Information entropy in complex systems: Mathematical foundations and their meaning

Karoline Wiesner
Institute of Physics and Astronomy
University of Potsdam

November 2021

In this talk

What is a complex system?

The role of information theory in complexity science

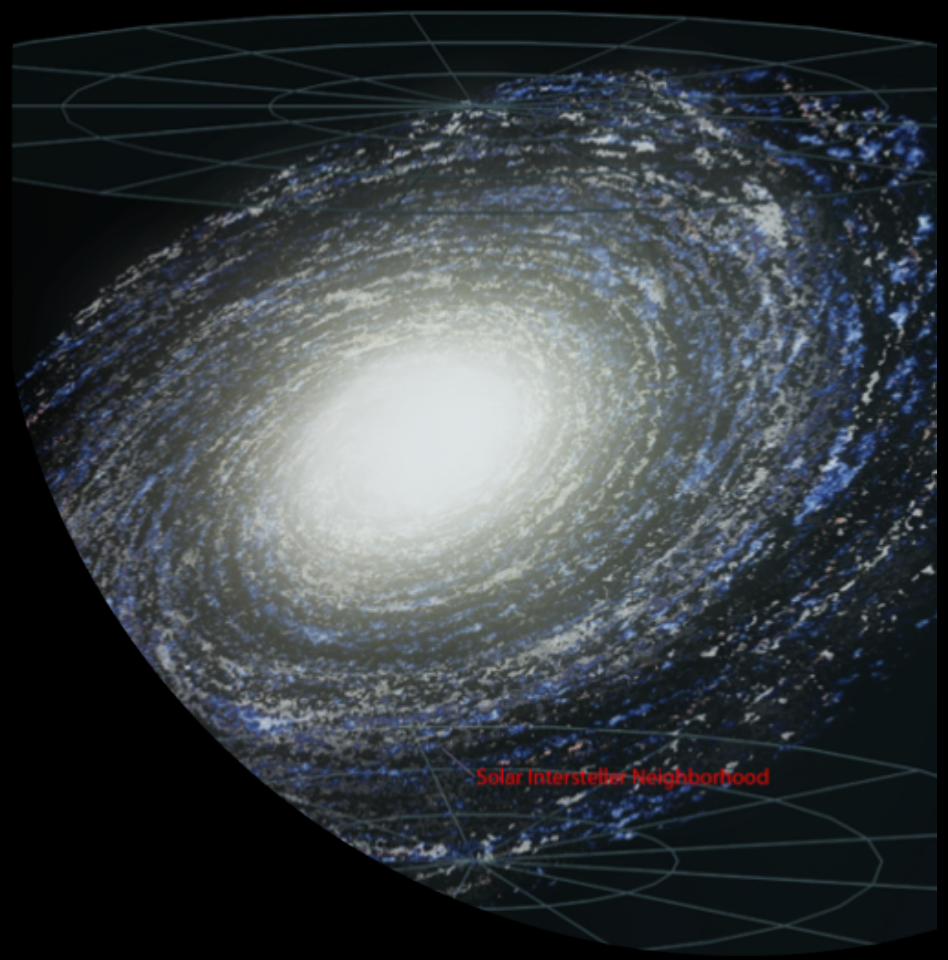
Examples in physics and biology

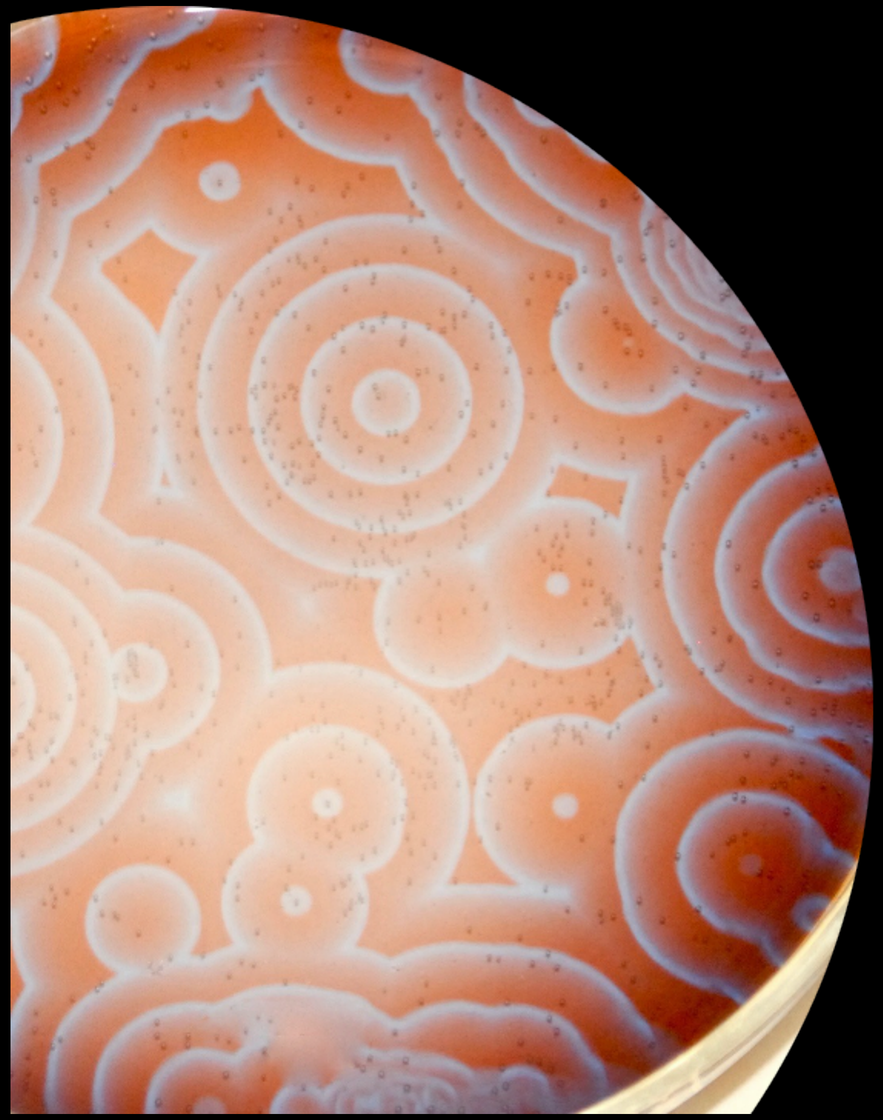
Cumulative Entropy and Complex Networks

What is a complex system?

“Many people might not bother to define complexity, thinking that we know it when we see it. Scientists and philosophers have no such luxury.”

Sean Carroll, Caltech (personal communication)






Longwave radiation
Lapse rate
Clouds
Water vapor
H_2O
Ocean circulation
Air-land CO_2 exchange and biogeochemical processes
Biogeophysical processes

Conditions for complexity

- **Numerosity**: complex systems involve many interactions among their components.
- **Disorder and Diversity**: the interactions in a complex system are not coordinated or controlled centrally, and the components may differ.
- **Feedback**: the interactions in complex systems are iterated so that there is feedback from previous interactions on a time scale relevant to the system's emergent dynamics.
- **Non-equilibrium**: complex systems are out of thermodynamic equilibrium with the environment and are often driven by something external.

Ladyman & Wiesner, What is a complex system?
Yale University Press (2020)

"In all complex systems the whole displays behavior that the individual parts cannot; this is called 'emergence'."

Philip Anderson, Science (1972)

Emergent features of complexity

- **Spontaneous order and self-organisation**: complex systems exhibit structure and order that arise out of the interactions among their parts.
- **Nonlinearity**: complex systems exhibit nonlinear dependence on parameters or external drivers.
- **Robustness**: the structure and function of complex systems is stable under relevant perturbations.
- **Nested structure**: there may be multiple scales of structure and clustering in complex systems.

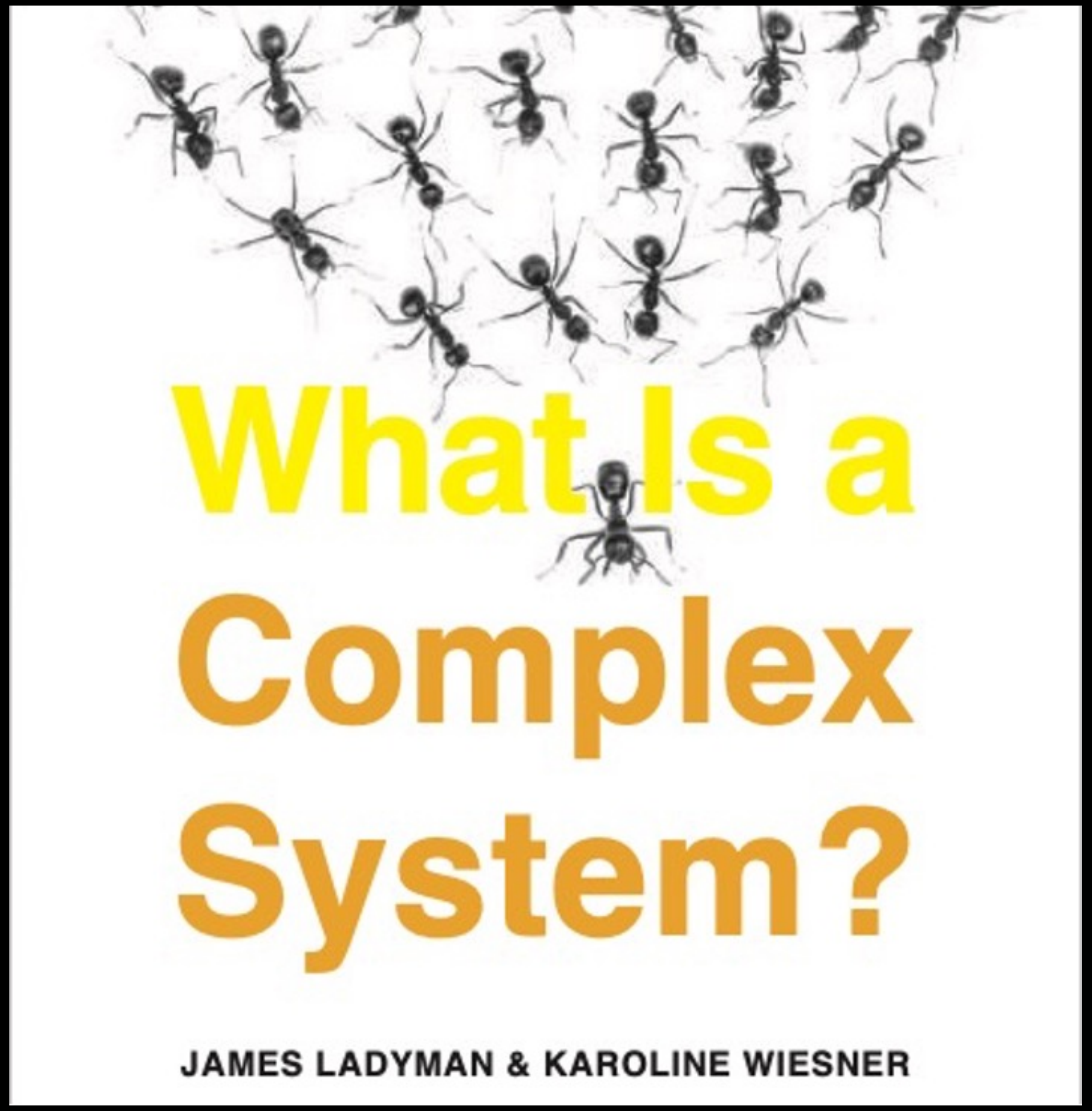
Ladyman & Wiesner, What is a complex system?
Yale University Press (2020)

Complexity in functional systems

- **Modularity**: there may be specialisation of function in complex systems.
- **History and Memory**: complex systems often require a very long his- tory to exist and often store information about history.
- **Adaptive behaviour**: complex systems are often able to modify their behaviour depending on the state of the environment and the predictions they make about it.

Ladyman & Wiesner, What is a complex system?
Yale University Press (2020)

A system is complex if it has some or all of…
… spontaneous order and self-organisation, nonlinear behaviour, robustness, history and memory, nested structure and modularity, and adaptive behaviour.



Book available at UP library as e-book and as paper copy at Golm library

Yale University Press (2020)

The role of information theory in complexity science

Shannon entropy measures randomness / disorder.

Shannon entropy of random variable X:

$$H(X) = -\sum_{x \in \mathcal{X}} P_X(x) \log P_X(x)$$

Mutual information measures correlations.

Mutual Information of two random variables X and Y:

$$I(X;Y) = \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} P_{XY}(xy) \log \frac{P_{XY}(xy)}{P_X(x) P_Y(y)}$$

Complexity is…

…disorder

…non-equilibrium

…numerosity

…diversity

…feedback

…nonlinearity

…robustness

…self-organisation

…nested structure

…adaptive behaviour

…memory

…modularity

To measure complexity is to measure…

Information theory can be used to measure…

…disorder

…non-equilibrium

…numerosity

…diversity

…feedback

…nonlinearity

…robustness

…self-organisation

…nested structure

…adaptive behaviour

…memory

…modularity

Complex systems are always correlated but rarely information processing

"There is a distinction between information processing – in the sense of encoding and transmitting a symbolic representation – and the formation of correlations (pattern formation / self-organisation).

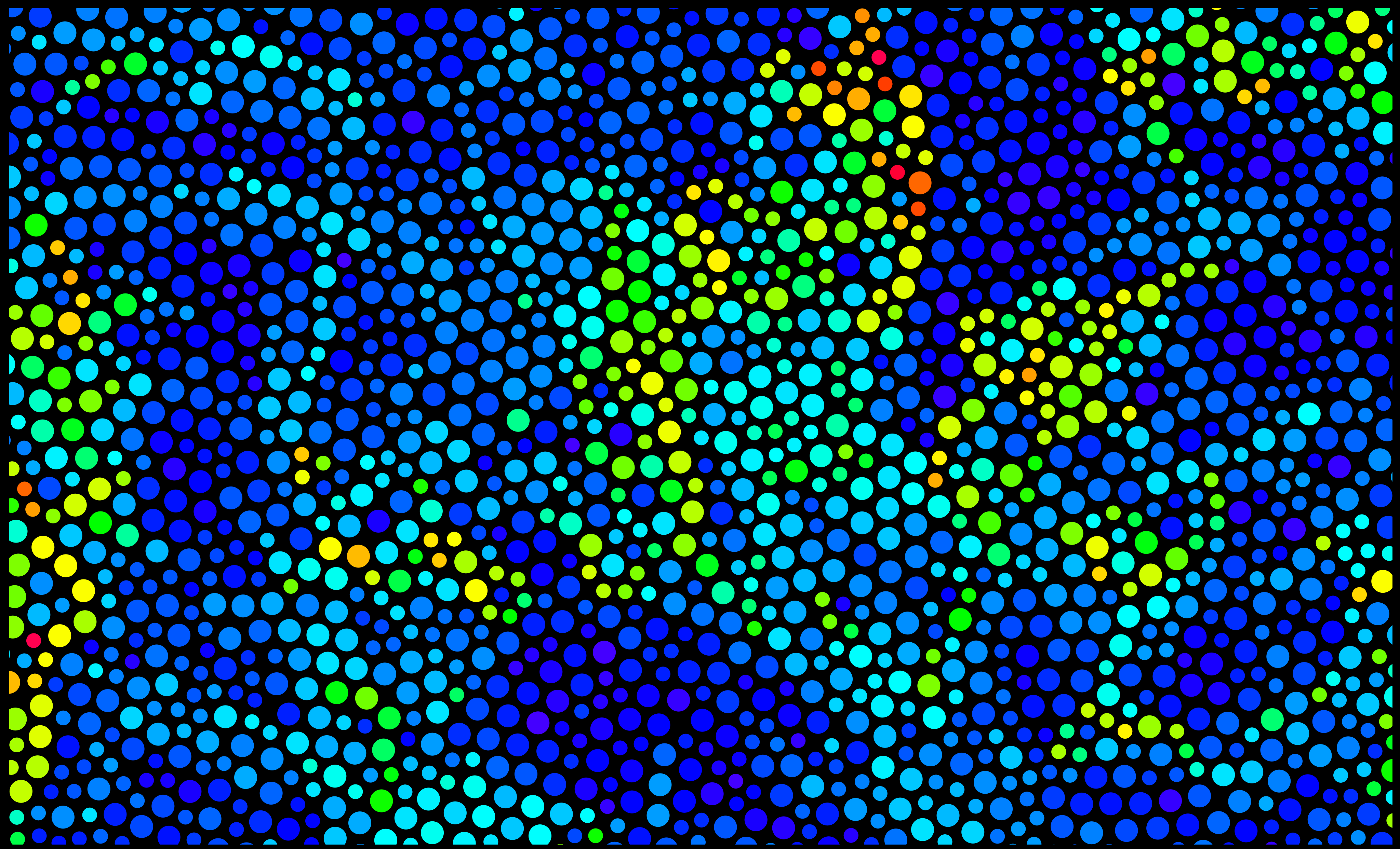
The study of both uses tools from information theory, but the purpose is very different in each case: explaining the mechanisms and understanding the purpose or function in the first case, versus data analysis and correlation extraction in the latter."

Karoline Wiesner and James Ladyman,
Journal of Physics: Complexity (in press).

Examples in physics and biology

Example 1

Finding a smoking gun for the onset of the glass transition in a colloidal system



A.J. Dunleavy, K. Wiesner, R. Yamamoto, and C.P. Royall. Mutual Information Reveals Multiple Structural Relaxation Mechanisms in a Model Glass Former. Nature Communications 6 *(2015).*

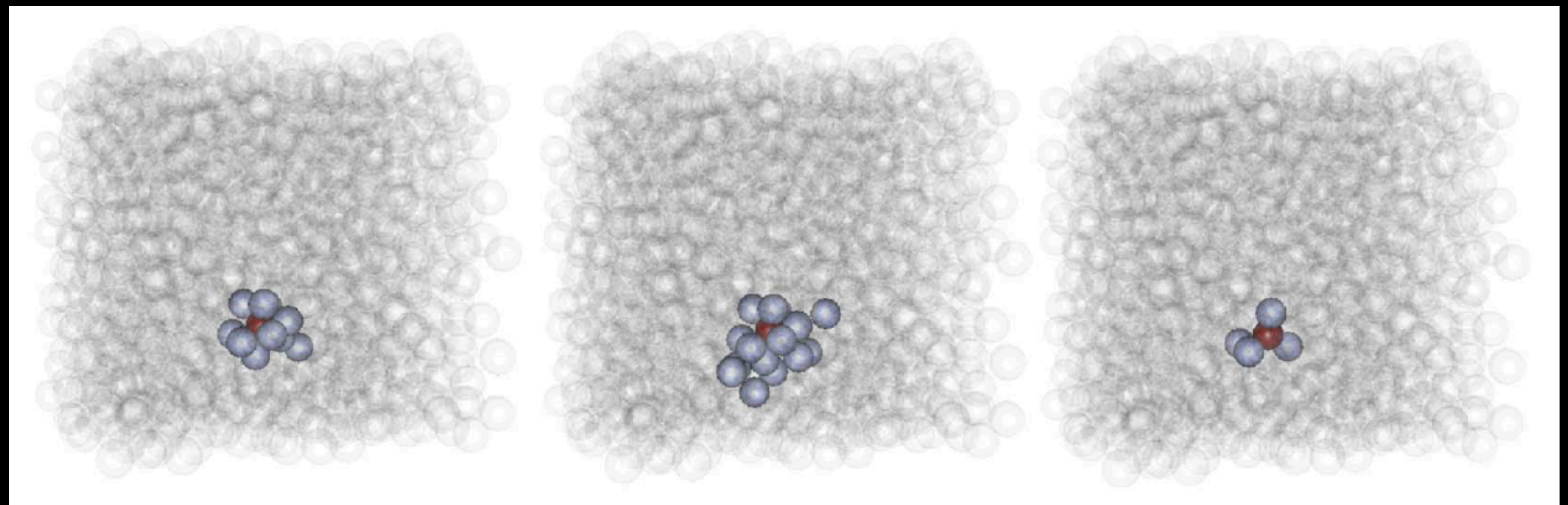
Engineering and Physical Sciences Research Council

Relaxation in a colloidal system is driven by correlations

probability density of displacement of particle i: $f_i(x_i)$

mutual information between particles i and j:

$$I_{ij} = \int f_{ij}(x_i x_j) \frac{f_{ij}(x_i x_j)}{f_i(x_i) f_j(x_j)} dx_i dx_j$$

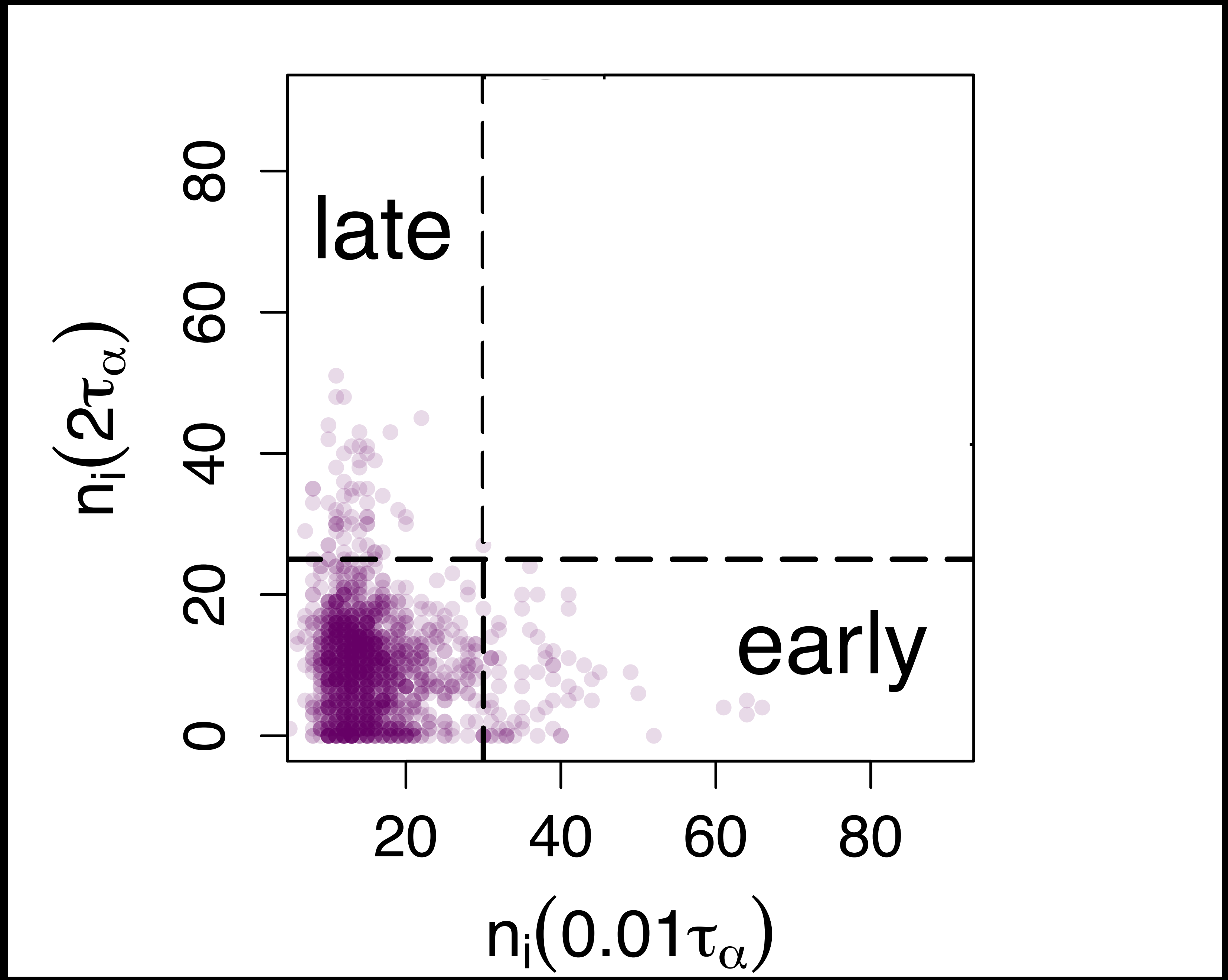


particles with
high correlation

Dunleavy, Wiesner,
Yamamoto, Royall
(*Nature Communications, 2015*)

time

Two types of particles: early movers and late movers

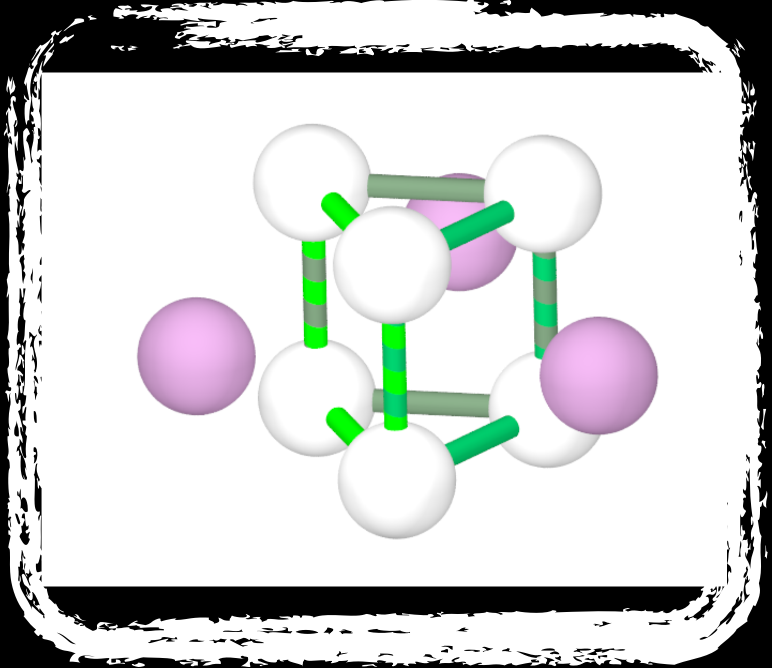


number of correlated partners later

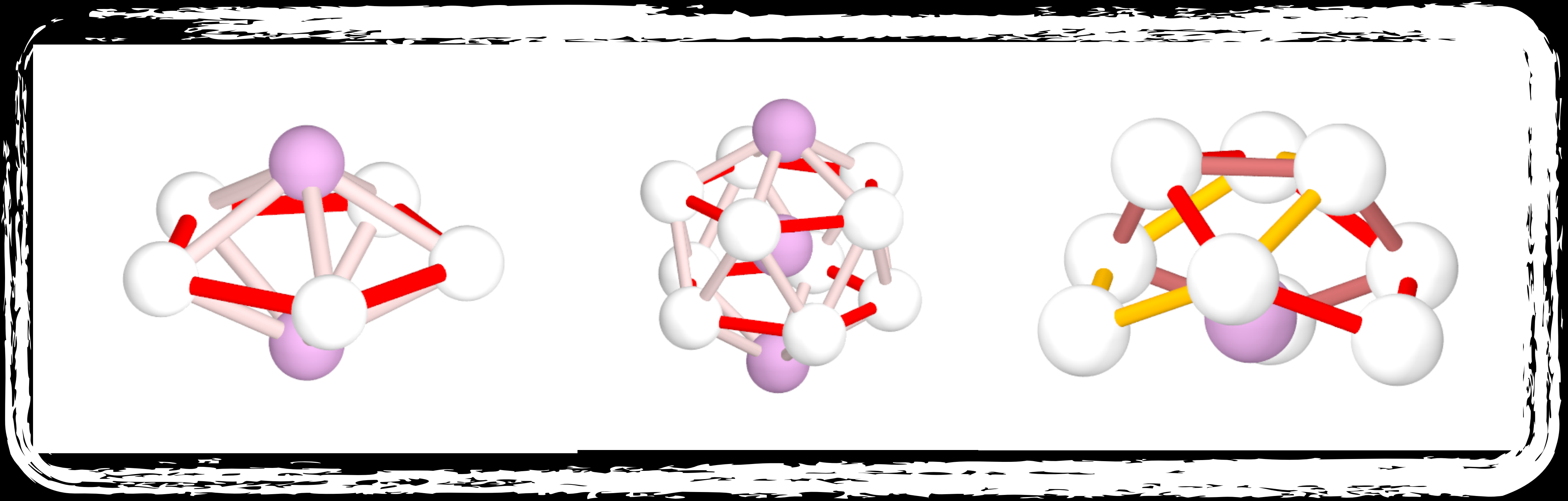
number of correlated partners early on

Dunleavy, Wiesner, Yamamoto, Royall (*Nature Communications, 2015*)

Initial configuration predicts players in relaxation mechanism



early movers

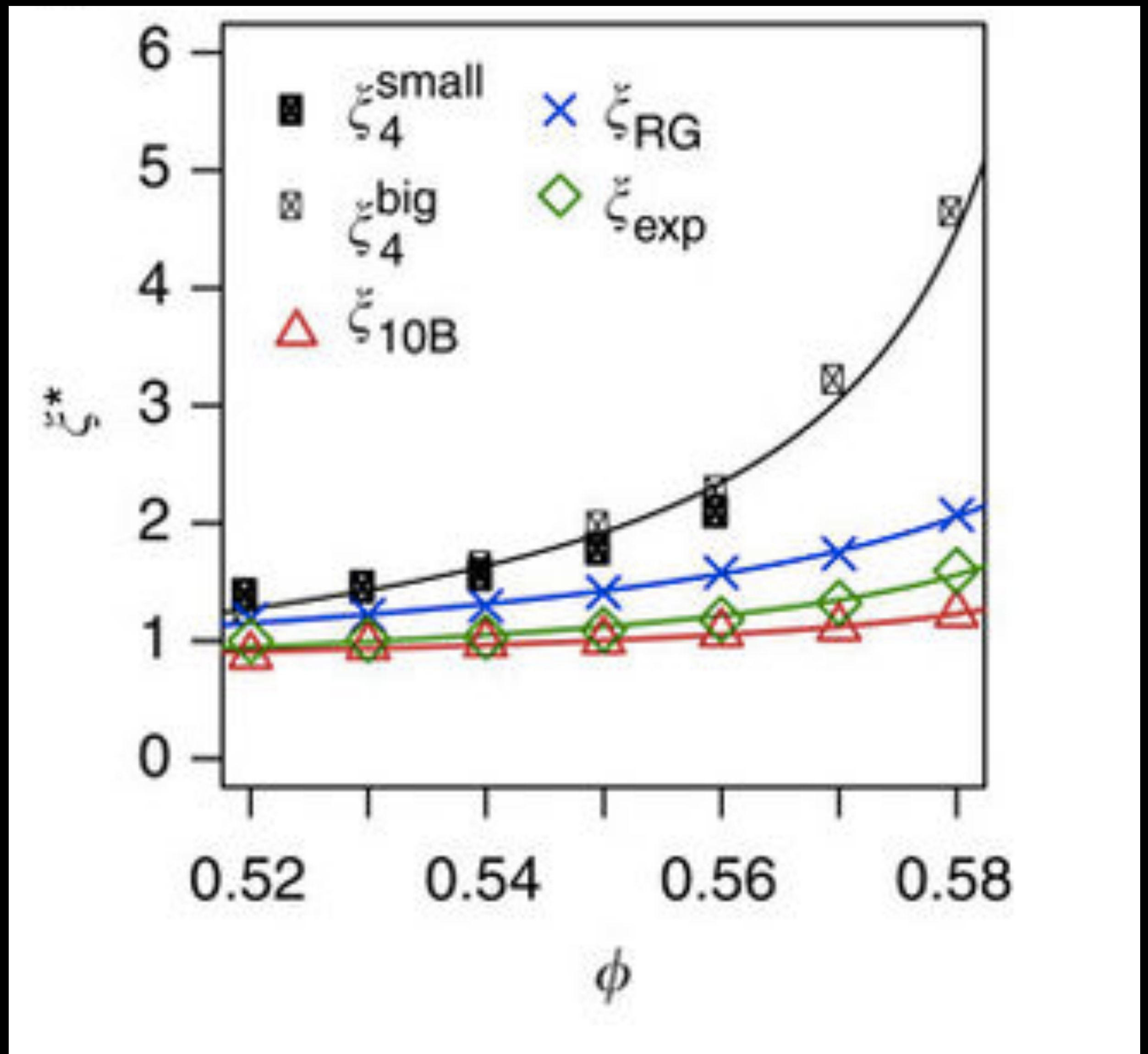


late movers

Dunleavy, Wiesner, Yamamoto, Royall (*Nature Communications, 2015*)

New length scale captures structure and dynamics

$$I(\mathbf{r},t) = \frac{\sum_{ij} I_{ij}(t)\delta(\mathbf{r} - |\mathbf{x}_i(0) - \mathbf{x}_i(0)|)}{\sum_{ij} \delta(\mathbf{r} - |\mathbf{x}_i(0) - \mathbf{x}_i(0)|)}$$



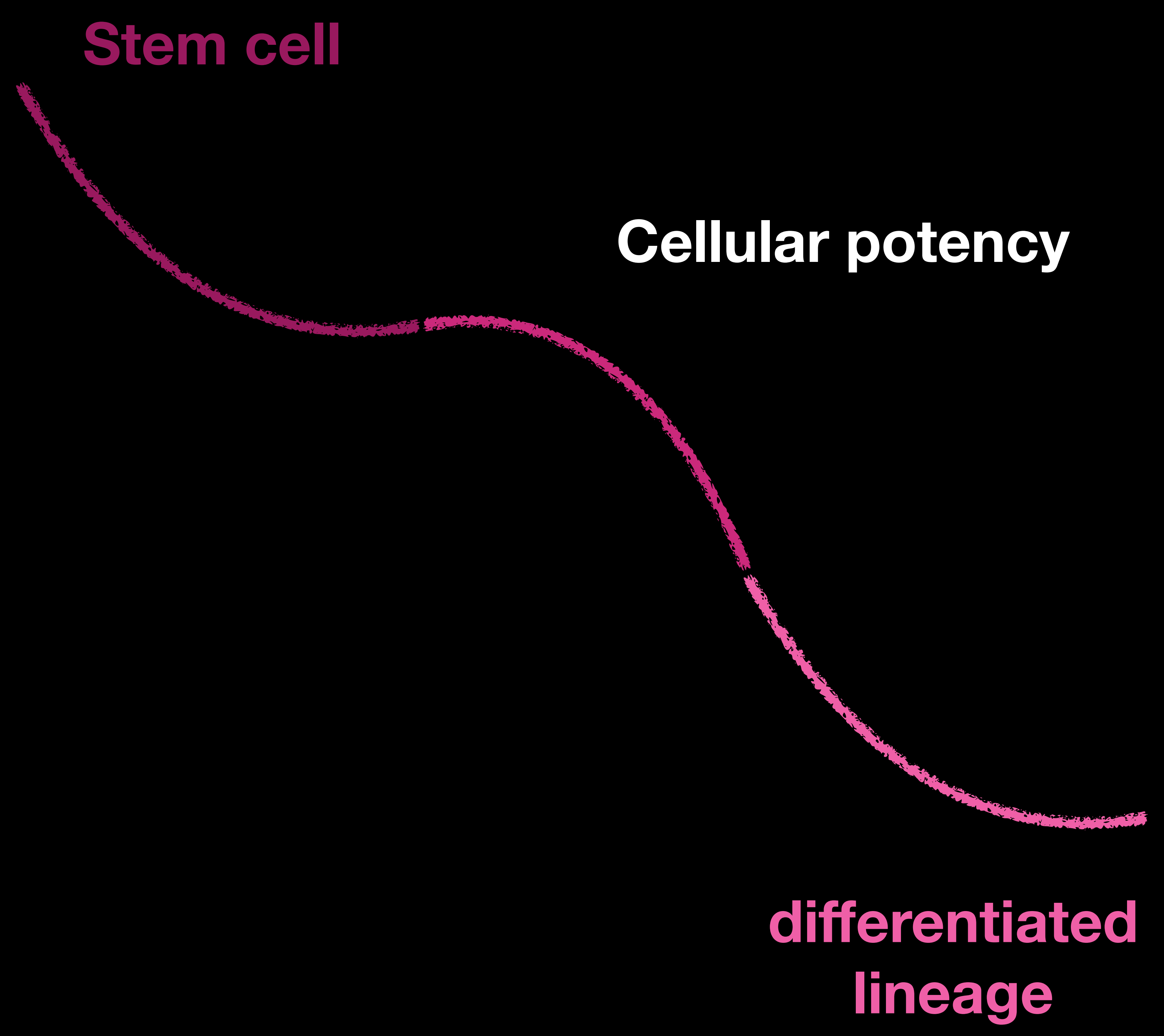
Fit an exponential function to define the length scale: ξ_{exp}

$$I(\mathbf{r},t) \propto e^{-\mathbf{r}/\xi_{exp}}$$

Dunleavy, Wiesner, Yamamoto, Royall (*Nature Communications, 2015*)

Example 2

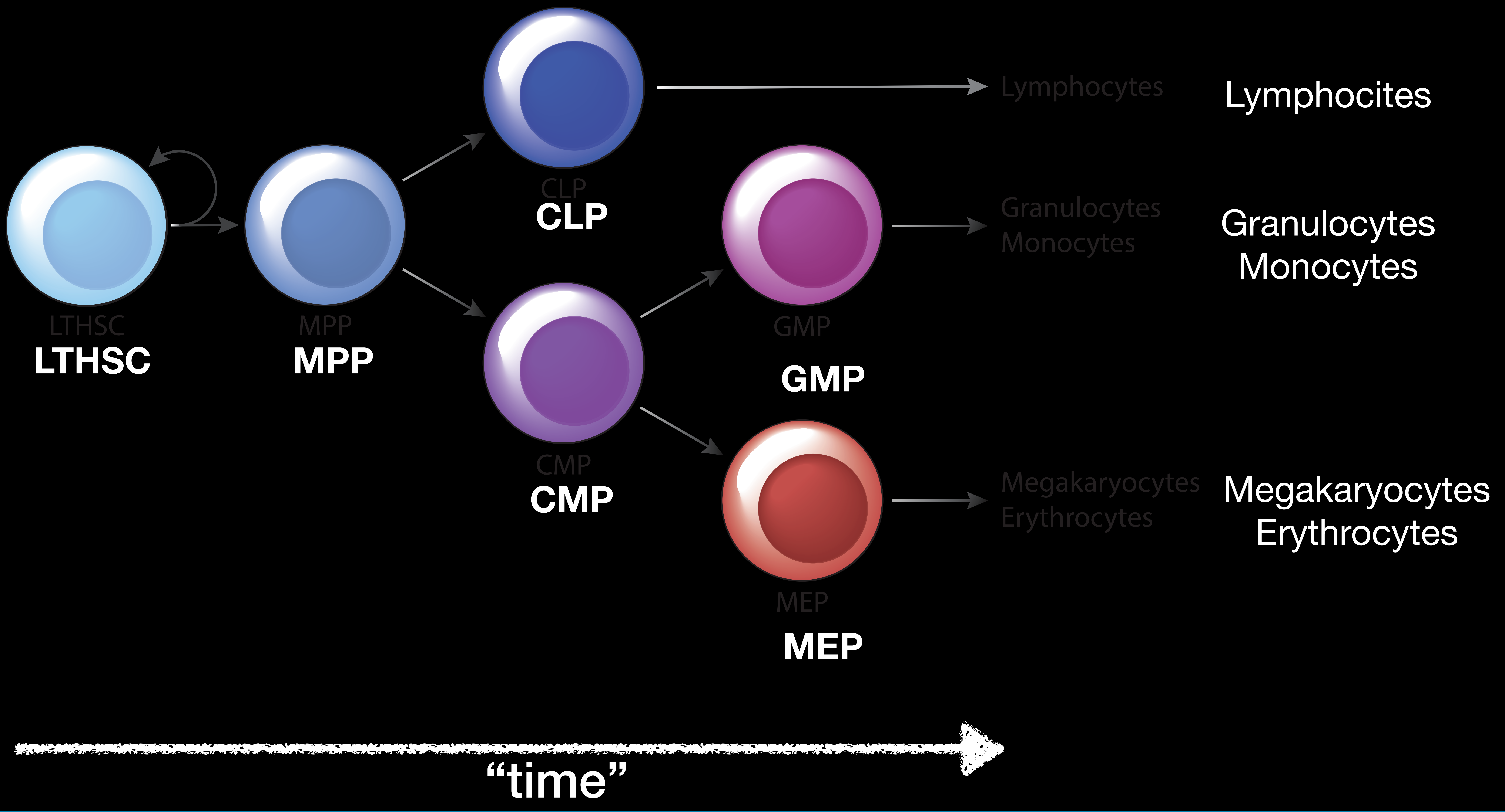
Finding the ‘point of no return’ in stem cell differentiation



Wiesner, K., Teles, J., Hartnor, M., & Peterson, C. (2018). Haematopoietic stem cells: entropic landscapes of differentiation. Interface focus, 8(6), 20180040.

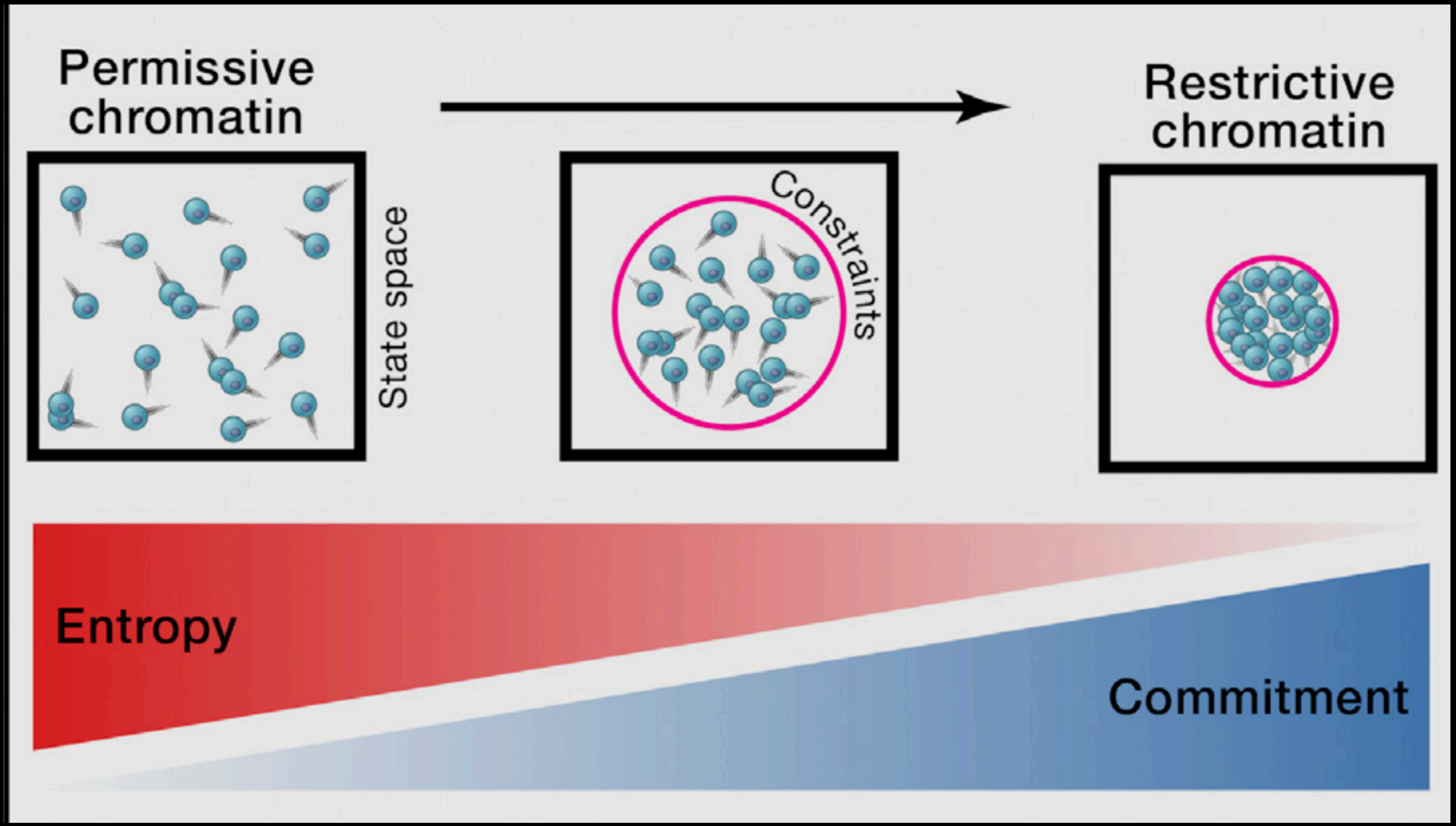
Engineering and Physical Sciences Research Council

Lineage tree of haematopoietic stem cell



Statistical mechanics analogy for stem cell development

Hypothesis by MacArthur et al. (Cell, 2013): Entropy monotonically decreases during differentiation



Experimental data for entropy measurements

Cell Stem Cell
Resource

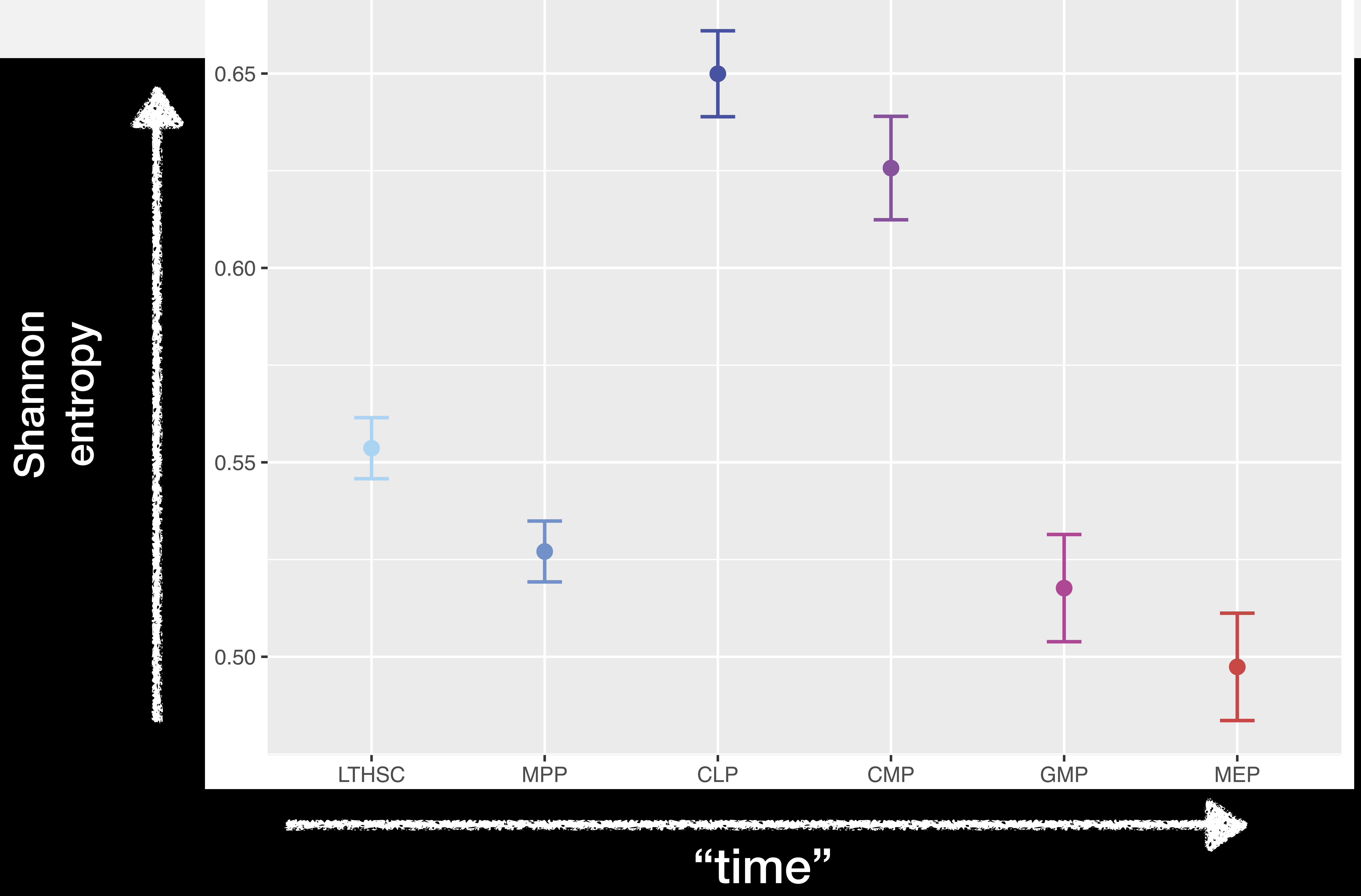
Mapping Cellular Hierarchy by Single-Cell Analysis of the Cell Surface Repertoire

Guoji Guo,[1] Sidinh Luc,[1] Eugenio Marco,[3] Ta-Wei Lin,[4] Cong Peng,[1] Marc A. Kerenyi,[1] Semir Beyaz,[1] Woojin Kim,[1] Jian Xu,[1] Partha Pratim Das,[1] Tobias Neff,[5] Keyong Zou,[6] Guo-Cheng Yuan,[3] and Stuart H. Orkin[1,2,*]

[1]Division of Pediatric Hematology/Oncology, Boston Children's Hospital and Dana-Farber Cancer Institute, Harvard Stem Cell Institute, Harvard Medical School, Boston, MA 02115, USA
[2]Howard Hughes Medical Institute, Boston, MA 02115, USA
[3]Department of Biostatistics and Computational Biology, Dana-Farber Cancer Institute, Harvard School of Public Health, Boston, MA 02115, USA
[4]Molecular Genetics Core Facility, Children's Hospital Boston, Boston, MA 02115, USA
[5]Pediatric Hematology/Oncology/BMT, University of Colorado, Aurora, CO 80045, USA
[6]Boston Open Labs, Cambridge, MA 02138, USA
*Correspondence: stuart_orkin@dfci.harvard.edu
http://dx.doi.org/10.1016/j.stem.2013.07.017

					Bax	Aebp2	CD63	Cdkn2a	Cdkn2c	CD48	Pax5	Gapdh	Cdkn2d	Hes5
					10.29	6.91	0	1.54	10.92	10.54	9.68	12.38	12.37	0
					8.6	6.13	0	0	7.93	4.18	11.62	11.36	9.58	0
					5.64	4.45	0	0	4.4	0	9.34	5.85	4.29	2.85
					7.78	4.38	0	5.41	0	7.57	9.92	10.65	7.97	0
					11.98	5.61	0	5.3	9.52	9.6	10.83	13.19	10.99	0
					9.77	4.4	0	6.56	0	10.74	8.13	11.28	0	0
					10.23	5.99	0	5.1	0	11.23	0	9.84	0	0
					8.38	3.31	0	0	10.23	9.62	0	10.66	10.54	0
					8.93	4.53	0	0.48	0	10.01	0	10.29	1.88	1.66
					9.38	3.37	0	0	8.41	9.61	0	9.04	7.98	0
					11	6.25	0	2.3	8.18	11.75	0	11.52	8.84	0
					10.47	5.89	7.62	7	0	10.21	0	10.97	0	3.12
					9.93	7.5	0	0	9.63	10.76	0	11.85	11.26	0
					9.62	6.69	0	3.46	0	9.95	8.35	11.13	7.94	0
					11.99	7.15	0	0	8.96	12.23	10.39	13.36	10.32	6.34
					9.29	5.11	0	3.58	8.7	10.15	0	12.04	10.82	0
					7.96	7.11	0	0	9.66	9.2	9.77	12.19	0	0
CLP	[illegible]	0	0	0	5.2	7.18	0	0	8.35	9.96	0	9.02	8.45	0
CLP	0	0	0	0	0	5.57	0	0	0	0	0	4.23	0	0
CLP	0	0	0	0	0	2.83	7.76	0	0	0	0	8.74	0	5.75
CLP	9.62	0	8	7.77	8.25	6.39	0	2.71	0	9.67	0	12.35	9.11	0
CLP	0	2.84	8.86	0.37	9.72	6.49	0	7.23	10.11	9.11	11.01	12.4	11.49	0
CLP	10.38	0	0	10.92	7.89	5.01	0	0	8.44	10.93	0	10.28	0	0
CLP	10.68	0	0	4.99	10.65	5.68	0	5.96	0	9.88	0	10.03	8.86	0
CLP	10.35	8.18	0	0	9.76	6.2	0	0	8.19	11.32	0	10.59	7.37	0
CLP	9.1	9.97	0	0	10.86	7.28	0	0	0	9	0	10.92	0	0
CLP	8.13	0	0	0	10.46	5.74	0	0	7.19	10.88	0	10.08	4.57	0
CLP	7.15	0	10.87	0.62	11.23	8.17	0	7.51	0	12.37	0	13.21	9.37	0
CMP	12.07	0	0	0	9.02	5.9	6.94	0	0	11.76	0	8.59	0	0
CMP	10.39	9.63	0	0	9.89	6	9.24	0	0	12.65	0	13.23	8.91	0
CMP	0	11.58	0	4.09	0	4.16	0	0	0	7.7	0	9.25	7.73	0
CMP	7.67	11.18	0	0	8.06	5.95	6.93	5.04	0	10.45	0	10.54	8.53	0
CMP	11.08	10.03	0	0	10.77	7.48	9.15	2.94	9.47	12.1	0	13.9	0	0

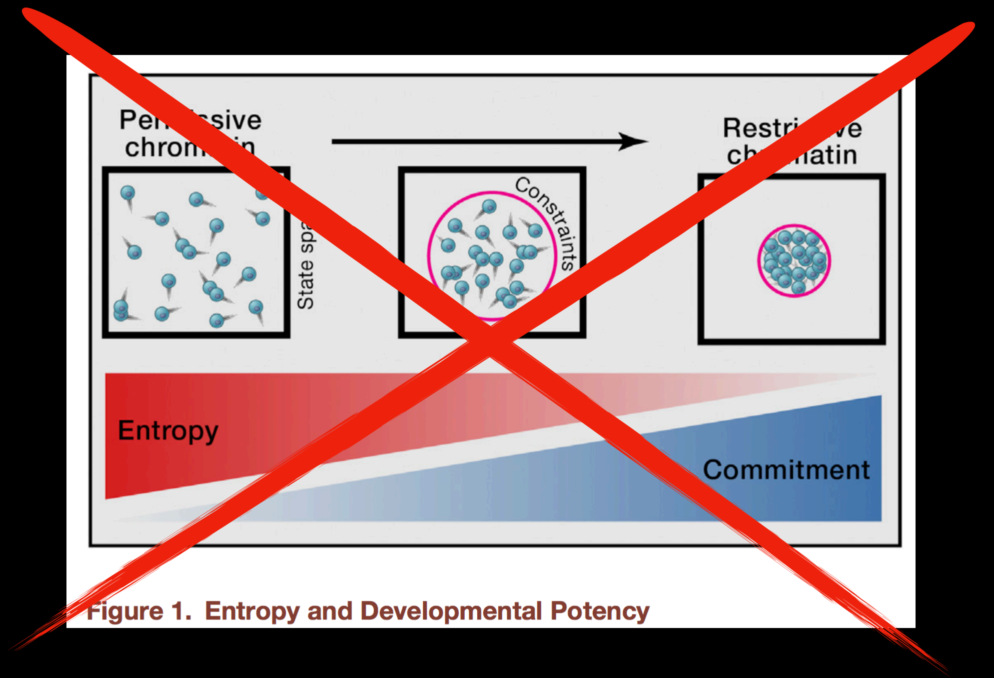
Entropy ‘peaks’ during differentiation.

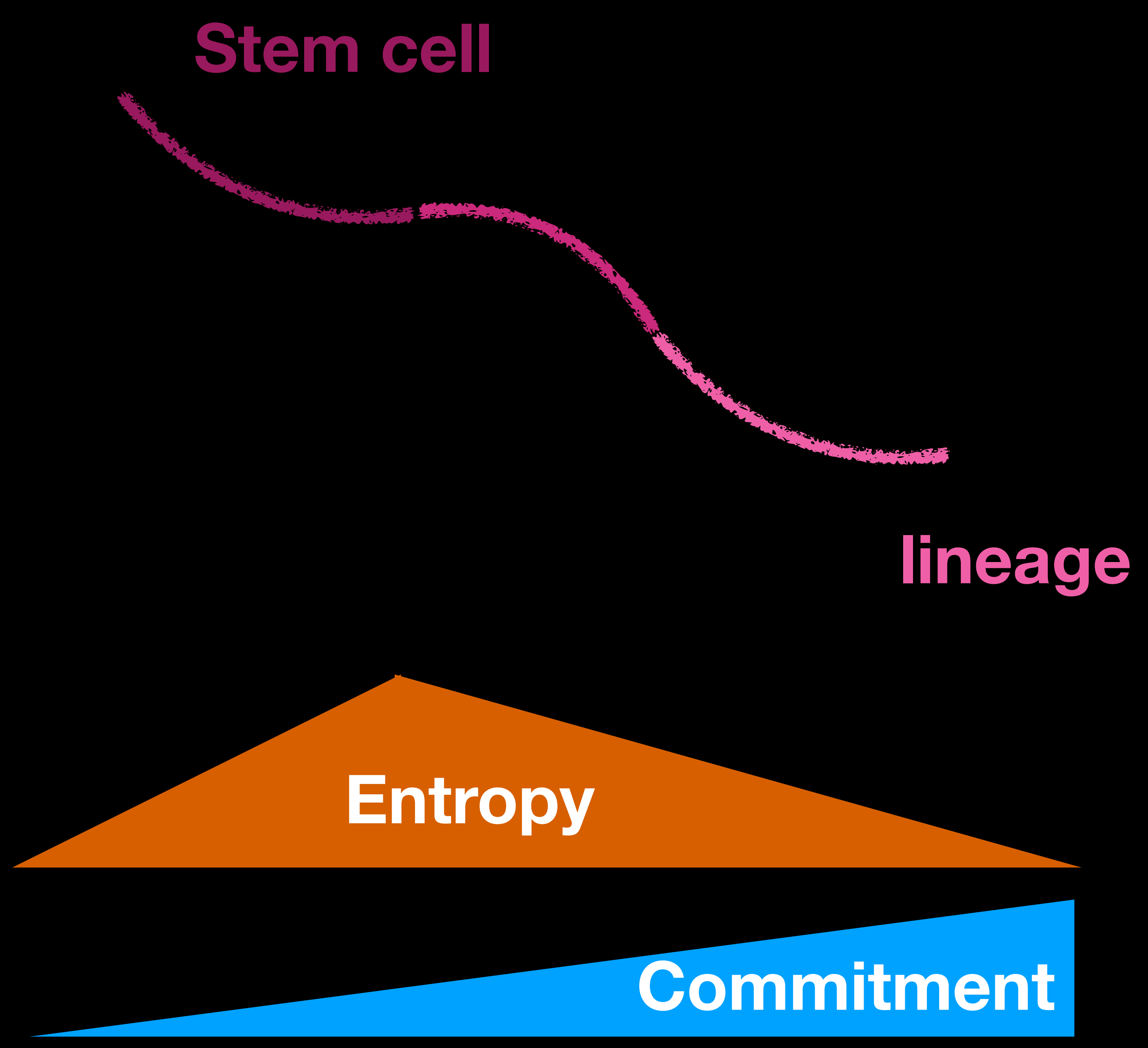


Wiesner et al., Interface Focus (2018)

Contrary to expectations: entropy goes through a maximum during differentiation

Biological interpretation: Opening up of several pathways toward final cell lineages.





Wiesner et al., Interface Focus (2018)

Example 3

Stability of networks

Is the Shannon entropy a good measure of network robustness?

Network robustness: Molloy-Reed criterion

'Critical fraction': fraction of nodes to be removed (on average) before network falls apart.

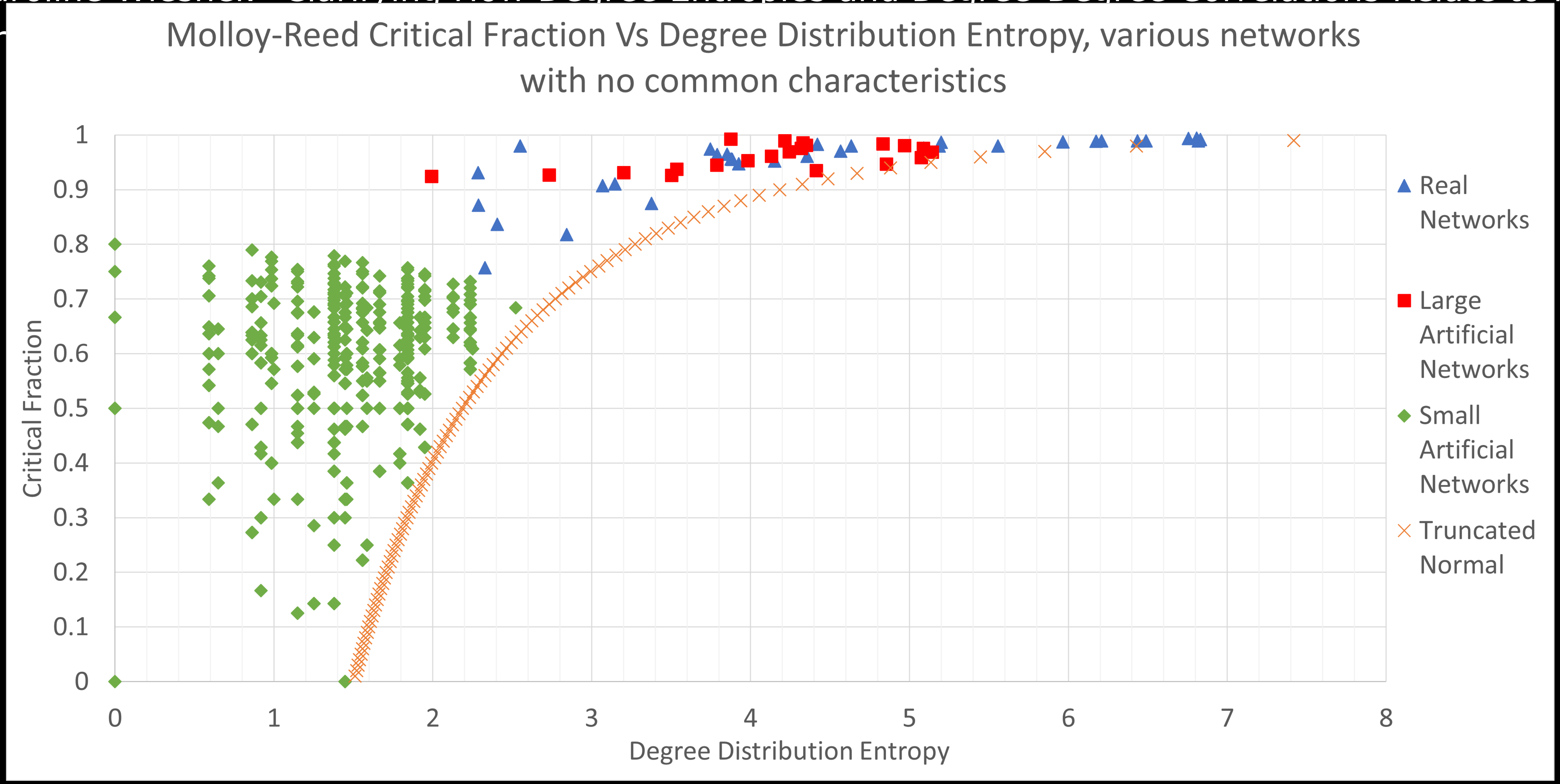
Average degree:

A randomly configured network will have a giant component, if

The critical fraction is then given by the formula

Degree distribution entropy gives lower bound to robustness

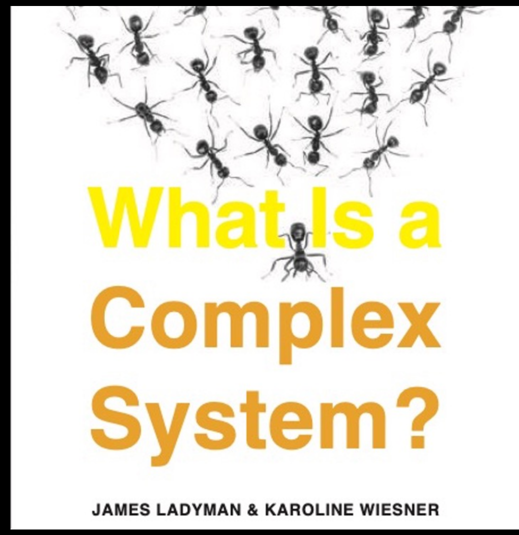
Jones, Chris, and Karoline Wiesner. "Clarifying How Degree Entropies and Degree-Degree Correlations Relate to Network Robustness." ar



Thank you

cumulative entropy

Wiesner, K. Cumulative entropy (working title). in draft form.

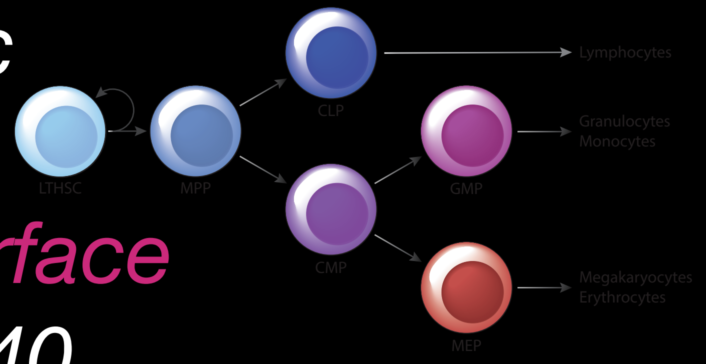


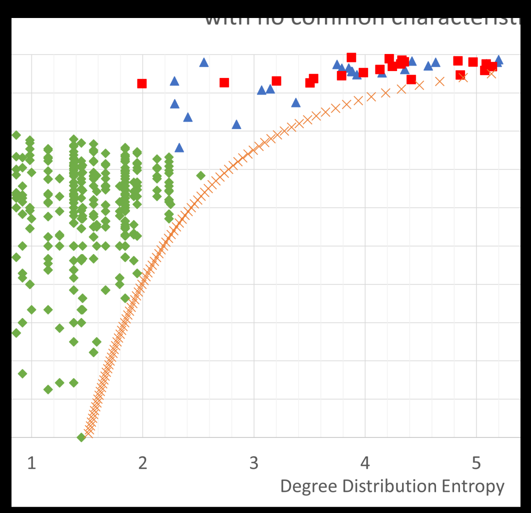
Ladyman, J., Wiesner, K.. What is a complex system? Yale University Press (2020).

information in complex systems

Wiesner, K., Ladyman, J.. Complex systems are always correlated but rarely information processing. Journal of Physics: Complexity in press.

Wiesner, K., Teles, J., Hartnor, M., & Peterson, C. (2018). Haematopoietic stem cells: entropic landscapes of differentiation. Interface focus 8(6), 20180040.





Jones, C., Wiesner, K.. Clarifying How Degree Entropies and Degree-Degree Correlations Relate to Network Robustness. YarXiv:2106.14784 (2021).

A.J. Dunleavy, K. Wiesner, R. Yamamoto, and C.P. Royall. Mutual Information Reveals Multiple Structural Relaxation Mechanisms in a Model Glass Former. Nature Communications 6 (2015).