Manubot Rootstock: nonequilibrium-barrier

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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.

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 the potential energy surfaces

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). To that end, we set out to explore the relationship between the shape of the potential energy surfaces and these properties. [1]

Optimization of a single surface for maximal flux

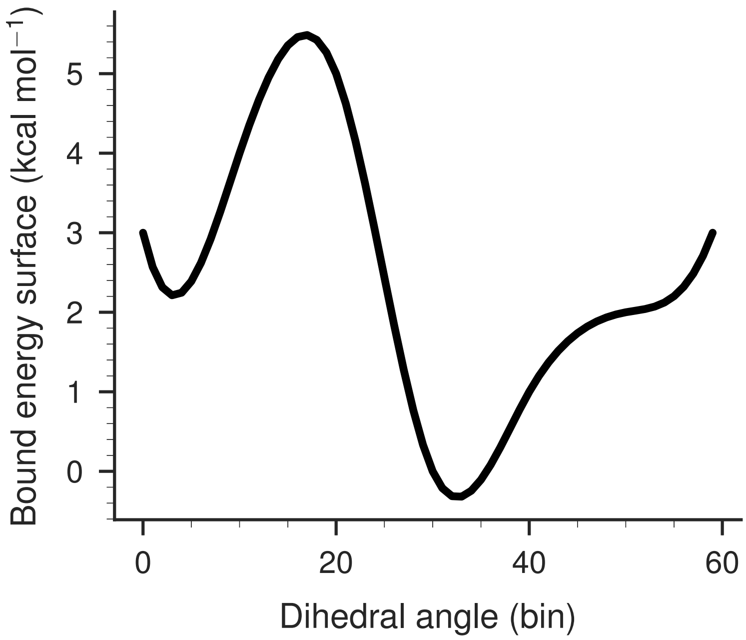

Figure 1: The fixed bound potential energy surface during optimization.

To start, let's begin with a fixed bound energy surface created by smoothing a sawtooth with six spline points 1.

This shows the results of Nelder-Mead optimization, also known as downhill simplex, which should be completely reproducible and deterministic.

There is something I still don't understand about this. The resutls do not seem to be completely reproducable 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. Betzig E, Patterson GH, Sougrat R, Lindwasser OW, Olenych S, Bonifacino JS, Davidson MW, Lippincott-Schwartz J, Hess HF. 2006 Imaging Intracellular Fluorescent Proteins at Nanometer Resolution. *Science* **313**, 1642–1645. See https://doi.org/10.1126/science.1127344.