# Achieving Energy Conservation in Poisson-Boltzmann Molecular Dynamics: Accuracy and Precision with Finite-Difference Algorithms

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Violation of energy conservation in Poisson-Boltzmann molecular dynamics, due to the limited accuracy and precision of numerical methods, is a major bottleneck preventing its wide adoption in biomolecular simulations. The widely-used Finite-difference scheme does not guarantee interface condition and can not remove charge singularity exactly. We explored the ideas of enforcing interface conditions by the immerse interface method and of removing charge singularity by rewriting equation set to improve the finite-difference methods. Our analysis of these ideas on an analytical test system shows significant improvement in both energies and forces. Our analysis further indicates the need for more accurate force calculation, especially the boundary force calculation.