BRODEA: An Efficient Brownian Dynamics Code Including Explicit Atoms

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A fast and efficient software solution so-called ***BRODEA*** (Brownian Dynamics program including explicit atoms) is presented for studying ion permeation and substrate translocation across nanopores, i.e., artificial or biological channels. ***BRODEA*** generalizes our previous hybrid molecular dynamics-Brownian dynamics scheme [1] in a such way that long simulation times are accessible at a low computational cost even when a large number of atoms along the permeation pathway undergoes thermal fluctuations. To achieve this goal, we devise several equilibrium and nonequilibrium simulation schemes by combining different boundary conditions and mean-field approximations. ***BRODEA*** was applied to study the ion diffusion across outer membrane porin OmpC from *E. Coli* as a test case. Equivalence between different simulation schemes was demonstrated and a significant reduction in the amount of CPU time, i.e., greater than 60% in most of cases, was observed as compared to the performance in our previous scheme. Remarkably, ***BRODEA*** simulations were able to reproduce the main features of ion current and free energy profiles as established by all-atom molecular simulations and experiments

References

[1] Solano, C. J. F.; Pothula, K. R.; Prajapati, J. D.; De Biase, P. M.; Noskov, S. Y.; Kleinekathöfer, U. *J. Chem. Theory Comput.* **2016**, 12, 2401–2417.