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Abstract for an Invited Paper for the SHOCK13 Meeting of the American Physical Society

Time Scales in Particulate Systems¹ DUAN ZHANG, Los Alamos National Laboratory

While there are many interests of studying interactions of individual particles, macroscopic collective behavior of particles are our main interest in many practical applications. In this talk, I will give a brief overview of the multiscale methods connecting the physics at individual particles to macroscopic quantities and averaged equations. The emphasis will be on dense dissipative particulate systems, such as powders. Unlike conservative particle systems, such as molecular systems, in a dissipative particle system the concept of thermodynamic equilibrium is not very useful unless in very special cases, because the only true thermodynamically equilibrium state in these systems is the state in which nothing moves. Other than idealized simple systems, mesoscale structures are common and important in many practical systems, especially in dissipative systems. Spatial correlations of these mesoscale structures, such as force chains in dense granular system, particle clusters and streamers in fluidized beds have received some recent attentions, partly because they can be visualized. This talk will emphasize the effects of time correlations related to the mesoscale structures. To consider time correlations and history information of the system, I will introduce the mathematical foundation of the Liouville equation, its applicability and limitations. I will derive the generalized Liouville equations for particulate systems with and without interstitial fluids, and then use them to study averaged transport equations and related closures. Interactions among the time scale of particle interactions, the time scale of the mesocale structures, and the time scale of the physical problem as represented by strain rate will be discussed. The effect of these interactions on the closure relations will be illustrated. I will also discuss possible numerical methods of solving the averaged equations, and multiscale numerical algorithms bridging the particle level calculations to continuum level calculations.

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