Abstract Submitted
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A New Approach in Processing Atomistic Simulations[1] LEOPOLD GRINBERG, GEORGE KARNIADAKIS, Brown University — Computing an ensemble average in unsteady flow simulations performed with the Molecular Dynamics or coarse-grained versions, e.g. the Dissipative Particle Dynamics method, typically requires phase averaging of numerical solution over large number of time periods and realizations. For faster and more accurate processing we propose a new approach based on the window-Proper Orthogonal Decomposition (WPOD) methodology developed by Grinberg et. al. (ABME, vol. 37, 2009). WPOD helps to extract components of the velocity fields with high correlation time, i.e., ensemble average, in a hierarchical manner. The method is very robust and easy to implement. It leads to at least ten-fold computational savings and is appropriate for steady and unsteady non-periodic in time flows. We will review the new technique and present results of 3D numerical simulations of unsteady flows in microvessels.

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