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Supporting Material

Roles of boundary conditions in DNA simulations: Analysis of ion distributions with the finite-difference Poisson-Boltzmann method

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Roles of boundary conditions in DNA simulations: Analysis of ion distributions with the finite-difference Poisson-Boltzmann method

Xiang Ye,¹ Qin Cai,^{1,2} Wei Yang,^{3,4,5} and Ray Luo^{1,2*}

*1. Department of Molecular Biology and Biochemistry
University of California, Irvine, CA 92697*

*2. Department of Biomedical Engineering
University of California, Irvine, CA 92697*

*3. Department of Chemistry and Biochemistry
Florida State University, Tallahassee, FL 32306*

*4. Institute of Molecular Biophysics
Florida State University, Tallahassee, FL 32306*

*5. College of Life Sciences
Nankai University, Tianjin 300071, P. R. China*

Supplementary Materials

Fig. S-1. Continuum ion distributions in the x-z plane for a t-RNA (310D). (a), (b), (c) are for the PBC simulations in the small, medium, and large boxes, respectively. (d) is for the NPBC simulation. See Fig. 1 for more details.

Fig. S-2. Continuum ion distributions in the x-z plane for a DNA-binding protein (1TSR). (a), (b), (c) are for the PBC simulations in the small, medium, and large boxes, respectively. (d) is for the NPBC simulation. See Fig. 1 for more details.

Fig. S-3. Continuum ion distributions in the x-z planes of 1BNA and 1TSR for the medium-sized box. (a) is for 1BNA with nonlinear FDPB in NPBC; (b) is for 1BNA with nonlinear FDPB in PBC; (c) is for 1TSR with nonlinear FDPB in NPBC; (d) is for 1TSR with nonlinear FDPB in PBC. See Fig. 1 for more details.

Fig. S-4. Correlation between relative electrostatic energies from linear FDPB and nonlinear FDPB for eight selected snapshots in one MC simulation trajectory of 1BNA.

Figure S-1

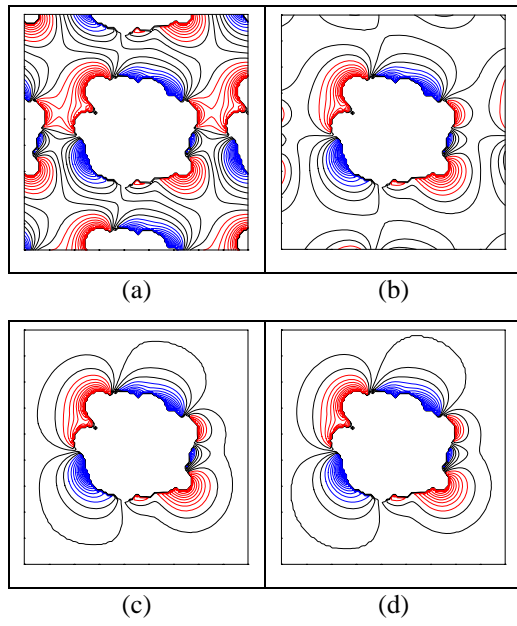


Figure S-2

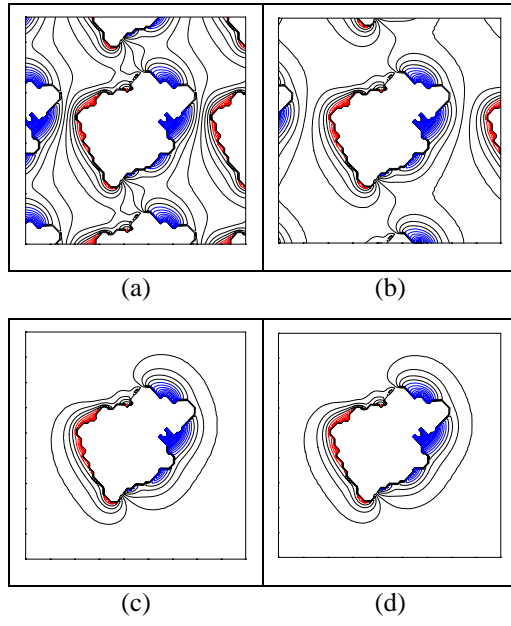


Figure S-3

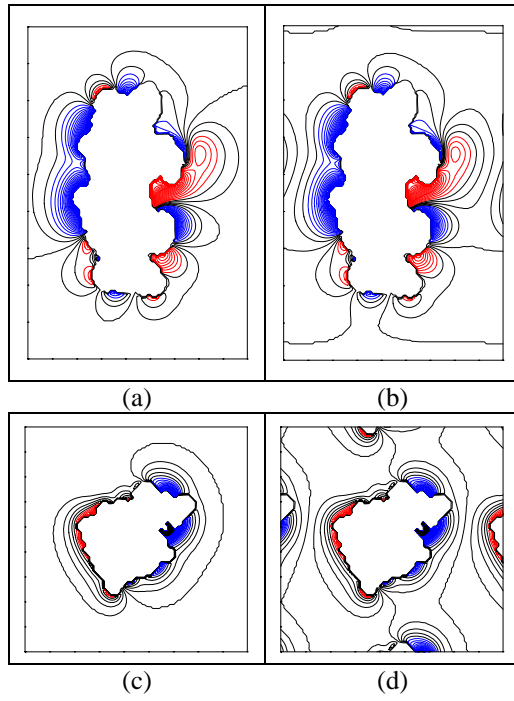


Figure S-4

