**Differential geometry based ion transport models**

Qiong Zheng, Zhan Chen and Guowei Wei

Department of Mathematics, Michigan State University, East Lansing, MI, 48824

---

**Introduction**

Ion channels are pore-forming proteins present in cell membranes, usually allowing specific ions to pass across membranes and maintaining proper intracellular ion compositions. They are crucial to cell survival and function, and are key components in many biological processes such as nerve and muscle excitation, action potential generation, and sensing, transduction, learning and memory, to name a few. Dysfunctional ion channels can cause many diseases, blindness, migraines, headaches, and cardiac arrhythmias. Ion channels are frequent targets for drug design.

---

**Governing equations obtained by variation**

Generalized Poisson-Boltzmann Equation:

\[ -\nabla \cdot \left( \kappa(S) \nabla \Psi \right) = (1 - S) \sum_a n_a \rho_a + S \sum_j Q_j(r - r_j) \]

\[ \kappa(S) = 1 - S \kappa_e + S \kappa_w \]

Electrochemical Potential:

\[ \mu_a(r) = \mu_{a,0} + k_B T \ln \frac{n_a(r)}{n_{a,0}} + \varphi_a(r) \]

Nernst-Planck equation:

\[ \frac{\partial n_a}{\partial t} - \nabla \cdot \left( D_a \nabla n_a + \frac{n_a}{k_B T} \nabla \varphi_a \right) = \sum_j Q_j(r - r_j) \]

Generalized Laplace-Young equation:

\[ \frac{\partial S}{\partial t} - \nabla \cdot \left( V_S \nabla S \right) + V_{LB} \]

where \( V_{LB} = -p + \kappa_S n_a + \frac{\kappa_a}{2} \nabla \varphi_a n_a + \phi \sum_j Q_j(r - r_j) \)

\[ -\frac{\kappa_a}{2} \nabla \varphi_a n_a - k_T n_a \]

---

**Simulation Results: II**

The electrostatic potential and ion concentration contours of K⁺ along the channel pore direction:

---

**Simulation Results: I**

Numerical simulations are carried out based on the molecular structure of Gramicidin A Channel which is one of the most widely studied channels and implicit membrane representation to study the ion transport. The surface defined by S is shown below:

---

**Conclusion**

The differential geometry based ion transport model is presented and numerical algorithms are developed for solving the coupled equations in the biomolecular context. Numerical convergence is validated and simulation results are compared well with experimental measurements.

---

**Acknowledgement**

This work was partially supported by NSF grants DMS-0616704 and CCF-0956600, and NIH grants R21CA127185 and R01GM-040208.

---

**References**

3. Qiong Zheng, Zhan Chen and Guo-Wei Wei, Differential geometry based ion transport models, submitted.

---

http://www.math.msu.edu/~wei/