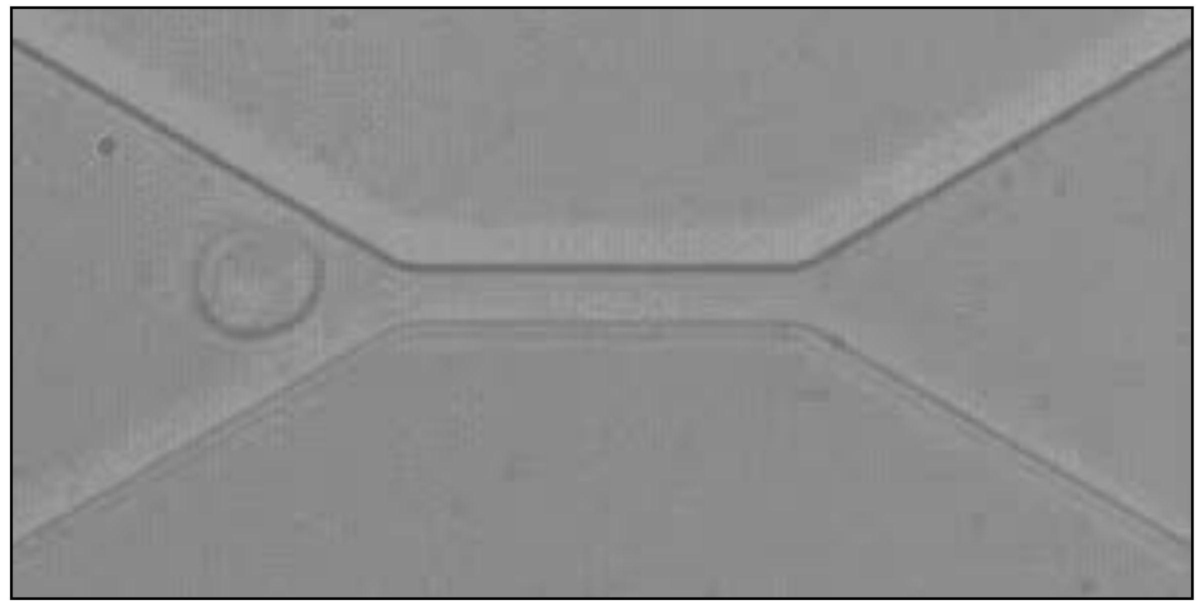

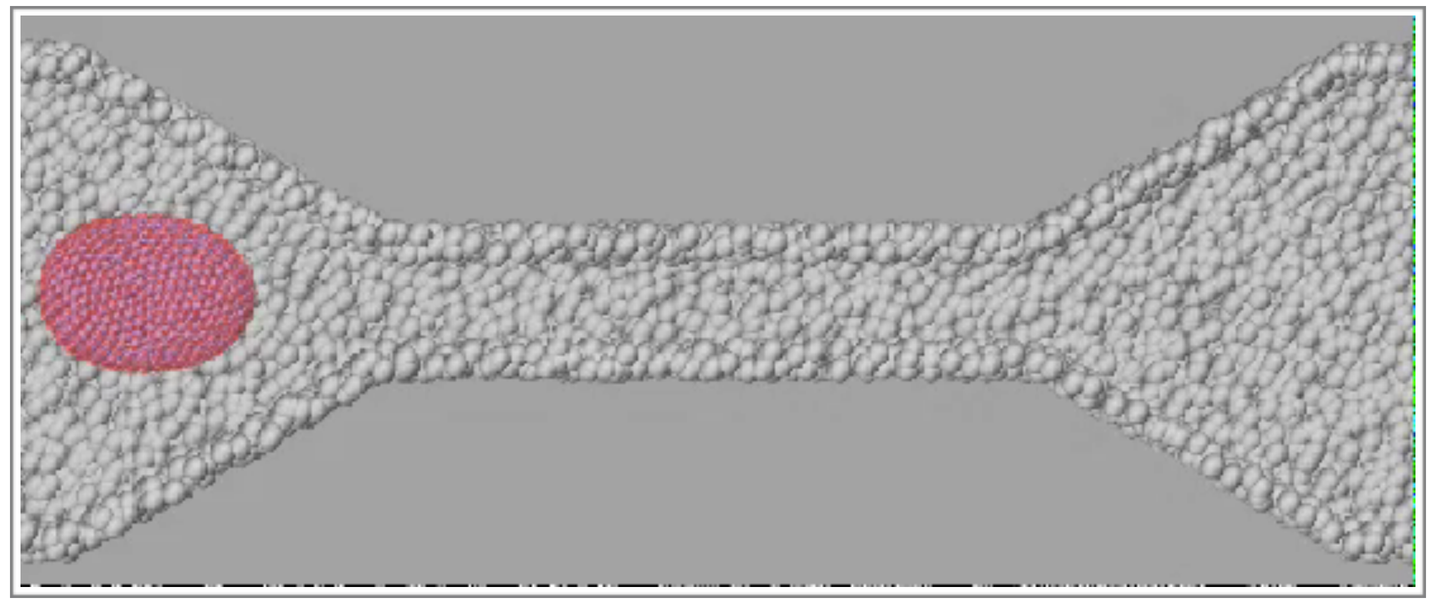

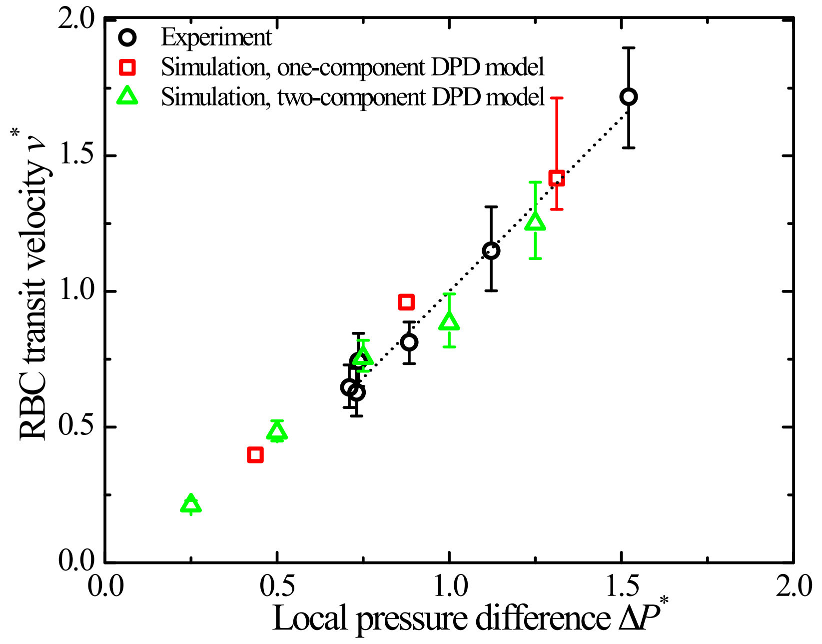

VALIDATION

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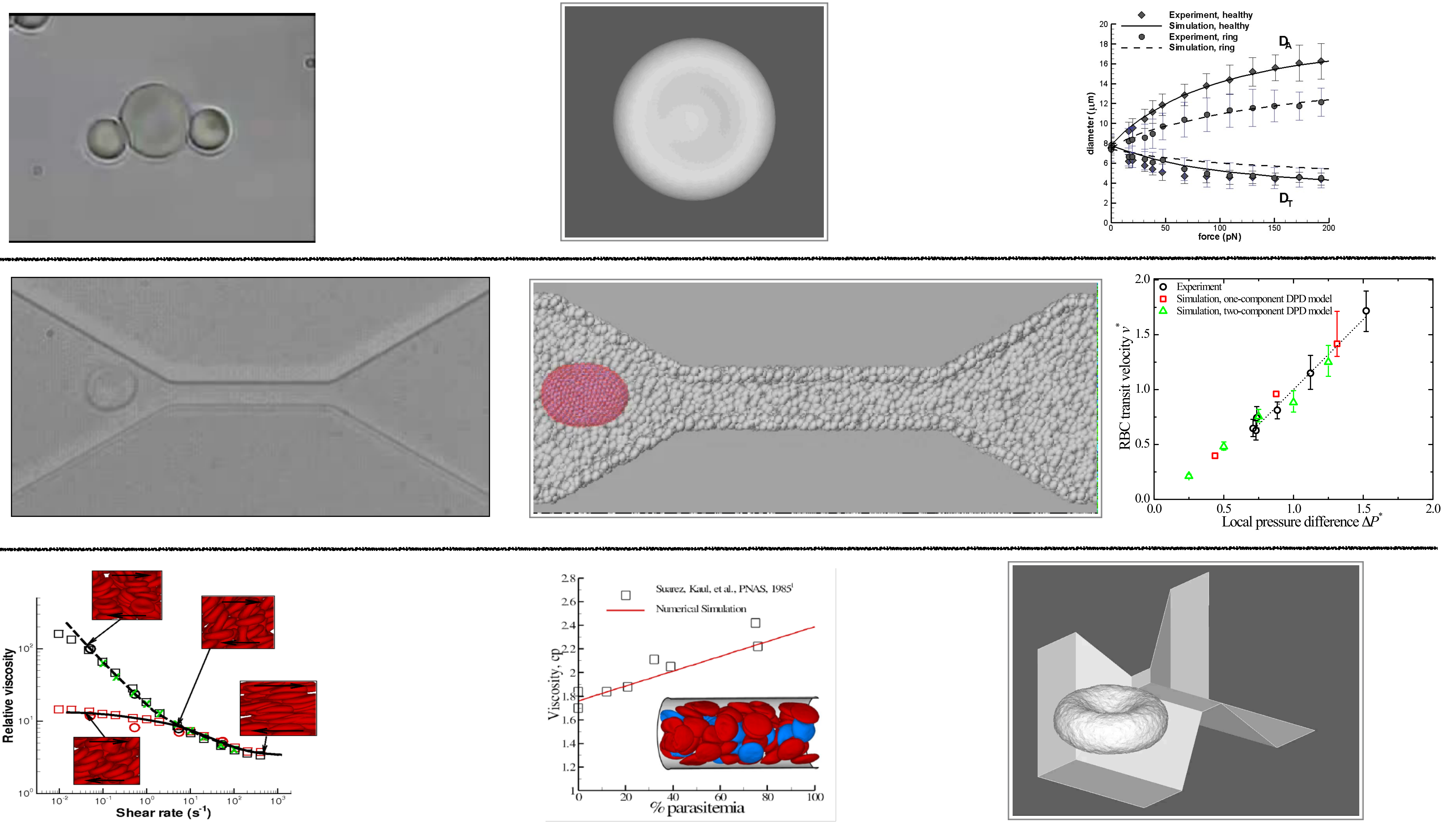

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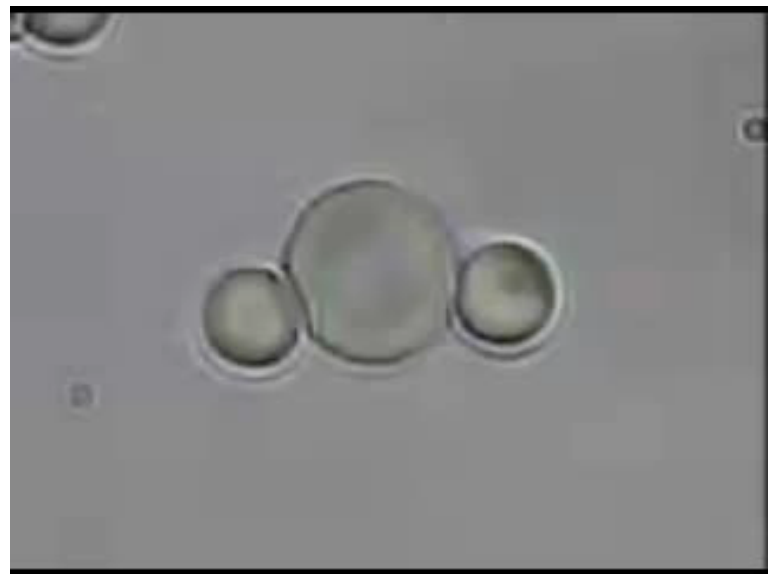
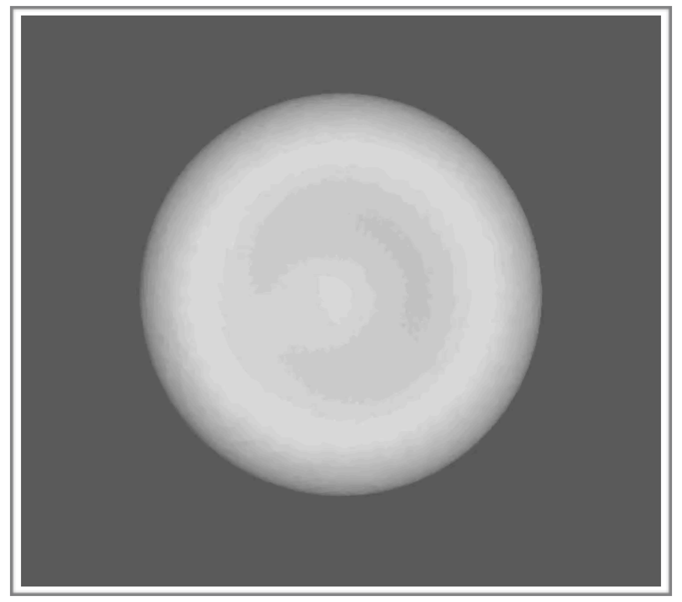
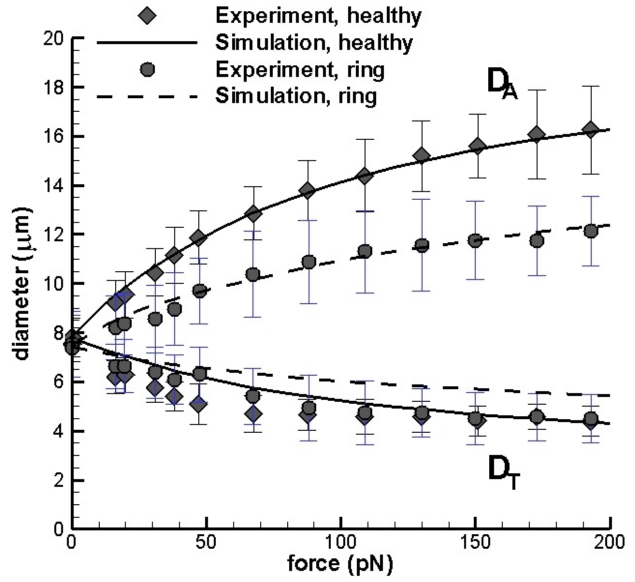
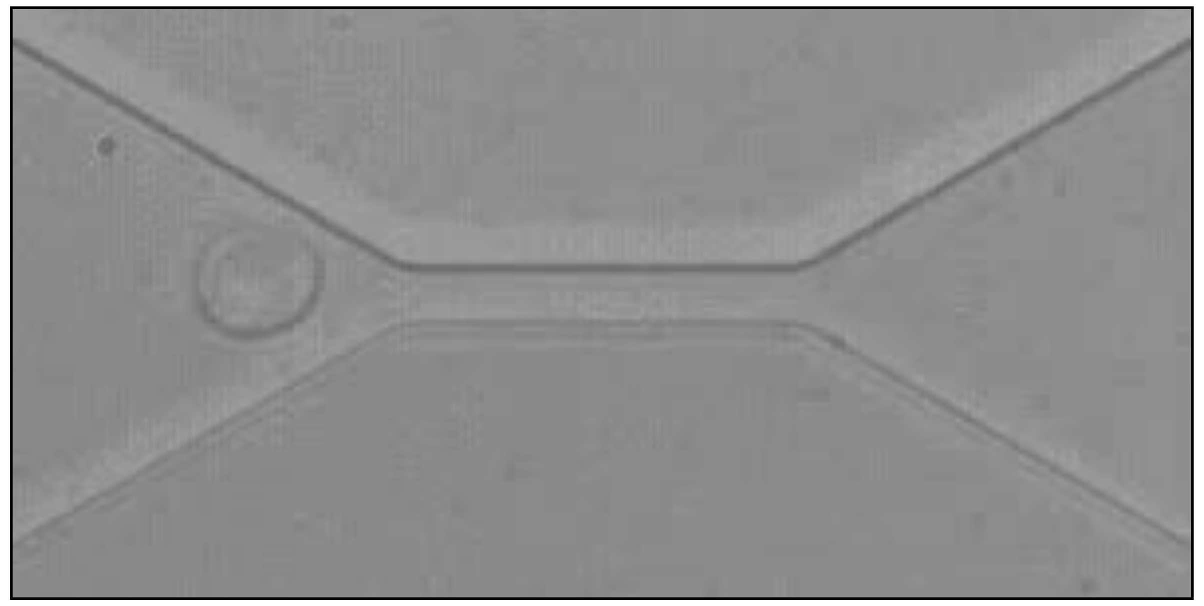
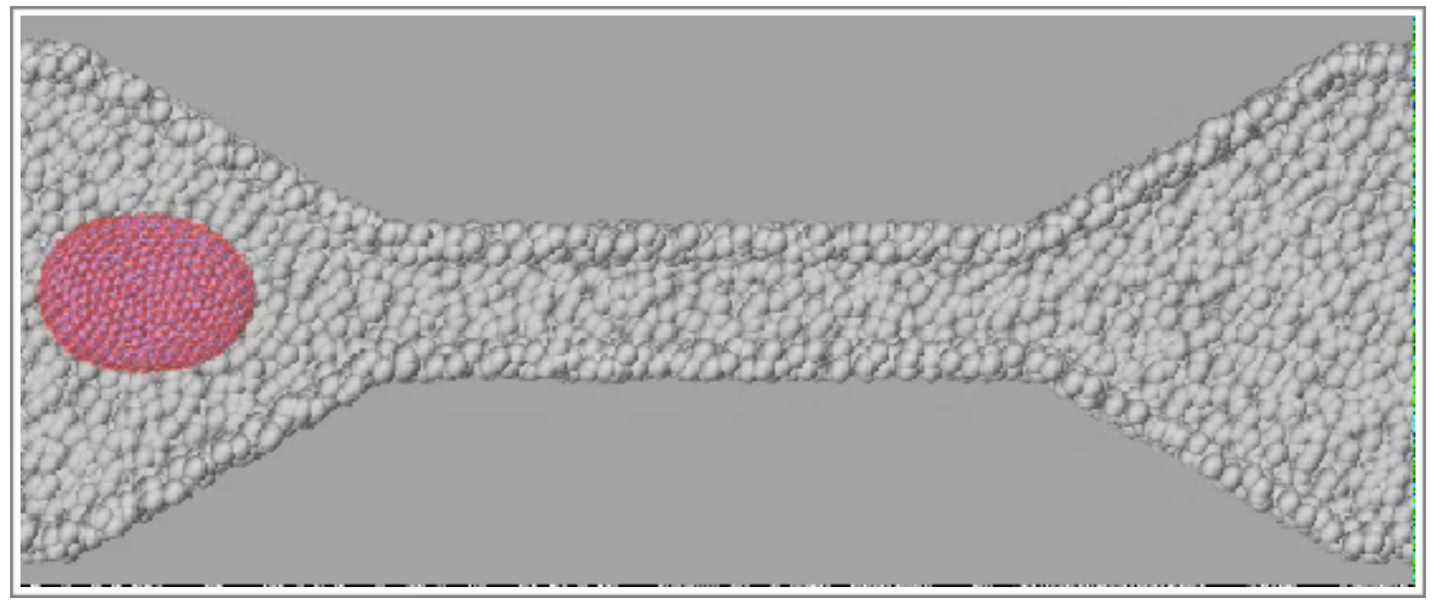
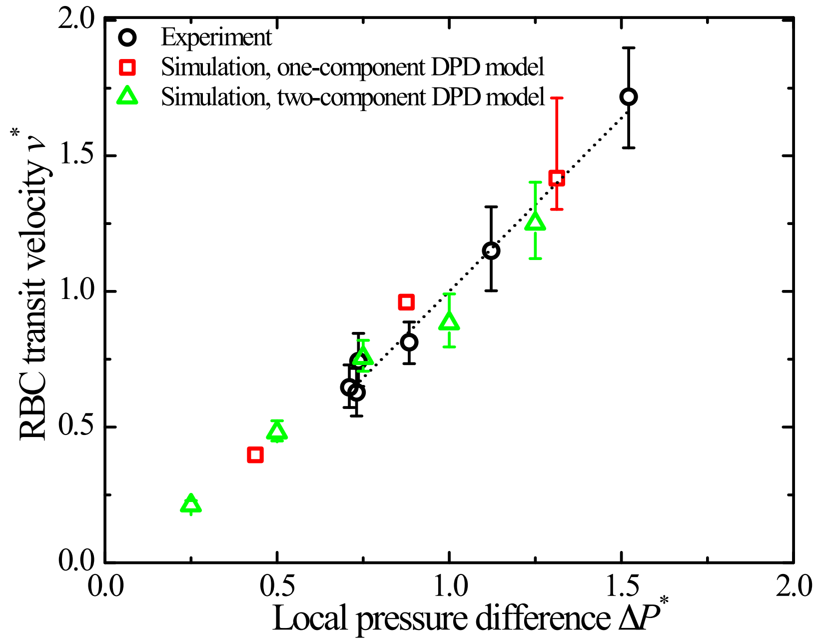


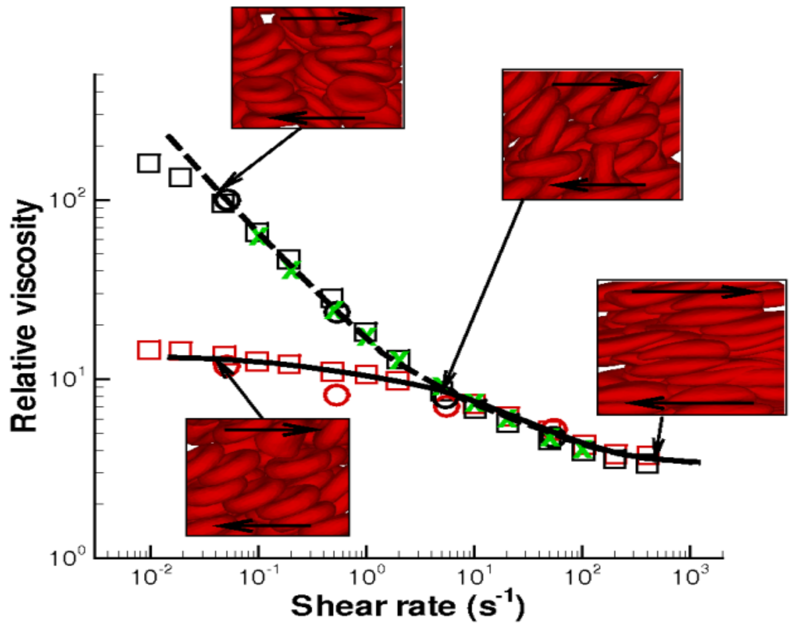


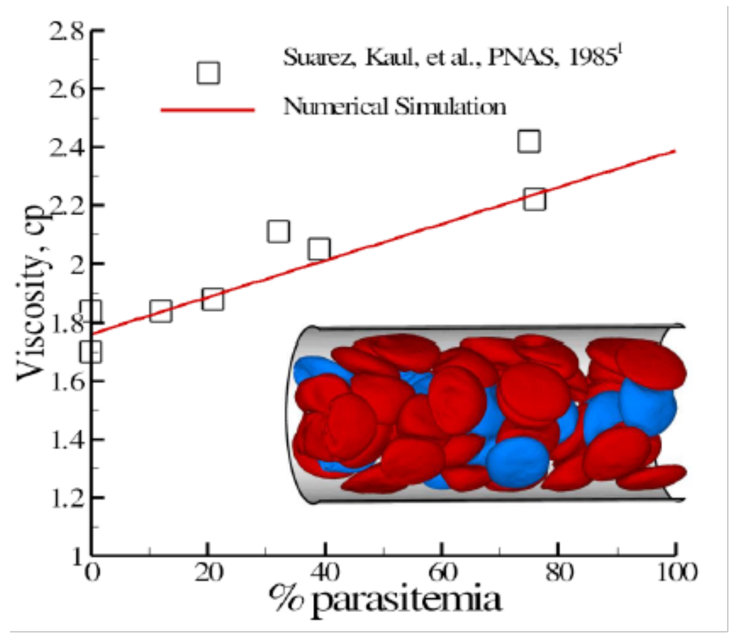


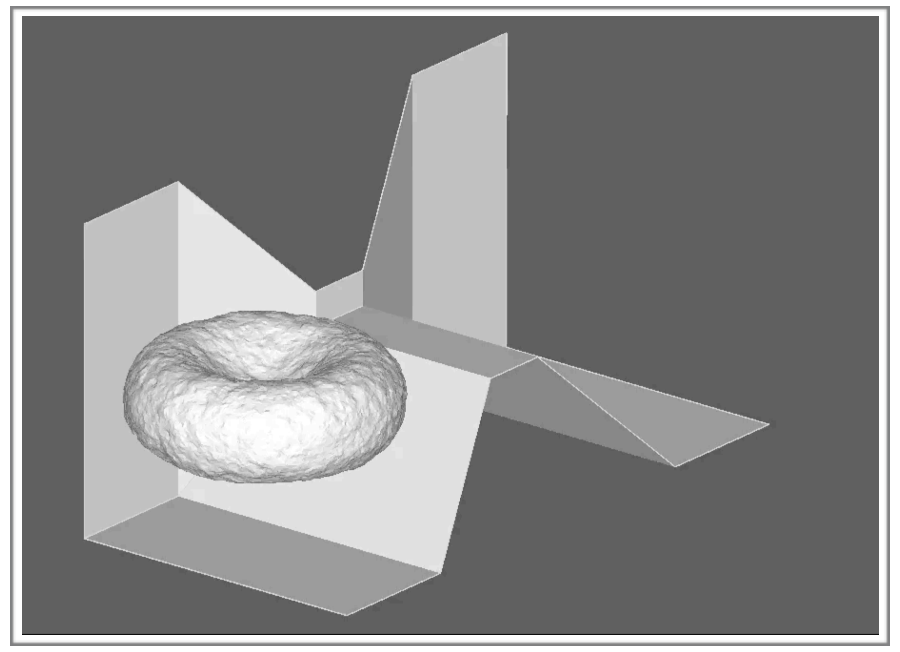


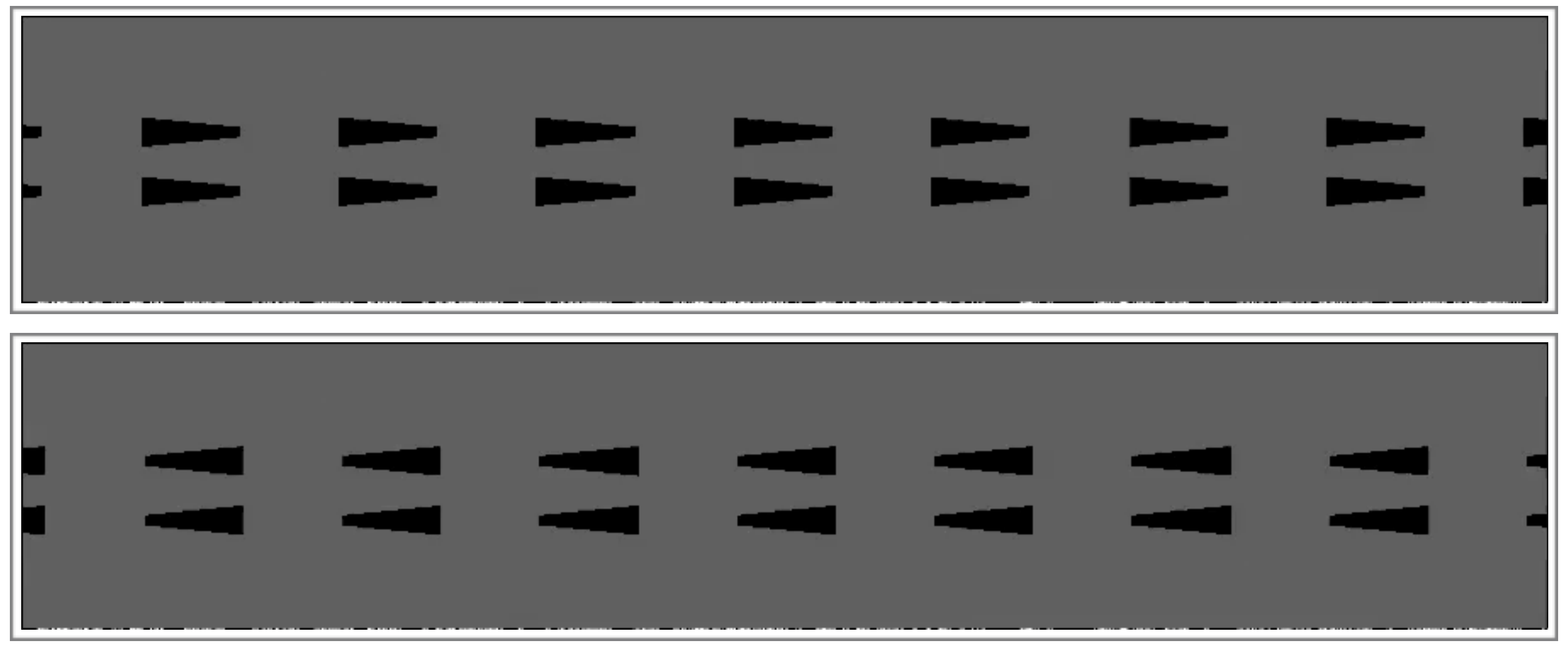


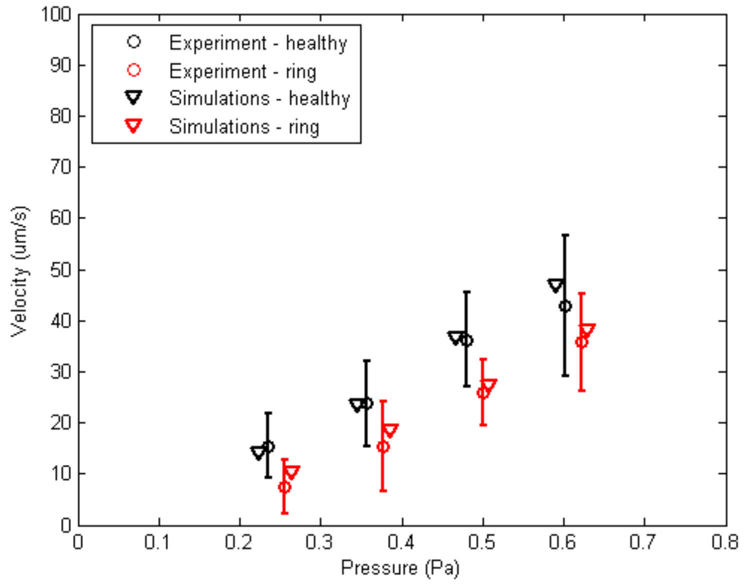


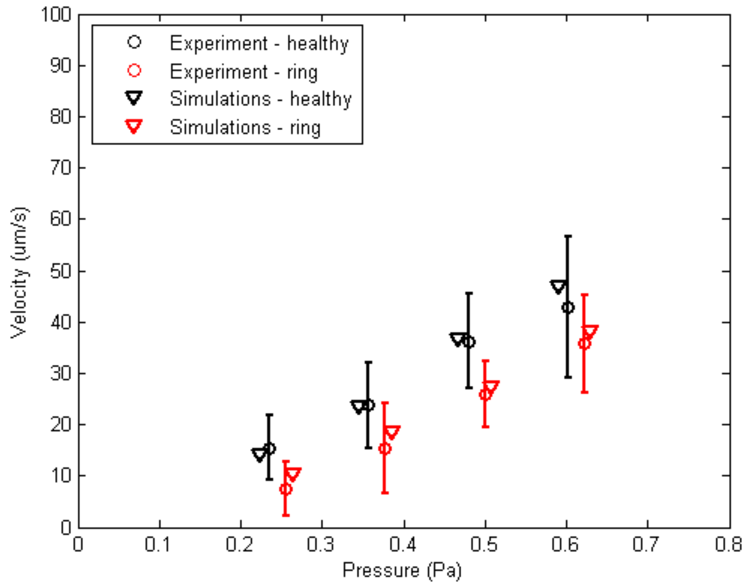






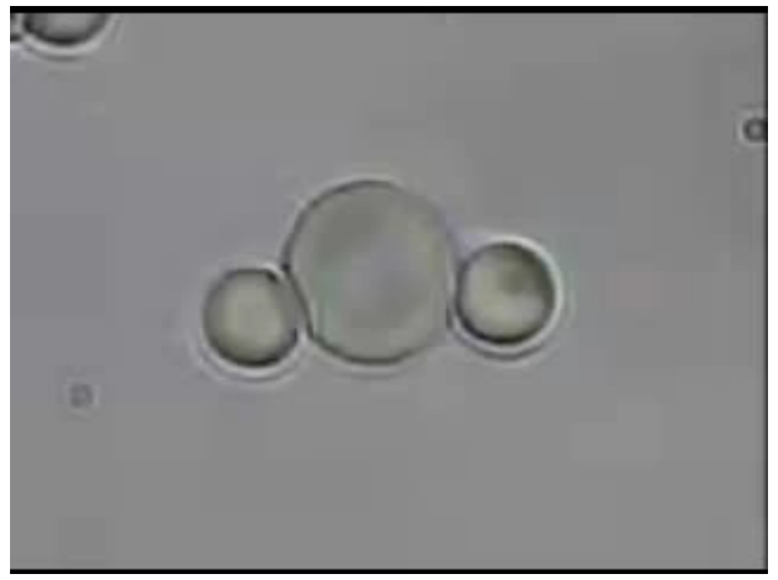


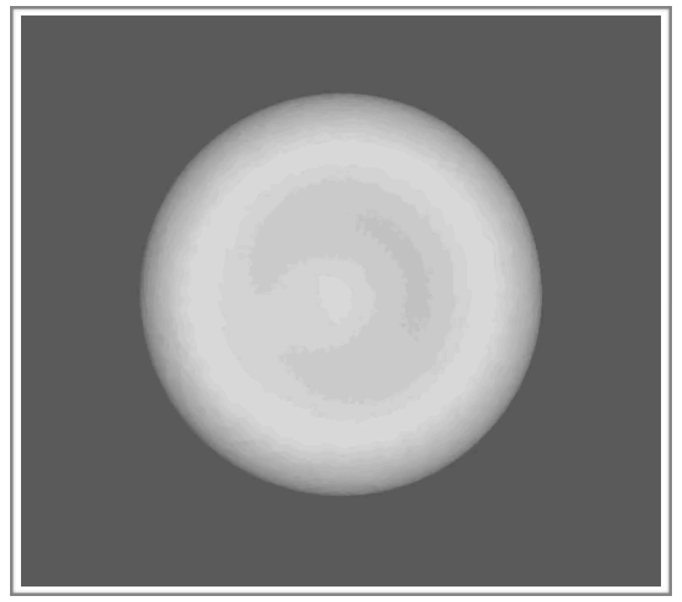


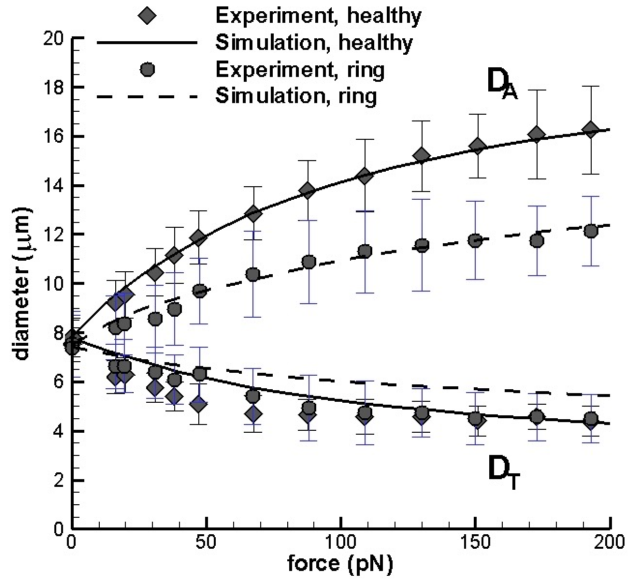


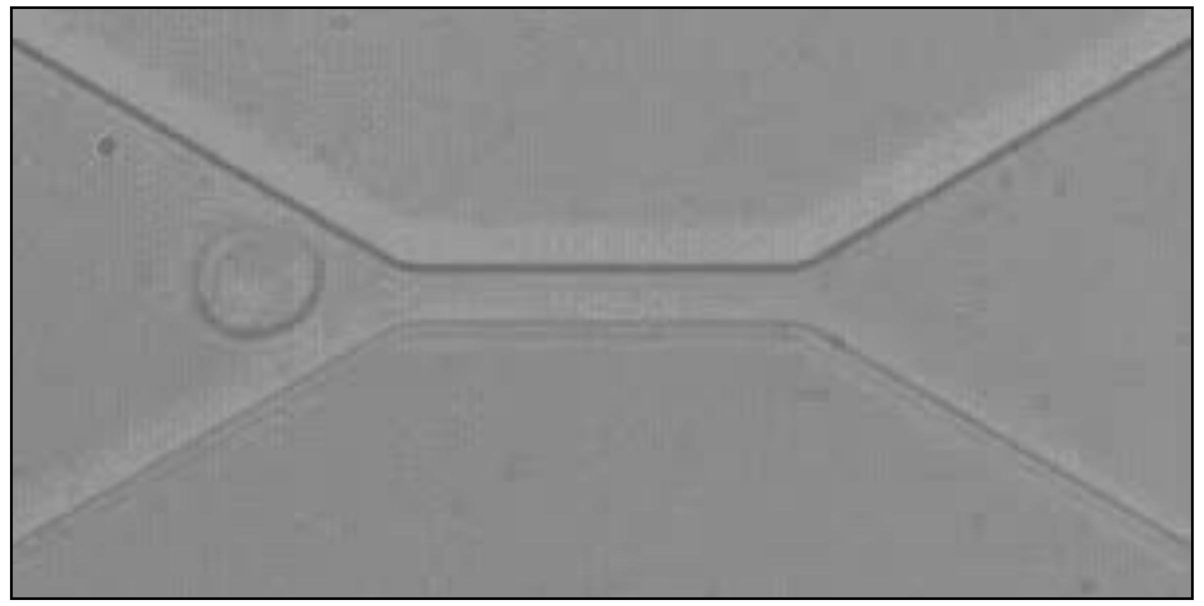
(Karniadakis Group)

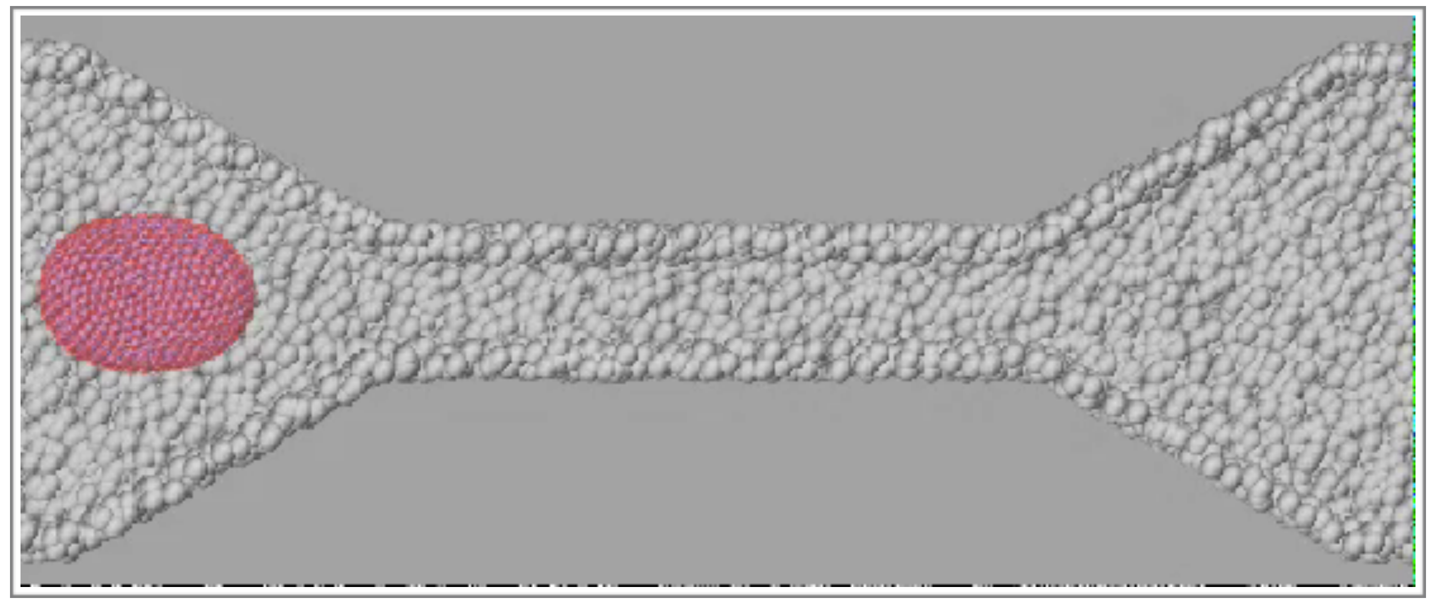
VALIDATION

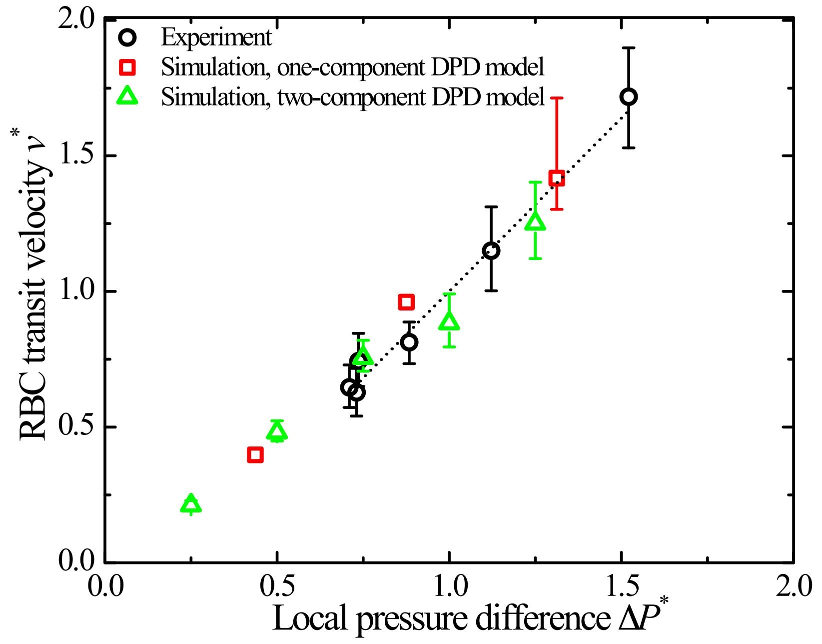


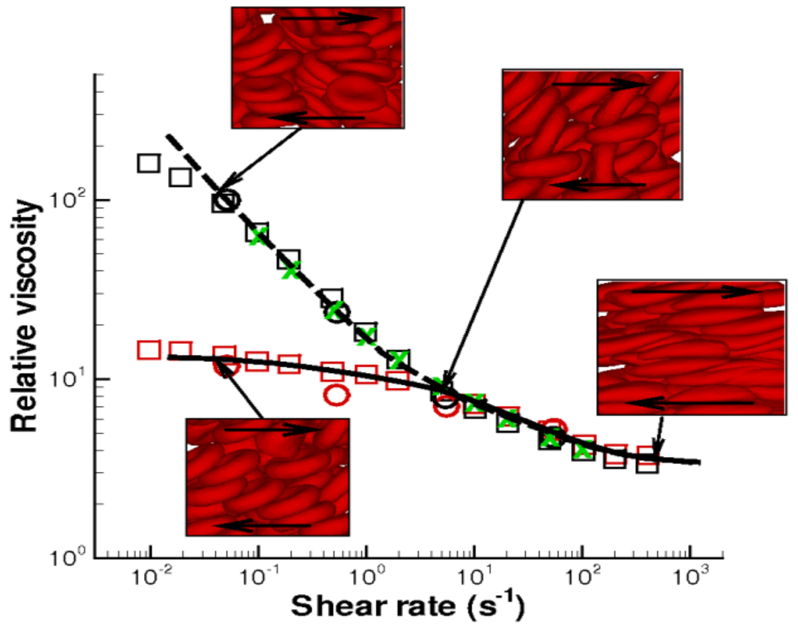


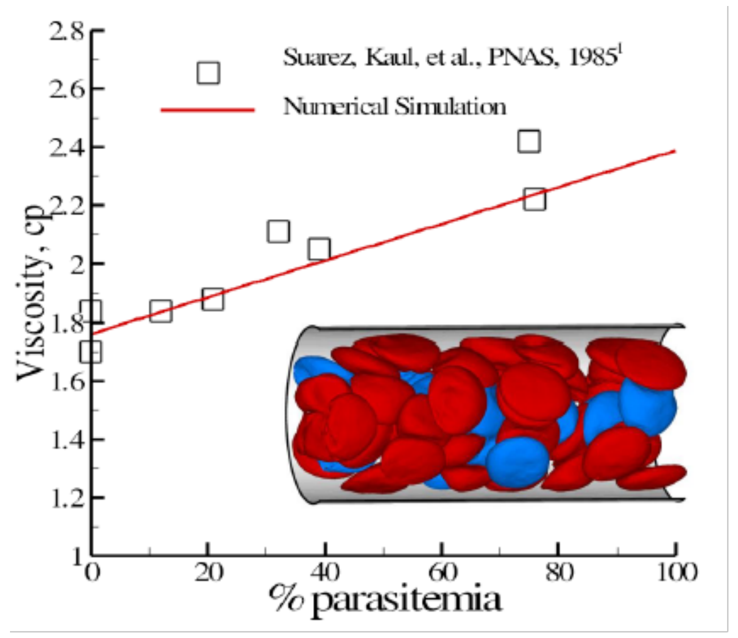


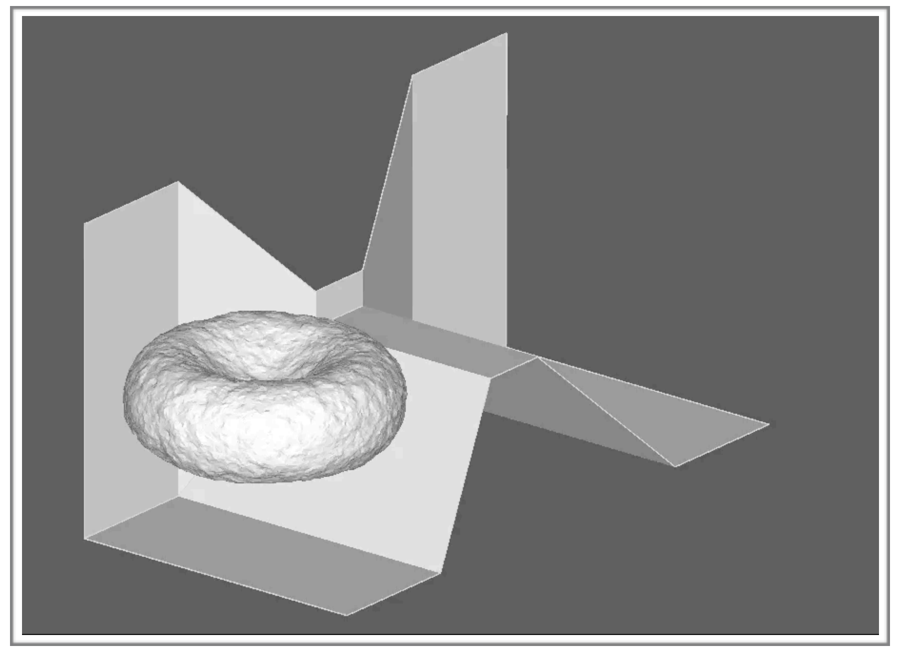


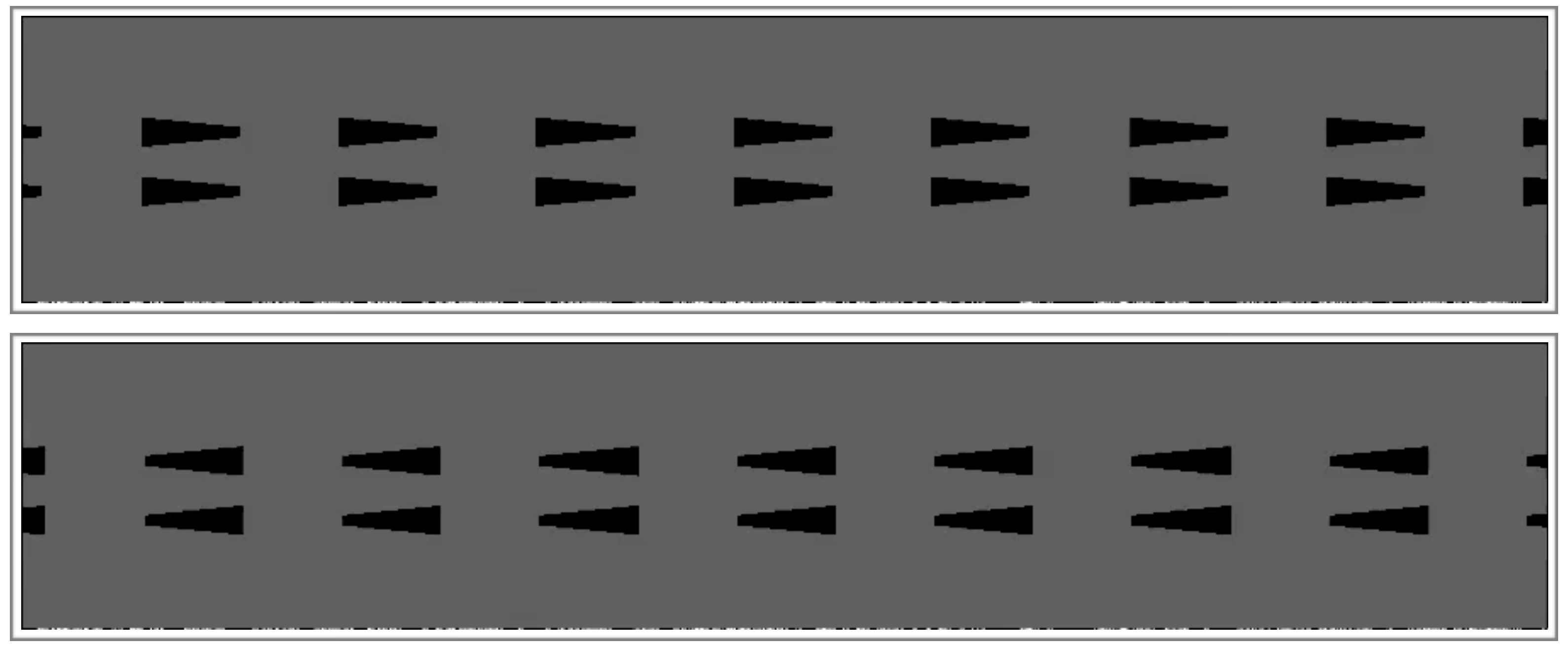


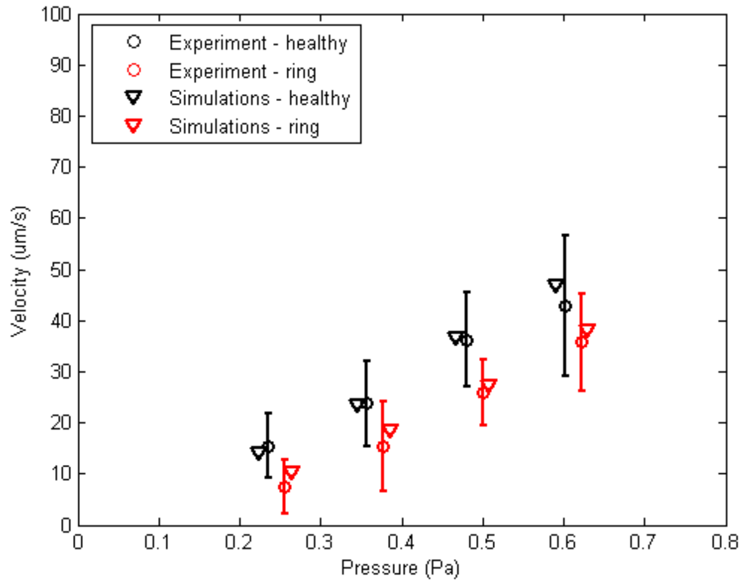


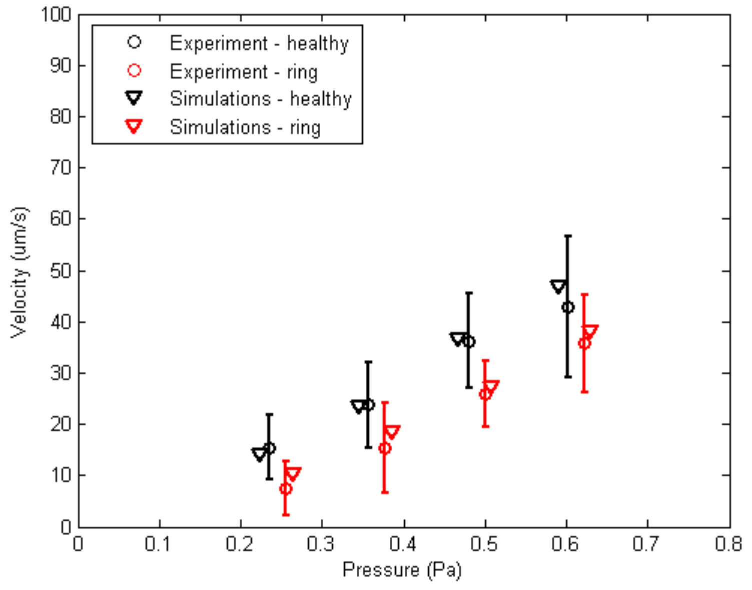






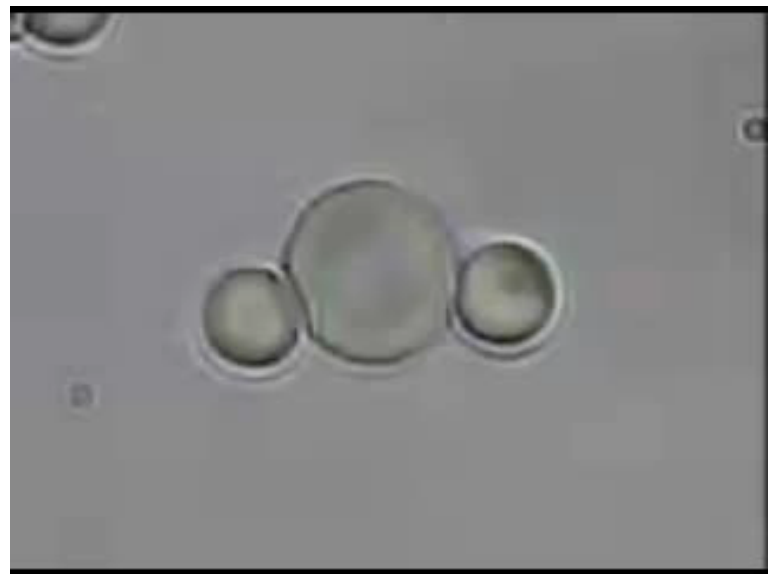


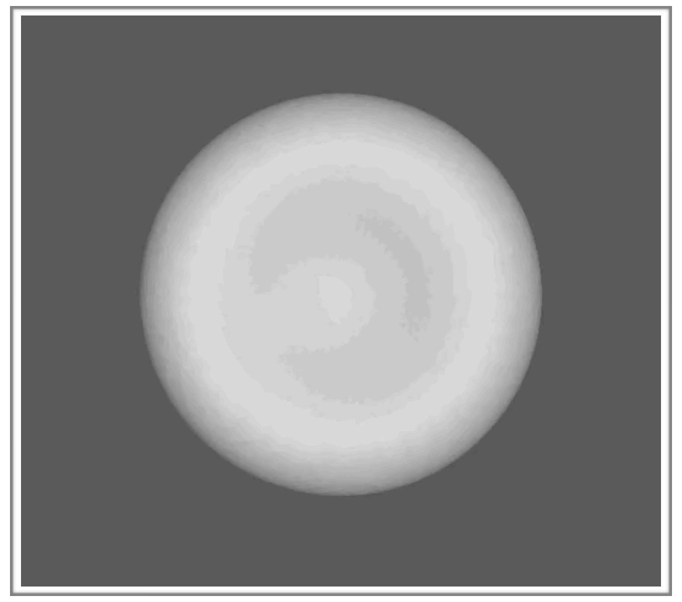


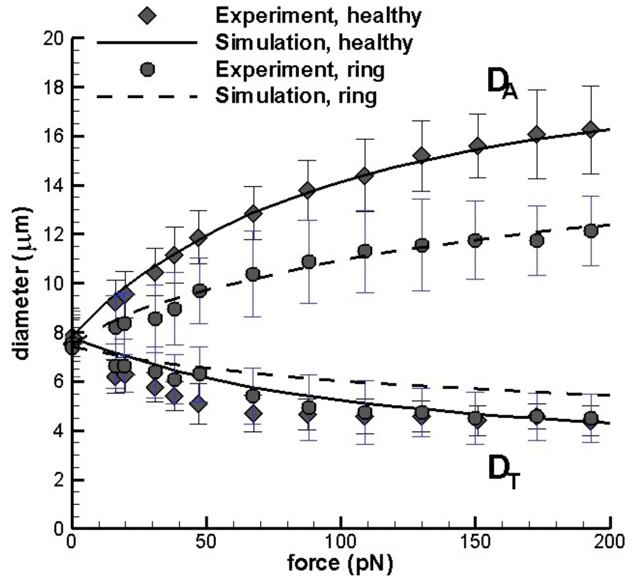


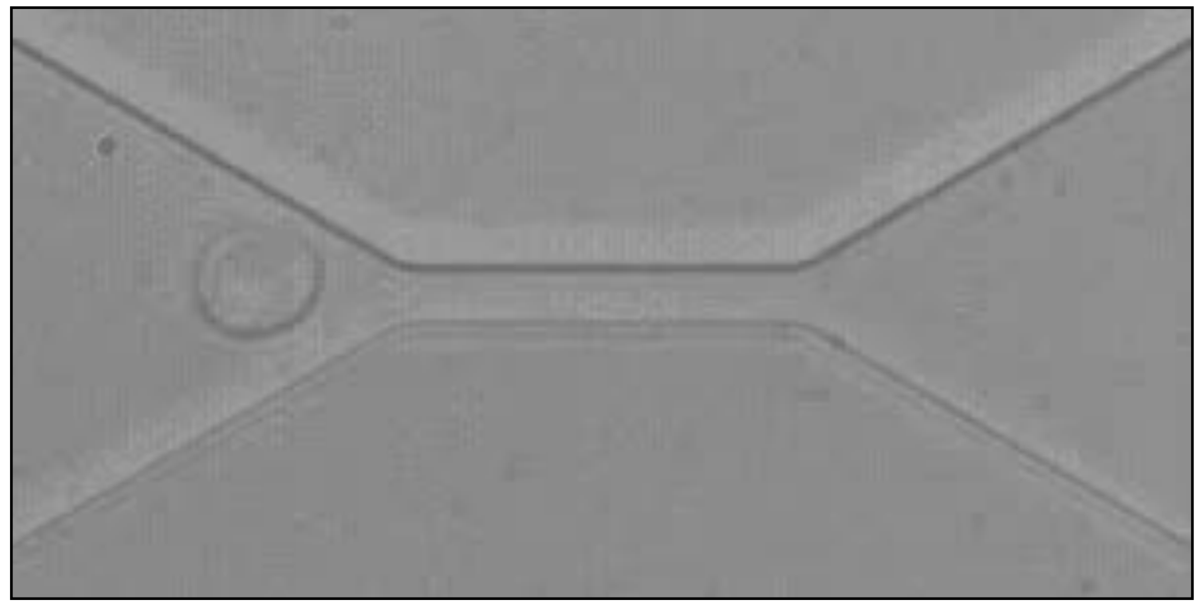
(Karniadakis Group)

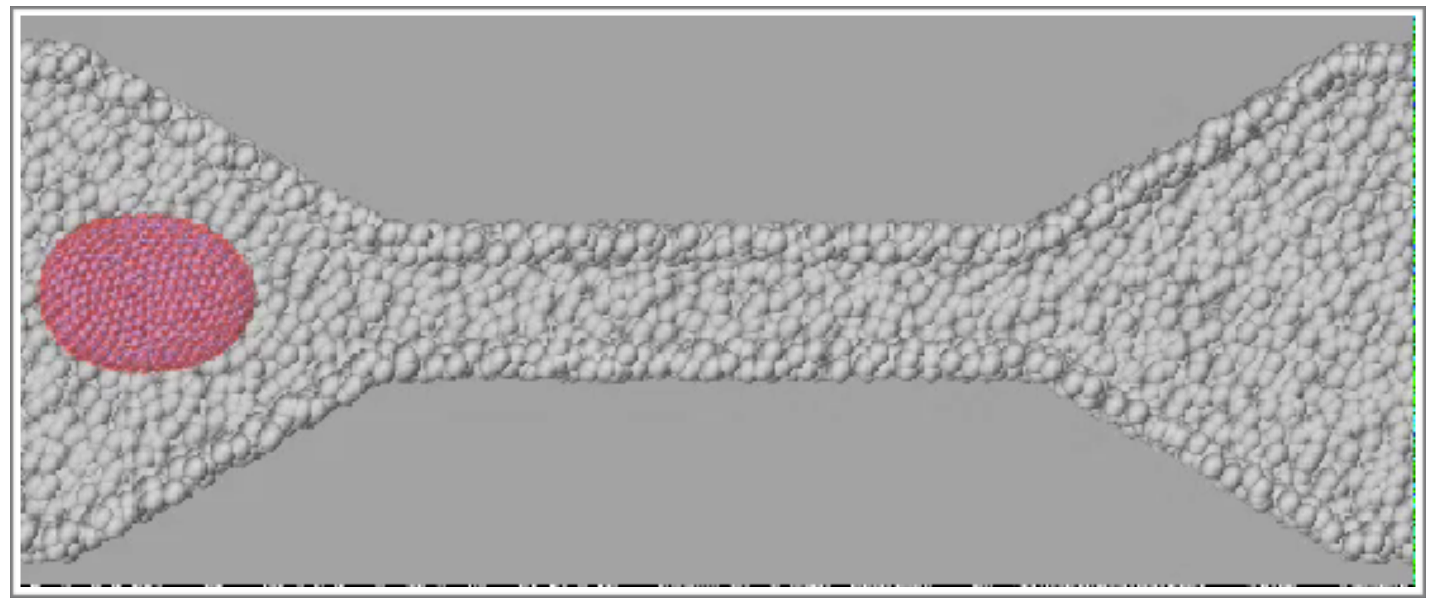
VALIDATION

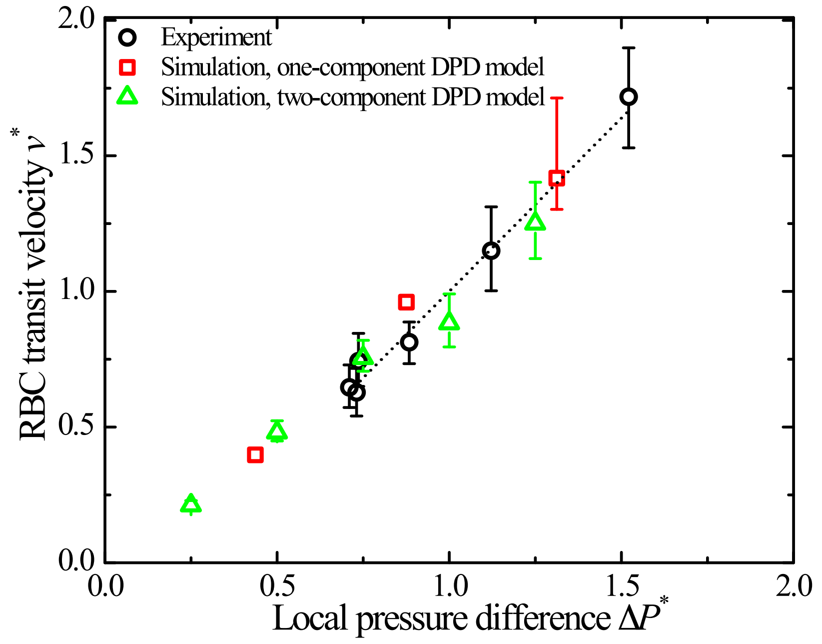


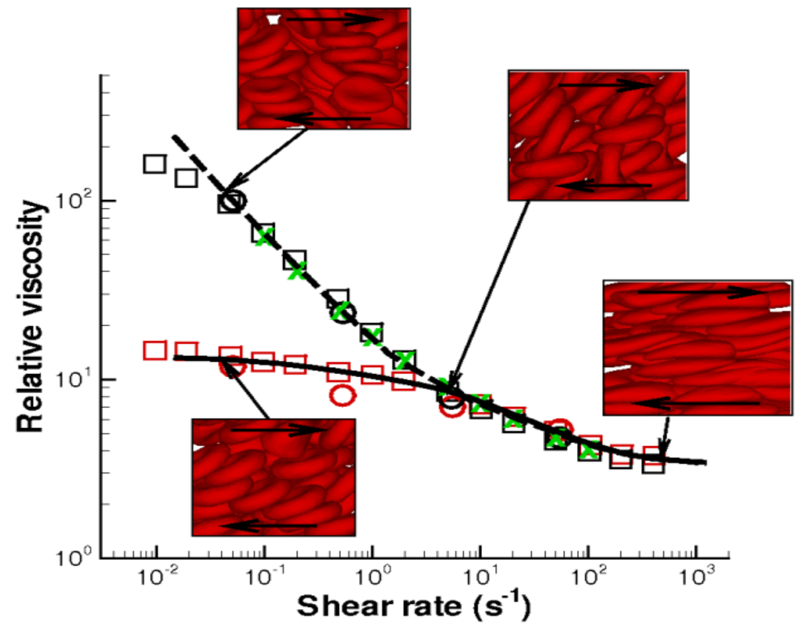


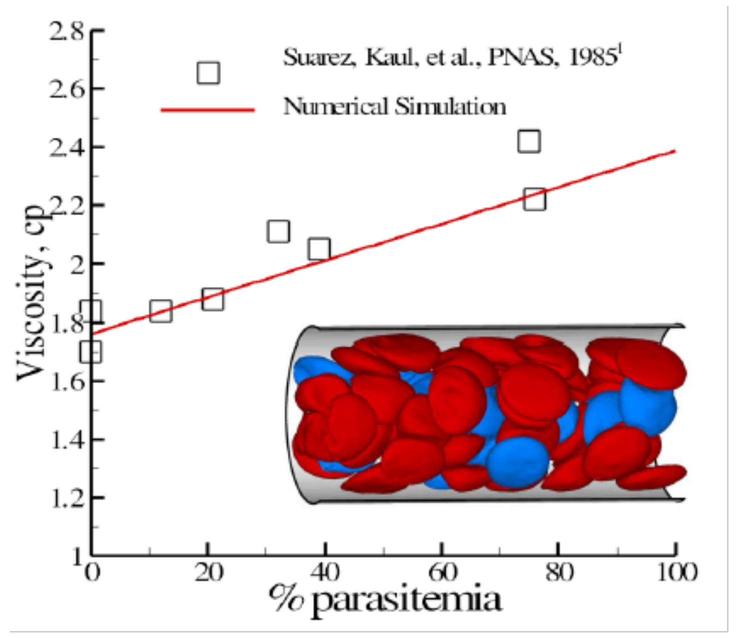


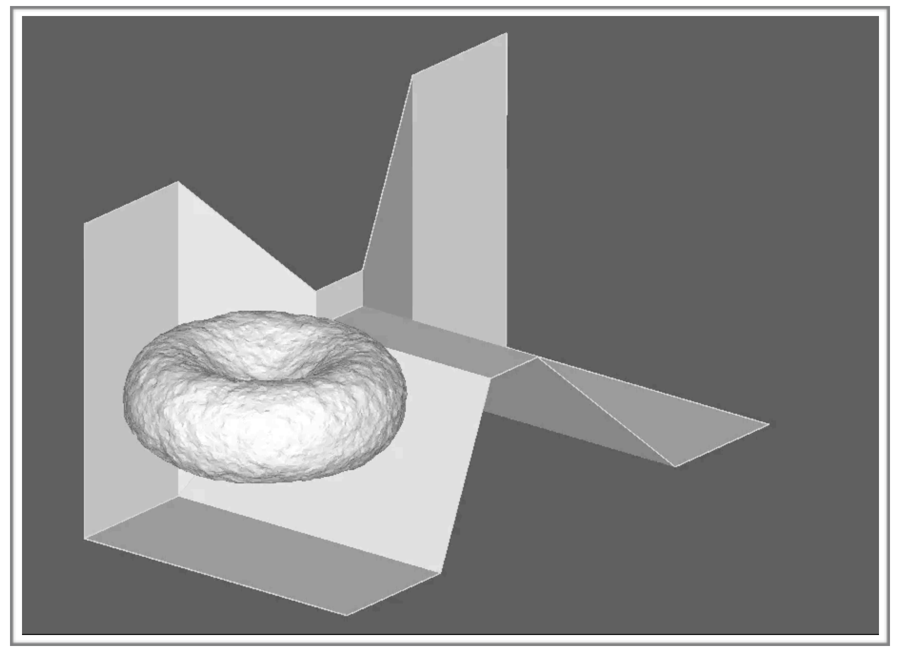


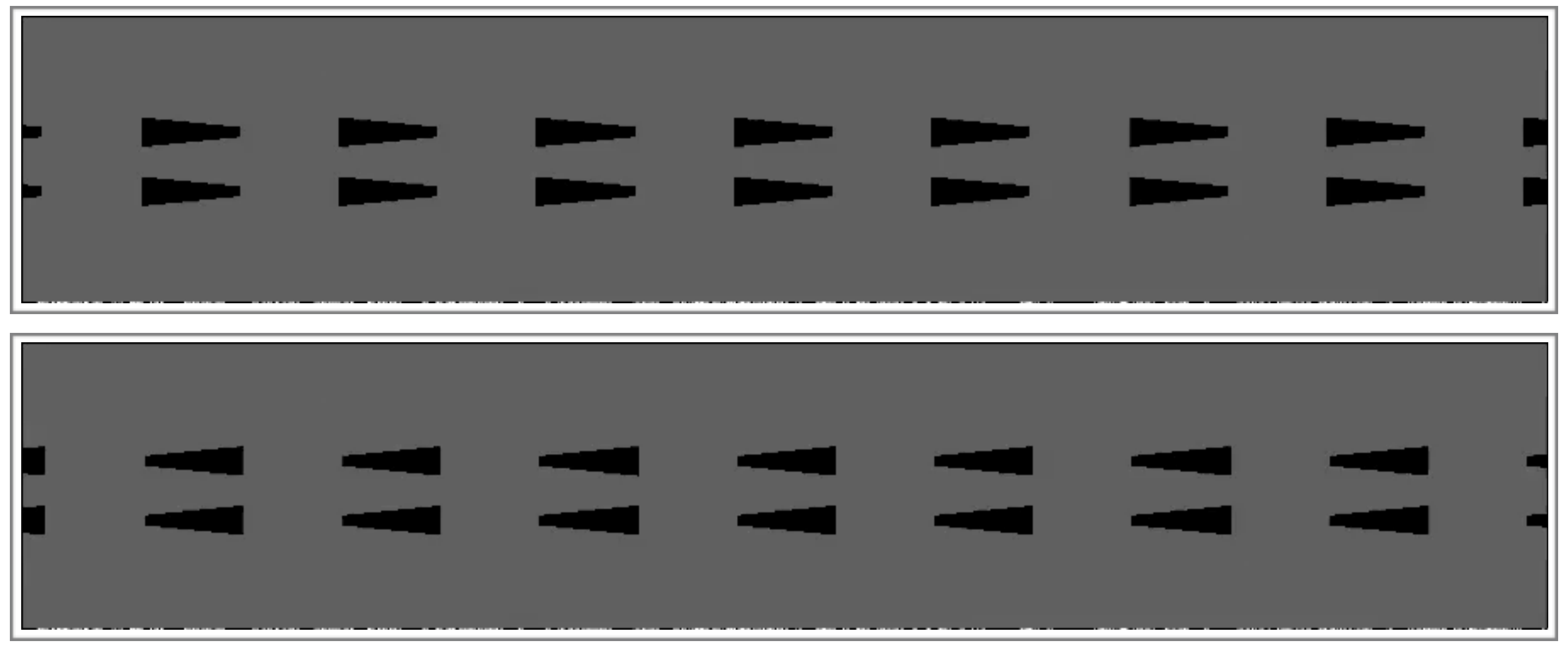


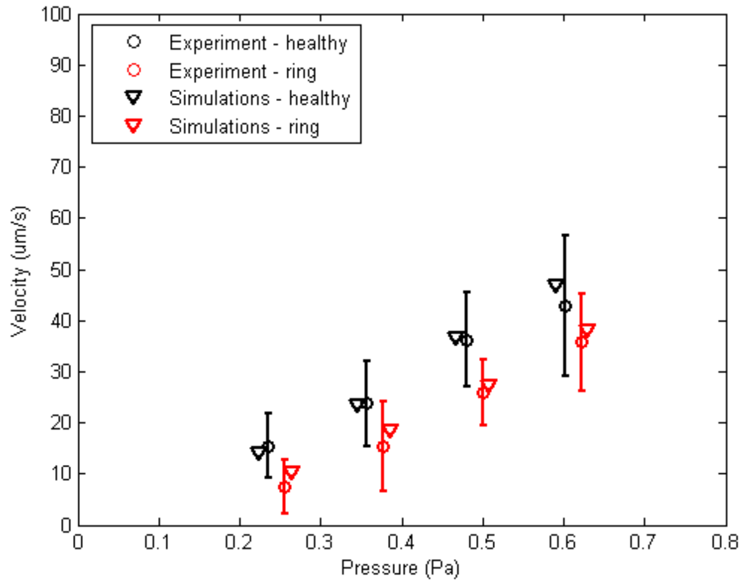


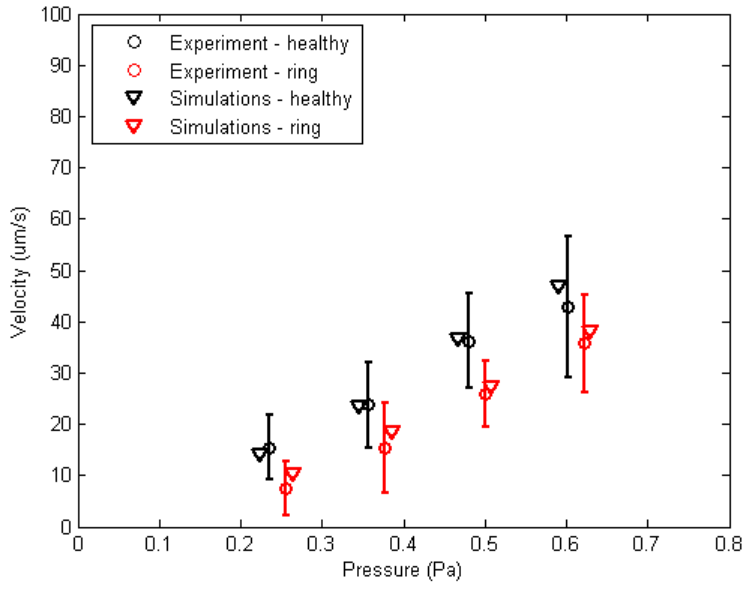












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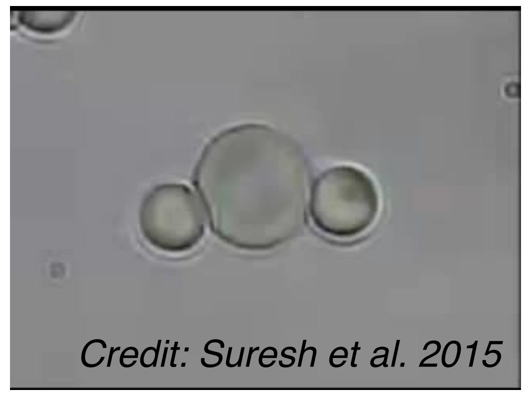
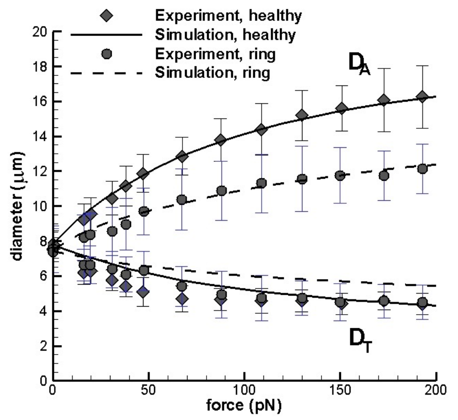
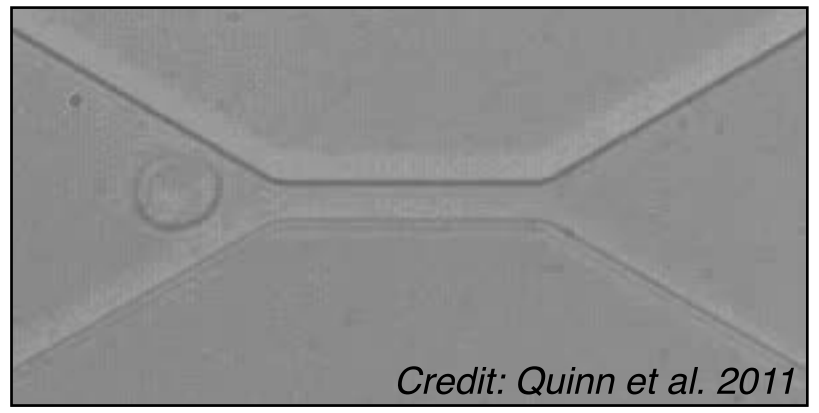
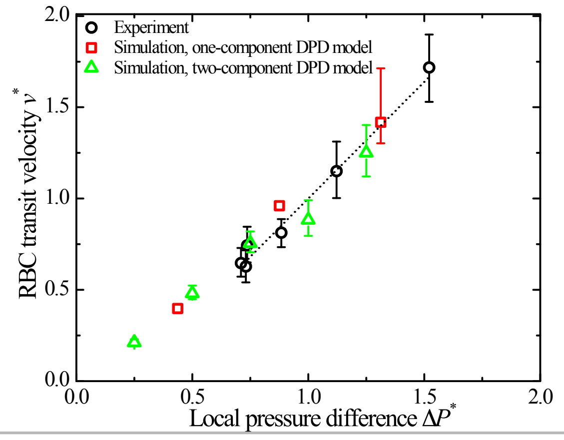
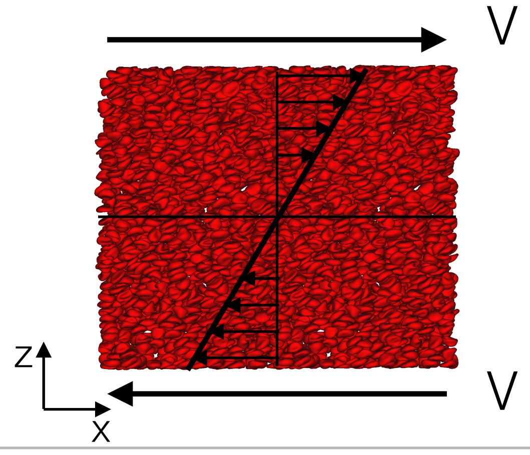
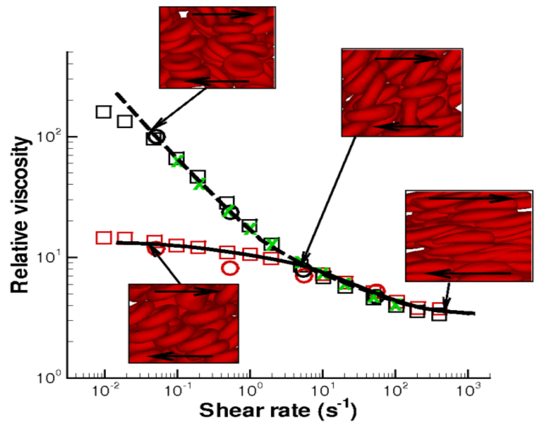
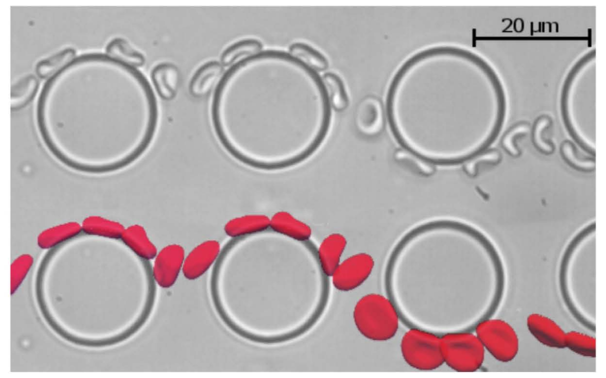
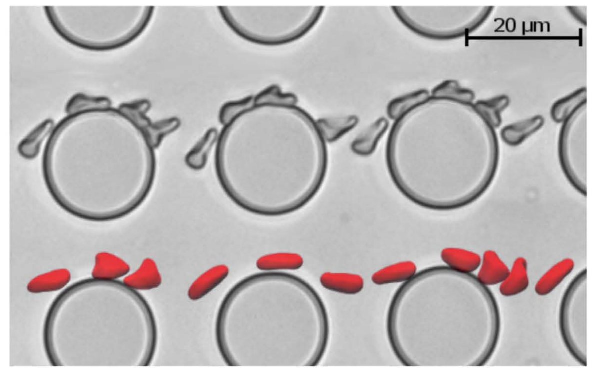
DPD validation: Different experiments - different model parameters

TEST CASE	Solvent Model / RBCmodel	Membrane rigidity	Membrane viscosity	Maximum spring extension	Persistence length	viscosity-contrast
stretching (Fedosov et al., 2010)  	DPD / stress-free	4.8E-19 [J]	0.022 [Pa.s]	1.23 e-6 [m]	1.99 e-9 [m]	1
squeeze in micro-channel (Bow et al., 2011)  	DPD / constant spring eq. length	7.5 E-19 [J]	varied to study its effect	3.17 e-7 [m]	1.08 e-7 [m]	1
shear of whole blood (Fedosov et al., 2011)  	DPD / stress-free	3.0 E-19 [J]	0.0144 [Pa.s]	1.3e-7 [m]	1.99 e-9 [m]	1
DLD device (Henry et al., 2016)  	SDPD+a / stress-free	4.8 E-19 [J]	0.022 [Pa.s]	1.23 e-6 [m]	1.99 e-9 [m]	5

THE PREDICTION GAME: MODELS & DATA

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- Models are imperfect representations of reality
- Computational models involve parameters

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- How to choose parameters and how much to trust them?
- How to integrate DATA ?

THE PREDICTION GAME: MODELS & DATA

- Models are imperfect representations of reality
- Computational models involve parameters

- Probability as the Logic of Science

- How to choose parameters and how much to trust them?
- How to integrate DATA ?

“**Theories**
have to be judged
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$$P(A|B)P(B) = P(B|A)P(A)$$

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$$P(A|B)P(B) = P(B|A)P(A)$$

$$\boxed{P(A|B) = \frac{P(B|A)P(A)}{P(B)}}$$

Bayesian Uncertainty Quantification: Models and Data

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$A \rightarrow$ Hypothesis/Model

$B \rightarrow$ DATA

Bayesian Uncertainty Quantification: Models and Data

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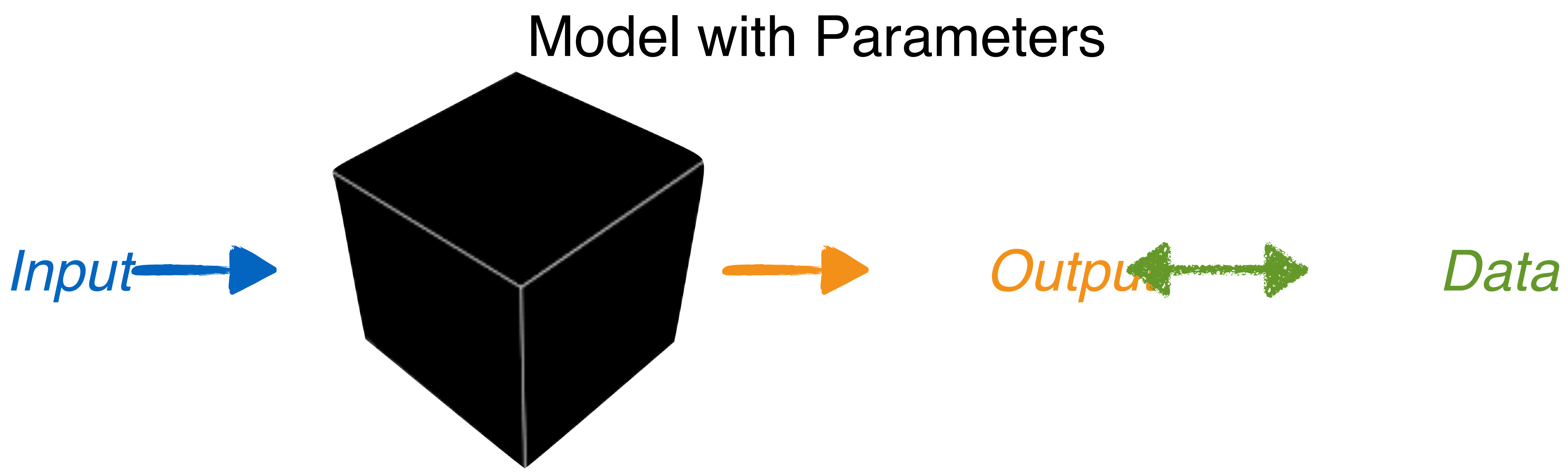
$$P(A|B)P(B) = P(B|A)P(A)$$

$$\underset{\text{posterior}}{P(A|B)} = \frac{\overset{\textit{likelihood}}{P(B|A)}\,\overset{\textit{prior}}{P(A)}}{P(B)}$$

$A \rightarrow$ Hypothesis/Model

$B \rightarrow$ DATA

Bayesian Uncertainty Quantification: Calibration and model selection



PARAMETER ESTIMATION

$$f\left(\theta_i|D,\mathcal{MD}_i\right)=\frac{f\left(D|\theta_i,\mathcal{MD}_i\right)\pi\left(\theta_i|\mathcal{MD}_i\right)}{f\left(D|\mathcal{MD}_i\right)}$$

Experiments

Physical limitations

Past studies

MODEL CLASS SELECTION

$$Pr\left(\mathcal{MD}_i|D\right)=\frac{f\left(D|\mathcal{MD}_i\right)Pr\left(\mathcal{MD}_i\right)}{f\left(D\right)}$$

Evidence of Model Class

$$f\left(D|\mathcal{MD}_i\right) = \int f\left(D|\theta_i,\mathcal{MD}_i\right)\pi\left(\theta_i|\mathcal{MD}_i\right)d\theta_i$$

- Bayesian inference : **large numbers of model evaluations**
- Each simulation : **computationally intensive**

Bayesian Uncertainty PROPAGATION:

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QUANTITIES OF INTEREST: **Posterior Robust Predictions: PDF**

$$f(q|D, \mathcal{MD}) = \int \underbrace{f(q|\theta, \mathcal{MD})}_{\text{Condition}} \underbrace{f(\theta|D, \mathcal{MD})}_{\text{Posterior}} d\theta$$

Sample Estimate:

$$f(q|D, \mathcal{MD}) = \frac{1}{N} \sum_{i=1}^{N} \underbrace{f\left(q|\theta^{(i)}, \mathcal{MD}\right)}_{\text{Condition}} \qquad \theta^{(i)} \sim f(\theta|D, \mathcal{MD})$$

Samples drawn from Posterior PDF

Bayesian Uncertainty PROPAGATION:

$$\theta \in \mathcal{R}^n \longrightarrow \boxed{\mathcal{MD}\ \text{Model class}} \xrightarrow{q(\theta|\mathcal{MD})} f(q|\theta, \mathcal{MD})$$

QoI

Conditional PDF

QUANTITIES OF INTEREST: **Posterior Robust Predictions: PDF**

$$f(q|D, \mathcal{MD}) = \int \underbrace{f(q|\theta, \mathcal{MD})}_{\text{Condition}} \underbrace{f(\theta|D, \mathcal{MD})}_{\text{Posterior}} d\theta$$

SAMPLING HIGH DIMENSIONAL INTEGRALS

Sample Estimate:

$$f(q|D, \mathcal{MD}) = \frac{1}{N} \sum_{i=1}^{N} \underbrace{f\left(q|\theta^{(i)}, \mathcal{MD}\right)}_{\text{Condition}} \qquad \theta^{(i)} \sim f(\theta|D, \mathcal{MD})$$

Samples drawn from Posterior PDF

Bayes' theorem

$$p(\boldsymbol{\vartheta} \,|\, \boldsymbol{d}, \mathcal{M}) = \frac{p(\boldsymbol{d} \,|\, \boldsymbol{\vartheta}, \mathcal{M}) \; p(\boldsymbol{\vartheta} \,|\, \mathcal{M})}{p(\boldsymbol{d} \,|\, \mathcal{M})}$$

Bayes' theorem

$$p(\boldsymbol{\vartheta} \,|\, \boldsymbol{d}, \mathcal{M}) = \frac{p(\boldsymbol{d} \,|\, \boldsymbol{\vartheta}, \mathcal{M})\, p(\boldsymbol{\vartheta} \,|\, \mathcal{M})}{p(\boldsymbol{d} \,|\, \mathcal{M})}$$

computational model

Bayes' theorem

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parameters of the computational model

computational model

Bayes' theorem

experimental data

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parameters of the computational model

computational model

Bayes' theorem

experimental data

posterior

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parameters of the computational model

computational model

Bayes' theorem

experimental data

prior

posterior

$$p(\boldsymbol{\vartheta} \,|\, \boldsymbol{d}, \mathcal{M}) = \frac{p(\boldsymbol{d} \,|\, \boldsymbol{\vartheta}, \mathcal{M})\, p(\boldsymbol{\vartheta} \,|\, \mathcal{M})}{p(\boldsymbol{d} \,|\, \mathcal{M})}$$

parameters of the computational model

computational model

Bayes' theorem

beliefs before seeing any data

prior

experimental data

posterior

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parameters of the computational model

computational model

Bayes' theorem

beliefs before seeing any data

experimental data

likelihood

prior

posterior

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parameters of the computational model

computational model

Bayes' theorem

uncertainties from simulation, experiment, model

beliefs before seeing any data

experimental data

likelihood

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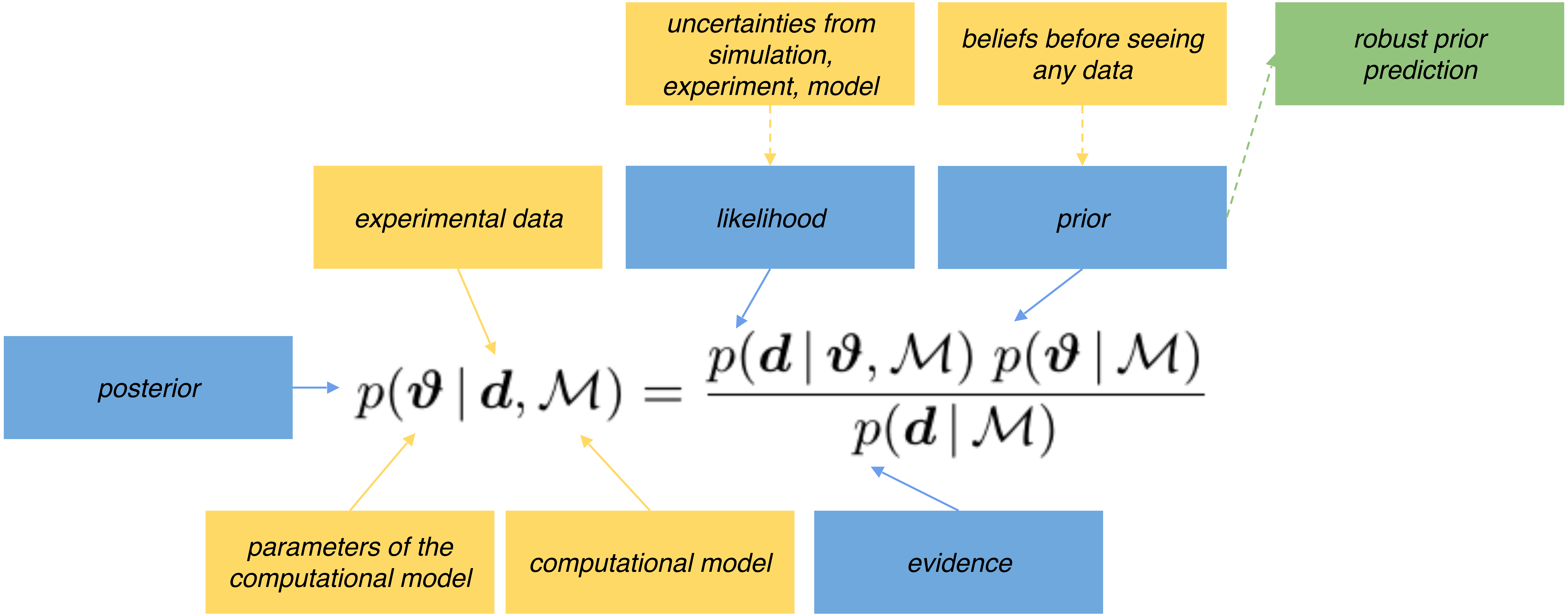
parameters of the computational model

computational model

evidence

Bayes' theorem



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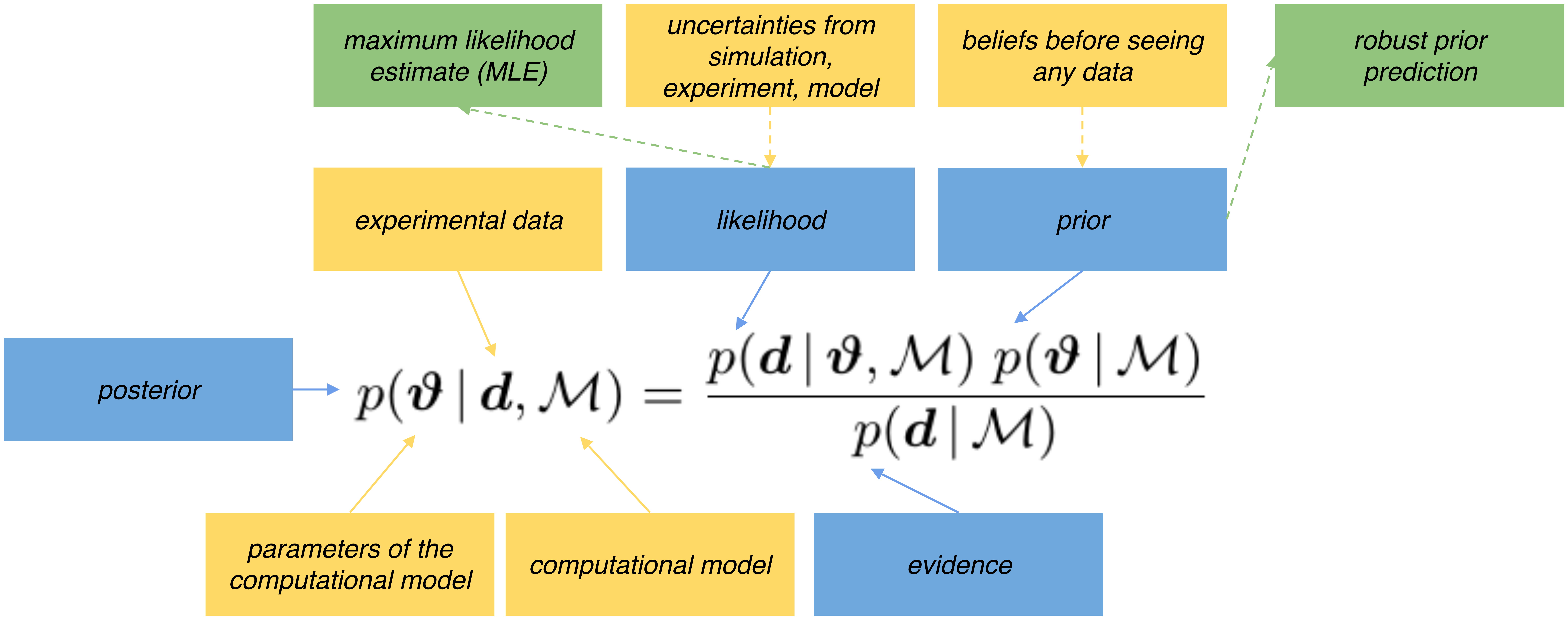
Bayes' theorem



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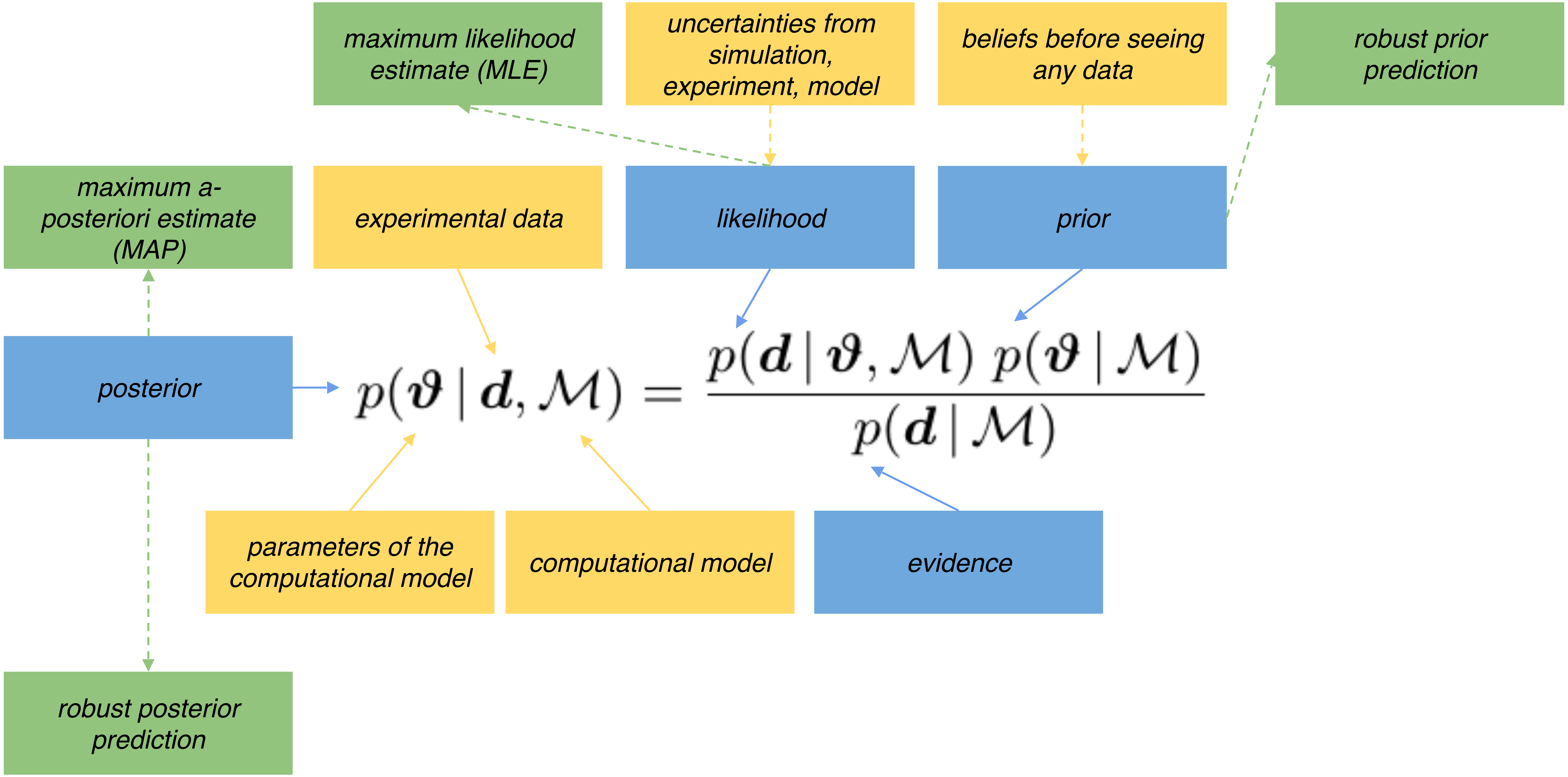

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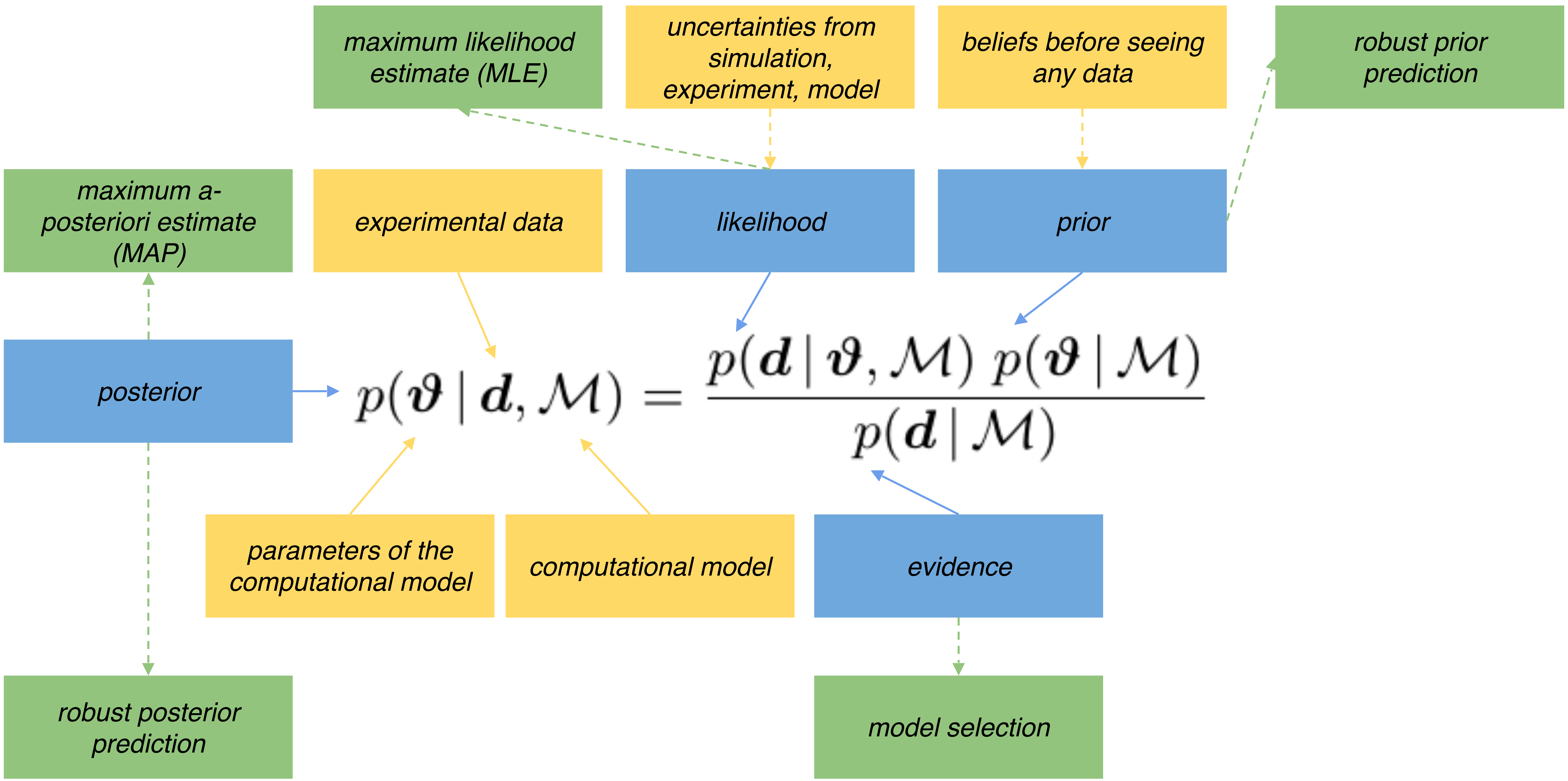

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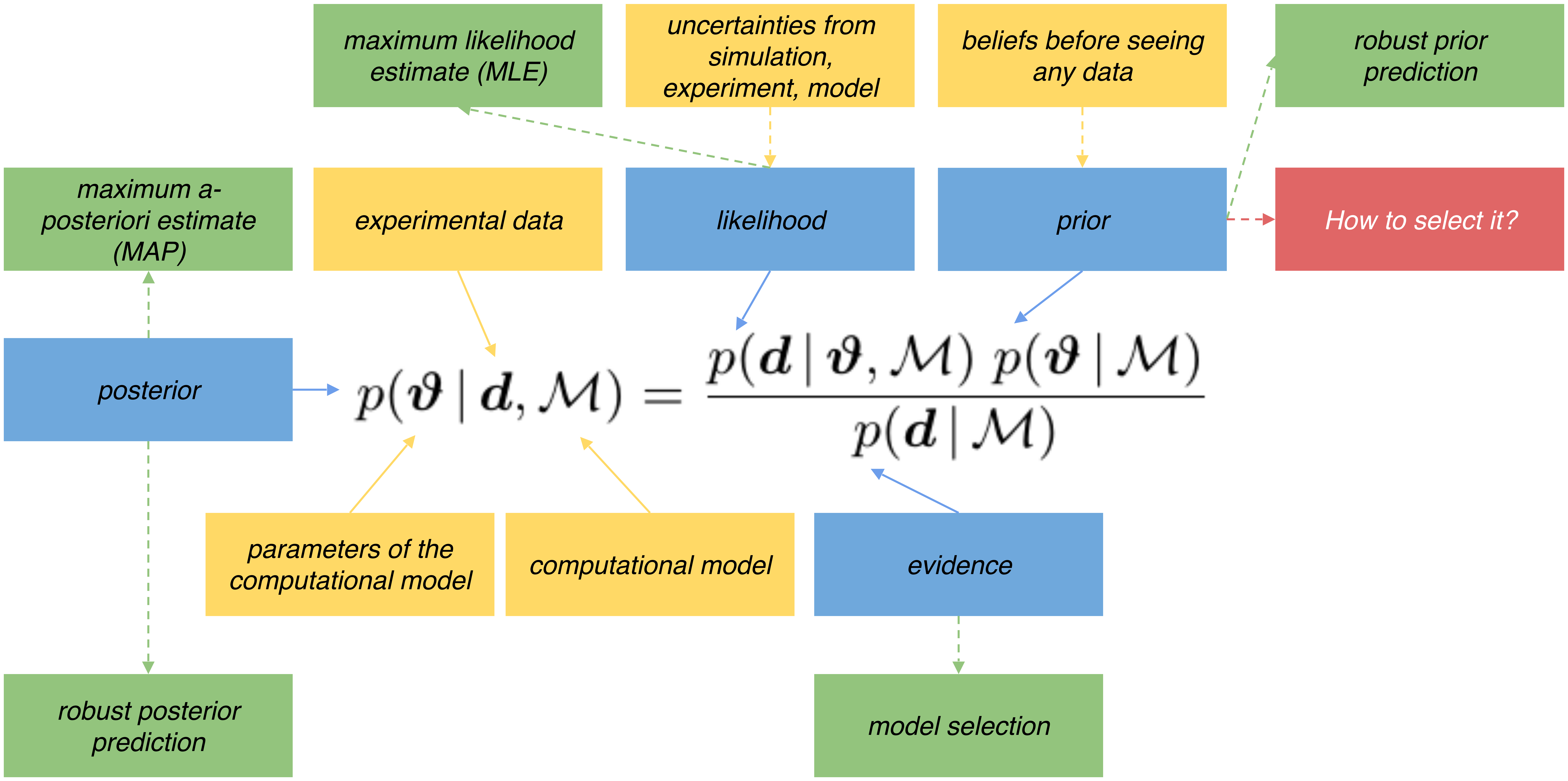

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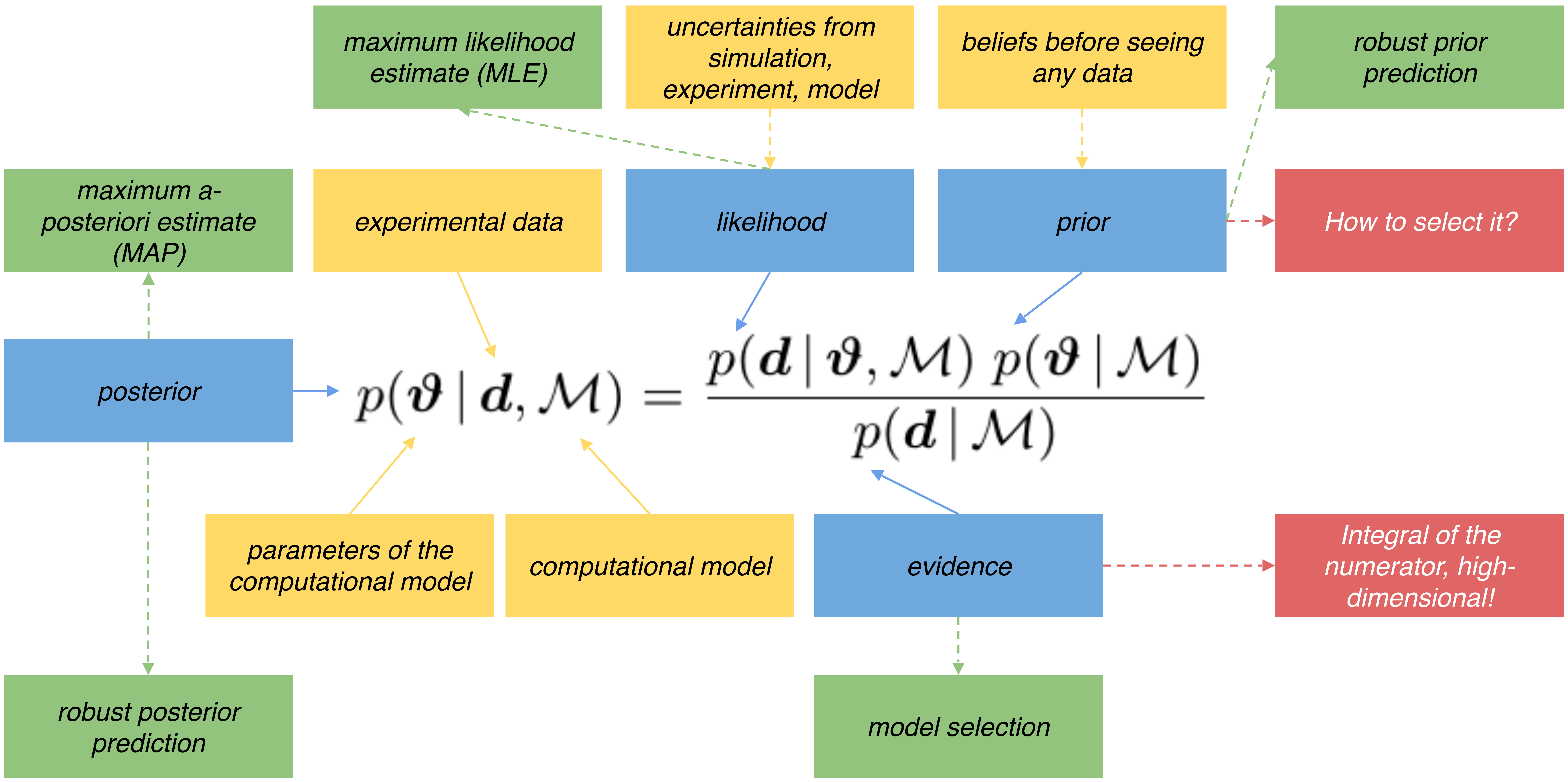

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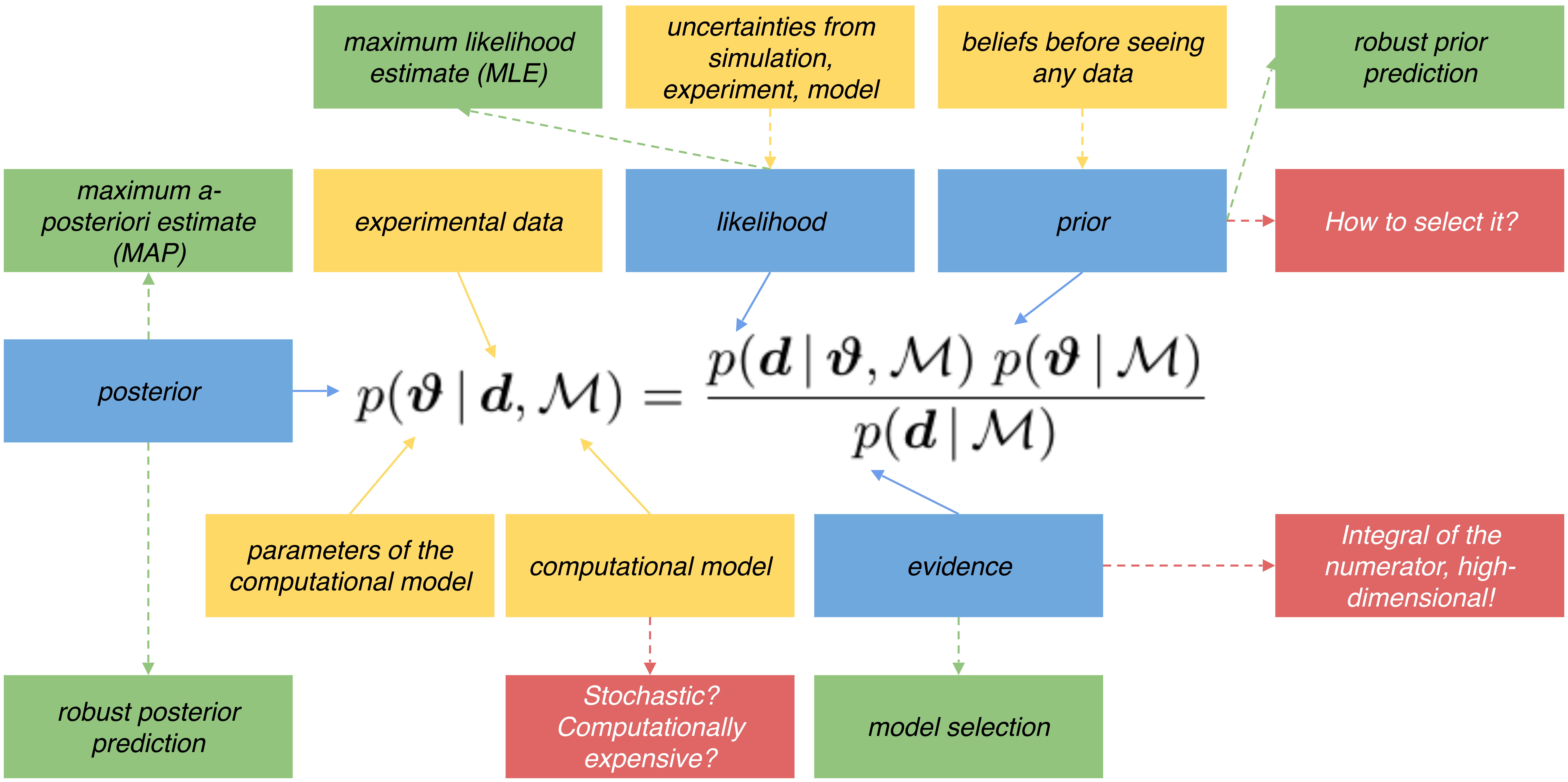

Bayes' theorem

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