Commun. Comput. Phys.
doi: 10.4208/cicp.101112.100413a

Vol. **15**, No. 1, pp. 93-125
January 2014

A Stabilized Finite Element Method for Modified Poisson-Nernst-Planck Equations to Determine Ion Flow Through a Nanopore

Jehanzeb Hameed Chaudhry[*,1], Jeffrey Comer[2], Aleksei Aksimentiev[2] and Luke N. Olson[3]

[1] *Department for Mathematics, Colorado State University, Fort Collins, CO 80523, USA.*
[2] *Department for Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA.*
[3] *Department for Computer Science, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA.*

Received 10 November 2012; Accepted (in revised version) 10 April 2013

Communicated by Bo Li

Available online 26 July 2013

Abstract. The conventional Poisson-Nernst-Planck equations do not account for the finite size of ions explicitly. This leads to solutions featuring unrealistically high ionic concentrations in the regions subject to external potentials, in particular, near highly charged surfaces. A modified form of the Poisson-Nernst-Planck equations accounts for steric effects and results in solutions with finite ion concentrations. Here, we evaluate numerical methods for solving the modified Poisson-Nernst-Planck equations by modeling electric field-driven transport of ions through a nanopore. We describe a novel, robust finite element solver that combines the applications of the Newton's method to the nonlinear Galerkin form of the equations, augmented with stabilization terms to appropriately handle the drift-diffusion processes.

To make direct comparison with particle-based simulations possible, our method is specifically designed to produce solutions under periodic boundary conditions and to conserve the number of ions in the solution domain. We test our finite element solver on a set of challenging numerical experiments that include calculations of the ion distribution in a volume confined between two charged plates, calculations of the ionic current though a nanopore subject to an external electric field, and modeling the effect of a DNA molecule on the ion concentration and nanopore current.

PACS: 82.20.Wt, 87.15.A-, 83.10.Rs, 87.10.Kn, 87.10.Ed

Key words: Steric effects, nucleic acids, ionic current, continuum transport theory, ion channels, PNP, SUPG, finite element method.

*Corresponding author. *Email addresses:* jehanzeb@colostate.edu (J. H. Chaudhry), jeffcomer@gmail.com (J. Comer), aksiment@illinois.edu (A. Aksimentiev), lukeo@illinois.edu (L. N. Olson)

1 Introduction

Beginning with the experiments that revealed the microscopic mechanisms of nerve cell excitation [1], measurements of ion currents through nanoscale channels and pores have become the basis of many experimental techniques in biology and biotechnology. In addition to permitting the study of the behavior of individual proteins that allow the passage of ions into and out of cells [2], ion current measurements through nanopores have been used to study the rupture of molecular bonds [3–5], to distinguish between similar molecules [6], and to determine the properties and sequences of nucleic acid molecules [7–11]. However, since direct experimental imaging of molecules within nanopores is extremely difficult, computation plays an important role in associating current with nanoscale phenomenon [12–19] (see [20, 21] for recent reviews of the field).

Equilibrium and transport properties of ionic solutions can be simulated using explicit ion methods such as all-atom molecular dynamics [16, 20] or Brownian dynamics [22–24], or by using continuum models such as the Poisson-Boltzmann and Poisson-Nernst-Planck equations [25, 26]. While the explicit ion methods provide the most accurate description of the system's behavior, both in spatial and temporal domains, they are stochastic in nature and thus require long, computationally expensive simulations to obtain average properties. Furthermore, the application of an explicit ion method usually requires the system to be described with the same resolution over the entire simulation domain. Often, this leads to a situation where a majority of the computational effort is applied to simulate a nearly uniform solution where quantities of interest exhibit little variation. In contrast, continuum methods allow different regions of the same system to be described at varying levels of detail, and thus focus the computational effort on regions that require a more precise description. In addition to being more computationally efficient, continuum models more easily incorporate certain types of boundary conditions that arise in physical systems, such as boundaries of fixed concentration or electrostatic potential.

The traditional continuum approach to modeling ionic transport is based on the Poisson-Nernst-Planck equations (PNPE). Although the PNPE have been applied successfully to model the electro-diffusion phenomena [27, 28], the equations are not without drawbacks. Within the PNPE approach, ions are modeled as mathematical points of negligible physical dimension, thereby allowing for accumulation of ions at unrealistically high concentrations in certain regions of the system. A modified formulation of the PNPE, called the modified Poisson-Nernst-Planck equations (MPNPE) [29], explicitly takes the physical dimensions of ions into consideration, which limits the maximum concentration that attained in the system. The advantage of using MPNPE over PNPE becomes apparent in the systems that contain regions subject to strong attractive potentials, for example, near charged surfaces.

In this work, we explore the MPNPE approach for modeling equilibrium and transport properties of ionic solutions in realistic three-dimensional geometries subject to realistic applied potentials. The finite difference method has been widely used to solve the