Coarse-grained molecular dynamics simulation of water diffusion in the presence of carbon nanotubes

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Abstract
Computational modeling of water diffusion in anisotropic media entails vital relevance to understand correctly the information contained in the magnetic resonance images weighted in diffusion (DWI) and of the diffusion tensor images (DTI). The effectiveness of DTI may be improved by the design of new Contrast Agents increasing the quality, resolution and specificity of the magnetic resonance images. We have previously shown that paramagnetic carbon nanotubes (CNTs) are able to perturb the diffusion of surrounding water molecules in an anisotropic manner, with larger effects in the longitudinal than in the transversal directions, constituting at present the first contrast agent for DTI [1]. In the present work we investigated the validity of a coarse-grained (CG) model to simulate water diffusion in a medium containing CNTs as models of anisotropic water diffusion behavior. The CG approach was chosen as it allows handling time and length scales of systems beyond what is feasible with traditional all-atom models. We report on the influence on water diffusion of various parameters such as length and concentration of CNTs, comparing the CG results with those obtained from a classic force field calculation. We show that water diffusion outside the CNTs follows Fick’s law, while water diffusion inside the CNTs is not described by a Fick’s behavior. Calculated water diffusion coefficients decreased in the presence of CNTs in a concentration dependent manner. We also observed smaller water diffusion coefficients for longer CNTs. Using the CG methodology we were able to demonstrate anisotropic diffusion of water inside the nanotube scaffold, but we could not prove anisotropy in the surrounding medium, suggesting that grouping several water molecules in a single diffusing unit may affect the diffusional anisotropy calculated. The methodologies investigated in this work represent a first step towards the study of more complex models with reasonable savings in computation time [2].

References
Figure 1. Models used for CG (A, B, C) and all-atoms simulations (D). In GG models, grey and blue beads represent CNTs and water molecules respectively: A) 1 CNT, B) 2 CNTs, C) 4 CNTs, D) all-atoms model.