PyGBe - LSPR

Python and GPU Boundary-integral solver for electrostatics.

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https://github.com/barbagroup/pygbe


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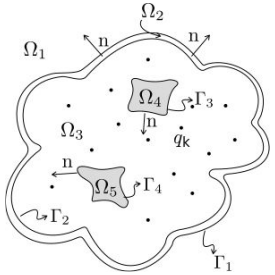
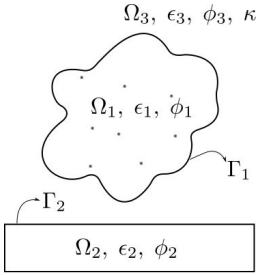
We use PyGBe for...

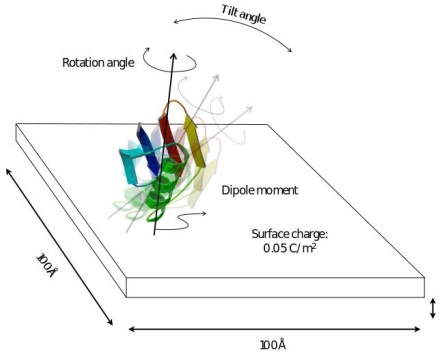
Poisson-Boltzmann equation of the [implicit-solvent](#) model in integral form.

Solvation energies for proteins modeled with any number of dielectric regions



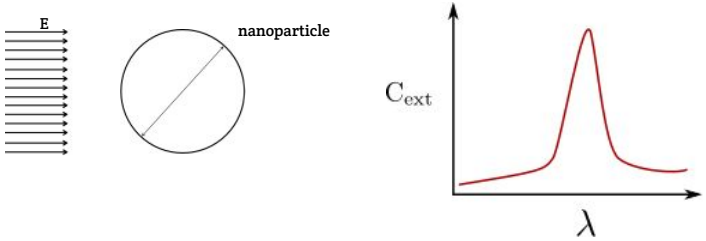


Protein surface interaction

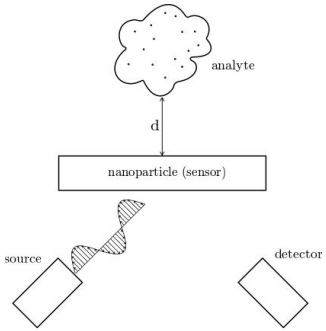


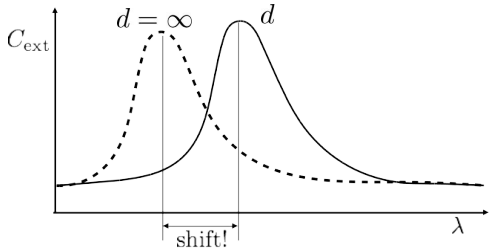
Probing protein orientation near charged nanosurfaces.

Localized surface plasmon resonance of nanoparticles.



Compute the extinction cross section of scatterers that are much smaller than the incident wavelength





How do we do it ...

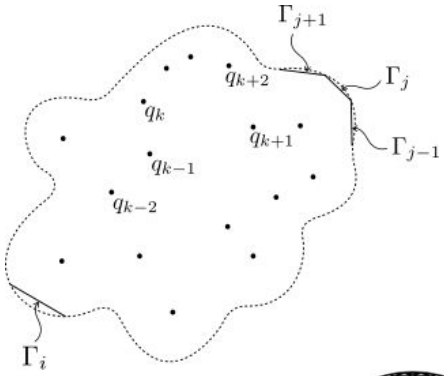
Boundary Element Method (BEM)

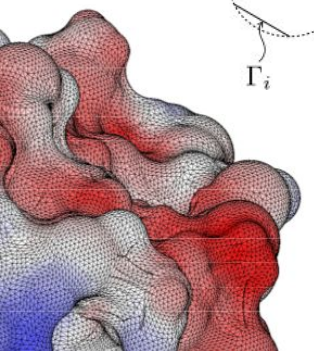
PDE

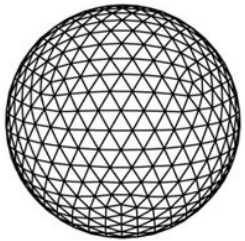
$$\nabla^2\phi = 0$$

BIE

$$\phi = \oint_\Gamma G\frac{\partial\phi}{\partial\mathbf{n}}\mathrm{dS} - \oint_\Gamma \phi\frac{\partial G}{\partial\mathbf{n}}\mathrm{dS}$$







Biomolecular Electrostatics

$$\begin{bmatrix} \frac{1}{2} + K_L^\Gamma & -V_L^\Gamma \\ \frac{1}{2} - K_L^\Gamma & \frac{\epsilon_1}{\epsilon_2}V_L^\Gamma \end{bmatrix} \begin{bmatrix} \phi_{1,\Gamma} \\ \frac{\partial}{\partial\mathbf{n}}\phi_{1,\Gamma} \end{bmatrix} = \begin{bmatrix} \sum_{k=0}^{N_q} \frac{q_k}{4\pi|\mathbf{r}_\Gamma - \mathbf{r}_k|} \\ 0 \end{bmatrix}$$

Localized Surface Plasmon Resonance

$\epsilon = \epsilon(\omega)$

$$\begin{bmatrix} \frac{1}{2} + K_L^\Gamma & -V_L^\Gamma \\ \frac{1}{2} - K_L^\Gamma & \frac{\epsilon_1}{\epsilon_2}V_L^\Gamma \end{bmatrix} \begin{bmatrix} \phi_{1s,\Gamma} \\ \frac{\partial}{\partial\mathbf{n}}\phi_{1s,\Gamma} \end{bmatrix} = \begin{bmatrix} Q \\ \frac{\epsilon_2 - \epsilon_1}{\epsilon_2}\frac{\partial\phi_i}{\partial\mathbf{n}} \end{bmatrix}$$

$$V_{L,ij}^\Gamma = \int_{\Gamma_j} G_L(\mathbf{r}_{\Gamma_i}, \mathbf{r}_{\Gamma_j})\mathrm{d}\Gamma_j$$

$$K_{L,ij}^\Gamma = \int_{\Gamma_j} \frac{\partial}{\partial\mathbf{n}}\left[G_L(\mathbf{r}_{\Gamma_i}, \mathbf{r}_{\Gamma_j})\right]\mathrm{d}\Gamma_j$$

How do we do accelerate it ...

BEM

Problem: Dense matrix, Gaussian elimination, $O(N^3)$ computations.

Integrals are approximated with gauss quadrature rules converting the mat-vec in an N body problem

GMRES

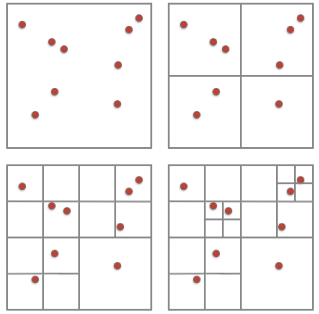
Krylov subspace iterative solver. It reduces computations to $O(N^2)$ per iteration.

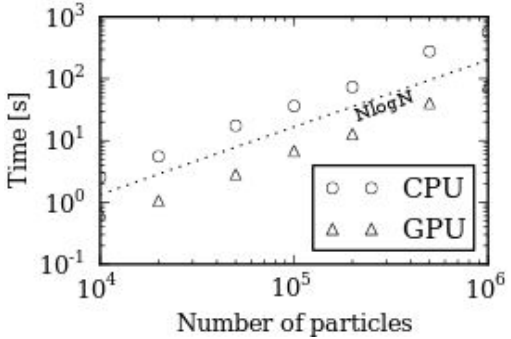
Barnes and Hut Treecode

Approximate far-away source-target interactions with a multipole expansion using Taylor expansions.

Potential due to point-sources (gauss points) of mass is calculated on target (collocation points) locations.

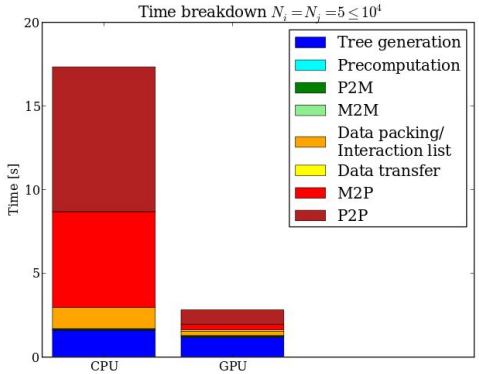
Reduces computations from $O(N^2)$ to $O(N\log N)$.



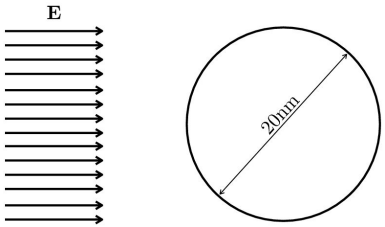


GPU

Consuming parts of the treecode M2P and the P2P interactions.



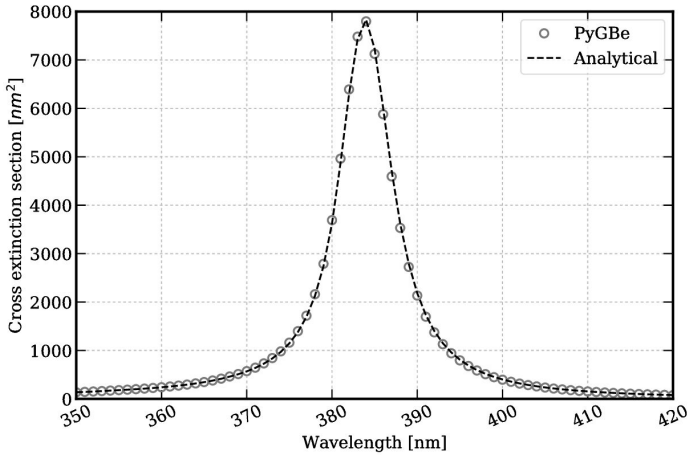
LSPR single NP verification



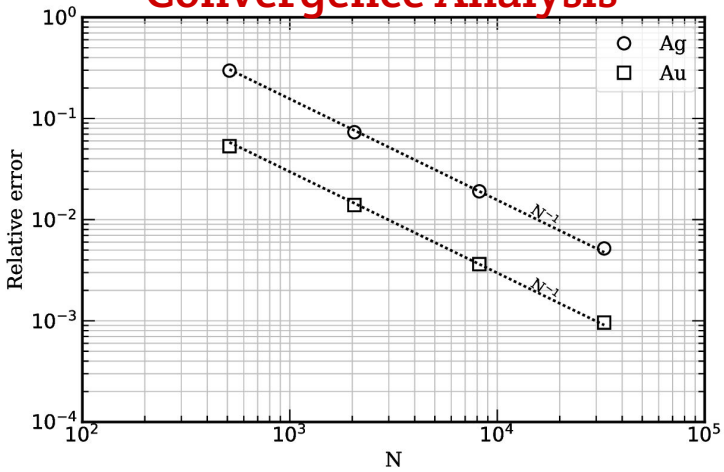
GPU - NVIDIA K40 (time per run)

N	% err_Ag	time_Ag [s]	% err_Au	time_Au [s]
512	29.73	2.35	5.328	2.10
2048	7.32	8.02	1.396	7.19
8192	1.91	62.83	0.363	53.33
32768	0.52	350.63	0.096	298.13

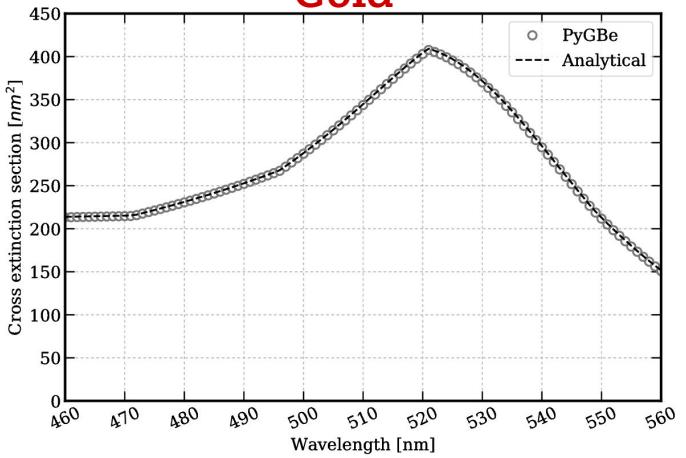
Silver



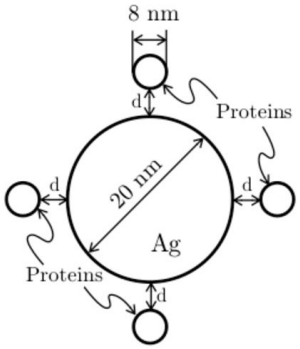
Convergence Analysis



Gold



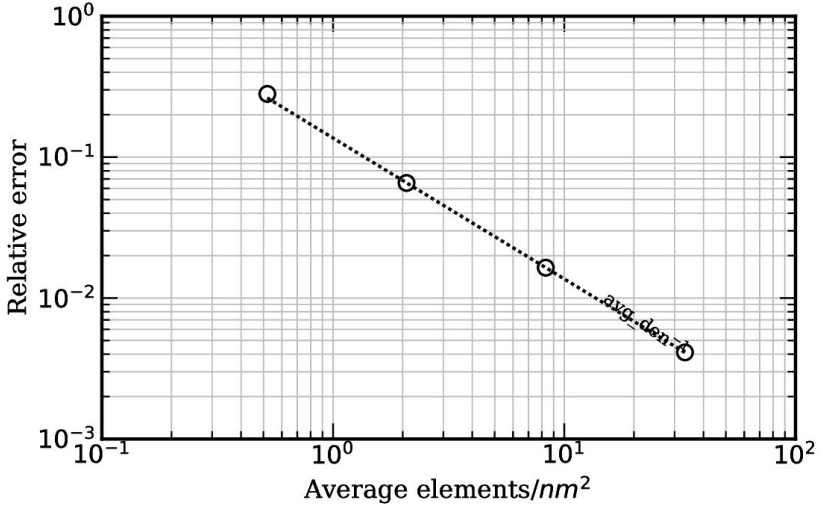
LSPR sensor response POC



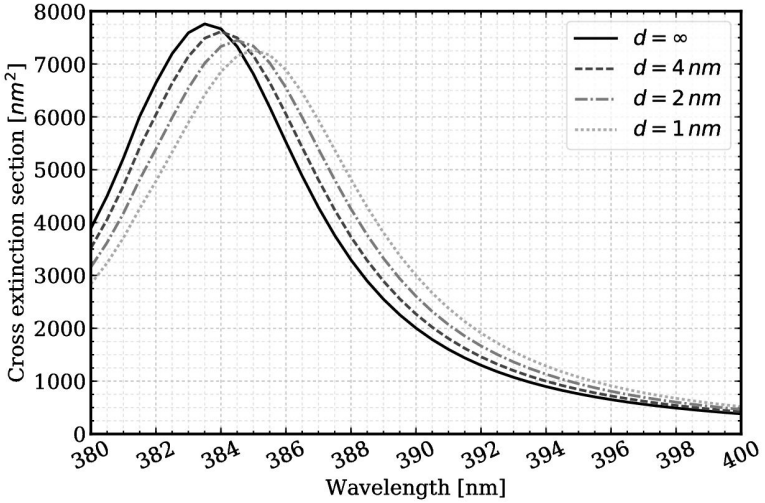
GPU - NVIDIA K40 (time per run)

avg_dens	% error	time [s]
0.52	28.09	24.72
2.08	6.56.	137.70
8.32	1.64	649.50
33.26	0.41	3695.76

Convergence Analysis



Silver - BSA



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