Nonequilibrium molecular motors: optimization and torque

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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.

Optimization of a single surface for maximal flux

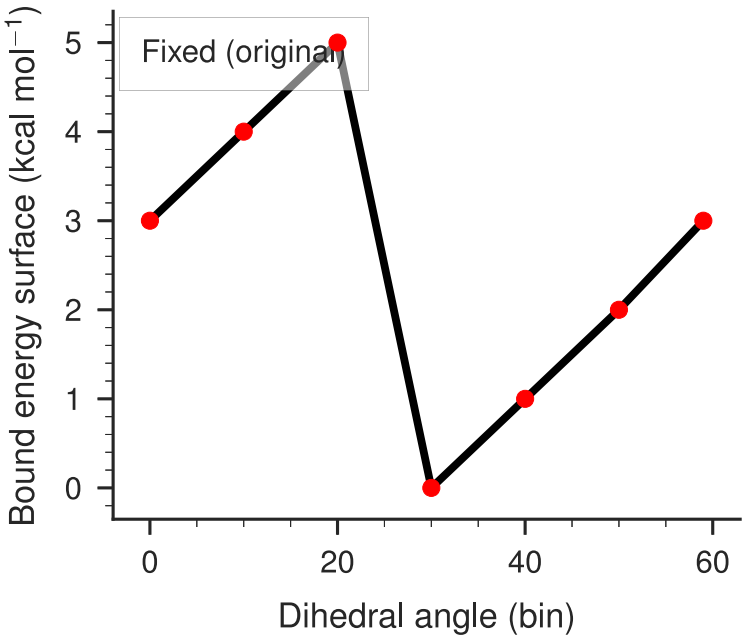

Figure 1: The fixed bound potential energy surface, based on a sawtooth wave. It is a little misleading, but this curve is actually only the seven points in red, drawn on a scale of 60, to show how the seven points map to the interpolated spline below. That is, the bound state is the curve consisting of the points `{(0, 3), (10, 4), (20, 5), (30, 0), (40, 1), (50, 2), (59, 3)}` interpolated to 60 bins using the spline.

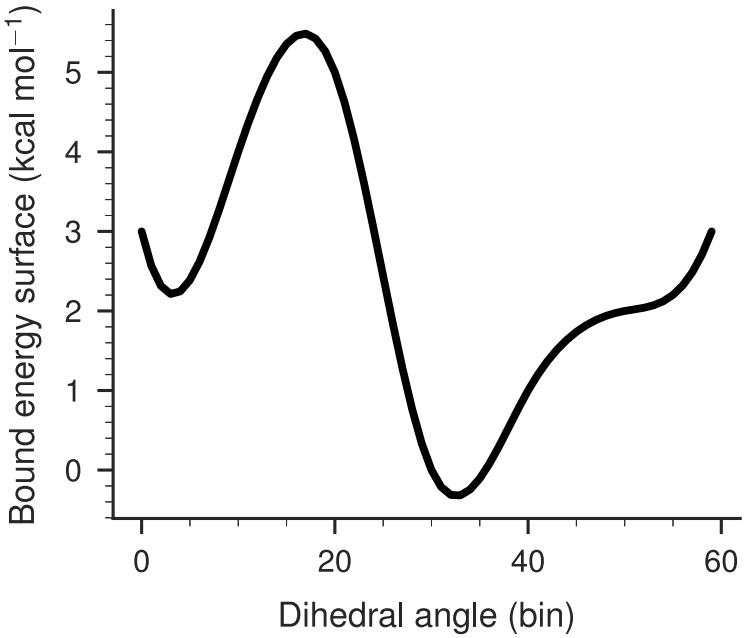

Figure 2: The fixed bound potential energy surface after splining.

To start, let's begin with a fixed bound energy surface created by smoothing a sawtooth with seven spline points (Figure 2). I couldn't find a way to spline across the periodic boundary, so the curve looks a little wonkier than expected. My first attempt was to use a downhill simplex method (Nelder-Mead optimization) to optimize the two surfaces together for flux. The results are not completely deterministic, even with with setting `np.random.seed(42)`, and I don't understand that.

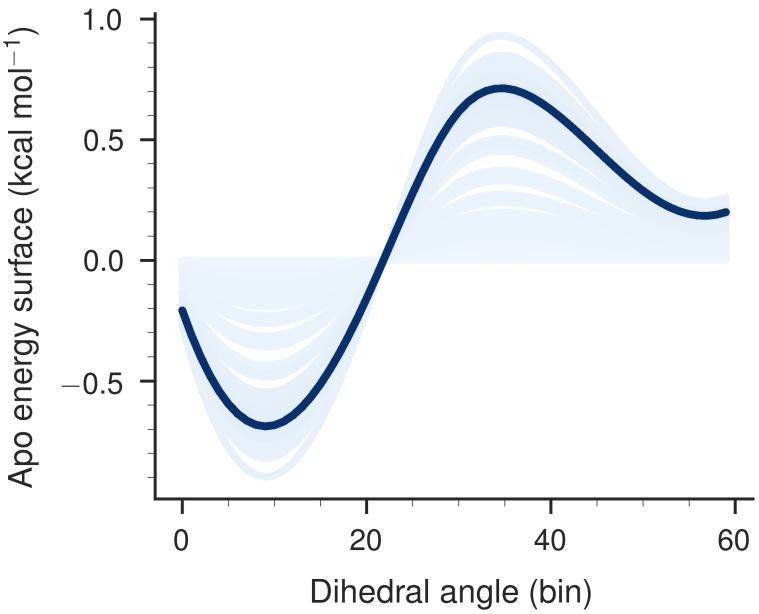

Figure 3: The result of the optimized apo potential energy surface.

After 1403 iterations, Nelder-Mead optimization results in the surface shown in Figure 3. Each blue line is an interation of the optimization. Lighter color correspond to earlier iterations. The final surface is darker because many lines are overlayed. I have not implemented bounds on the optimization because Nelder-Mead does not allow bounds, as far as I know. The result of this optimization is that the flux approaches $-0.050 \text{cycle s}^{-1}$ quickly and stays there.

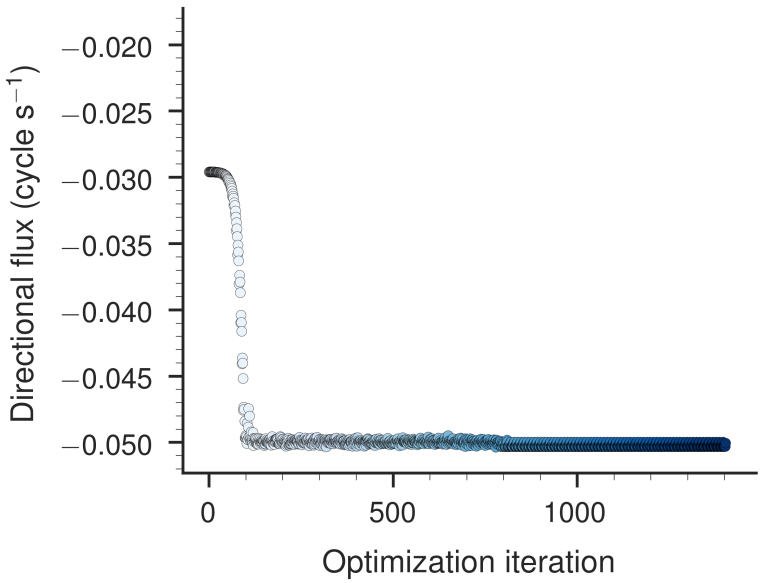

Figure 4: The flux during optimization.

COBYLA and Powell's method result in better optimization than simplex downhill.

Optimization of both surfaces for maximal flux

COBYLA in particular handles the bounds and produces highly optimized surfaces after just a few iterations.

Optimization of a surface for maximum force

The force on a barrier

It is interesting that in most places $F = 0$.

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.