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Continuum versus Particle Simulation of Model Nano-Pores

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INTRODUCTION

The class of biological macromolecules known as ion channels are becoming of great interest to physical scientists and engineers, as well as biophysicists and pharmacologists. Long term stability and the wide range of properties displayed by this large group of proteins, makes them one of the most popular contenders to bridge the gap between solid state and biological systems. However, many of the most basic properties of sub-nanometre pores are poorly understood.

We present a comparison between continuum and discrete simulation methods in model sub-nanometre pores. We demonstrate that continuous methods are not sufficient to model simple pore structures.

SIMULATION METHODOLOGY

In order to make comparison as accurate as possible, all simulations were carried out on identical model structures (a 6Å square channel model pore is shown in Fig. 1). Materials are represented by blocks of either, ion accessible or in-accessible regions. In order to obviate effects from the geometry of the simulation domain, a single dielectric constant of 80 is applied to all regions of the simulation.

Continuous simulations have been performed using the commercial 3D Drift Diffusion (DD) simulator, Taurus [1]. Particle simulations were performed using the Glasgow self-consistent Brownian dynamics (BD) simulator [2]. Particle simulations with exact ions and ion splitting in micro particles (BDM) [3] were carried out to better compare with continuous methods. All simulations were performed using a bulk concentration of mobile Potassium ions of 1M and a continuous background charge density ensuing electro-neutrality of the solution.

RESULTS

Due to the discrete nature of ions, the effect of inter-particle interactions becomes significant in channels with dimensions comparable to the characteristic length of the Coulomb interactions. Fig. 2 shows the single filing of ions in a model pore with 3Å cross-section. By comparing the temporal correlation in pore occupancy, we can attempt to quantify the impact of single filing on the permeation of ions through the pore.

Fig. 3 shows that the magnitude of the conduction mediated by single filing is strongly dependant on the diameter of the pore.

Single filing reduces the overall occupancy of the pore, which produces a drop in the conductivity when compared with continuous calculation. Fig. 5 shows a comparison between the calculated current using DD, BD and BDM. In a 3Å pore BD shows ~60% less current compared to DD. As expected the BDM simulations of the same structure show much closer agreement with DD. Fig. 5 and

Fig. 6 show the difference in average charge density through pores of 3Å and 12Å when compared to DD. Note that the BDM simulation compares well with DD but BD shows a very different charge distribution.

CONCLUSIONS

While continuous methods are both efficient and accurate in many situations, great care must be taken when modelling particular transport through very small structures such as nano-pores. Due to the discrete nature of ionic transport continuum results can differ widely from discrete particle methods.

REFERENCES

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[3] C.Millar, A.Asenov and S.Roy, *Self-Consistent Particle Simulation of Ion Channels*, Journal of Theoretical and

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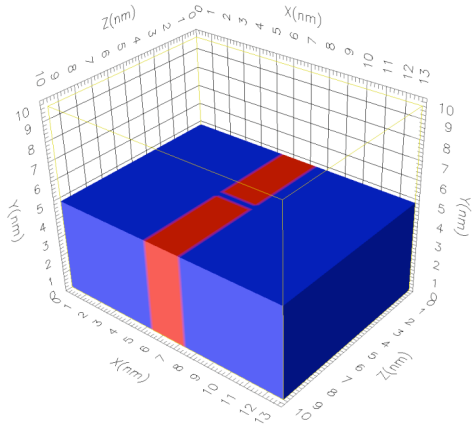

Fig. 1. The model pore simulation structure for a 6Å square channel pore. Ion accessible water is shown in blue, inaccessible material is shown in red. Particle and electrostatic boundaries are applied at x=0nm and x=12.8nm.

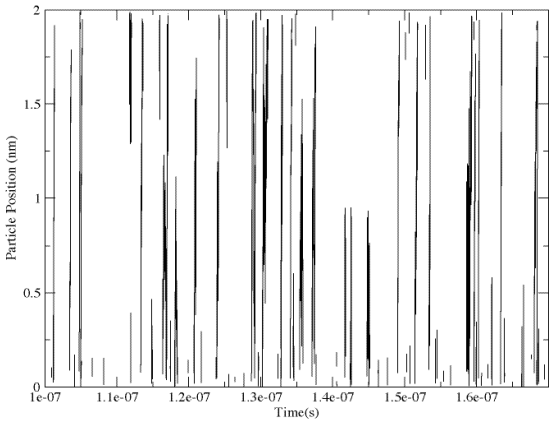

Fig. 2. Single filing of Potassium in a 3Å pore

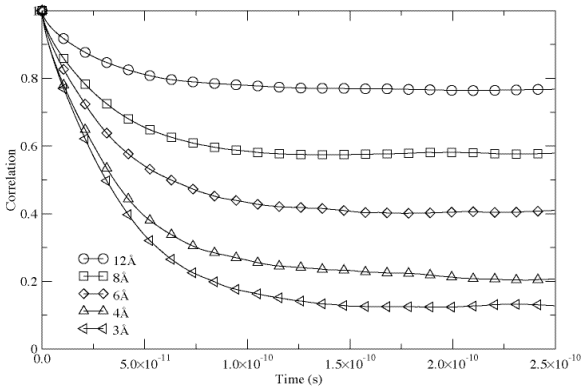

Fig. 3. Time correlation of model pore ion occupancies.

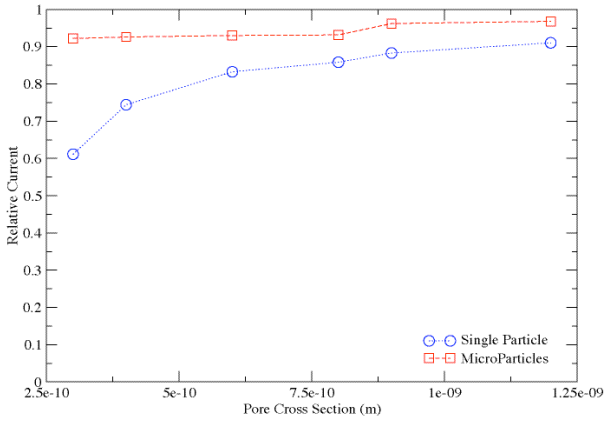

Fig. 4. Model pore current relative to Taurus drift diffusion simulation

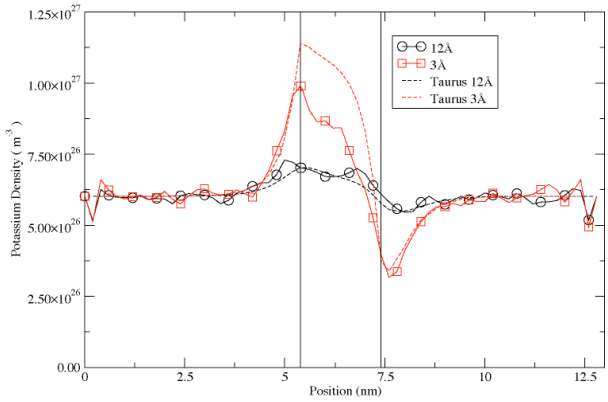

Fig. 5. Single particle Brownian simulation. Charge densities through the pore are compared to continuum simulation.

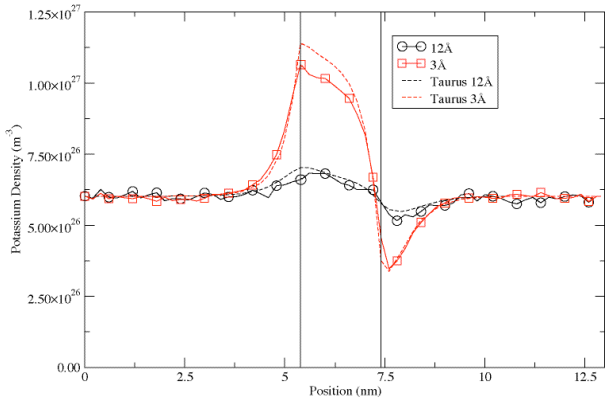

Fig. 6. Micro-particle simulation charge densities compared to continuum.