Numerical experiments on 2D strongly coupled complex plasmas

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Abstract. The Brownian Dynamics simulation method is briefly reviewed at first and then applied to study some non-equilibrium phenomena in strongly coupled complex plasmas, such as heat transfer processes, shock wave excitation/propagation and particle trapping, by directly mimicking the real experiments.

1. Introduction
Laboratory generated complex (dusty) plasma is a suspension of micron-sized charged dust particles in a weakly ionized plasma with electrons, ions, and neutral atoms or molecules. These dust particles usually acquire a few thousand electron charges by absorbing surrounding electrons and ions and/or by secondary electron/photoelectron emission, float over the lower electrode in the discharge chamber due to the plasma sheath electric field, and interact with each other via a dynamically screened Coulomb potential while undergoing Brownian motion due primarily to fluctuations of local field and frequent collisions with the neutral molecules. When the interaction potential energy between charged dust particles significantly exceeds their kinetic energy, they become strongly coupled and can form ordered structures comprising liquid and solid states that are observable even with naked eyes. Since the motion of charged dust particles in complex plasmas can be directly observed in real time by using a video camera, such systems have been generally regarded as a promising model system to study many phenomena occurring in solids, liquids and other strongly-coupled systems at the kinetic level, such as phase transitions, transport processes, and collective dynamics [1, 2].

The complex plasma physics has now grown into a mature research field with a very broad range of interdisciplinary facets [2]. In addition to usual experimental and theoretical study, computer simulation in complex plasma has been playing an important role in bridging experimental observations and theories and in understanding many interesting phenomena observed in laboratory. The present contribution is intended to demonstrated the basic ideas of numerical experiments on strong coupled complex plasmas (SCCPs) and will focus on a class of non-equilibrium computer simulations that mimic the real complex plasma experiments in laboratory (i. e., numerical experiment). The simulation method, i. e., the so-called Brownian Dynamics methods, is reviewed in Sec. 2 and then examples, such as simulations of heat transfer and shock wave propagation in two-dimensional (2D) dust solids and liquids, are presented in Sec. 3 and Sec. 4, respectively. A short summary is given in Sec. 5.
2. Brownian dynamics method

In a typical experiment, charged dust particles are immersed in very weakly ionized plasmas, where absolute majority of components is the neutral gas atoms/molecules. Therefore it is not surprising to see that many (if not all) dynamic processes are heavily influenced by neutral gas, for example, melting of plasma crystal, collective dynamics and transport processes. On one hand the neutral gas provides a viscous/dissipative media, which takes away extra kinetic energy of dust particles and cools down the system, while on the other hand neutral gas molecules frequently collide with dust particles and set them into Brownian motion. Behaviors of dust particle are therefore better simulated by Brownian dynamics method, which may be regarded as a generalization of the usual Molecular Dynamics (MD) method and is based the Langevin equation and its integral (or Kramers equation written in Hamilton form) [3, 4, 5],

\[
\frac{d}{dt} \mathbf{r} = \mathbf{v} \\
\frac{d}{dt} \mathbf{v} = -\gamma \mathbf{v} + \frac{1}{m} \mathbf{F} + \mathbf{A}(t). \tag{1}
\]

Here, as usual, \(m\), \(\mathbf{v}\) and \(\mathbf{r}\) are respectively the mass, velocity and the position of a Brownian particle, and \(\mathbf{F}\) is the systematic (deterministic) force resulting from external sources and/or from the inter-particle interactions in a many-particle system of Brownian particles interacting with the ambient gas of light particles. What is different from Newton’s equations is the appearance of dynamic friction, \(-\gamma \mathbf{v}\), and the stochastic (Brownian) acceleration, \(\mathbf{A}(t)\). It should be stressed here that the Brownian acceleration may include either internal random kicks from surrounding gas molecules or any external heating sources that can be represented or approximated by a Gaussian white noise, such as fluctuations of local field, a scanning laser beam or other instabilities in the system. When the system is in thermal equilibrium, the friction and the stochastic acceleration are related to the ambient temperature via fluctuation-dissipation theorem. Note that the friction coefficient \(\gamma\) is usually regarded as constant [3].

The Langevin equation (1) may be integrated numerically in a manner similar to that used for Newton’s equations in MD simulations. The most popular algorithms are the so-called Euler-like (EL) method, and Beeman-like (BL) method [3]. However, the above two methods has first-order and second-order accuracy, respectively, and very small time-steps is needed, in order to maintain a necessary accuracy and to conserve the system energy, especially when the damping is very small (say \(\gamma < 0.05\), which is a common parameter range in complex plasma experiments). Therefore a Gear-like (GL) method [4, 5], which has higher orders of accuracy, excellent stability, and a negligibly small energy drift on the long time scales, is developed recently to circulate this issue. The Gear-like BD method will therefore be used in all the following simulations.

3. Heat transfer

The first example [6] is to study the heat conduction in 2D dust solids and liquids, motivated by recent experiments on thermal conduction in 2D SCCPs [7, 8] in both crystalline and solid/liquid mixture states. Typically, \(N = 10000\) particles are simulated in a rectangular area with periodical boundary condition in \(y\) direction and confining boundary condition in \(x\) direction. Particles interact with each other via pairwise Yukawa potential [9]:

\[
\Phi(r) = \frac{Q^2}{r} \exp(-r/\lambda_D), \tag{2}
\]

with \(Q\), \(r\) and \(\lambda_D\) being the particle charge, interparticle-distance and screening length, respectively. Such a system can be fully characterized by three parameters, i.e., the Coulomb coupling parameter, \(\Gamma = Q^2/(aT)\), the screening parameter, \(\kappa = a/\lambda_D\), and the damping
rate, $\nu/\omega_0$, due to the neutral gas, where $T$ is the system temperature (in energy units), $a = (\pi \sigma_0)^{-1/2}$ the Wigner-Seitz radius, and $\sigma_0$ the equilibrium dust number density. The dust plasma frequency is defined by $\omega_0 = \left[2Q^2/(ma^3)\right]^{1/2}$. $\Gamma$ and $\gamma$ are varied to realize different equilibrium states and different damping rates, while $\kappa = 1$ is kept constant throughout our simulation and in subsequent discussions, because $\kappa \sim 1$ is the most typical value found in experiments and, moreover, no substantial effects of varying $\kappa$ are expected in the features to be discussed in the following.

Our simulation is directly reproducing recent experiments [7, 8], and is different from the usual method of non-equilibrium simulation for heat conduction [10]. The system is firstly brought to an equilibrium with desired temperature ($T_0$) in either liquid or solid state. The
melting point for $\kappa = 1$ is at $\Gamma^* \approx 180$ [11], and we’ll denote the corresponding temperature as $T^*$. Then the right half of the system ($x > 0$), is heated to a higher temperature ($T_1$) by applying a Gaussian white noise with desired strength. The evolution of the, system structures, temperature profile and also the heat flux are recorded. In particular, Fig. 1 depicts the time evolution of temperature profile and system structure in the first 1000 time units of heating. A steady state is approached after a substantially long period.

The microscopic heat flux for ith particle is defined as:

$$J_i(t) = v_i E_i + \frac{1}{2} \sum_{j=1, j \neq i}^{N} \mathbf{r}_{ij} \cdot \mathbf{F}_{ij} - \mathbf{r}_i \cdot \mathbf{F}^\text{ext}$$

where $E_i = (1/2)(mv_i^2 + \sum_{j=1, j \neq i}^{N} \Phi_{ij}) + \phi^\text{ext}$ is the particle energy. The total flux in a region is then a summation of the microscopic flux

Figure 2: Stationary temperature profiles for: (a) $\gamma = 0.05\omega_0$ but different system states and temperature gradients and; (b) $T_0 = 0.36T^*$ and $T_1 = 3.6T^*$ but different damping rate. In both figures, symbols are simulation results while solid lines are fits according to Eq. (3). For (a), $\lambda = 0.35\omega_0k_B$, and for (b) different $\lambda$ values (given in the inserted plot) are obtained. Copyright (2009) by Institute of Physics Publishing [6].

Figure 3: Heat flux for different system states and different temperature gradients with $\gamma = 0.05\omega_0$. Symbols are simulation results, solid lines are fits according to Eq. (3), using $\lambda = 0.35\omega_0k_B$, and dash lines in the two panels on the left are direct linear fits of the heat flux with $\lambda = 1.2\omega_0k_B$. Copyright (2009) by Institute of Physics Publishing [6].
of all particles therein divided by its area $A$, i.e., $\mathbf{J}(t) = (1/A) \sum_{i \in A} \mathbf{J}_i(t)$. We are mainly interested in the $x$-component of the heat flux $J_x$. The three terms on the right-hand-side of above equation correspond to respectively contributions from: (1) the particle migration, which is believed to be the main mechanism of heat transport in gas and is denoted as $J_{kx}$ hereafter, (2) particle interactions, i.e., phonon scattering, which is dominant in solids and is denoted as $J_{px}$ hereafter, and (3) the external force. Since the external force acts on only a few rows of particles around the two confining boundaries, its direct influence on the heat flux is localized. Neglecting the external contribution will bring it back to the standard one [12, 13].

**Analytical model:** The heat transfer in our specific case can be described by Fourier’s law: $\mathbf{J} = -\lambda \nabla T$ together with energy balance between heat conduction and energy dissipation due to damping: $\nabla(\lambda \nabla T) = 2 \gamma n (T - T_0) k_B$ [8], where $\lambda$ is the heat conductivity. According to [8], the heat conductivity $\lambda$ is almost a constant in a wide range of coupling strength that covers both liquid and solids states. We therefore assume that $\lambda$ a constant in the following derivation of analytical model and one has,

$$T(x) - T_0 = \frac{T_1 - T_0}{2} e^{\sqrt{2\nu_0 k_B} x}, (x < 0); \quad T(x) - T_1 = \frac{T_0 - T_1}{2} e^{-\sqrt{2\nu_0 k_B} x}, (x > 0). \quad (3)$$

Expressions for heat flux may be obtained in a straightforward way, and we omit the results here. Since $\lambda$ is the only unknown parameter in Eq. (3), it may be measured by fitting the stationary temperature profile (STP) to Eq. (3). It should also be mentioned that the Fourier’s law could break down for low dimensional crystalline systems [13], largely due to a slow decay of equilibrium correlations of the heat current and a divergence of the finite-size conductivity. However, both of them may be avoided in complex plasmas because of the finite damping effect.

Figure 2 (a) shows examples of STPs for different system states and temperature gradients with $\gamma = 0.05 \omega_0$, which is close to the experimental condition of [8]. Symbols are measurements from simulation, while solid lines are analytical fits according to Eq. (3). These fits give a constant heat conductivity, $\lambda = (0.35 \pm 0.05) \omega_0 k_B$, or in terms of thermal diffusivity $D_T$: $D_T \approx 22 \text{mm}^2/\text{s}$ using parameters from Ref. [8]. This value is between the experimental measurement for crystalline state ($30 \text{mm}^2/\text{s}$) [7] and that for solid/liquid mixture phase ($9 \text{mm}^2/\text{s}$) [8]. Fits for high temperature (e.g., the two upper-most curves) suggest a slightly smaller $\lambda$. Nevertheless, the value is in the range of the error bar for the present measurement.

Figure 2 (b) shows STPs for different damping rate with other parameters fixed. Fits with Eq. (3) give a damping-dependent heat conductivity, as is shown in the inserted plot that $\lambda$ rises slightly with the decrease of $\gamma$. Note that this tendency is contradictory with that given by the analytical model in [14], which predicts an increase of $\lambda$ with increase of damping rate and was confirmed by their experiment [14]. However, this model is based on an empirical relation between diffusion and heat conduction coefficients obtained by fitting simulation results for three-dimensional (3D) simple liquid without damping, and their experiment was also performed in a 3D complex plasma liquid [14]. Whereas in our simulation we study 2D systems covering both liquid and solid states and/or with a liquid-solid mixture phase. So the discrepancy could have been caused by the different dimensionality and system states, as is known that transport processes depends much on these two factors. In our simulation, the damping effect is taken into account self-consistently and increase of $\lambda$ with decrease of $\gamma$ may be intuitively understood as follows. It has two effects on heat conduction: direct energy dissipation and indirect suppression of phonon propagation. The first one is only related to kinetic energy of the system, and had been explicitly taken into account in Eq. (3), whereas the second one affects the collective modes and is not included in Eq. (3). Therefore decrease of $\gamma$ means less damping of phonon propagation, more efficient heat transfer through phonon scattering and consequently a higher heat conductivity.
Figure 3 shows distributions of $J_x$, $J_{px}$ and $J_{kx}$ for different system states and temperature gradients, together with the analytical result derived from Eq. (3). Firstly, it may be seen that the kinetic part $J_{kx}$ and the phonon part $J_{px}$ have different weights in different system states. As expected, $J_{px}$ is clearly dominant for solid state and low temperature liquid state, while $J_{kx}$ dominates for high temperature liquid. The critical temperature where the two parts become equal is about $6T^*$. Secondly, the heat flux is not symmetrical about the heating interface. The decay of heat flux on the low-temperature side is slower and one needs a smaller slope, consequently a larger $\lambda$ to fit $J_x$ on this side, indicating a higher heat conductivity for lower temperature. Thirdly, the agreement between analytical results and simulation depends closely on system states. One generally observes a better agreement on the high temperature side and for higher temperature. These features suggest that $\lambda$ becomes temperature-dependent.

![Figure 3: Distributions of $J_x$, $J_{px}$ and $J_{kx}$ for different system states and temperature gradients, together with the analytical result derived from Eq. (3).](image)

Figure 4: Density profiles of the wave for subsequent $100\tau_0$, when $\Gamma = 20$. Copyright (2008) by the American Physical Society [15].

4. Simulation of dust-density wave propagation and particle trapping
The second example [15] is to study the propagation of large amplitude dust-density waves (DDWs) [16] in 2D SCCPs and particle trapping therein, motivated by recent experimental observations of particle-wave interactions in SCCPs [17, 18]. In our simulation, we use a rectangular geometry with confining boundary conditions in the $x$ direction (also the wave propagation direction) and periodic boundary conditions in the $y$ direction, and consider 3000 dust particles interacting via Yukawa potential Eq.(2). We use again $\kappa = 1$ throughout our simulation. Under these conditions, we have a rectangular system with a length of $160a$ (approximately) ($x \in [-80a, 80a]$) and width $80a$ ($y \in [-40a, 40a]$). Such a geometry could prevent a perfect triangular crystal to form at very large $\Gamma$, and consequently introduce some defects around the confining boundary in deep solid state. To reduce influence from these effects, we perform most of our simulations in liquid state or high-temperature solid state ($\Gamma = 800$ is the highest coupling strength). To further reduce the boundary effect, we make our analysis of trapping (which could be affected by defects) in a much smaller region (approximately $x \in [-45a, 45a]$). So the margin between the geometrical boundaries ($x = -80a$ and $80a$) and the
Figure 5: Time dependent (a) wave amplitude ($A_\phi = \sigma_n/\sigma_0$), (b) wave width $W_\phi$ [(defined by $0.5(\sigma_n - \sigma_0)$, and normalized by $a$)], (c) wave speed $v_\phi$ (normalized by $v_s$), and (d) number of trapped particles, when $\Gamma = 20$. Note here that the record for particle trapping starts from $t = 35\tau_0$ in order to avoid any possible boundary effect and effect from initial excitation (for example numerical heating during the wave excitation). Copyright (2008) by the American Physical Society [15].

The simulation starts by generating an equilibrium system with an expected temperature, then pulse waves are excited at one confining end. As for the wave-excitation, one may imagine that there is a piston moving back and forth periodically about the left boundary at $x = -80a$, and the motion of the piston follows a symmetrical triangular function with a constant speed ($v_p = 0.8v_s$) and period ($\tau_p = 110\tau_0$). When the piston is moving forth, it compresses particles in front it and so launches the pulse wave. We have observed that the so-excited wave reaches its maximum amplitude in a few $\tau_0$ of the excitation, and detaches from the piston once the wave speed exceeds that of the piston. After that, the wave propagates freely along the $x$ direction as a soliton [19], as is shown in Fig. 4: the evolution of density profiles $\sigma_n$ (normalized by $\sigma_0$) for subsequent $100\tau_0$.

We see that particles in the wave region is highly compressed, as the compressional rate is always larger than unity, i.e., $\sigma_n/\sigma_0 > 1$. The highest compression rate is reached at the very beginning and is around $\sigma_n/\sigma_0 = 2.2$, which is comparable to the recent experimental realization [19] in 2D plasma crystals. The wave amplitude $A_\phi$ (defined by the peak height of
Figure 6: Snapshots of potential energy contour (normalized by $\phi_0 = (Ze)^2/a$) in a plane parallel to the dust layer with a distance $h = 0.8a$ for different $\Gamma$ (from top to bottom $\Gamma = 20$, $\Gamma = 200$ and $\Gamma = 800$, respectively). Copyright (2008) by the American Physical Society [15].

Figure 7: (a) Periodogram of 4 successive pulse waves, and samples of trajectories for trapped and untrapped particles, when $\Gamma = 20$. Here dots show the time-dependent wavefronts (defined by the peak positions in Fig. 4); the (blue) dash-dot line shows the averaged trajectory of particles, whose initial positions fall into the range $-32a > x > -42a$; other numbered lines are trajectories for 6 different particles: the line 1 [(blue) thin dash-line] is an example of trajectories for untrapped particles; and lines 2-6 are examples of trapped-particle trajectories. Note here that, for clarity, only one of the trapped-particle trajectories, line 2, is shown for whole range, with the (black) thin solid-line for untrapped time and (red) heavy solid-line(s) for the time around trapped period. Copyright (2008) by the American Physical Society [15].
the compressional rate) continuously decays, with the time marching on. According to another experimental observation in 2D plasma crystal [20], the nonlinearity becomes pronounced when \((\sigma_n - \sigma_0)/\sigma_0 > 0.1\). So one can immediately conclude from Fig. 4 that the wave here is strongly nonlinear in most of the time. And the dissipation of the pulse wave may be attributed to the Epstein damping [19] as well as the viscous heating of the equilibrium particles, and the latter is then responsible for the continuous broadening of the wave-width \(W_\phi\) [defined by the width at half-amplitude \(i.e., 0.5(\sigma_n - \sigma_0)\)], as is clearly shown in Fig. 4. Less obvious is that the wave speed \(v_\phi\) also decreases continuously during the wave propagation and is found proportional to the wave amplitude or local density. More quantitative illustrations of these wave properties are given in Fig. 5. Similar tendencies had also been observed in previous experiments [19, 20].

In the following, we illustrate the microscopic process of wave propagation and wave-particle interaction by analyzing the dynamics of individual particles. A microscopic view of wave propagation in the dust layer is given in Fig. 6: snapshots of the potential energy (including the Hartree part of the energy) [11] over the plane. Note here that 0.8\(a\) is the root of \(mv_\phi^2/2 = \phi(r)\), i.e., the interparticle distance at which the interaction potential energy between two particles equals their kinetic energy when they have relative speed \(v_\phi\). Such a treatment is mainly to remove the singularity of potential distribution in the dust plane, and consequently to obtain a better visualization.

The three figures in Fig. 6, from top to bottom, give wave propagation in three different equilibrium states, \(\Gamma = 20\): a high temperature liquid state, \(\Gamma = 200\): a state close to the liquid-solid phase transition and, \(\Gamma = 800\): a solid state, respectively. Particle positions can be readily identified from those small circles or spots. All the three figures are divided into two distinct zones with sharp boundaries indicated by the enhanced brightness around \(x/a = 18\), which actually give roughly locations of the wavefront (defined by the peak positions of density profiles shown in Fig. 4). Obviously, the waves are propagating from left to right of the plane. On the right hand side, the system is not affected yet and are in their respective equilibria, whereas on the left, where the waves just swept by, the systems are in a great disorder.

A small number of particles are observed traveling along with the wave for certain periods of time. Fig. 7 shows the periodogram (wavefront position v.s. time) of 4 successive pulse waves, together with trajectories (only component in \(x\) direction) of typical trapped and untrapped particles, and averaged trajectory as well. The curvature of the wavefront with time indicates the variation of the wave speed, as shown above in Fig. 5 (b). As in a classical wave-particle interaction picture, most of the particles just bounce forward and backward when the wavefront is approaching and leaving this area, such as the trajectory #1 in Fig. 7. Such a tendency may be seen more clearly in the averaged trajectory (dash-dot line), which oscillates back and forth during the passage of the wave front. Note here that there is a net shift in the averaged trajectory toward the wave propagation direction. We found that this shift is proportional to the amplitude of the wave and that it might be related to those particles which are carried along by the wave for a considerable distance: the trapped particles. Lines 2 – 6 in Fig. 7 are examples of trapped trajectories. Comparing with an untrapped trajectory (Line #1) and averaged trajectory (dash-dot line), the trapped ones (Lines 2 – 6) are characterized by extended periods during which the trajectory lines are parallel to the wavefront curves. This shows that these particles have a speed very close to the wave speed and travel together with the wave. The corresponding trajectories in \(v_\phi - x\) phase space are also shown in Fig. 7 (b) and (c), from which one can see that the trapping picture is different from the classical one in a sinusoidal potential well. Since the wave here is in the form of a pulse-wave or soliton, the trapping occurs in front of a single moving potential barrier. The trapped particles usually have extended trajectories in phase space, while untrapped ones making local circles. The similar tendency had also been observed in recent experiment [18].

It should be pointed out that in the simulation, all particle trajectories are recorded, but
only those particles, which lie in a very narrow region ($5\lambda_D$ wide in $x$ direction) around the moving wavefront and at the same time have an $x$-component of velocity above 90% of local wave speed, i. e., when $v_x > 0.9v_\phi$, are defined as trapped particles. Typically, there are a few hundreds (about 300 when $\Gamma = 20$ and less for higher $\Gamma$) of particles are trapped during the 4 successive pulse-wave propagations shown in Fig. 7. Trapped particles have a finite lifetime (trapping time), and will lose their energy and become detrapped very soon (If $v_x$ of a trapped particle decreases to below 0.9$v_\phi$, we say the particle is detrapped.), mainly due to the collisions with surrounding particles. The time interval, during which $v_x > 0.9v_\phi$, is then defined as the trapping time, for the convenience of later discussion. Typical trapping time is around a couple of $\tau_0$ and fewer particles can be trapped for longer period and vice versa. In our observation, the longest trapping time is about 12$\tau_0$.

As is shown above that the trapping picture is quite different from a classical one that we are familiar with in ordinary ion-electron plasmas. The differences mainly come from nonlinear effect associated with large amplitude waves and the pronounced interparticle interaction due to strong-coupling effect in our system. The former makes it possible to trap a large number of particles in the main part of the distribution (near $v = 0$), instead of only “resonant particles” with speed very close to the wave speed, and it may still be explained by the classical trapping condition, while the latter poses new condition for trapping to happen. The short-range interaction or correlation between particles must also be included by introducing the concept of “caging” potential formed by all surrounding particles. Now trapping of a particle needs not only enough energy to accelerate it to wave speed, but also enough energy to overcome the “caging” potential barrier. In other words, the strong coupling effect makes the trapping harder to happen in SCCPs than in ordinary weakly coupled plasmas, while on the other hand, makes the detrapping more significant and frequent.

5. Summary

Thus we have demonstrated the basic ideas of numerical experiments on strongly coupled complex plasmas through two examples, i. e., the heat transfer and shock wave propagation and particle trapping, by directly mimicking the real experiments. This kind of numerical simulation will be helpful to explain many phenomena observed in real experiments and to explore more details of physical pictures that an real experiment cannot easily obtain.

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