Large-scale Molecular Dynamics Simulations of Dense Plasmas

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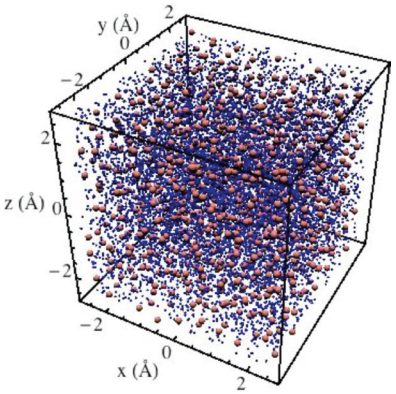
Fusion reactivities are typically computed using a binary collision picture in which two charged particles collide to form fusion-reaction products. Here, we have examined how that basic result is modified due to nearby particles that are present in dense-plasma environments. We have utilized the massively parallel molecular dynamics code ddcMD, which we have recently ported to the Cielo supercomputer, to study these dense-plasma effects in the context of fast ignition. We illustrate the effects of the dense-plasma environment by comparing our data against predictions given by a simple theory for low-density plasmas.

Dense plasma physics plays a central role in a wide variety of astrophysical settings and laboratory experiments. The microphysical properties of such systems can be accurately computed using molecular dynamics (MD) simulations, which correctly capture the N-body collisions inherent to strongly coupled (highly collisional) plasmas by self-consistently following time evolution of individual plasma particles in a 6D phase space (see Fig. 1). We have recently ported the Gordon Bell prize-winning, massively parallel MD code ddcMD [1] to Cielo, which is currently the sixth-largest supercomputer in the world. The ddcMD code was originally developed at LLNL and has been recently adapted to dense-plasma physics by a multi-institutional team including the authors of this review. It utilizes a highly optimized particle-particle-particle-mesh (PPPM) algorithm in order to efficiently handle the Coulombic interaction between the N particles in the simulation domain [2].

Fig. 1. A typical MD simulation box containing particles of two species. Individual atoms of the higher-density, lower-charged species are shown in blue and the lower-density, higher-charged species are shown in red. Data is extracted from the MD simulation by averaging the particle positions and velocity distributions as the simulation advances in time.



Our initial investigations have involved the exploration of structural properties of many-body Coulomb systems, and their implication for fusion burn at the National Ignition Facility (NIF). In particular, we wish to understand the role of charged-particle impurities on thermonuclear burn characteristics of the dense thermonuclear fuel. Under typical NIF burn conditions the fuel is composed of a mixture of charged particles which create, and are affected by, local charge density fluctuations. These fluctuations exert forces on individual plasma ions and change the likelihood of the rare event in which a pair of atoms are close enough to one another to achieve fusion. A fundamental understanding of this process is central to understanding the subtleties inherent to the fusion process.

Two-particle events are modified in the presence of the surrounding dense plasma. To observe these effects, we examine the pair correlation function (g(r)) of the plasma system. This function is formally defined as the probability of finding a particle within in a shell of width dr at a distance r from a reference particle; a simple cartoon of this is shown in Fig. 2. The simplest measure of g(r) for an ensemble of plasma particles is known as the "bare" result, $g_0(r)$, which considers an idealized system of only two particles interacting with each other through an unscreened potential. This model serves as a baseline to which we can compare the pair correlation data obtained directly from ddcMD simulations. The MD data contains the pair correlation effects of all the N-body interactions within the system, thus we can obtain the enhancement due to the screening inherent to the dense plasma system by defining the enhancement factor as the limit as r goes to zero of $E(r) = g(r)/g_0(r)$ [3]. In the context of fusion plasmas, enhancements greater than unity as r approaches zero indicate an increased likelihood of a fusion event occurring because particles are more likely to be close together than in an idealized system.

To illustrate the importance of the enhancement in dense plasma systems, we have run an MD simulation of a plasma with initial parameters relevant to fast ignition processes [4]. In fast ignition, a spherical deuterium-tritium (D-T) fuel pellet is first compressed and then ignited by separate laser pulses. A thin gold cone is often inserted into the D-T pellet to allow the ignition beam to more efficiently deposit its energy into the center of the pellet by "guiding" the beam and keeping this channel clear of the D-T plasma that is formed by the heating beam. As such, we have modeled a homogenous D-T mix at 100 eV and

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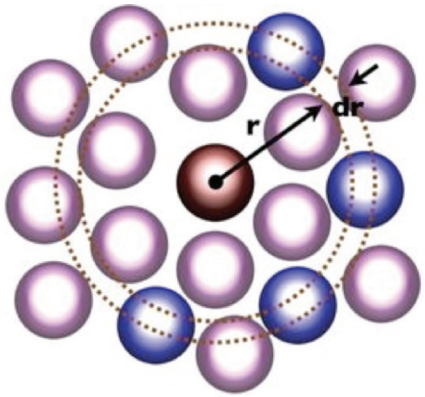
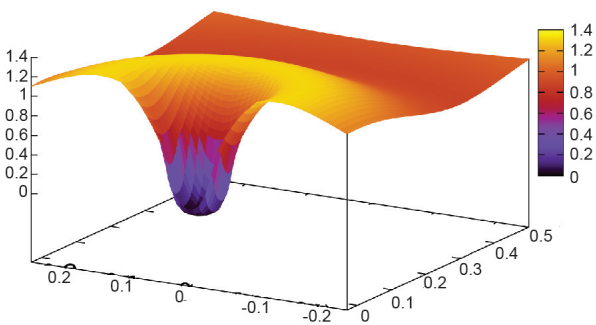


Fig. 2. Cartoon illustrating the pair correlation function g(r). Also known as the radial distribution function, g(r) is a measure of the probability of finding an atom in an annulus of width dr at a distance r from a particular atom, taken to be at the origin.

300 g/cc with a 5% (by number density) dopant of gold atoms at the same temperature. Under these conditions, we expect very strong coupling to occur between the gold atoms, as well as enhancements to g(r) at small r for the hydrogenic species. While we have successfully run plasma simulations on Cielo with 5 million atoms on ~4500 processors, and on LLNL's Blue Gene with 2.8 billion atoms on ~278,000 processors [1] in this example we have used 11,000 atoms on 10 processors–this corresponds to a cube of homogenous plasma with an edge length of 5.25 Å. The self-consistent evolution of the particles was followed for 450,000 time steps (350 fs) to reach an equilibrium configuration and collect sufficient particle statistics to construct the pair correlation function for the hydrogenic species shown in Fig. 3. The structure following the sharp incline in the radial distribution can be attributed to the presence of the gold atoms in the system.

Figure 4 shows the enhancement factor E(r) obtained from this simulation. The asymptotic enhancement value of ~6 as r approaches zero indicates that the likelihood of a fusion event occurring is increased by this amount relative to the result predicted by the binary interaction theory. This increase can be attributed directly to the influence of the dense-plasma environment. We note that the data is noisy at small r–this is to be expected because particles passing quite close to each other are rare events. We have recently developed a technique that allows us to easily sample these rare events, and as such, can measure the enhancement factor at extremely small r-values quite accurately [5]. This simple example clearly demonstrates both the influence of dense plasma effects on fusion-plasma environments and the extended (and new to LANL) capability of the MD code ddcMD.

Fig. 3. Pair correlation function g(r) for D and T atoms for an 11,000-atom simulation of typical fast ignition parameters. To better illustrate the physical meaning of the pair correlation function, we have here plotted g(r,θ).



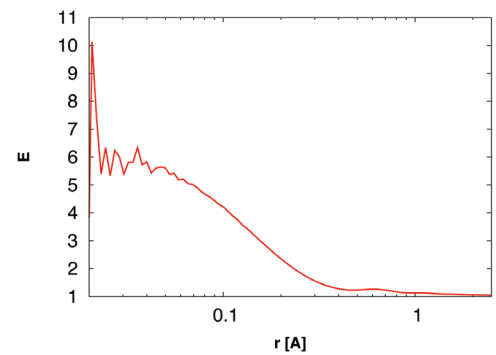


Fig. 4. The enhancement factor E(r) obtained using typical fast ignition parameters. Since like-charged particles repel each other, there are few statistics at small values of r; this leads to the noise observed in E(r).

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