Abstract

This thesis presents a computational study of large scale hydrodynamic flows in strongly coupled liquids using “first principles” classical molecular dynamics (MD) simulations. The prototype model used in the study is a Yukawa liquid. As is well known, Yukawa liquids are ubiquitous in nature and well known examples include complex or “dusty” plasmas, colloids and certain astrophysical systems such as giant planetary interiors and cometary tails, to mention a few. The components of a typical Yukawa liquid such as a complex plasma are electrons, positive ions, neutrals and negatively charged dust grains. Such a complex plasma can exist in a state of strong coupling where the ratio of average interparticle potential energy per dust grain can significantly exceed the average kinetic energy. It is important to note that the mutual influence of the components determines the physical state of the system, for eg. the grain-plasma interaction can lead to the charge on a given dust grain to be a function of time i.e \( Q = Q(t) \). Hence, a complex plasma cannot, in general, be described by thermodynamic potentials and are as such thermodynamically open systems. As can be expected, an ideal description of complex plasma amounts to modeling grain-grain interactions including the dynamics of electrons, ions and neutrals. Such a description is clearly a formidable challenge even with the availability of modern day computers. One can, however, construct a near ideal “exact” description of complex plasma by considering only one charged species, namely the dust grains and assuming that both the grain charge and the background plasma do not evolve in time. This allows the grain dynamics to be modeled by a screened Coulomb or a Yukawa potential \( U(r) = (1/r)\exp(-r/\lambda_D) \), where \( \lambda_D \) is the Debye length of the background plasma. The resulting \( N \) body
problem is numerically solved using a classical MD simulation.

Using “first principles” classical MD simulations, the present thesis reports the onset, growth and nonlinear saturation of large scale hydrodynamic instabilities in strongly coupled Yukawa liquids. To this end, a massively parallel Multi Potential Molecular Dynamics (MPMD) code has been developed as part of this thesis. The code is extensively benchmarked against known results. The thesis begins with a study of Kelvin Helmholtz instability (KH) in parallel shear flows of a strongly coupled Yukawa liquid. At a given coupling strength, a subsonic shear profile is superposed on an equilibrated Yukawa liquid and an instability is observed. Linear growth rates directly computed from MD simulations are seen to increase with strong coupling and vortex roll formation in the non-linear regime is observed. The most interesting feature noticed here is the increase of instability growth rate with strong coupling. Interestingly, it is also observed that KH destabilized modes undergo inverse cascade leading to formation of giant coherent vortices. The emergence of such coherent vortices in the nonlinear regime of KH destabilized flows motivates one to investigate the stability of an isolated coherent vortex. The thesis also reports a comparison between growth rates directly obtained from MD simulations and a phenomenological generalized hydrodynamics (GH) model.

Following the study on parallel shears flows, we undertake a study on the evolution of axisymmetric flows in a 2D strongly coupled Yukawa liquid using MD simulations and report the emergence of coherent tripolar vortices in the nonlinear regime. Our MD simulations reveal that the tripolar vortices persist over several turn over times and hence may be observed in strongly coupled liquids such as complex plasma, liquid metals and astrophysical systems like white dwarfs and giant planetary interiors, thereby making the phenomenon universal. It is also seen that under certain conditions a tripolar vortex can spontaneously decay into a pair of dipolar vortices propagating in mutually opposite directions. Linear growth rates directly obtained from MD simulations are compared with a generalized hydrodynamic model. It is indeed very tempting to study if it is possible to excite such dipolar vortices from generic initial conditions and study their interactions in a laboratory
produced complex plasma. For this we undertake a study on evolution of jets in a strongly coupled Yukawa liquid using MD simulations. The initial state for this study is a sub-sonic jet profile superposed on a thermally equilibrated Yukawa liquid. A dipolar vortex is then seen to emerge from the self-organization of this jet profile. This dipole is seen to be very robust and, in general, shows a nonlinear relationship between vorticity and stream function. Starting from two jets injecting linear momentum in mutually opposite directions, we report on the centered head-on collisions between two dipolar vortices. It is seen that the inertial effects needed for the sustenance of dipolar vortices are rapidly quenched by gas friction. Hence, such dipolar vortices may be observed in a laboratory complex plasma at low gas friction.

In each of the foregoing flow studies, we noticed a significant heat generation close to the shear layers. This motivated us to perform a detailed study of molecular heat generation in shear flows of Yukawa liquids. To this end, we superposed a subsonic shear profile on an equilibrated Yukawa liquid and observed a KH instability. Inverse cascade leads to formation of giant coherent vortices. It is seen that while this inverse cascade leads to a continuous transfer of flow energy towards the largest scales, at the smallest scale there is also a simultaneous transfer of flow energy into the thermal velocities of grains. The latter is an effect of velocity shear and thus leads to the generation of a nonlinear heat front. We notice that the heat front is seen to propagate at speed much lesser than the adiabatic sound speed of the liquid in the linear regime. Hence, the spatio-temporal growth of this heat front occurs concurrently with the inverse cascade of KH modes.

The MD studies reported in the present thesis results are exact numerical solutions to the $N$ body problem and hence “first principles” in nature. The results are “to scale”, for eg. in a typical laboratory dusty plasma, the dust plasma frequency $\omega_{pd} \sim 100$ Hz. A typical growth rate (normalized to $\omega_{pd}^{-1}$) in the studies presented so far, falls in the range $10^{-3} - 10^{-2}$ and corresponds to $[0.1 - 1]$ Hz’s in physical units. Typical system size used in our studies, for eg. $L = 640$ (in units of Wigner Seitz radius $a$) corresponds to 26 cm approximately for $a = 0.4$mm. Hence the hydrodynamic phenomena addressed in the thesis should be observable in laboratory experiments on
complex "dusty" plasma.