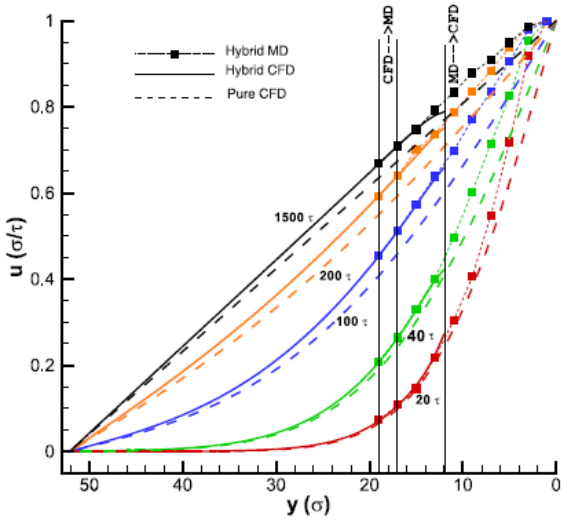
Scale-bridging Simulator for Non-Equilibrium Processes involving BioMaterials

Outcome: Louisiana State University Professors Dimitris Nikitopoulos, Dorel Moldovan, and Shantenu Jha with postdoctoral researchers Nayong Kim, Jeff Ko and Brian Novak have developed a tool generically coupling Continuum CFD and MD simulation codes for the study of non-equilibrium flow phenomena in mixed-scale domains (mm to atomistic) involving biological materials. Under this grant, a graduate student, Kasra Hesary, working with the group has successfully used the tool to couple LAMMPS to a commercial continuum code (ANSYS/Fluent) and verified the results for simple test problems. He is now working with computer science LaSiGMA colleagues (under LSU Professor Ram Ramanujam) to leverage use of CPU and GPU computing to dramatically accelerate the CFD/MD coupled simulations.

Impact: The impact of this work is expected to be significant. It will enable exploration of non-equilibrium phenomena in both purely biological and hybrid non-bio/bio systems, which are inherently multi-scale, through efficient high-performance simulations, which would otherwise not be possible. Furthermore, it will revolutionize the design capabilities of such systems and processes.

***Motivation*:** Many interesting and significant phenomena in processes involving both purely biological and hybrid non-bio/bio systems occur at material interfaces and on the molecular level, while influenced by more "bulk" processes taking place on a much larger scale. Bio-molecules, such as mononucleotides or DNA fragments, interacting with natural, or functionalized/chemically modified wall surfaces in bio-analytical mixed-scale (micro/nano) fluidic instruments is a relevant example involving both bio and non-bio materials. To design such systems one must understand and resolve molecular interaction processes at material interfaces while resolving bulk transport and this necessitates the coupled simulation capabilities pursued by the present work. This work will leverage force-field development efforts also under the LaSiGMA grant to enable multi-scale simulations involving interactions between biomaterials for which such force-fields are unknown.



Results from a test problem solved with the coupled ANSYS CFD/LAMMPS simulation tool developed. The system simulated is a Lenard-Jones (L-J) fluid between two L-J solid surfaces one of which (at y=0) has a strong interaction with the fluid and is impulsively set in motion with fixed velocity at t=0. The figure shows velocity profiles at different times from the initiation of the impulsive motion of one of the plates. The influence of the strong molecular interaction of the fluid with the moving surface material permeates into the continuum flow domain. The conditions of the problem are such that the continuum and pure MD solutions over the entire domain are both valid when interaction with both wall surfaces is consistent with a no-slip condition.