

Manubot Rootstock: nonequilibrium-barrier

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Manubot Rootstock: Molecular motors with barriers

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Abstract

TBD

Outline

1. Surface with and without a barrier
2. Family of curves showing force on the barrier as a function of height and position of the barrier.
3. Optimization of a surface for flux and force with and without a barrier. [1]

Ideas

1. MD and umbrella sampling of a Feringa-type motor.
2. pH change can be modeled as a change in substrate concentration, for our purposes.
3. Can the experimental groups synthesize motors based on an energy surface?
4. CD can be a platform -- a scaffold -- for building, but it will be hard to figure out the appropriate assays.

Optimization of a surface for maximum probability flux

It would be nice to be able to design -- or suggest -- how to design a molecular motor for specific properties (speed, force, torque, gearing, ability to work against a load, resistance to being forced backwards, or something else).

Two surfaces, starting with

Starting with a fixed bound surface □

There is something I still don't understand about this. The results do not seem to be completely reproducible even with setting `np.random.seed(42)`. I have consistently gotten between 1300 and 1400 iterations, but not always the same number.

Two surfaces, both optimized (?)

Optimization of a surface for maximum force

1. Slochower DR, Wang Y-H, Tourdot RW, Radhakrishnan R, Janmey PA. 2014 Counterion-mediated pattern formation in membranes containing anionic lipids. *Advances in Colloid and Interface Science* **208**, 177–188. See <https://doi.org/10.1016/j.cis.2014.01.016>.