Mathematical Biosciences and Engineering

MBE, 17(6): 6259–6277.
DOI: 10.3934/mbe.2020331
Received: 29 June 2020
Accepted: 06 September 2020
Published: 21 September 2020

http://www.aimspress.com/journal/MBE

Research article

A Newton-like iterative method implemented in the DelPhi for solving the nonlinear Poisson-Boltzmann equation

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Supplementary

An example is provided in below to numerically verify that the SOR method and the NWT method are equally efficient and accurate when solving the LPBE.

Example S1. This example is the 1st basic example borrowed from DelPhi's online examples http://compbio.clemson.edu/delphi. In this example, a single charged atom is placed in a continuum media (subplot in Figure S1). This atom carries charge $Q = 10.0e$ ($e = 1.602176565 \times 10^{-19}$ C is the elementary charge) with radii $r = 3.0$ Å. A low dielectric constant $\varepsilon_{\text{in}} = 2.0$ inside the atom and a higher dielectric constant $\varepsilon_{\text{out}} = 80.0$ in water are used. The electrostatic component of solvation energy (corrected reaction field energy) $\Delta G^{\text{sol}} = -4566.23$ KT can be explicitly calculated by the Born formula with the vacuum permittivity $\varepsilon_0 = 8.8541878176 \times 10^{-12}$ F/m [27,34].

The LPBE is solved by both the SOR and NWT methods with the scale varying from *scale* = 2.0 (number of grids per direction = 21) to *scale* = 9.0 (number of grids per direction = 91). DelPhi returns three energies, G_g, G_r, and G_c. The remaining energies, G_ρ and G_r, G_0, and G_i, are not produced since the LPBE, instead of the NLPEB, is solved. $G_c = 0.0$ KT is found in all tested cases, while resulting G_g and G_r are presented in Figure S1a, and CPU time is presented in Figure S1b. It can be seen that both methods produce completely identical energies and cost almost the same time in all tested cases. In particular, the numerically calculated ΔG^{sol} converges to −4566.22 KT ($\log(|-4566.22|) \approx 3.6595568$), which is very close the its exact value obtained by the Born formula.

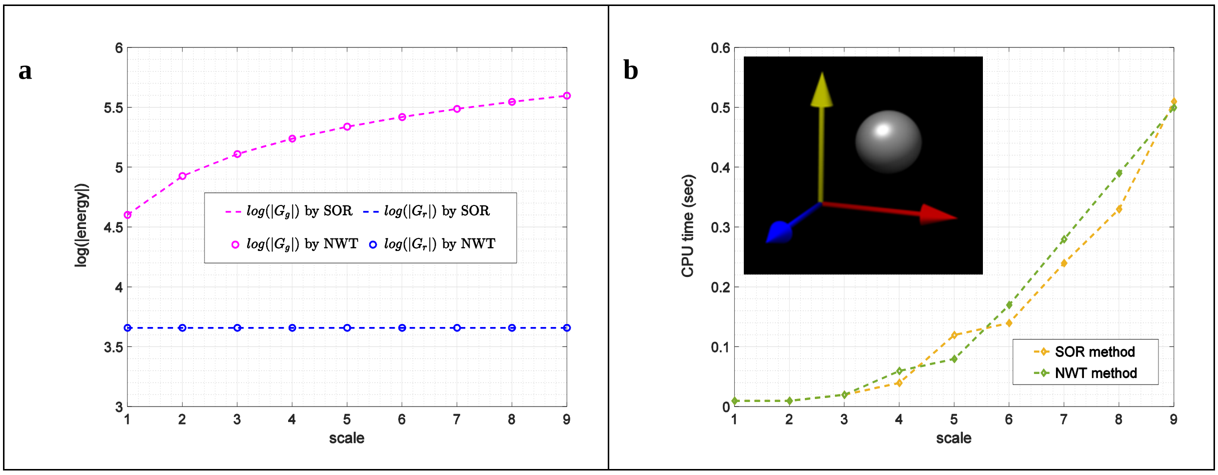

Figure S1. Benchmarks in Example S1. (a) Energies. (b) CPU time.