Implementation of SMC averaging method in a channeled molecular flow of liquids and gases

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Abstract
This paper proposes the application of SMC (SAM-Modified-CAM) method of averaging, formerly developed by Karimian et al, in a channelled molecular flow. While they have used periodic boundary conditions in all three directions, in this paper wall boundary condition is used in one direction and in the other two directions, periodic boundary conditions are applied. In order to verify the results obtained from SMC averaging method for the above boundary conditions, velocity profile extracted here is compared to the one obtained by Sofos et al. Results show that very good agreement is achieved. In addition, same trends reported in the work of Sofos et al for the change of velocity magnitude with the spring stiffness and also with the interaction ratio ($\varepsilon_f/\varepsilon_w$), have been observed in the present study as well. It is worth to mention that the velocity profile calculated by the present averaging method is much smoother than the one obtained by Sofos et al. This approves that SMC averaging method is capable of being used for cases with wall boundary conditions. To check whether the simulation has reached equilibrium, "convergence history" of maximum velocity in the channel is plotted using both SMC and CAM methods of averaging. A comparison between the two proves that SMC yields a much smoother graph which is more suitable for determination of the time step in which the equilibrium occurs. It can be concluded that SMC method of averaging is a reliable way of data sampling in molecular dynamics simulations.