Functional Dynamics in Out-of-Equilibrium Allosteric Assemblies

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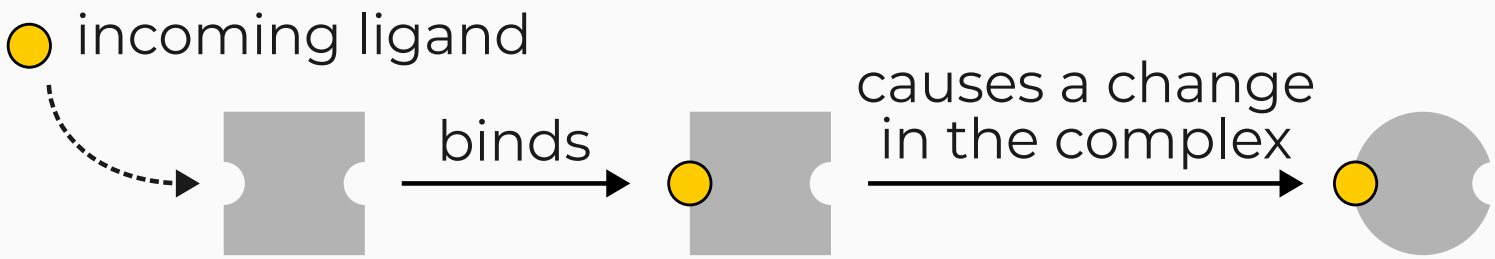
poster number: 2

[†] indicates equal contribution

Allostery – interactions between distant sites on a complex



Notable examples:

- Cooperative binding in Haemoglobin [1]
- Allosteric regulation in the Ribosome [2]

Multiple established equilibrium models:

- Monod-Wyman-Changeux (MWC)[3]
- Koshland-Nemethy-Filmer (KNF)[4]

(1) M. I. Stefan et al., *PLOS Computational Biology*, 2013, **9**, e1003106.
(2) T. M. Makarova et al., *Biochemistry. Biokhimiia*, 2017, **82**, 1557–1571.
(3) J. Monod et al., *Journal of Molecular Biology*, 1965, **12**, 88–118.
(4) D. E. Koshland et al., *Biochemistry*, 1966, **5**, 365–385.

What does out-of-equilibrium allostery allow

But there are out-of-equilibrium allosteric systems:

- KaiC circadian clock[1]
- DNA Clamp Loader[2]

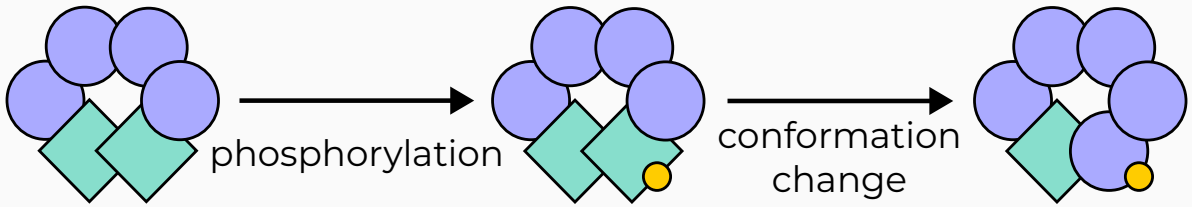
What classes of new behaviour are possible in out-of-equilibrium allostery?

(1) J. S. van Zon et al., *Proceedings of the National Academy of Sciences*, 2007, **104**, 7420–7425.
(2) B. A. Kelch et al., *Science (New York, N.Y.)*, 2011, **334**, 1675–1680.

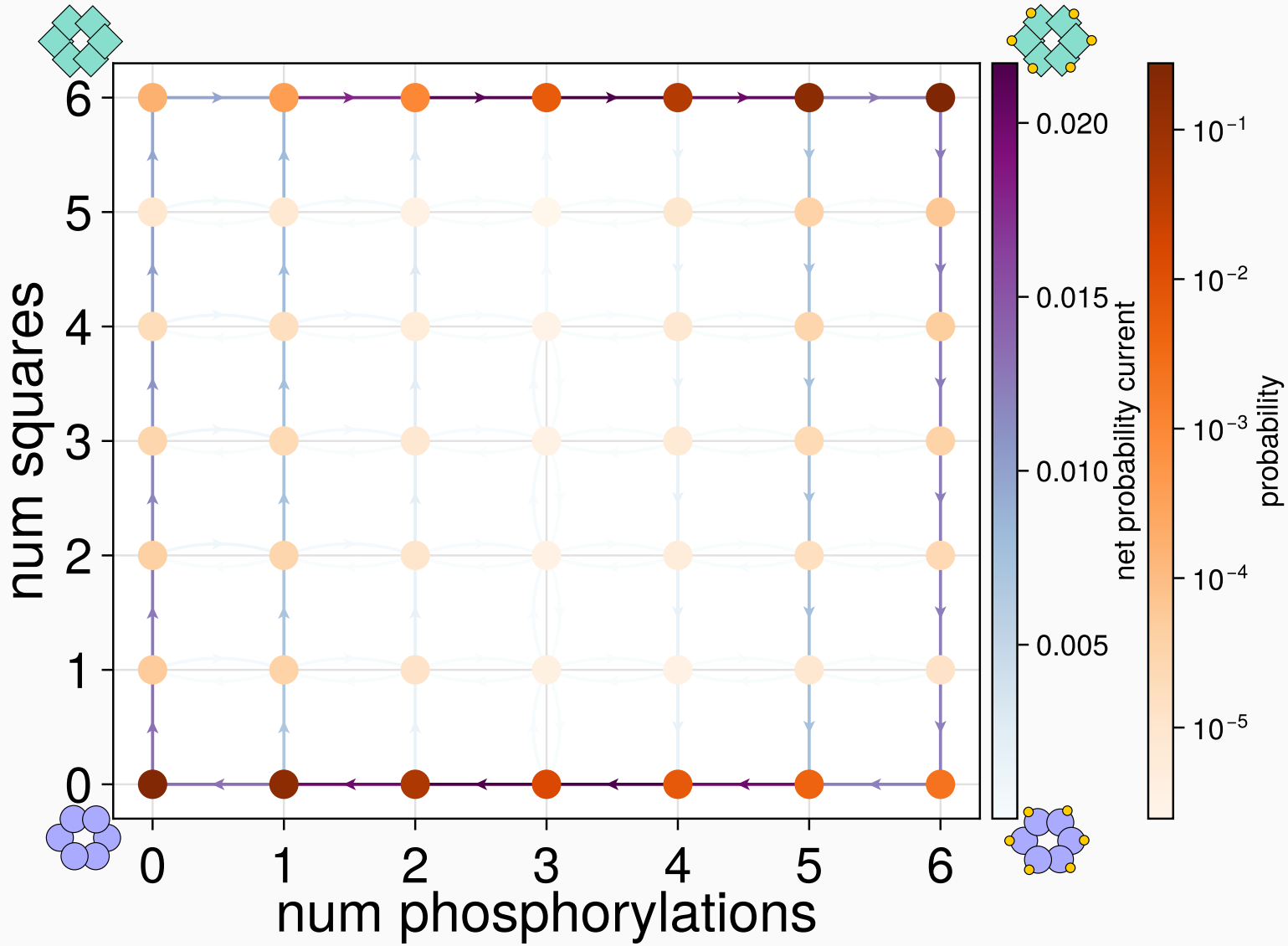
We construct minimal models capable of allostery

Core ingredients in our approach

- Systems made of identical subunits
- Local interactions (nearest-neighbor)
- Thermodynamically consistent (local detailed balance)

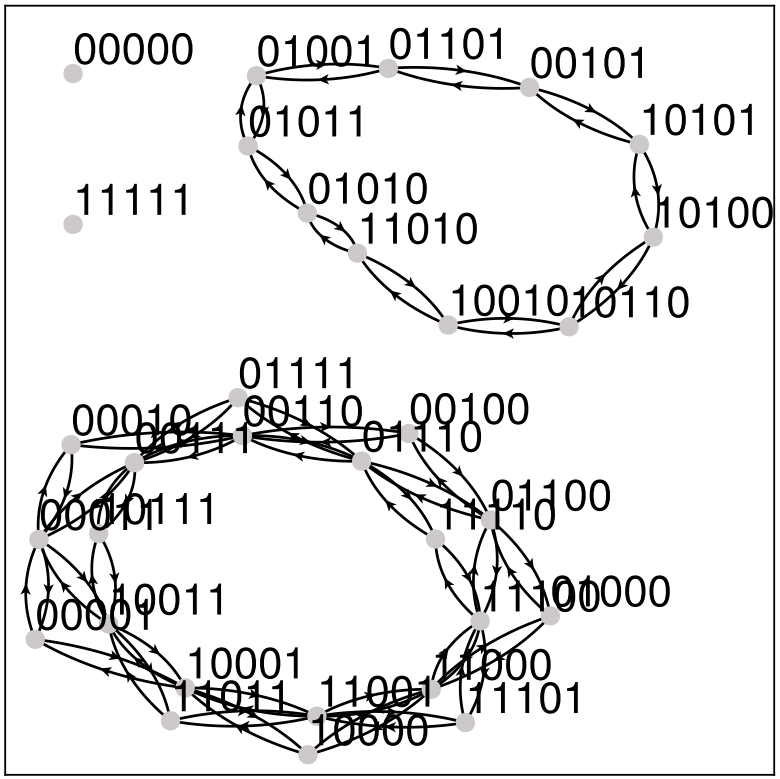


Topologically protected dynamic states?

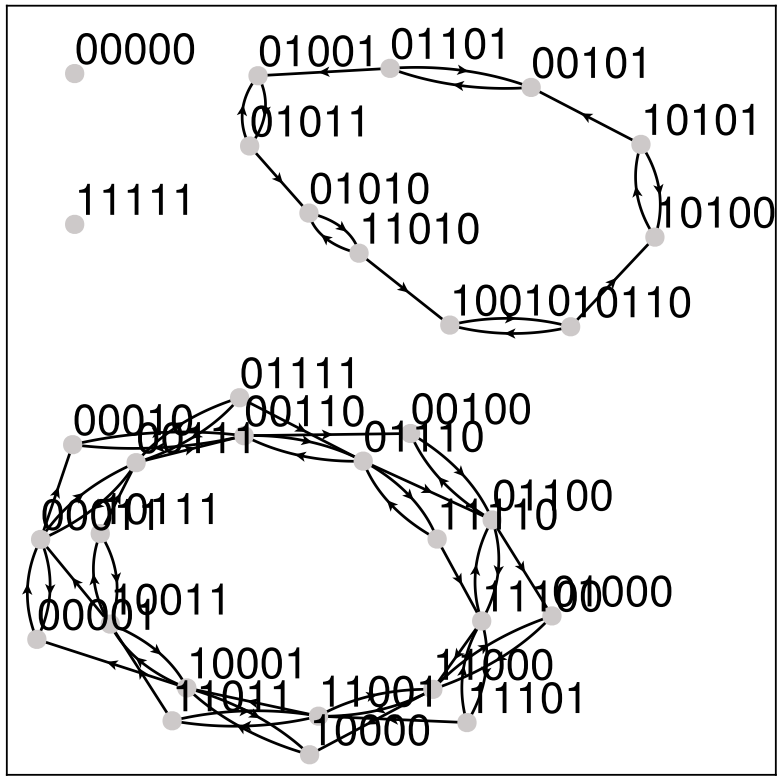


Each node is a measurable group of states, their colours denoting steady state probability, and the arrows are the steady state probability currents.

Chirality induced by out-of-equilibrium drive



(a) Equilibrium ruleset, diffusion on loops



(b) Non-equilibrium ruleset, directed currents

Thank you for your attention

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