Study of Differential Diffusion Using Backward Trajectories in Turbulence

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Abstract

Molecular diffusion due to turbulent dispersion plays a crucial role in pollutant spreading and flame stabilization. Molecules in fluid flow undergo Brownian motion at a rate determined by their molecular diffusivity or Schmidt number (Sc). In this research we investigate differential diffusion of molecules for two sets of molecular pairs, one in high diffusivity regime (Sc of 0.001 and 0.01) and one in the low diffusivity regime (Sc of 100 and 1000) that provides us statistical relations between properties of each diffusing substance due to different molecular diffusivities. Direct numerical simulation with parallel computing is first used to track a large population of molecules forwards in time. Then, we follow their trajectories backwards by utilizing a Lagrangian approach and analyze the molecular trajectories on the Stampede2 supercomputer.

Some interesting results include the linear growth in time of mean square separation for molecular pairs of low Sc. The growth is quadratic for pairs of high Sc, with the initial growth rate being close to six times the sum of the molecular diffusivities. Molecules of low Sc show similar behavior only at much earlier times due to the dominance of molecular diffusion over advective transport by the velocity field. The probability density function (PDF) characterizing the likelihood of samples in different ranges of initial separation was calculated for both groups of molecules. The distribution of samples follows a quadratic growth but sharply drops towards 0 for large values of initial separation. The statistics of backward separation are conditioned upon the initial backwards separation. As for fluid particles, backward dispersion is faster than forward, but the differences diminish for molecules of high diffusivity. Therefore, this study has helped highlight some of the distinctive differences between dispersion of entities subject to molecular diffusion and the dispersion of fluid elements constituting the fluid itself.

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