MARY PUGH, Mathematics, University of Toronto

A Variable Step Size Implicit-Explicit Scheme for the Solution of the Poisson-Nernst-Planck Equations

The Poisson-Nernst-Planck equations with generalized Frumkin-Butler-Volmer boundary conditions (PNP-gFBV) are equations which describe ion transport with Faradaic reactions and have applications in a wide variety of fields. In this talk, we develop a variable step size implicit-explicit time stepping scheme for the solution of the PNP-gFBV equations. We test our chosen numerical scheme on a simplified "toy" version of the PNP-gFBV equations, with special care paid to how we extrapolate the coupled nonlinear terms in the boundary condition. We evaluate various ways of incorporating the boundary condition into the scheme, and a method based on ghost points is chosen for its favorable numerical properties compared to the alternatives. We also observe a thresholding in the time step values, which we found to occur when we temporally extrapolate terms in the boundary condition. With the method we develop, we are able to run simulations with a large range of parameters, including any value of the length scale parameter ϵ. This is joint work with Dave Yan and Francis Dawson (both from Electrical and Computer Engineering, University of Toronto).