PyGBe: Python, GPUs and Boundary elements for biomolecular electrostatics

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Summary

PyGBe—pronounced *pigbē*—is a Python code to apply the boundary element method for molecular-electrostatics calculations in a continuum model. It computes solvation energies for proteins modeled with any number of dielectric regions. The mathematical formulation follows Yoon and Lenhoff (1990) for solving the Poisson-Boltzmann equation of the implicit-solvent model in integral form.

PyGBe achieves both algorithmic and hardware acceleration. The solution algorithm uses a Barnes-Hut treecode from Barnes and Hut (1986) to accelerate each iteration of a GMRES solver to O(N logN), for N unknowns. It exploits NVIDIA GPU hardware on the most computationally intensive parts of the code using CUDA kernels in the treecode, interfacing with PyCUDA (see Klöckner et al. (2012)). Some parts of the code are written in C++, wrapped using SWIG.

References

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