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PyGBe-LSPR: Python and GPU Boundary-integral solver for electrostatics

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Summary

PyGBe—pronounced *pigbē*—is a Python library for applications in biomolecular electrostatics and nanoparticle plasmonics. The previous code release, reported in Christopher D. Cooper et al. (2016), solves the Poisson-Boltzmann equation for biomolecules immersed in an ionic solvent, using the boundary integral method. It computes the solvation energy, which is the free energy spent in moving a biomolecule from vacuum to its dissolved state. This quantity is used for assessing binding affinity, protein-surface interactions (Christopher D Cooper, Clementi, and Barba (2015)), and other mechanisms at this scale.

This PyGBe release makes the following contributions: (1) it updates the exisiting library presented in Christopher D. Cooper et al. (2016) to Python 3, (2) it introduces a new capability to solve problems in nanoplasmonics, and (3) it includes better regression tests using pytest and a redesign of the convergence tests.

The largest contribution in this release is extending PyGBe to nanoplasmonics, by treating localized surface plasmon resonance (LSPR) quasi-statically (see Mayergoyz and Zhang (2007)). LSPR is essentially a miniaturization of SPR: the resonance of the electron cloud on a metallic surface, excited by incident light. It is an optical effect (see Bohren and Huffman (1983)), but electrostatics is a good approximation in the long-wavelength limit. This leads to a coupled system of Poisson equations on complex dielectric regions. We use an integral formulation (see Jung et al. (2010)), making the existing boundary integral approach suitable. The code exploits algorithmic speedup via the Barnes-Hut treecode (Barnes and Hut (1986)), as detailed in Christopher D. Cooper, Bardhan, and Barba (2014). The complex scenario required adapting the linear solver (a GMRES algorithm), modifying the right-hand side, and being able to use the existing treecode separately on the real and imaginary parts of the resulting system.

PyGBe's LSPR computations measure the scattered electromagnetic field on a detector that is located far away from a nanoparticle. For nanoparticles smaller than the wavelength of incident light, PyGBe can compute the extinction cross-section of absorbing and non-absorbing media Mishchenko (2007).

To our knowledge, PyGBe is the only open-source software that uses a fast algorithm—O(N logN), for N unknowns—and hardware acceleration on GPUs to compute the extinction cross-sections of arbitrary geometries. We plan to use PyGBe-LSPR research related to nanobiosensors and to explore nanophotonics applications.

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