Play. Pause. Rewind. Measuring local entropy production and extractable work in active matter

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Ro, Guo, …, **SM**, PRL, 129 (22), 220601 (2022)
Anand, … **SM***, Cheng*, arXiv:2308.08421 (2024)

What defines nonequilibrium?

We must start by defining equilibrium systems:

(a) intensive properties are independent of time

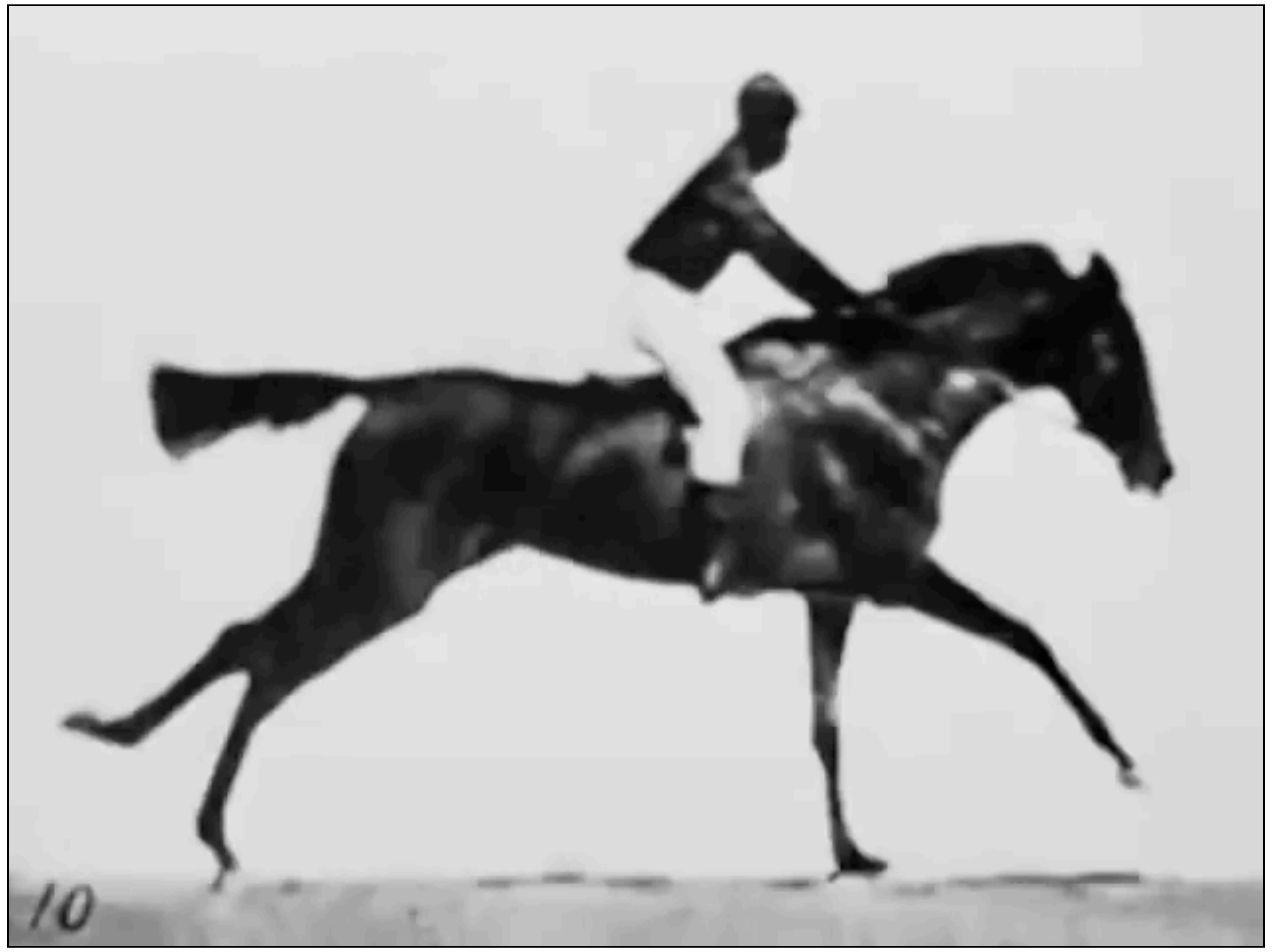
(b) no current of matter or energy exists in the system's interior or at its boundaries

Kirkwood, J.G., Oppenheim, I. (1961)

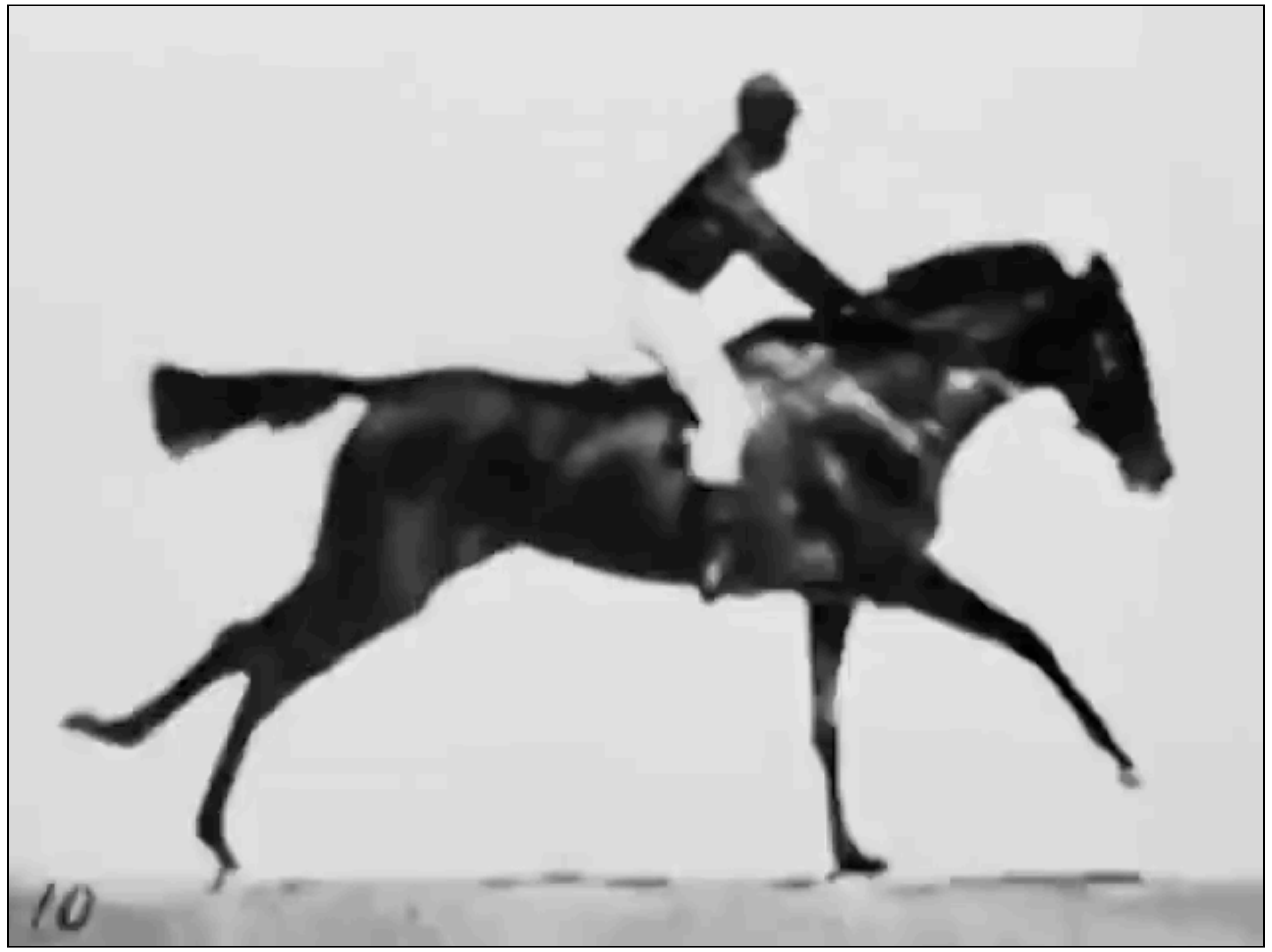
So, being out of equilibrium means that these conditions do not hold, but is there a quantifiable signature of how far from equilibrium a system is?

Time reversal symmetry breaking (TRSB)

Forward trajectory $\overrightarrow{X}$



Reverse trajectory $\overrightarrow{X}^R$



$$\frac{P(\overrightarrow{X})}{P(\overrightarrow{X}^R)} = e^{\Sigma(\overrightarrow{X})/k_B} > 1$$

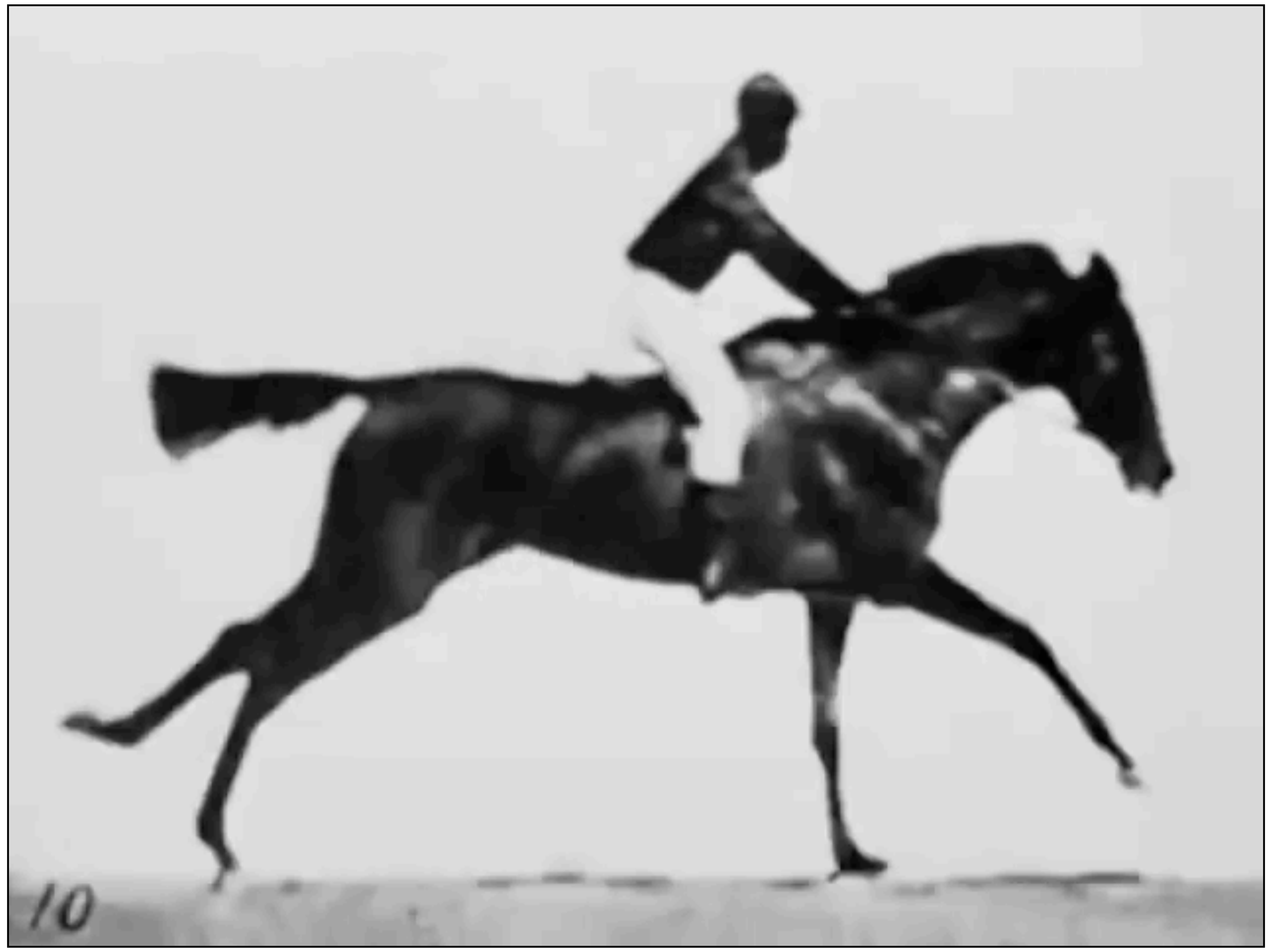
Fluctuation theorem

$$\Sigma(\overrightarrow{X}) > 0$$

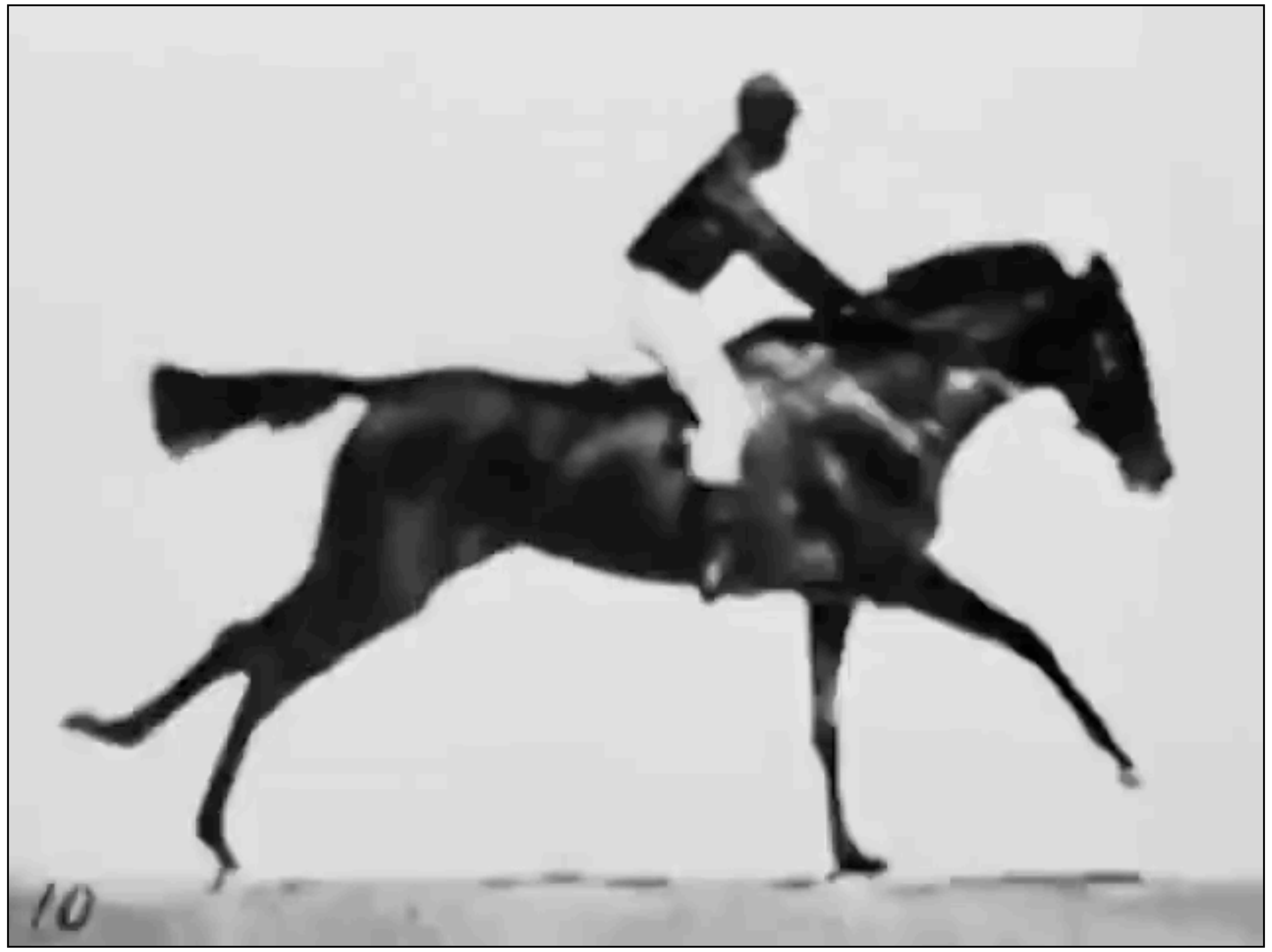
The Horse in Motion, Eadweard Muybridge, 1878

Time reversal symmetry breaking (TRSB)

Forward trajectory $\vec{X}$



Reverse trajectory $\vec{X}^R$



Entropy production quantifies departure from equilibrium, degree of TRSB, and the thermodynamic cost of maintaining the system out of equilibrium

$$\Sigma(\vec{X}) > 0$$

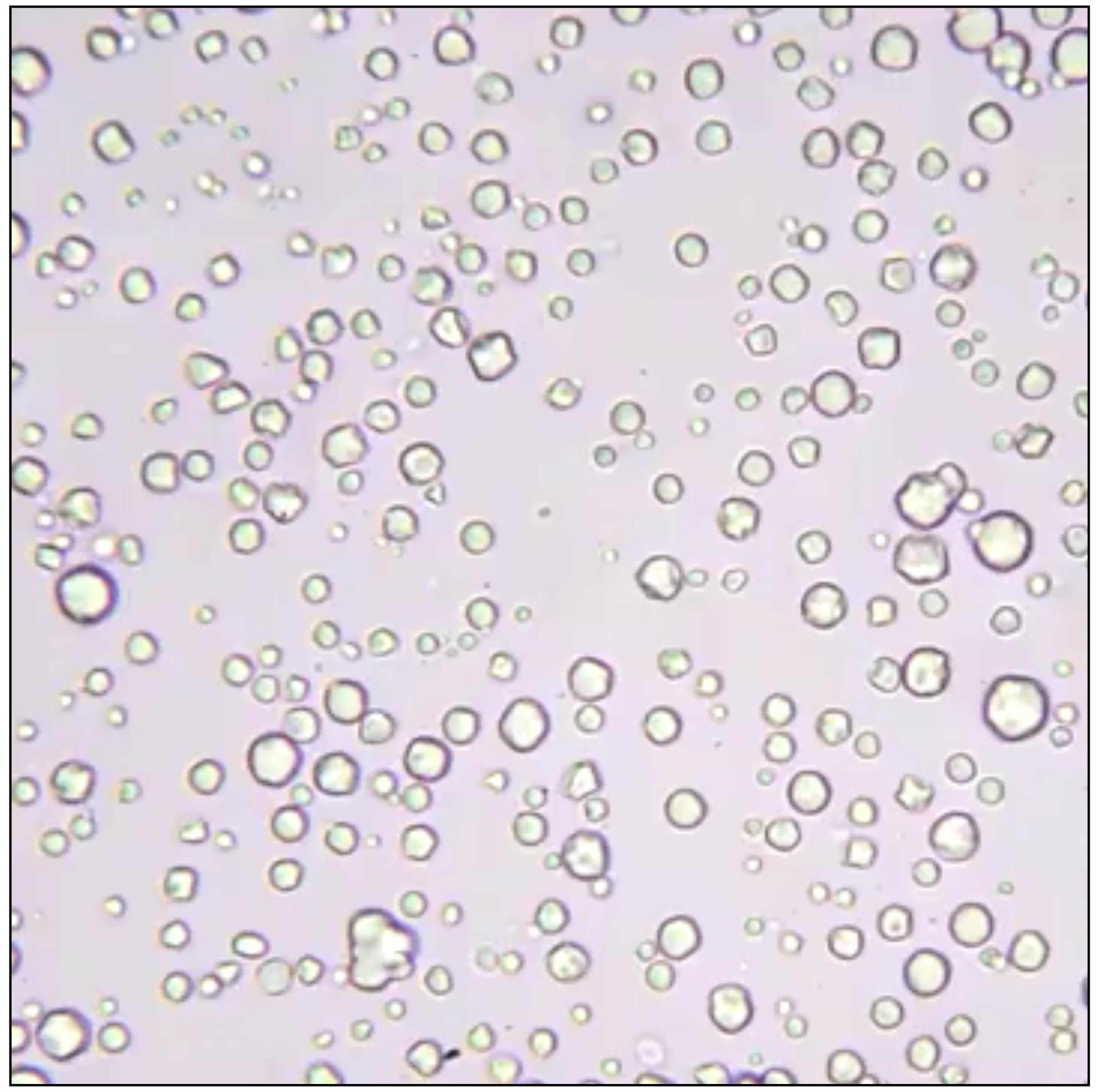
The Horse in Motion, Eadweard Muybridge, 1878

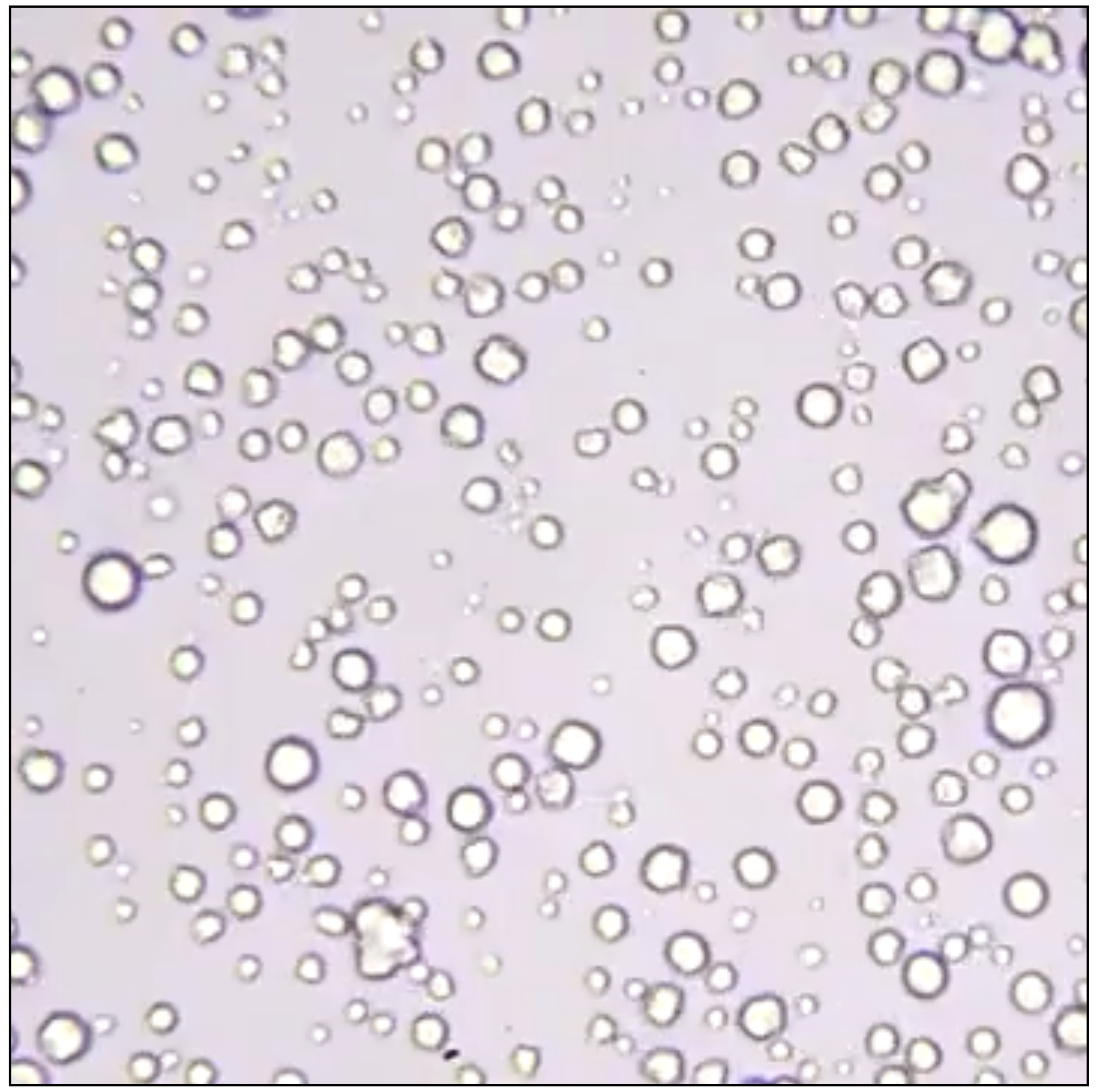
Play. Pause. Rewind.

For an equilibrium system

Forward trajectory

$\overrightarrow{X}$





Reverse trajectory

$\overrightarrow{X}^R$

$$\frac{P(\overrightarrow{X})}{P(\overrightarrow{X}^R)} = e^{\Sigma(\overrightarrow{X})/k_B} = 1$$

Entropy production $\Sigma(\overrightarrow{X}) = 0$ since dynamics are symmetric under time reversal

(i.e., forward and backward trajectories are indistinguishable)

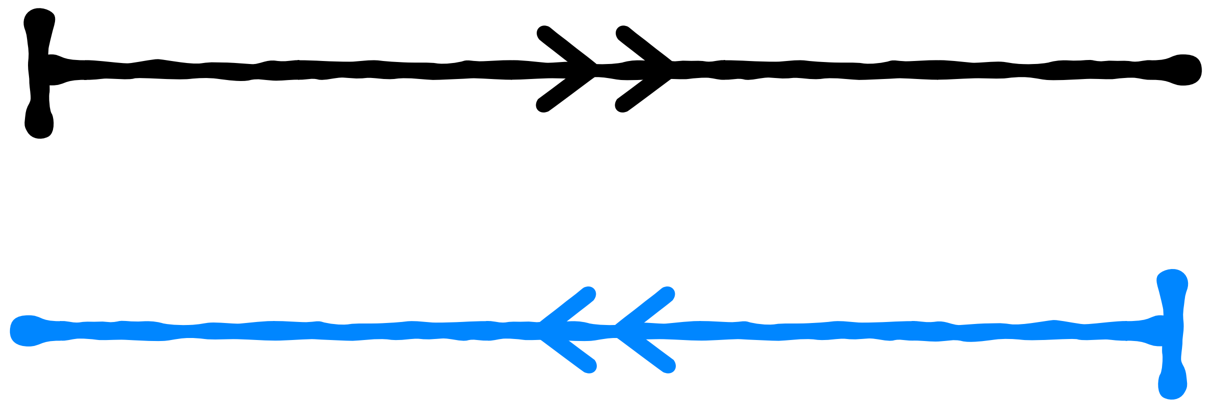
Paul Baker, Brownian Motion of Fat Globules, 2019

Quantifying time reversal symmetry breaking

Relative Entropy/KL Divergence

Forward sequence $\overrightarrow{X}_1^n$ $P(\overrightarrow{X})$

Time-reversed sequence $\overleftarrow{X}_n^1$ $P(\overrightarrow{X}^R)$



KL divergence

$$D_{\mathrm{KL}}(P(\overrightarrow{X})||P(\overrightarrow{X}^R)) = \frac{1}{n}\sum_X P(\overrightarrow{X})\log\frac{P(\overrightarrow{X})}{P(\overrightarrow{X}^R)}$$

$$= \underbrace{H[P(\overrightarrow{X}), P(\overrightarrow{X}^R)]}_{\text{Cross entropy}} - \underbrace{H[P(\overrightarrow{X})]}_{\text{Entropy}}$$

Measure of time reversal symmetry breaking

← Remember!

$$D_{\mathrm{KL}}(P(\overrightarrow{X})||P(\overrightarrow{X}^R)) = \frac{1}{n}\left\langle \ln\frac{P(\overrightarrow{X})}{P(\overrightarrow{X}^R)}\right\rangle = \frac{1}{n}\langle\Sigma(\overrightarrow{X})\rangle$$

Entropy production

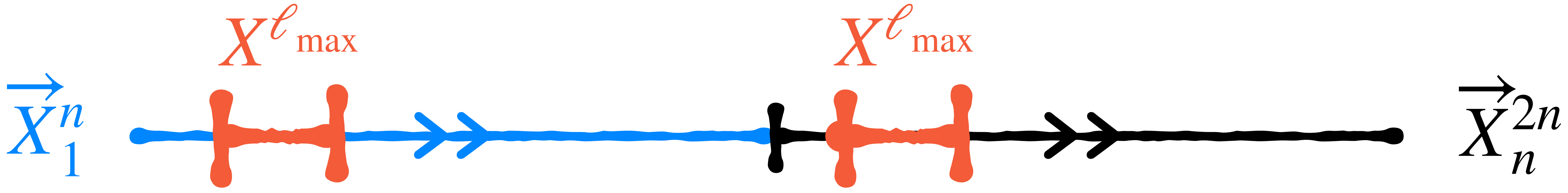
Seifert, PRL **95**, 040602 (2005)

Kawai et al., PRL **98**, 080602 (2007)

Quantifying time reversal symmetry breaking

A symmetric estimator

Take a sequence and split it in half



$$D_{\mathrm{KL}}(\overrightarrow{p} \| \overleftarrow{p}) = \hat{H}(\overrightarrow{X}_n^{2n} \| \overleftarrow{X}_n^{1}) - \hat{H}(\overrightarrow{X}_n^{2n} \| \overrightarrow{X}_1^{n})$$

Entropy

Pattern matching estimator

$$\hat{H} = \frac{\log n}{\langle \ell_{\max} \rangle}$$

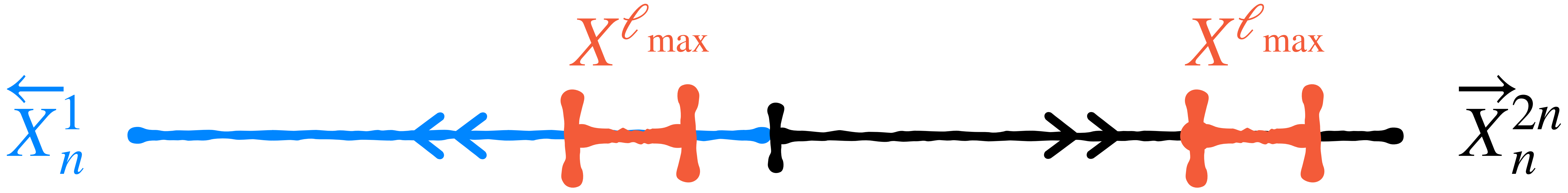
Ro et al., in preparation

Ro, …, **SM,** PRL, 129 (22), 220601 (2022)

Quantifying time reversal symmetry breaking

A symmetric estimator

Take a sequence and split it in half



$$D_{\mathrm{KL}}(\overrightarrow{p}\,\|\,\overleftarrow{p}) = \hat{H}(\overrightarrow{X}_n^{2n}\,\|\,\overleftarrow{X}_n^{1}) - \hat{H}(\overrightarrow{X}_n^{2n}\,\|\,\overrightarrow{X}_1^{n})$$

Cross entropy

Pattern matching estimator

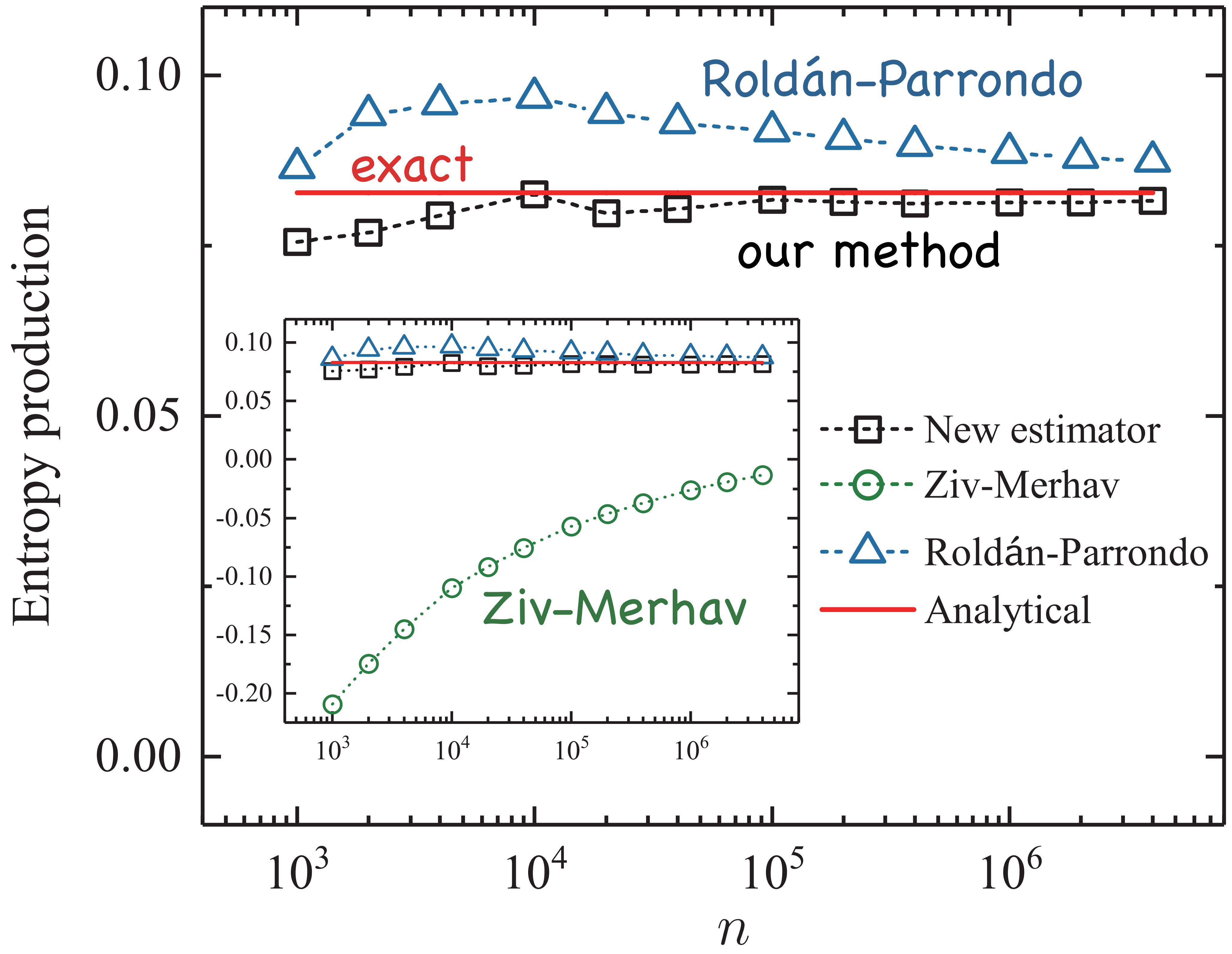
$$\hat{H} = \frac{\log n}{\langle \ell_{\max} \rangle}$$

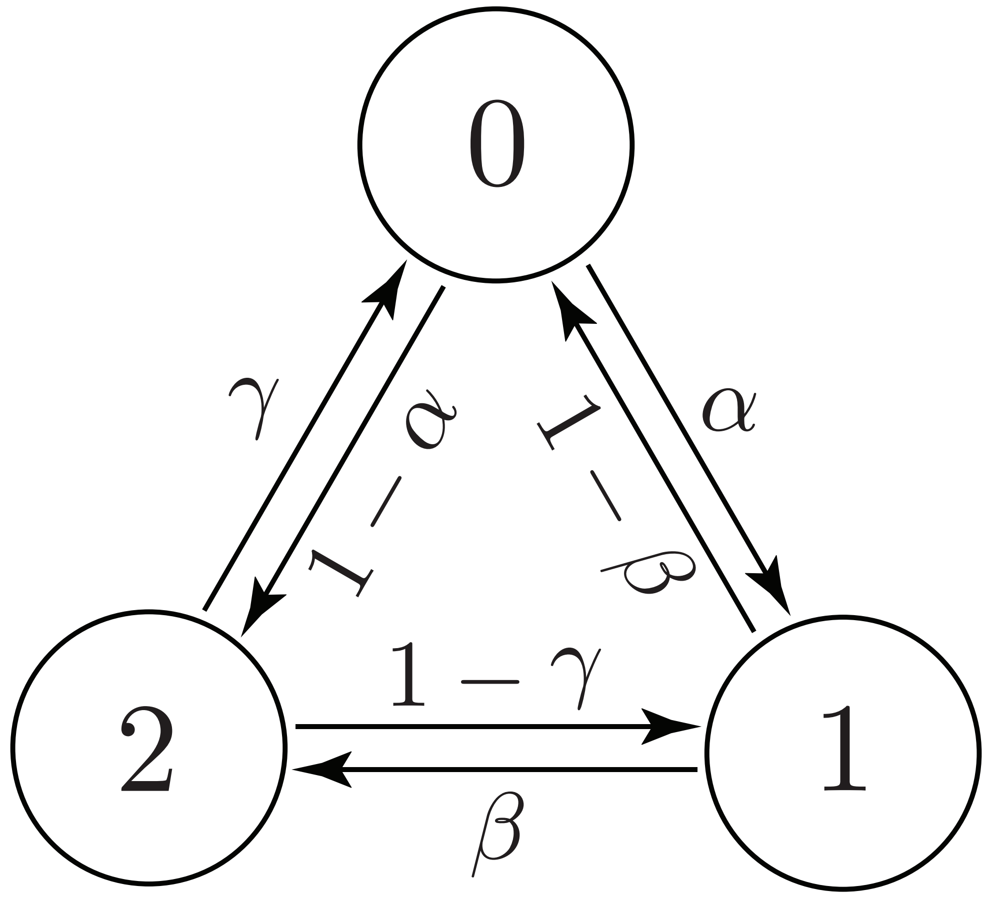
Ro et al., in preparation

Ro, ..., **SM,** PRL, 129 (22), 220601 (2022)

Quantifying time reversal symmetry breaking

A symmetric estimator





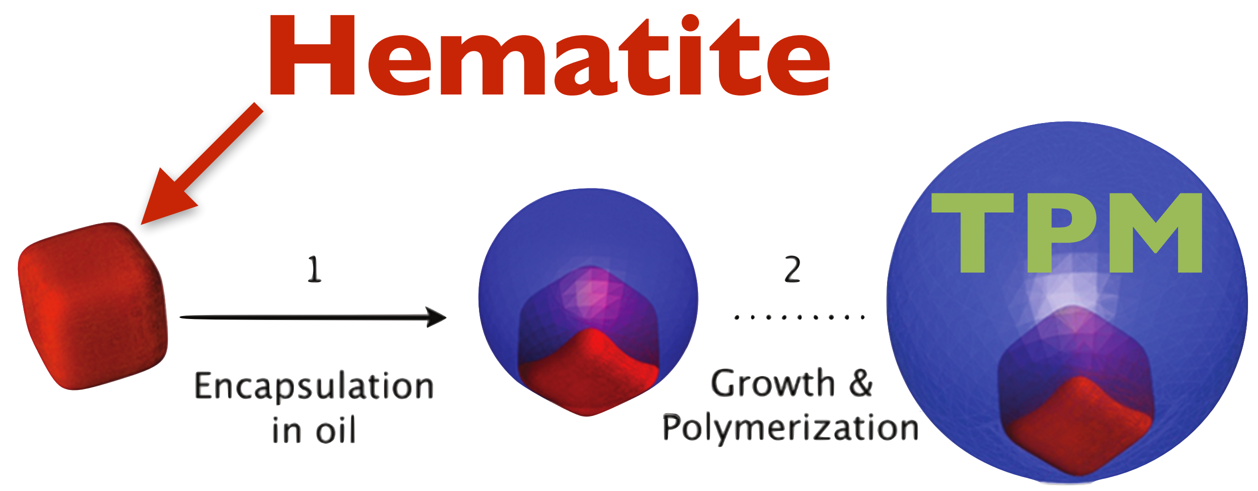
$\alpha = 0.5, \beta = 0.7, \gamma = 0.6$

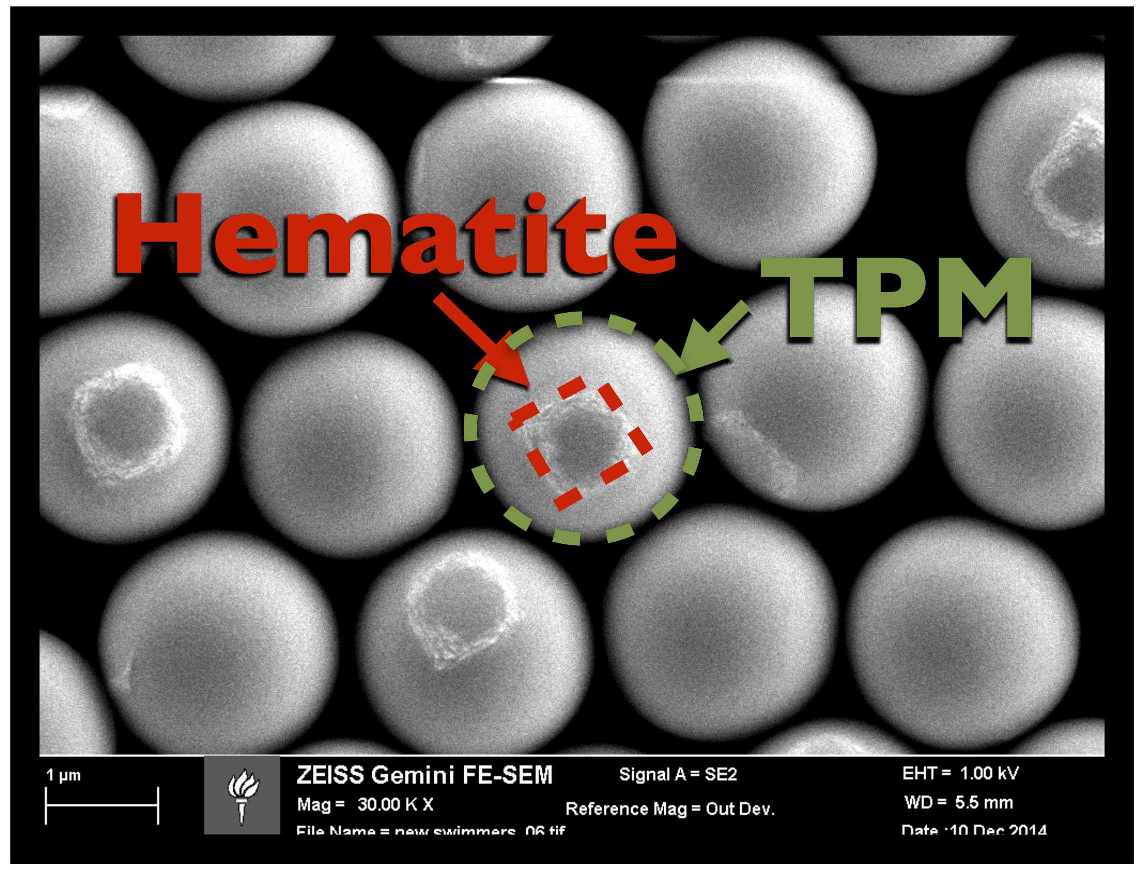
Our symmetric estimator of KLD converges much more rapidly (at least $10^3 \times$ on 3-state MM) than those proposed by Ziv & Merav, and Roldán & Parrondo.

Roldán & Parrondo, PRE, **85**, 031129 (2012)
Ziv & Merhav, IEEE Trans. Inf. Theory, **39**, 1270 (1993)

Motility Induced Phase Separation of Active Colloids

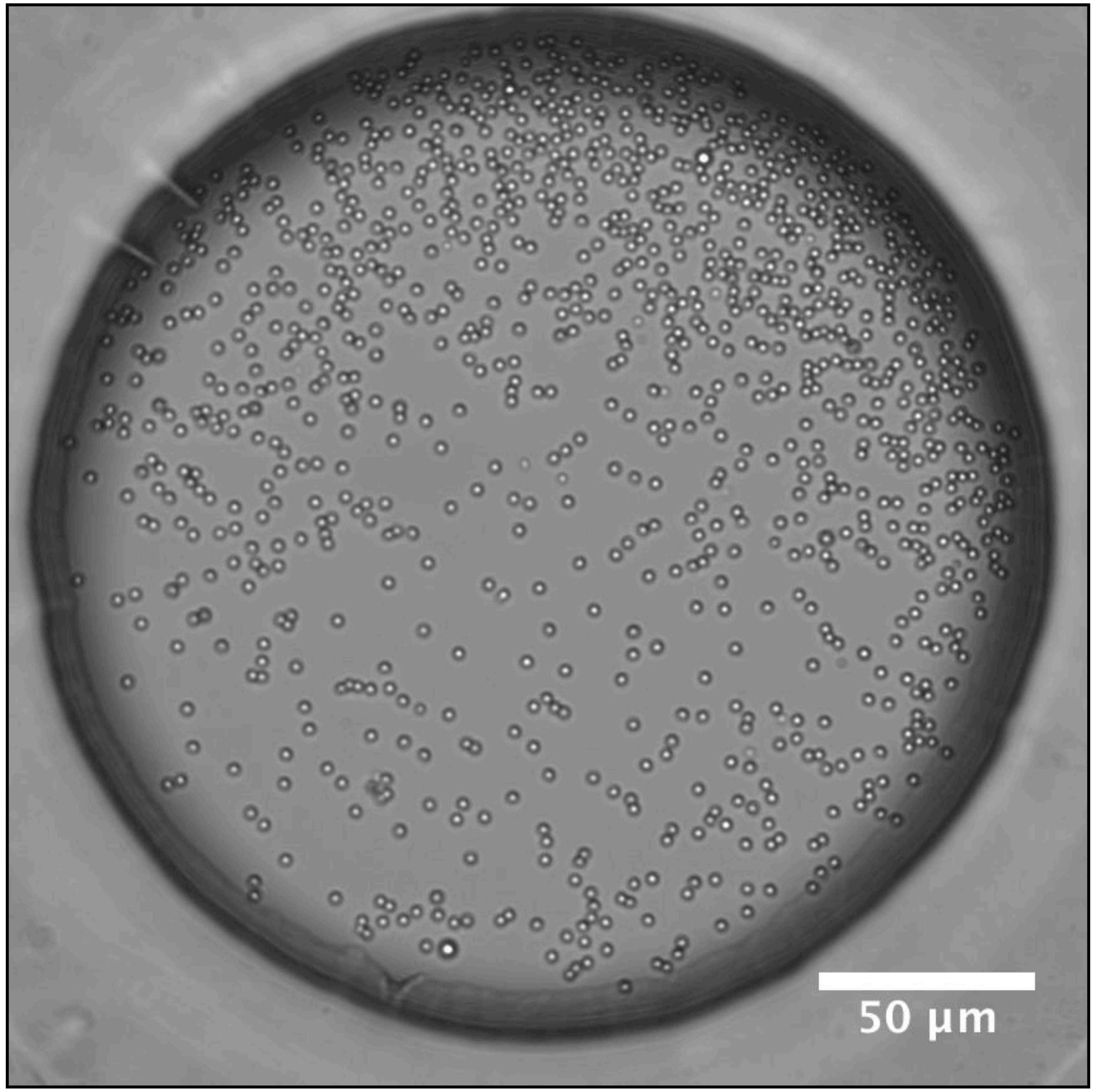
Interacting assemblies of self-propelled colloids give rise to cohesive states of matter in the absence of cohesive forces





TPM = 3-(Trimethoxysilyl)propyl methacrylate

Sacanna et al., JACS (2012)

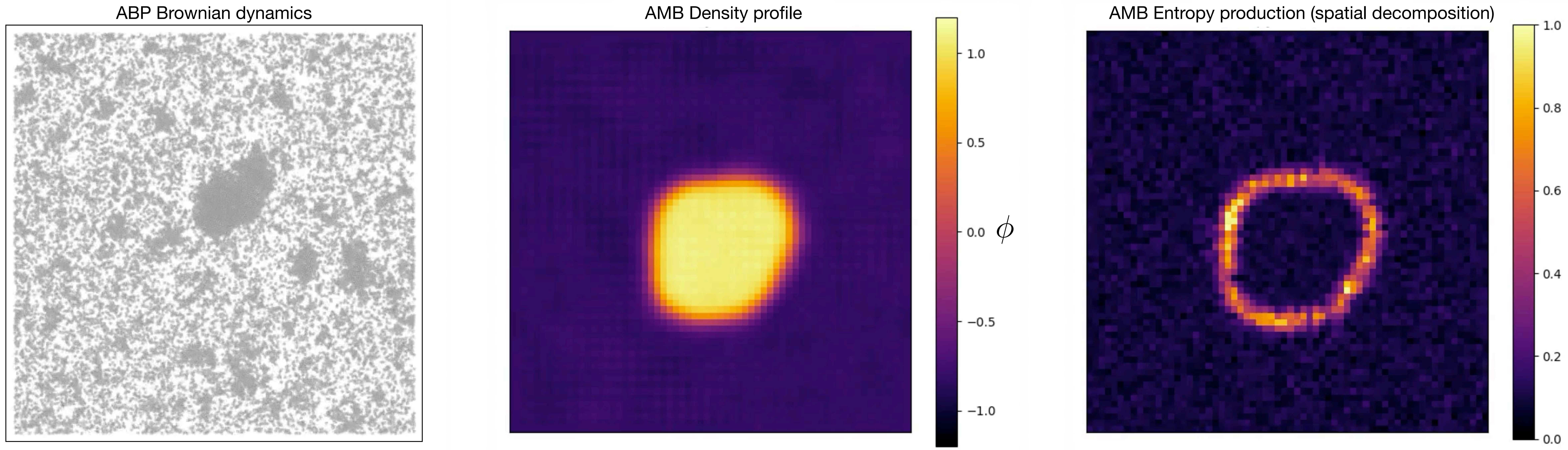


Light activated
μm swimmers propelled by photocatalytic decomposition of hydrogen peroxide

Experiments by M. Ferrari, S. Sacanna, P. Chaikin (NYU)

Active Model B (MIPS)

On large scales behavior akin to equilibrium phase separation, but...



$$\frac{\partial \phi}{\partial t} = -\nabla \cdot \left(\mathbf{J} + \sqrt{2DM}\boldsymbol{\Lambda}\right)$$

$$\mathbf{J} = -M\nabla\mu$$

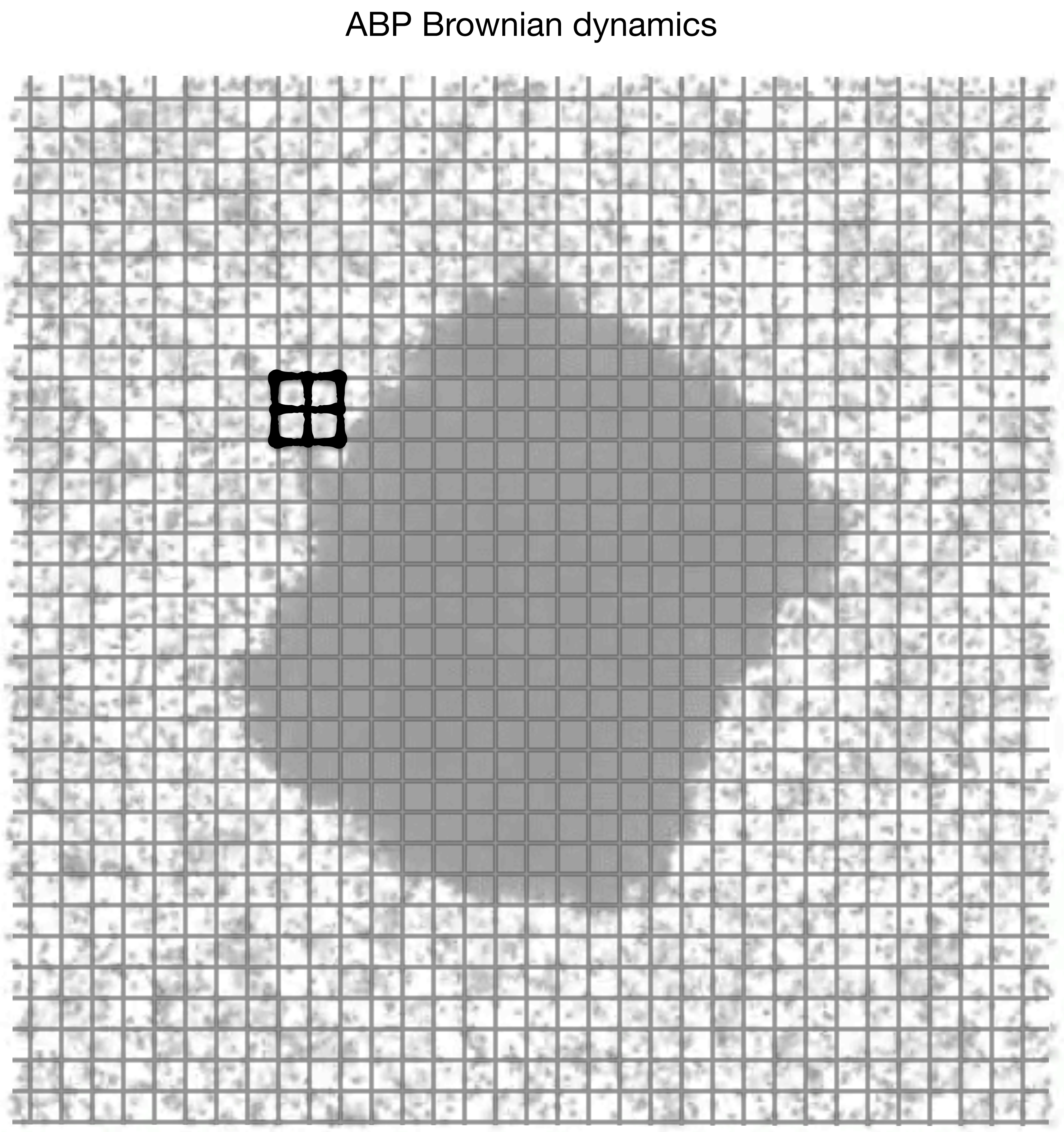
$$\mu = \mu_{eq} + \mu_A$$

Ro, …, **SM,** PRL, 129 (22), 220601 (2022)

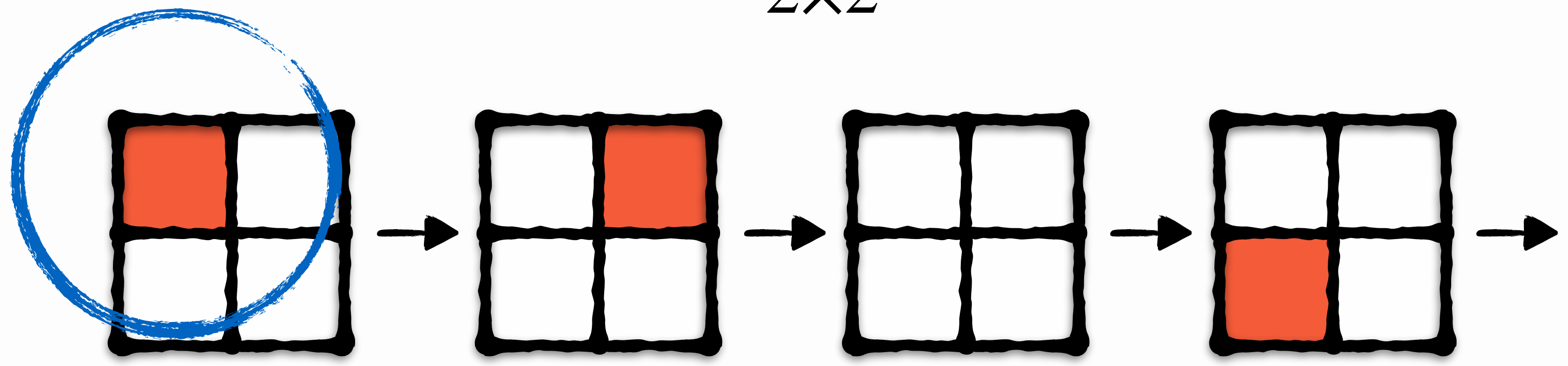
Nardini et al., PRX **7** 021007 (2017)

Spatially decomposing entropy production

An information theoretic approach



$\overrightarrow{\mathbf{x}}_{2\times 2}$

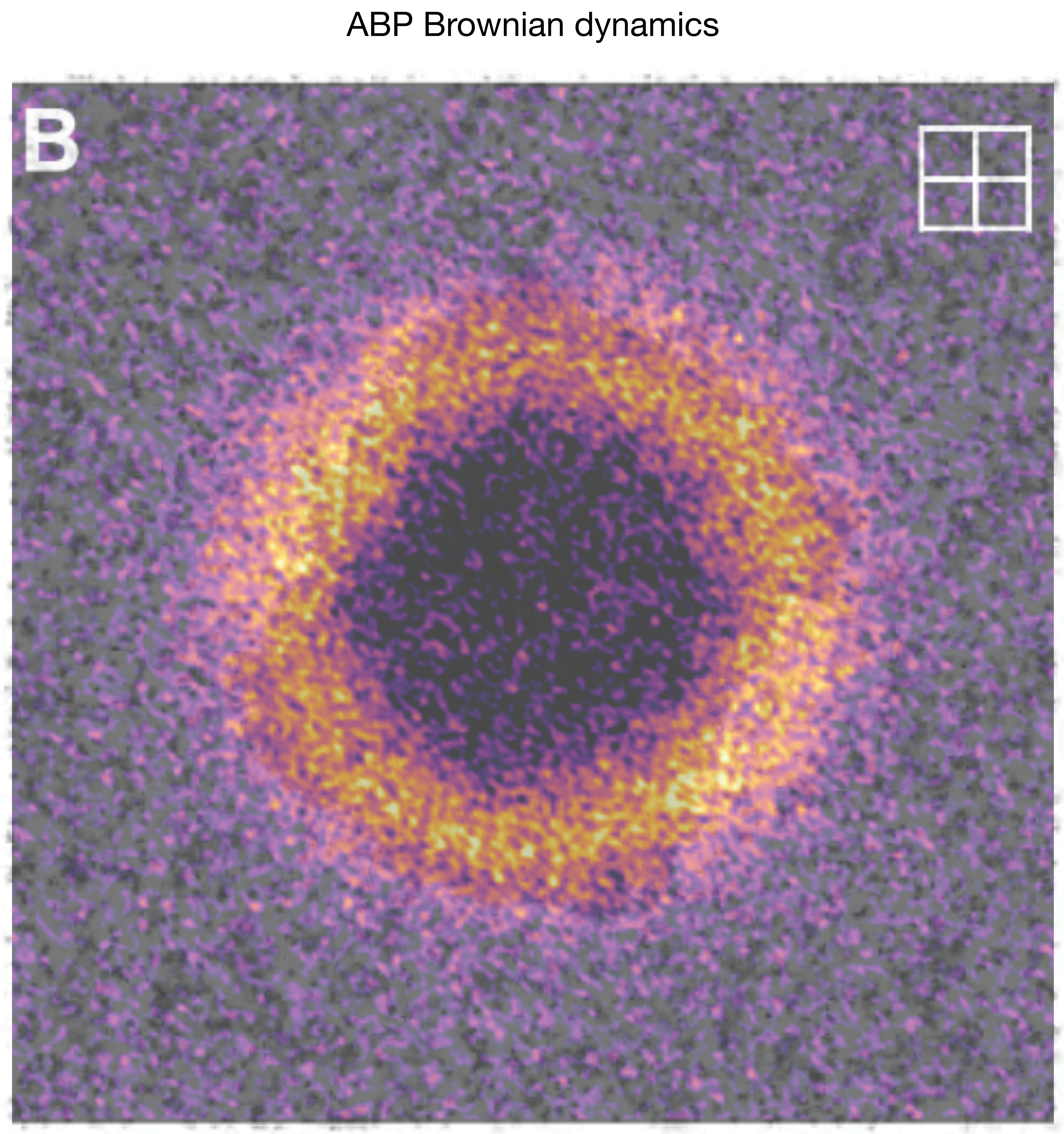


$$D_{KL}(\overrightarrow{\mathbf{x}}_{2\times 2}\|\overleftarrow{\mathbf{x}}_{2\times 2}) = \hat{H}(\overrightarrow{\mathbf{x}}_{2\times 2}\|\overleftarrow{\mathbf{x}}_{2\times 2}) - \hat{H}(\overrightarrow{\mathbf{x}}_{2\times 2}\|\overrightarrow{\mathbf{x}}_{2\times 2})$$

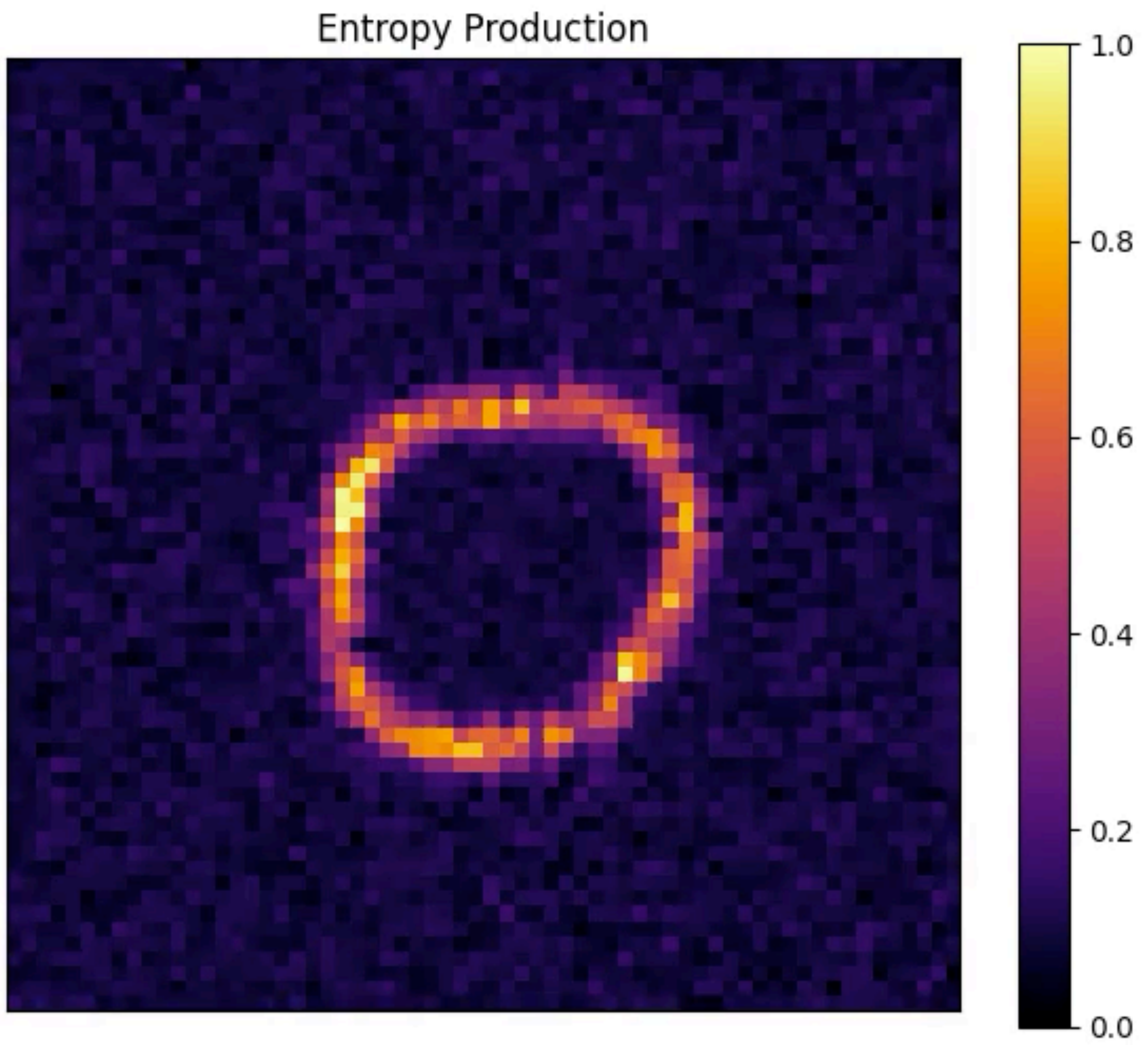
Ro, ..., **SM,** PRL, 129 (22), 220601 (2022)

Spatially decomposing entropy production

An information theoretic approach



Model-free Measurement

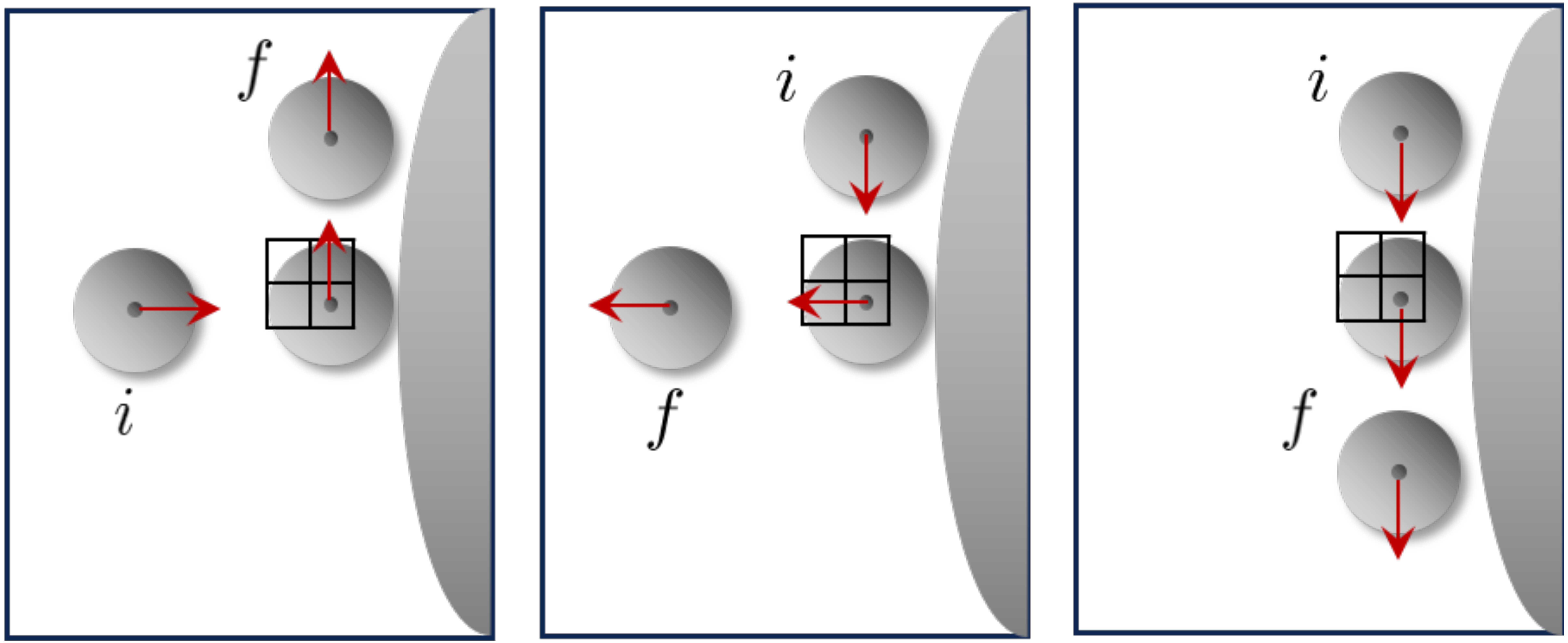


Field Theory

Ro, …, **SM,** PRL, 129 (22), 220601 (2022)

Spatially decomposing entropy production

TRSB at the single particle level near interfaces



Forward

Reverse
(less likely)

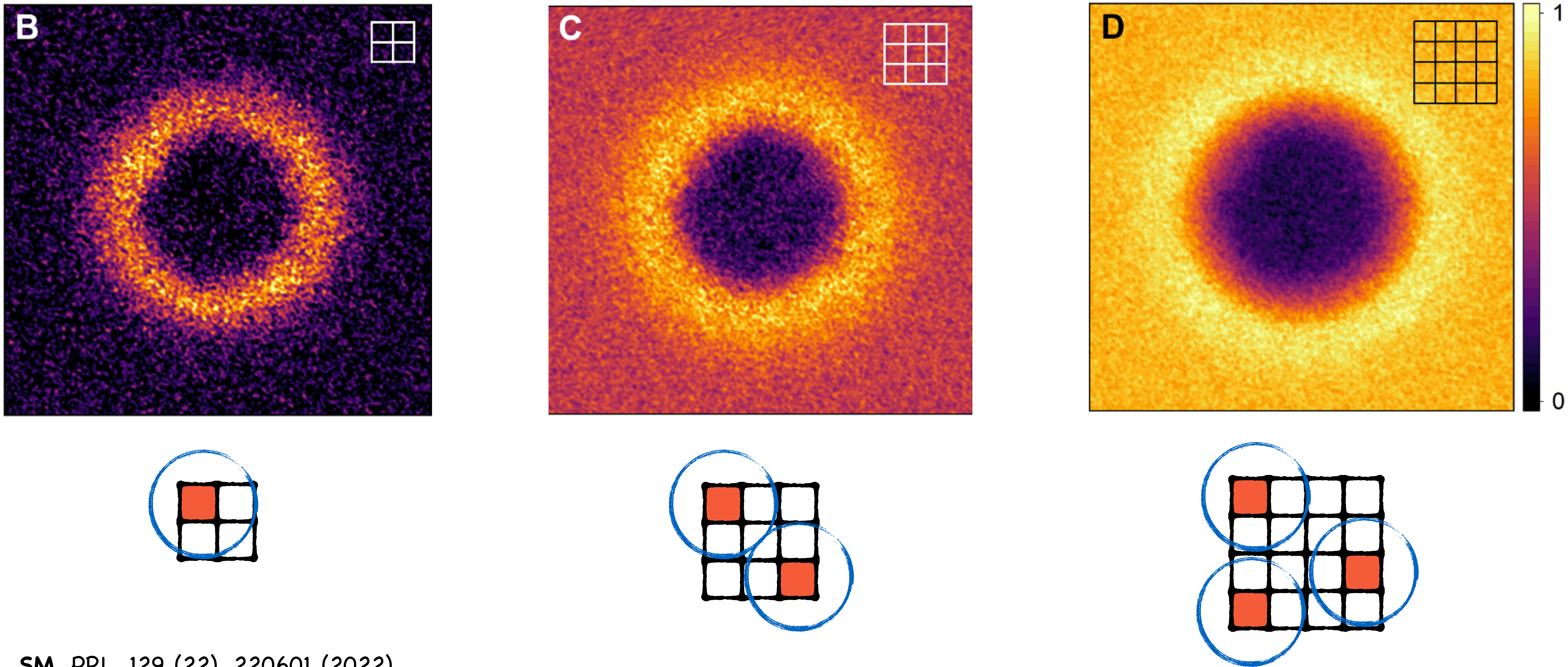
Typical
trajectory

Ro, ..., **SM,** PRL, 129 (22), 220601 (2022)

Spatially decomposing entropy production

Dependence on length scale

$D_{KL}(\overrightarrow{\mathbf{x}}_{2\times 2} \| \overleftarrow{\mathbf{x}}_{2\times 2})$ $D_{KL}(\overrightarrow{\mathbf{x}}_{3\times 3} \| \overleftarrow{\mathbf{x}}_{3\times 3})$ $D_{KL}(\overrightarrow{\mathbf{x}}_{4\times 4} \| \overleftarrow{\mathbf{x}}_{4\times 4})$



Ro, ..., **SM,** PRL, 129 (22), 220601 (2022)

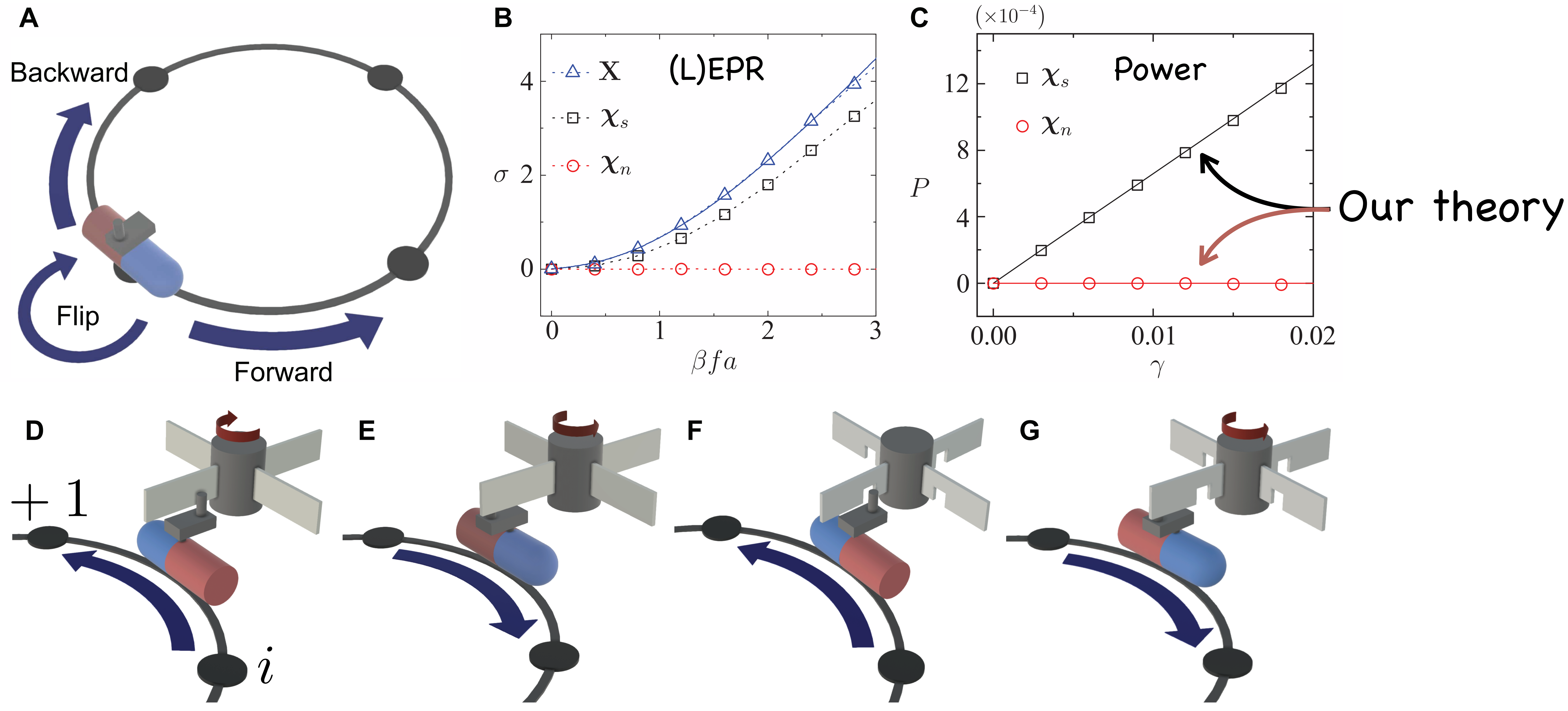
Work extraction

By weakly coupling a given d.o.f. to a work extraction mechanism we show that average power recorded by the mechanism is

$$\langle P \rangle = \frac{\gamma}{2} \langle \sigma(\chi) \tilde{W}(\chi) \rangle_{\chi}$$

Extractable work is 0 if EP is 0

RTP on a track

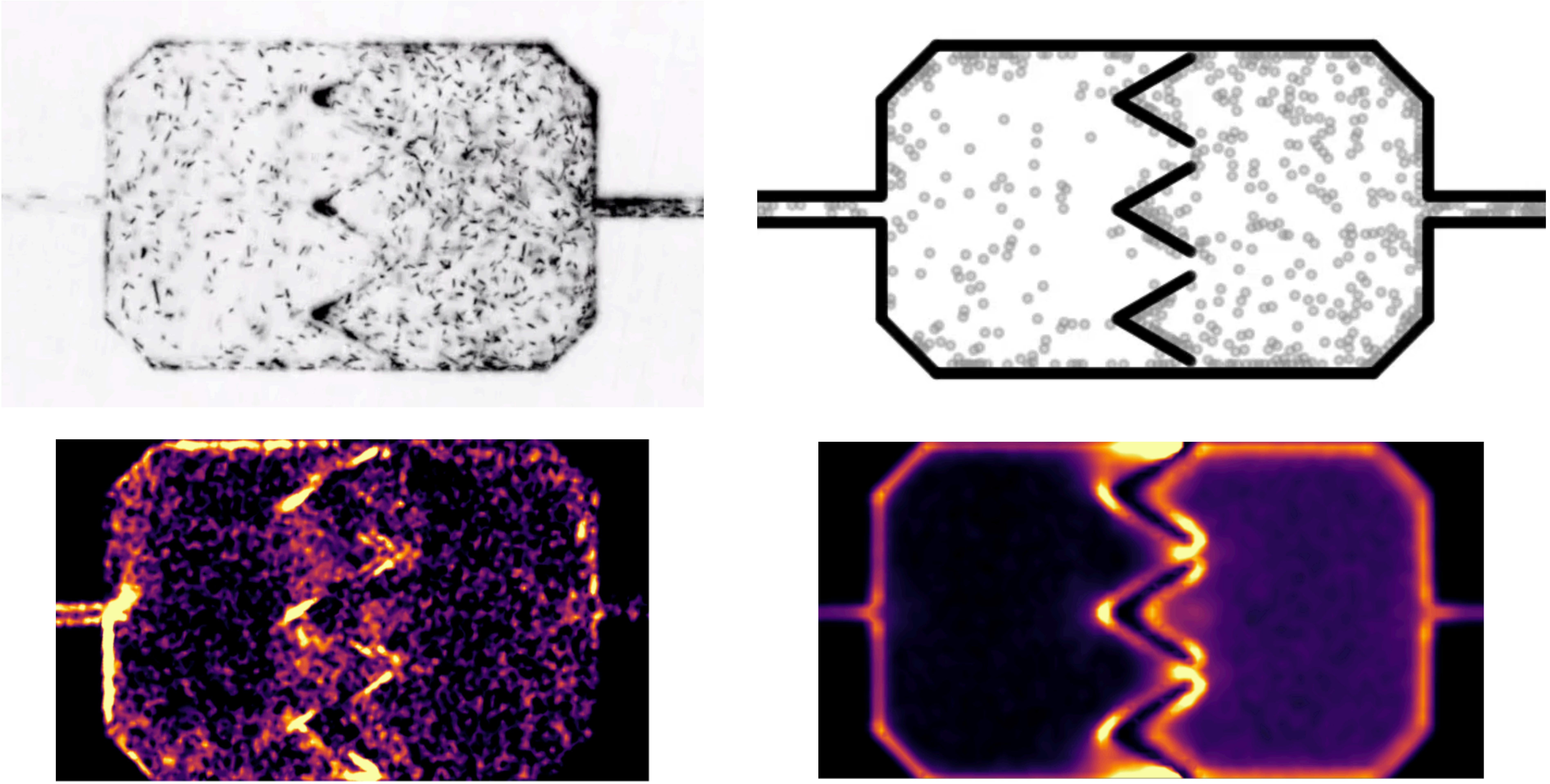


$$\chi_n = (|s_i|, |s_{i+1}|) \qquad \chi_s = (s_i, s_{i+1})$$

Ro, ..., **SM,** PRL, 129 (22), 220601 (2022)

Rectification in active matter

The asymmetry emerges from spatial symmetry breaking (provided by the wall) accompanied by time-reversal asymmetry in the trajectories

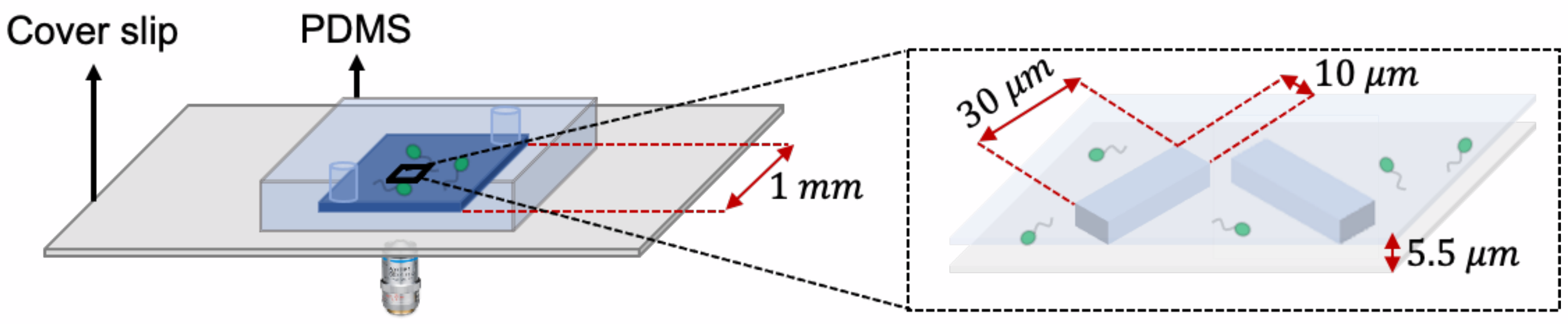


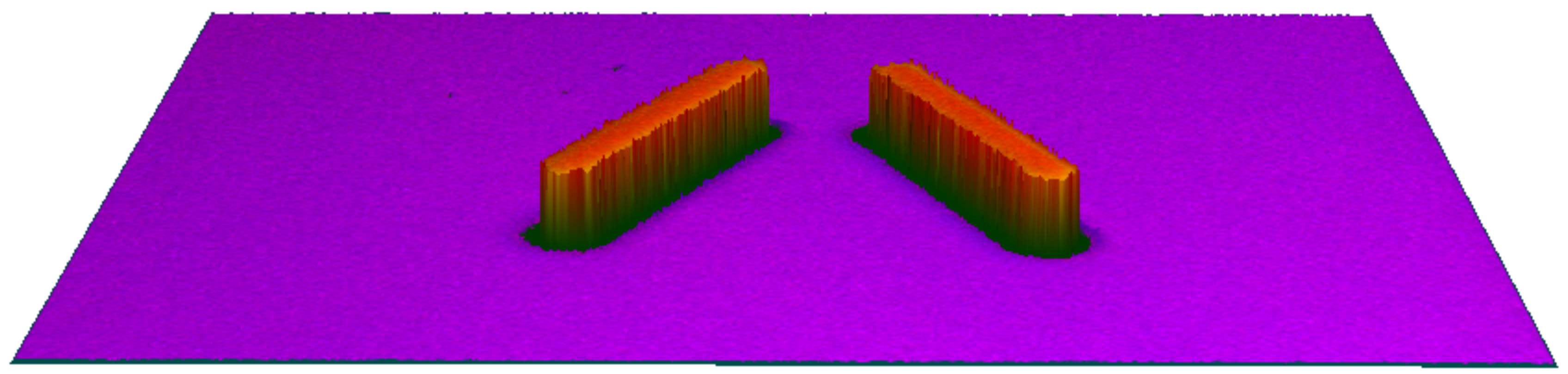
Ro, ..., **SM,** PRL, 129 (22), 220601 (2022)

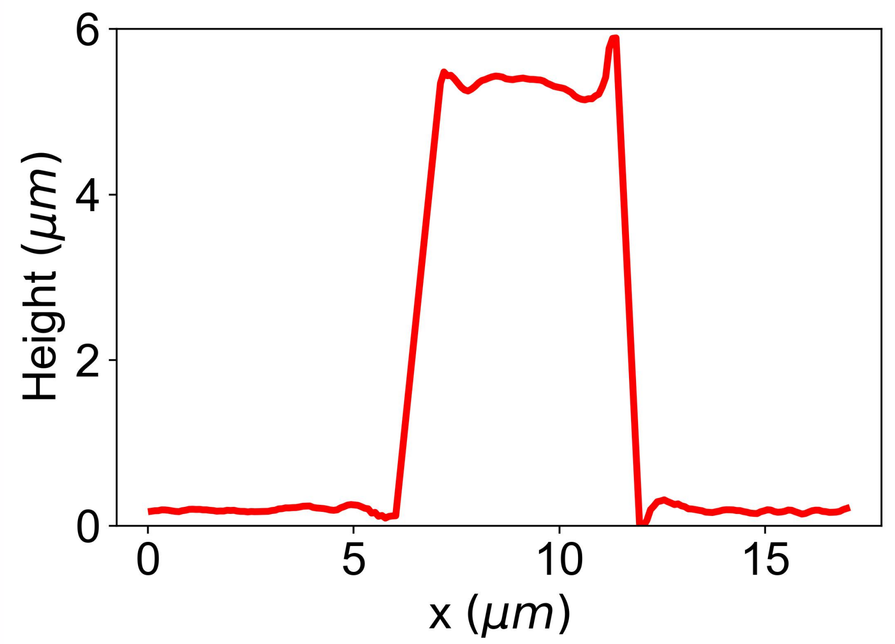
Experiments: A. Phan and R. Austin (Princeton)

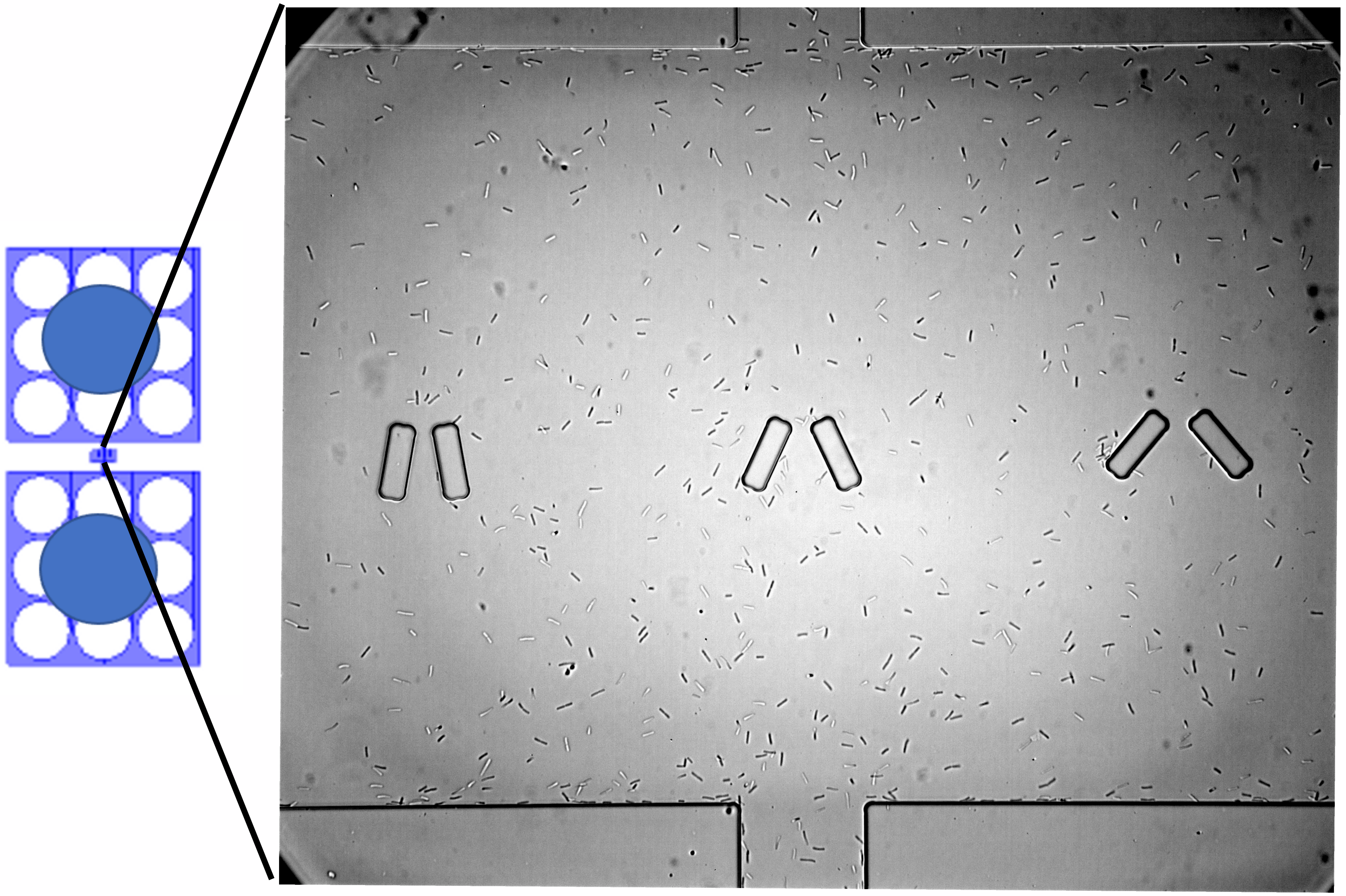
A mechanical model of rectification in active matter

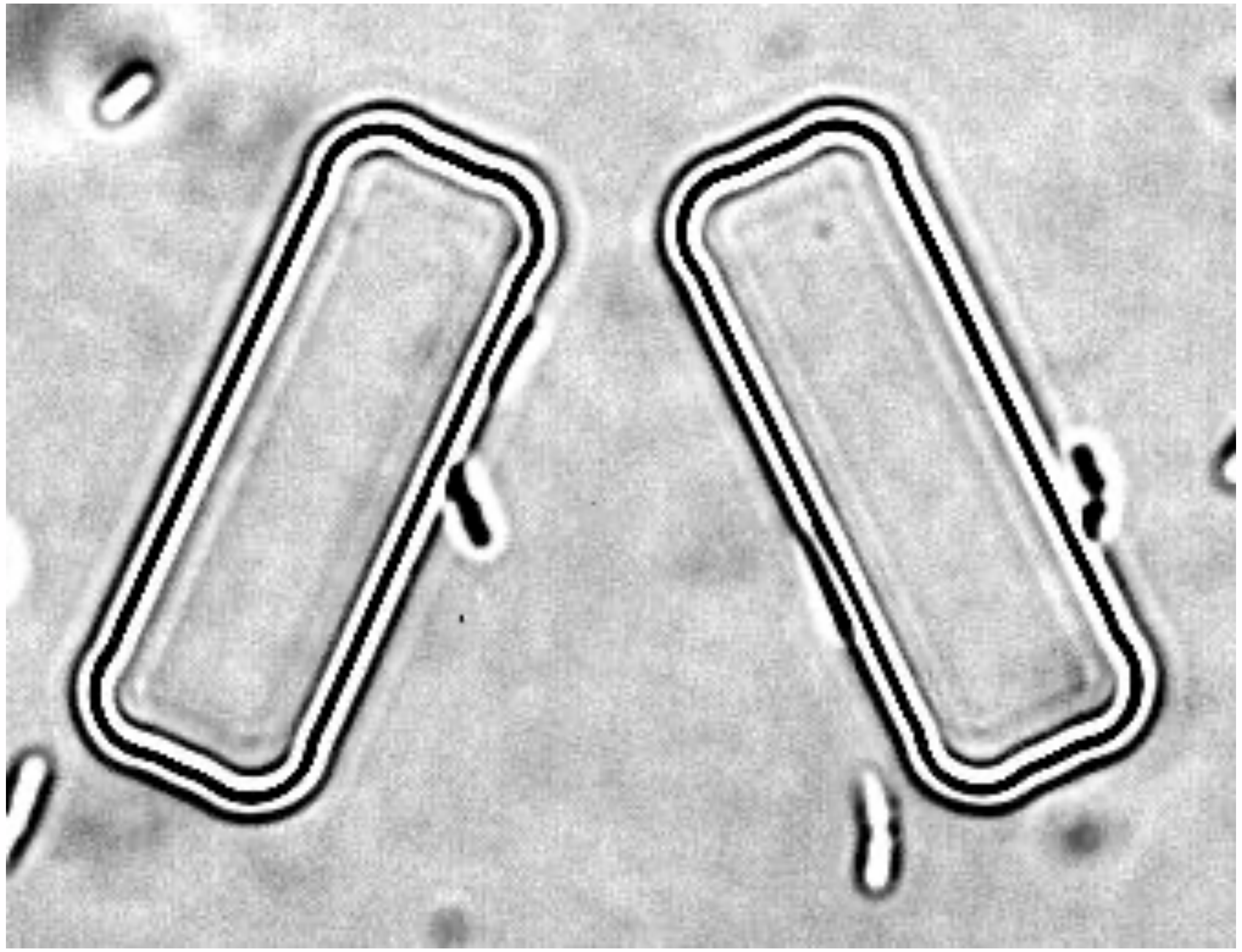
Experimental setup







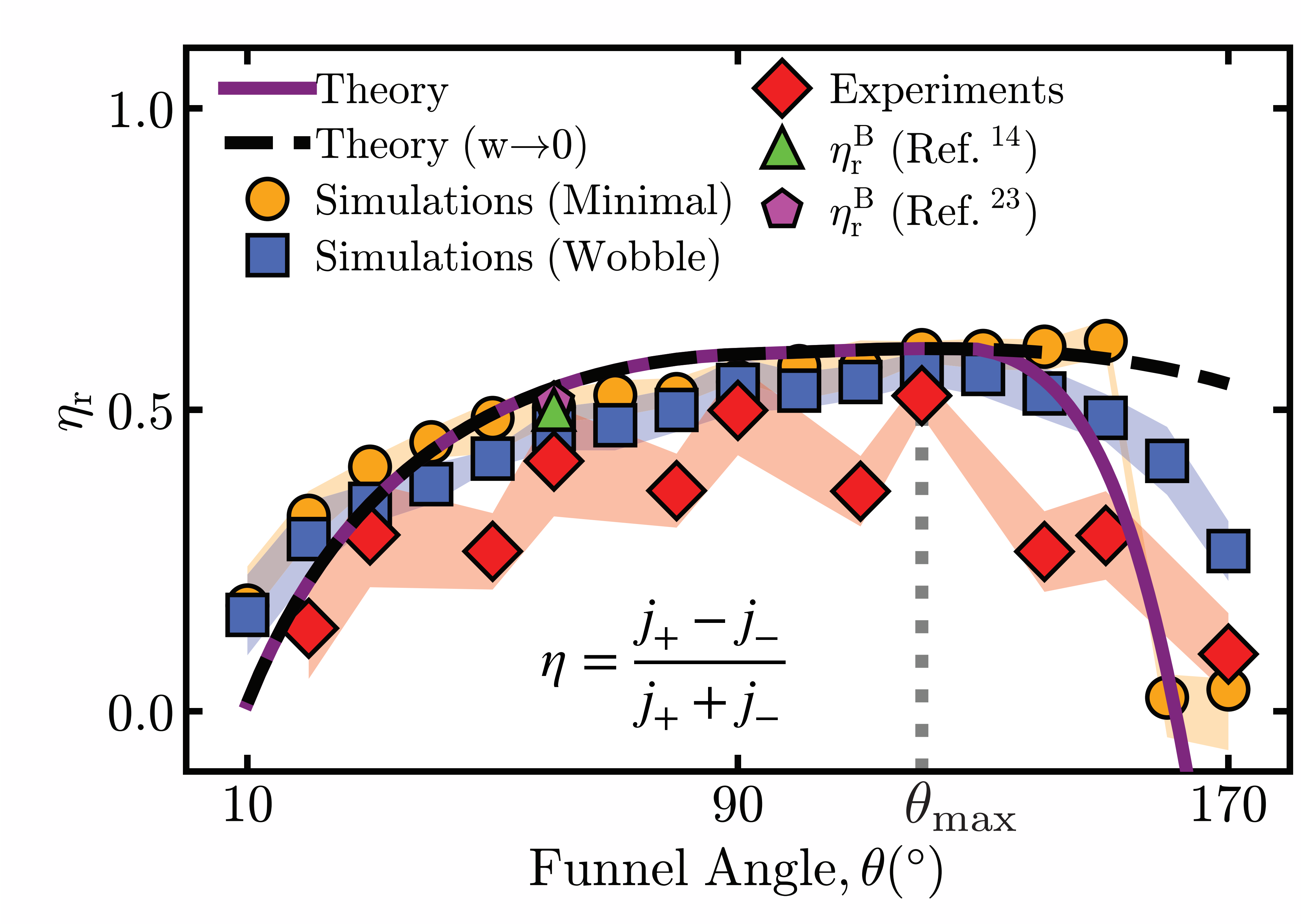




Anand, … **SM***, Cheng*, arXiv:2308.08421

A mechanical model of rectification in active matter

Parameter-free analytical model

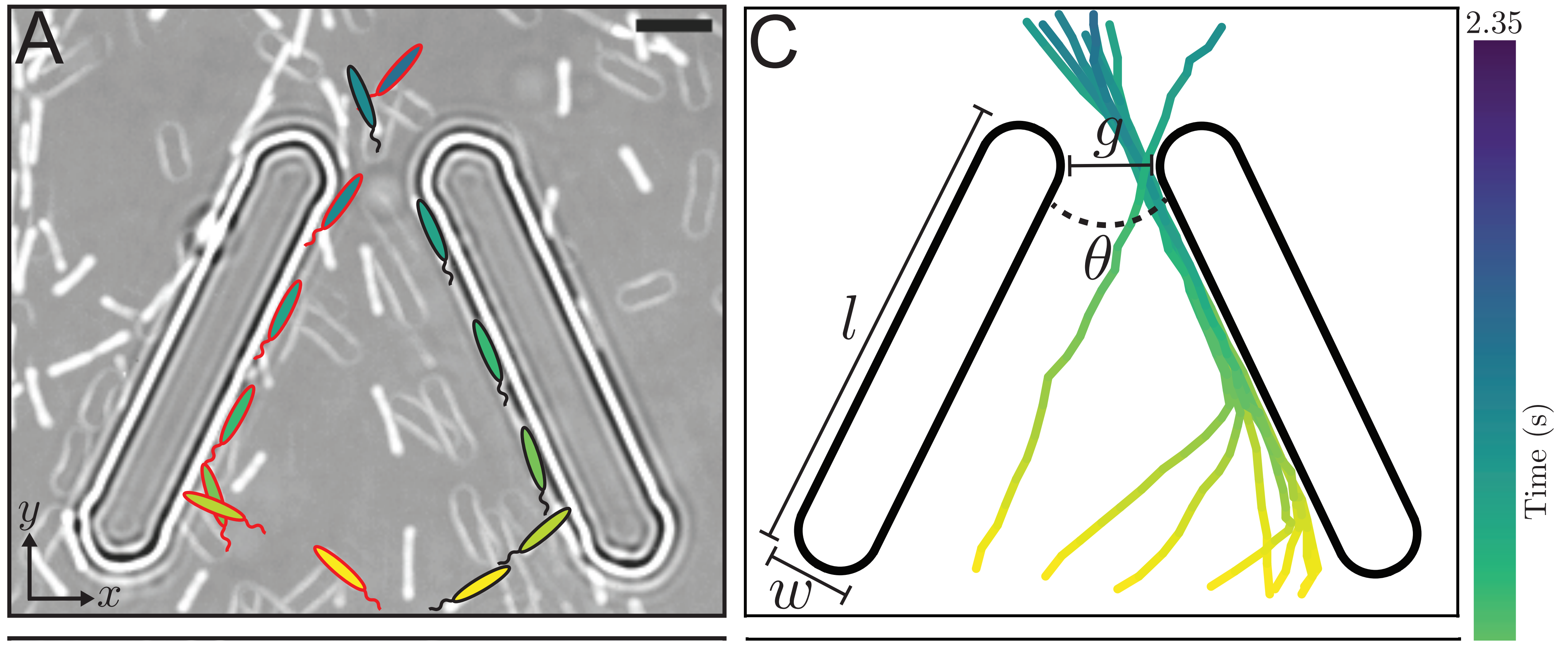


3 factors control bacterial rectification:

> A universal distribution of self-propulsion angles at gate

> Realignment along solid boundaries

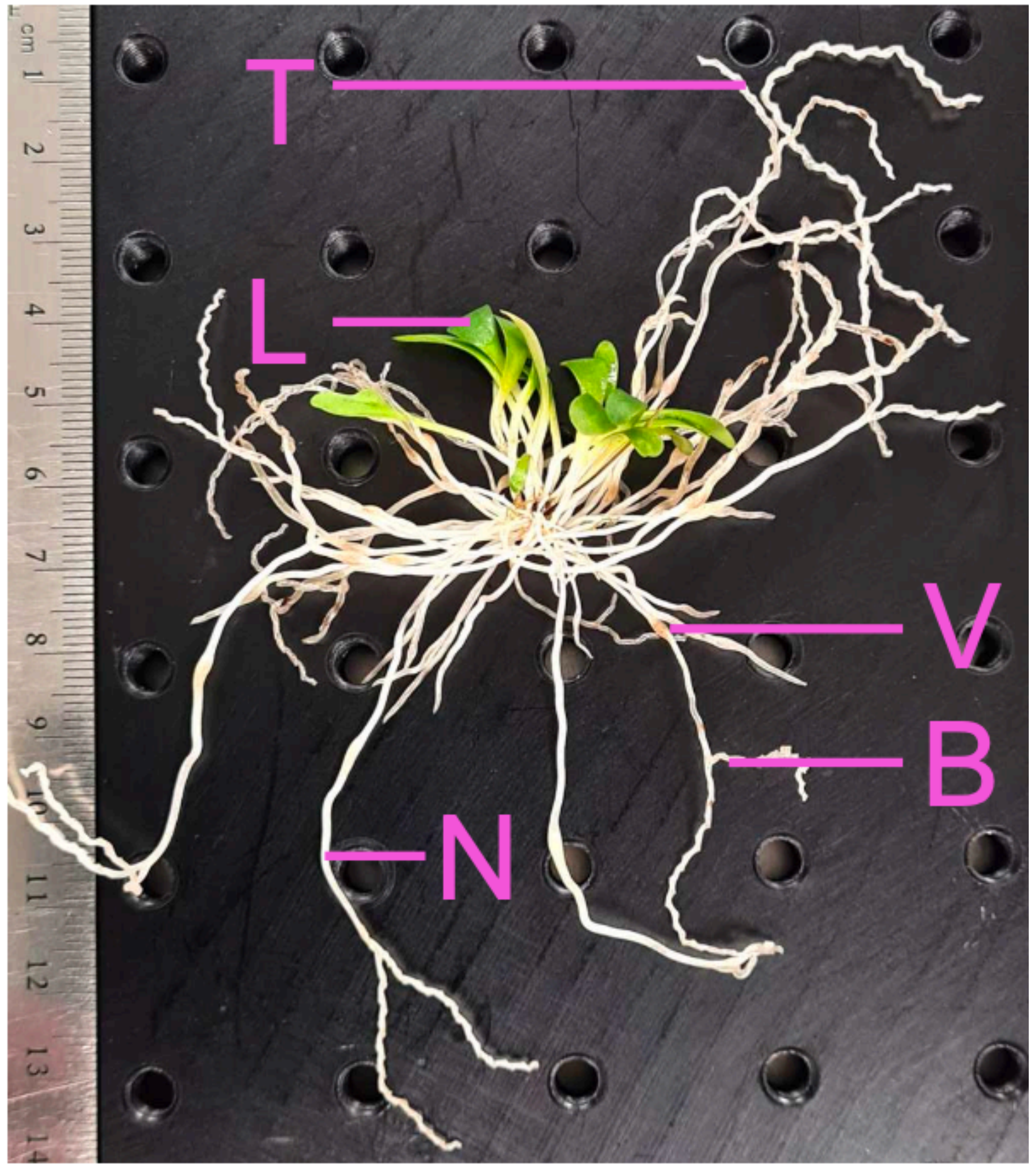
> Bacterial wobbling

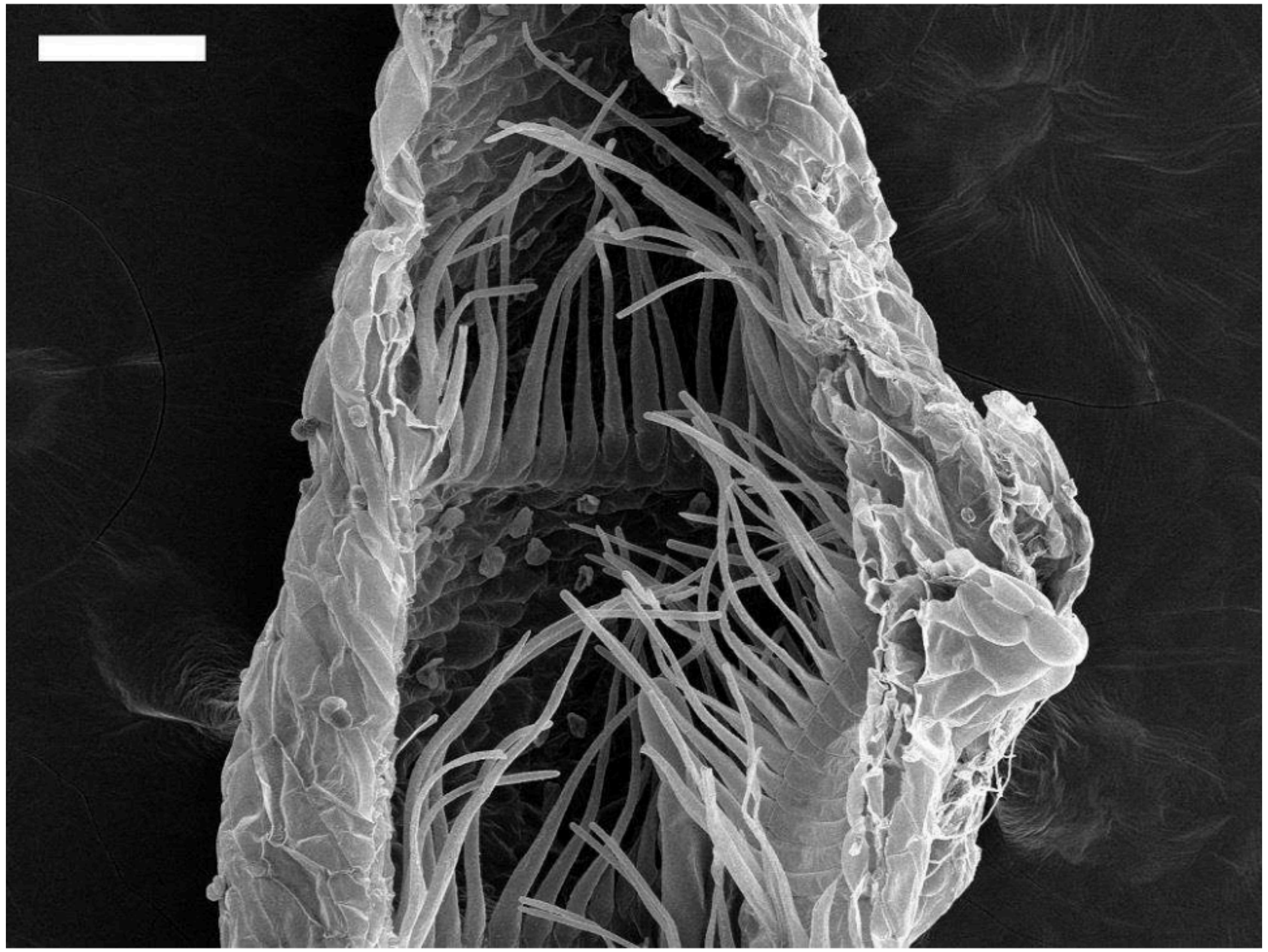


We can thus build a parameter-free model that predicts experimental and simulation results

Anand, … **SM***, Cheng*, arXiv:2308.08421

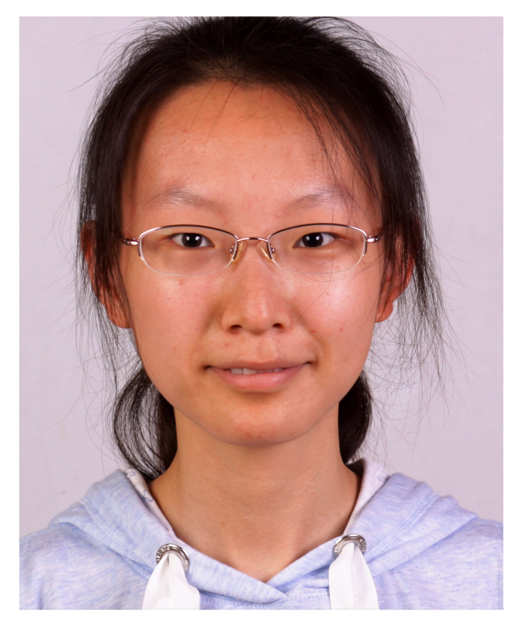
Active rectification is leveraged by carnivorous plants





Genlisea uses modified subterranean leaf structures (rhizophylls) to feed on microorganisms in the soil. The interior of rhizophylls present hairs with a 45–70° half angle, consistent with the 60° optimum that we predicted.

Martin-Roca et al., arXiv:2310.08216


Buming Guo
NYU


Satyam Anand
NYU


Aaron Shih
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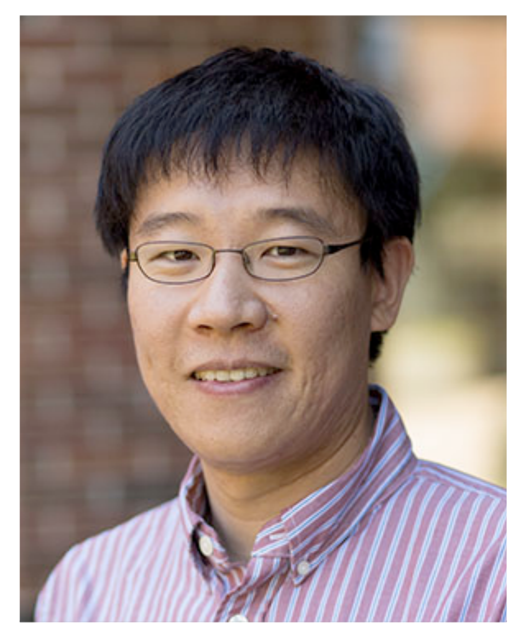
SIMONS FOUNDATION

NIH

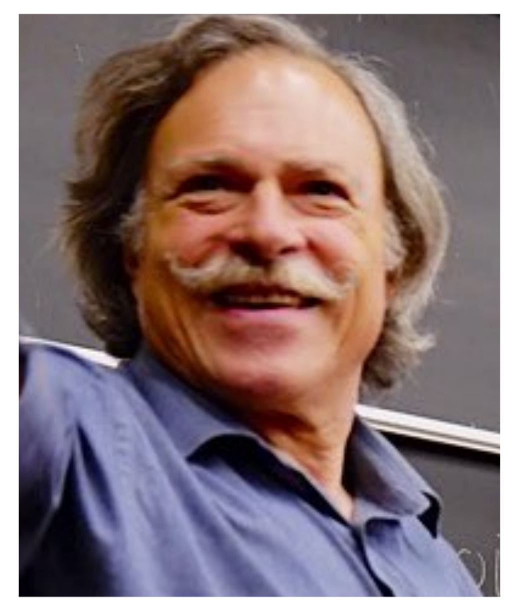
NSF


Sunghan Ro
Harvard


Xiang Cheng
UMN


Bob Austin
Princeton


Dov Levine
Technion


Paul Chaikin
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Daan Frenkel
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