Running to-do

# August 22, 2016

* Rewrite C\_intrasurface in terms of the diffusion coefficient, D. Namely .
* Look at the MSD of Gaussians (in the iterative method) and compare this to the MSD for the butane torsion. Make sure the MSD is independent of the number of bins. Then we can say that we’re properly modeling the diffusion equation.
* Look at finding the spline (perhaps 20 points) that gives maximum flux or maximum stall force. Consider genetic algorithm.
* Look at the parameter scans in the PPT for different files to see if the maxima (or inflection points) are at different values.
* Look at intersurface flux (sloshing).
* Calculate the M-M . Specifically
* Look for a bump (or deflection) around the stall force in the flux vs. applied load graph.
* Investigate the mechanism of myosin: how is the power stroke initiated? Is it the rotation of one or a few amino acid torsions?
* Look at simulating an extended and collapsed alpha helix to generate a minimal 2-state model for torsion histograms.
* Make a graph for ATP concentration of zero.

# Uncategorized notes on the primary paper

* Re-read Andrew’s PNAS entropy-enthalpy paper (Fenley, Muddana et al. 2012) for ideas on how to appeal to a general audience.
* What is remarkable about molecular motors is that they exhibit directional motion: myosin, F1 ATPase, flagella, and so on. It’s not clear how that asymmetry emerge and we tend to associate that sort of motion with motors. That may not be the case.

References

* Fenley, A. T., et al. (2012). "Entropy-enthalpy transduction caused by conformational shifts can obscure the forces driving protein-ligand binding." Proc Natl Acad Sci U S A **109**(49): 20006-20011.
* Molecular dynamics simulations of unprecedented duration now can provide new insights into biomolecular mechanisms. Analysis of a 1-ms molecular dynamics simulation of the small protein bovine pancreatic trypsin inhibitor reveals that its main conformations have different thermodynamic profiles and that perturbation of a single geometric variable, such as a torsion angle or interresidue distance, can select for occupancy of one or another conformational state. These results establish the basis for a mechanism that we term entropy-enthalpy transduction (EET), in which the thermodynamic character of a local perturbation, such as enthalpic binding of a small molecule, is camouflaged by the thermodynamics of a global conformational change induced by the perturbation, such as a switch into a high-entropy conformational state. It is noted that EET could occur in many systems, making measured entropies and enthalpies of folding and binding unreliable indicators of actual thermodynamic driving forces. The same mechanism might also account for the high experimental variance of measured enthalpies and entropies relative to free energies in some calorimetric studies. Finally, EET may be the physical mechanism underlying many cases of entropy-enthalpy compensation.