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電子擴散系統的快速計算法(1/3)

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本計畫今年進行十分順利，關於第一年之 Linearized Poisson-Boltzmann 方程之 spectral method 已完成，論文也已撰寫完畢。

A Spectral Method for Two-Dimensional Linearized Poisson-Boltzmann Equation

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Abstract

We consider a circular macromolecule immersed in an ionic water solvent. A concentric ring is formed around the circular molecular surface. This ring is an ionic exclusion layer. The dielectric coefficient is discontinuous across the molecular surface, whereas the Debye parameter is also discontinuous across the outer boundary of the ionic exclusion layer. As the Debye strength is strong, the system can be approximated by a linear Poisson-Boltzmann equation. Using boundary integral method, we solve a 2×2 systems of integral equations numerically. The ingredients of our numerical methods include: (i) a spectral discretization, (ii) a desingularization technique, (iii) a wavelet compression for matrix-vector multiplication. The method is fast and robust.

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