Project 1: Numerical Analysis and Simulation for Nernst-Planck Model

Charge transport is one of the most important processes in nature and man-made devices. Charge transport is a physical process where charge carriers interact with an electric field, so that their transport not only affects the configuration of other charge carriers, but also has a global influence on the electric field. Ion channel refers to porous proteins across cell membranes controlling various biological functions ranging from signal transfer in the nervous system to regulation of secretion of hormones. One crucial problem in molecular biophysics is to understand the mechanism of ionic flows within a channel as a function of ionic concentration, membrane potential, and the structure of the channel. In this project, the primal-dual weak Galerkin (PDWG) scheme will be proposed for the Nernst-Planck (NP) equations which are transport equations with diffusion. The advantages of using the PDWG for NP model include: (1) the algorithm is applicable for any polygonal or polyhedral meshes flexible and beneficial for highly irregular molecular shapes; (2) it preserves the conservation property of the original PDEs; (3) there holds the discrete maximum principles so that the positivity of the ion concentrations is retained, and (4) it is applicable to discontinuous solutions as the weak formulation requires no continuity at all on the numerical solution.

Timeline: Week 1: Background information on PDWG algorithm and fast solvers. Weeks 2-3: Derive an error estimate for PDWG scheme and establish possible maximum principle and non-negativity estimates for the PDWG solution; Weeks 4-6: Design parallel/fast solvers for solution of discrete problem, validate the numerical solutions in the application to the ion transport. Weeks 7-8: Verify NP model through a very accurate approximation of the equations and write paper.

References

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