Calculating energy of ‘Saltation’ using the Gaussian module in DelPhi

The physiological ionic strength within living cell is 0.15 M. A realistic and more accurate estimate of binding energy upon interaction of two protein chains should ideally take into account this physiological ionic strength by considering the contribution of mobile ions in the water phase (without a definite solute-solvent boundary). To that end, delphi invokes its Gaussian-based smooth dielectric function, which, treats mobile ions via a Boltzmann distribution with an added desolvation penalty. The effect is known as ‘Saltation’ (Please see for reference, the following paper).

Jia, Z.; Li, L.; Chakravorty, A.; Alexov, E. Treating Ion Distribution with Gaussian-Based Smooth Dielectric Function in DelPhi. J. Comput. Chem. 2017, 38 (22), 1974–1979.

In this example, we demonstrate how to calculate the ‘energy of saltation’ in case of a protein-protein binding. Take the example of the protein-protein complex, ‘COLICIN E9 Dnase Domain with its Cognate Immunity Protein Im9’ (PDB ID: 1EMV) involving the interaction of two helical (all-α) chains, A and B. Implementing the Gaussian approach, first, the ‘total grid energy’ is to be computed for both the free chains (A, B) as well as the complex (A-B), twice; first, at ‘zero’ salt and then at physiological salt (0.15 M). Let these terms be ΔGnz_AB, ΔGnz_A, ΔGnz_B (for A-B, A and B chains at non-zero salt), ΔGz_AB, ΔGz_A, ΔGz_B (at zero salt). Then, the energy of ‘saltation’ would be:

ΔΔG_saltation = ΔΔGsalt_AB - (ΔΔGsalt_A + ΔΔGsalt_B)
where,
ΔΔGsalt_AB = ΔGnz_AB - ΔGz_AB
ΔΔGsalt_A = ΔGnz_A - ΔGz_A
ΔΔGsalt_B = ΔGnz_B - ΔGz_B

How to Run:

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bash ./run.sh
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The script runs delphi on six consecutive files and computes quantities mentioned in above equations from the output files obtained from DelPhi runs, these vales are as below.

Salt: Zero

Energy> Total grid energy : 63971.15 kT

Energy> Total grid energy : 24138.68 kT

Energy> Total grid energy : 39785.12 kT

Salt: Non-Zero

Energy> Total grid energy : 62767.11 kT

Energy> Total grid energy : 23693.72 kT

Energy> Total grid energy : 39008.93 kT

ΔΔGsalt_AB = delG0_complex (G0_nonzero - G0_zero): -1204.04

ΔΔGsalt_A = delG0_mol1 (G0_nonzero - G0_zero): -444.96

ΔΔGsalt_B = delG0_mol2 (G0_nonzero - G0_zero): -776.19

ΔΔG_saltation: 17.11