How taking ”Issues in Scientific Computing” has changed my life...

YOUR NAMES*

April 7, 2013

*Department of ...., Virginia Tech, Blacksburg, VA 24061

Abstract

A brief, matter of fact description of the main results and conclusions. 300 words MAXIMUM. The first sentence or two sets the stage, shows importance.

Keywords: Laplace Daemon, dynamic instability, molecular surface, folding funnel, etc.;

1 Introduction

One or two pages most.

Start by introducing the problem. Why is it important? What was done before? A brief literature review.

Then give a brief layout or ”road map” of the paper – 1/4 of a page at most. It serves to orient the reader, to show him what to expect.

2 Results and discussion

This is the meat of the paper. Present your results. Use subsections. Briefly state what each result means and how it supports your hypothesis. See subsection examples below. Some of the subsections may be the "Deliverables"from your midterm presentation. Try to limit yourselves to 4 pages, not counting "Methods", "Conclusions" and "Code description".

2.1 Effect of T_m on dN/dS

2.2 Effect of GC content on dN/dS

Example of a picture set-up:

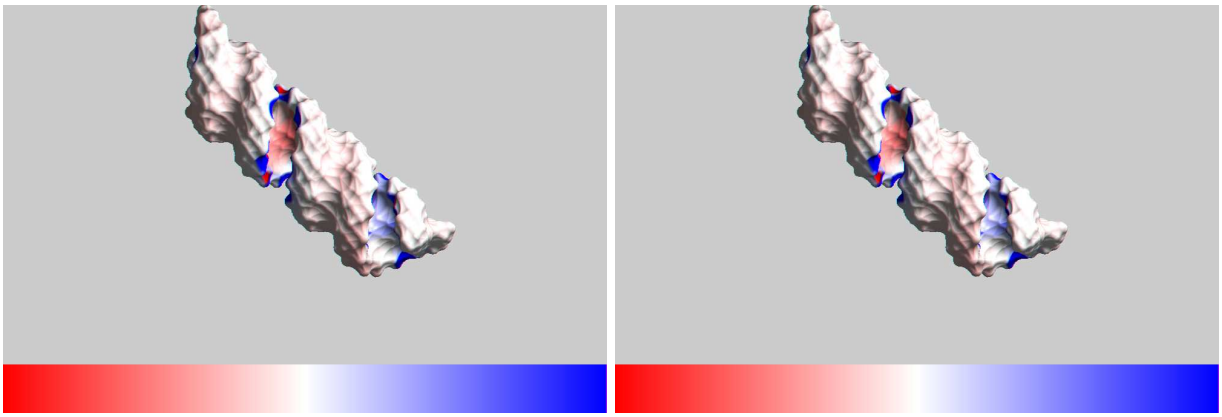

Figure 1: **Left:** Distribution of electrostatic potential around RNA. **Right:** Effective radii in thioredoxin computed, for each atom, with GB^{HCT} (black squares) and GB^{OBC} I (red circles) models vs. calculated by the PB. An exact match between GB and PB models is indicated by the diagonal line.

example of a table:

Table 1: The change in electrostatic part of solvation free energy, $\Delta G_{\mathrm{el}}(N) - \Delta G_{\mathrm{el}}(U) [Kcal/mol]$, of apo-myoglobin and protein-A in going from the unfolded (U) to the native (N) states calculated with PB and GB models based on Bondi radii set. (Since a perfect GB model would correspond to zero grid size PB, and since we observe a decrease in $\Delta G_{\mathrm{el}}(N) - \Delta G_{\mathrm{el}}(U)$ upon reducing the grid size from 1 Å to 0.5 Å, we adjust the parameters of GB^{OBC} to produce values of $\Delta G_{\mathrm{el}}(N) - \Delta G_{\mathrm{el}}(U)$ slightly below the PB predictions based on 0.5 Å grid spacing.)

	Electrostatic Model				
	PB(1 Å)	PB(0.5 Å)	GB^{OBC} set I	GB^{OBC} set II	GB^{HCT}
(apo)myoglobin, pH=2	−2082.0	−2088.8	−2089.9	−2093.8	−2161.1
protein-A, pH=7	+143.9	+143.0	+145.1	+142.9	+131.1

3 Methods

HERE you describe the computational methods used. Succinctly, matter-of-fact. But make sure there is enough detail so that every calculation or computer experiment can be reproduced by someone knowledgeable of the field, but unfamiliar with this particular work.

3.1 Structures

The set of apo-myoglobin structures used in optimization of the GB model parameters was prepared from the holo-Mb coordinate set (PDB ID 2Mb5) by heme removal and simulated acid-unfolding in explicit solvent, as described elsewhere.[1] The native state is represented by 50 consecutive snapshots (2 ps apart from each other) with near-native radius of gyration, $\sim$ 16 Å, taken from the beginning of the acid-unfolding simulation. The unfolded state is represented by 50 consecutive snapshots from the end of that simulation, at which point the radius of gyration has approached $\sim$ 30 Å – as is experimentally observed in the unfolded state. Protein-A structures were prepared from the NMR average coordinate set (PDB ID 1BDD, residues 10-55). This structure was used as a starting point for all MD simulations reported here. The native-state ensemble is represented by 50 consecutive snapshots (2 ps apart from each other) from the implicit solvent simulation protocol described below, and deviations from the native coordinates are less than 2 Å for C_α atoms. The unfolded state was prepared by heating the protein to 450 K for 1 ns in an implicit solvent environment, and 50 consecutive snapshots with average RMSD from the native structure of no less than 15 Å were chosen to represent this state. Protein L (PDB ID 1PTL) is represented by 215 snapshots from an explicit solvent high-temperature unfolding simulation, spanning various degrees of compactness, from close to native to largely unfolded. The villin head-piece is represented by 120 structures that model compact near-native, compact misfolded, and extended conformations, produced from the native coordinate set (PDB ID 1VII). The ubiquitin native structure is PDB ID UBQ, and thioredoxin is PDB ID 2TRX. Barnase/Barstar complex is given by X-ray coordinate set PDB ID 1AY7, which is also used to prepare the unbound state by translating Barstar relative to Barnase.

3.2 Poisson-Boltzmann calculations

All PB solvation energies were computed using DELPHI-II with a cubic box. The grid spacing used in each case is given in the main text. The dielectric constant for protein interior is 1 and the ionic strength is zero.

4 Conclusions

Briefly outline what was done in the paper. Then present your conclusions. In the end, you can speculate (just a bit) about what potential implications your results might have – something that you have not proved, but believe is likely.

Acknowledgments

Acknowledge people who helped you.

5 Project assessement

Please summarize your over-all impression of the project, in 1/2 page or so. What did you like/dislike? What would you change to make it a better experience for the students next year?

References

[1] Onufriev, A., Bashford, D., and Case, D. Exploring protein native states and large-scale conformational changes with a modified generalized born model. Proteins 55:383–394, 2004.

6 Computational Tools Developed

If any codes were developed, please briefly describe EACH code. That is what it does, the algorithm, the input structure, the output. Give enough details so that an intelligent user can run the code. The source must have ample comments around the critical parts. Please give a couple of examples of usage, e.g: `energy -sorted molecule` etc.