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ADAPTIVE RESOLUTION OF ATOMISTIC PROTEIN IN MULTISCALE WATER

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In this talk, an adaptive resolution simulation of atomistic protein in multiscale water will be presented. We couple atomistic water around the protein with mesoscopic water, where four water molecules are represented with one coarse-grained bead, farther away. The water molecules change their resolution from four molecules to one coarse-grained particle and vice versa adaptively on-the-fly. We observe within our error bars no differences between the properties of our protein in the adaptive resolution approach compared to the fully atomistically solvated model. Our multiscale approach bridges the hydrodynamics from the atomic to mesoscopic scale and enables the study of biophysical phenomena that are beyond the scope of either atomistic or mesoscopic simulations.

REFERENCES

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