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Integration of Computational Biochemistry Tools and Device Design Tools To Design Molecular Device Components for Nanotechnology

Aluru, Narayana R., Chen, Dairui, Jakobsson, Eric, Joseph, Sony, Kathawaia, Gulzar, Mashl, R.J., Qiao, Rui, Ravaioli, Umberto, van der Straaten, Trudy, Varma, Sameer
University of Illinois at Urbana-Champaign, Urbana, IL, USA

As miniaturization moves the size of engineered devices down to the nanometer scale of biological macromolecules, theoretical concepts and computational algorithms and software developed in the context of molecular biophysics are increasingly applicable to device design, and vice versa. This paper reports on advances in integrating theory, algorithms, and software developed in the dual contexts of biophysics and device design to develop design tools for dealing with ion conduction and fluid flow for nanoscale devices. In particular, we show the adaptation of the biomolecular computational program Gromacs, the Poisson-Boltzmann solvers UHBD and APBS, and the device design program MOCA into integrated protocols for computing ion and fluid conduction in protein channels and synthesized channels of human design. Exemplary computations to be presented include ion flow through decorated nanotubes, gramicidin, and bacterial porins, water flow and structure in nanotubes (including the unexpected finding of geometrically induced high temperature water freezing in nanotubes, which may provide a basis for switching behavior), and fluidic behavior in confined nanochannels that could impact the design of biomimetic devices. The protocols are being integrated into a multi-functional nanoscale design portal.

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