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Radiation in Particle Simulations

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Abstract

Hot dense radiative (HDR) plasmas common to Inertial Confinement Fusion (ICF) and stellar interiors have high temperature (a few hundred eV to tens of keV), high density (tens to hundreds of g/cc) and high pressure (hundreds of Megabars to thousands of Gigabars). Typically, such plasmas undergo collisional, radiative, atomic and possibly thermonuclear processes. In order to describe HDR plasmas, computational physicists in ICF and astrophysics use atomic-scale microphysical models implemented in various simulation codes. Experimental validation of the models used to describe HDR plasmas are difficult to perform. Direct Numerical Simulation (DNS) of the many-body interactions of plasmas is a promising approach to model validation but, previous work either relies on the collisionless approximation or ignores radiation. We present four methods that attempt a new numerical simulation technique to address a currently unsolved problem: the extension of molecular dynamics to collisional plasmas including emission and absorption of radiation. The first method applies the Lienard-Weichert solution of Maxwell's equations for a classical particle whose motion is assumed to be known (section 3). The second method expands the electromagnetic field in normal modes (plane-waves in a box with periodic boundary-conditions) and solves the equation for wave amplitudes coupled to the particle motion (section 4). The third method is a hybrid MD/MC (molecular dynamics/Monte Carlo) method which calculates radiation emitted or absorbed by electron-ion pairs during close collisions (section 5). The fourth method is a generalization of the third method to include small clusters of particles emitting radiation during close encounters: one electron simultaneously hitting two ions, two electrons simultaneously hitting one ion, etc.(section 6). This approach is inspired by the Virial expansion method of equilibrium statistical mechanics.

1.) INTRODUCTION

Inertial fusion research aims to achieve self-sustaining nuclear reactions by compressing DT fuel to high particle densities. Fusion ignition requires ion temperatures T_i above 2 - 10 keV. In these hot plasmas electron and ion temperatures may be unequal. There may be impurities of higher Z material mixed with the DT fuel. We can expect the D, T ions to be fully-ionized, but high-Z impurities may retain some bound

electrons. As fusion reactions begin, highly energetic reaction products (e.g., 3.5 MeV DT fusion alphas) will add energy to the hot plasma, sustaining or raising the temperature.

This paper describes recent work aimed at developing a new fundamental tool for particle simulation of hot dense plasmas near the ignition threshold for fusion. At present the specific challenge is to add emission and absorption of radiation to molecular dynamics (MD) particle simulations. In the future we plan to include nuclear reactions and reaction-products in the simulations.

Inertial fusion plasmas have long been modeled by elaborate calculations using hydrodynamic models which typically include various forms of energy transport. The size-scale of these simulations is the $\sim 10^{-2}$ cm size of the target capsules. The models assemble theoretical formulas to describe the many underlying physical processes. The formulas are obtained from kinetic theories of varying complexity and *a priori* we expect that most of the formulas are good approximations. Hydrodynamic simulations have been compared to a variety of experiments at conditions below the ignition threshold, and have generally succeeded to describe or even predict experimental results.

However, in most cases the formulas were derived by assuming simplified initial conditions or boundary conditions, or by considering one process at a time, and it is always possible that some unexpected interaction between two microscopic phenomena could make a significant modification in the plasma behavior. In particular, radiation processes are typically studied separately from charged-particle energy-exchange, nuclear reactions and hydrodynamic processes (e.g., diffusive mixing of materials or viscosity effects on flow gradients).

Accurate and detailed experiments on burning plasmas might reveal unexpected couplings between the different processes but even with large new facilities now being prepared, sufficiently detailed experiments will be difficult to perform and diagnose. Despite many years of research on fusion science it is still not true that all the models for all the important basic process have been tested with adequate diagnostics at the relevant (extreme) conditions.

Fortunately, microscopic particle simulation offers an additional methodology. Particle simulation is based on known fundamental laws: Newtonian particle mechanics under the Coulomb pair-forces, a known coupling to the radiation field and (eventually) known cross-sections for nuclear reactions. Particle simulation automatically includes any nonlinear interaction between the fundamental couplings, and offers the possibility to see how the "macroscopic" energy-exchange coefficients emerge from the atomic-scale interactions.

Particle simulations do not need to make the typical approximations of kinetic theory, such as predicting three-body correlations by an integral over two-body distribution functions. A particle simulation with enough particles will generate many-particle correlations without theoretical assumptions and can test the validity of results

from kinetic theories. Another important advantage of particle simulation is that the diagnostics are accurate and comparatively inexpensive, although they also encounter questions of signal and noise.

Molecular Dynamics (MD) and Monte Carlo (MC) particle simulations have already provided a great deal of useful information about dense plasmas, especially in the low-temperature strongly-coupled range. However to the best of our knowledge radiation processes have never been included in atomic-scale MD or MC particle simulations.

There should be no doubt that radiation is important to ignition physics. The radiation energy-density may significantly exceed the matter energy-density at temperatures 2-10 keV, and the process of converting plasma energy into radiation competes with the possibility of heating to fusion conditions. (The conversion is rapid for low-energy photons and slower for high energy X-rays and that difference of rates can have a large effect on plasma energetics.)

The energy-density of ideal black-body radiation in vacuum is (T_{keV} is the temperature in keV units):

$$U = aT^4 = 13.7 \text{ MJ/cm}^3 T_{\text{keV}}^4 \quad (1)$$

In comparison the energy-density of ideal-gas DT plasma can be written

$$\rho E_{\text{mat}} = 116 \text{ MJ/gram } \rho_{\text{g/cc}} T_{\text{keV}} \quad (2)$$

The larger numerical coefficient in Eq. (2) should not obscure the higher power of temperature in the radiation energy density. At ignition temperatures, if the radiation is anything like a black-body field, the radiation energy is dominant. Likewise the equilibrium radiation pressure easily exceeds the material pressure. There are two important questions here: 1.) Is the radiation anything like a black-body (Planck) distribution? and 2.) Are the ideal-gas estimates too crude? The first question is about reaching equilibrium and the second questions is about non-ideal corrections due to coupling between particles, waves and radiation. Because the ideal equilibrium radiation pressure and energy are large, even modest corrections might play an important role for plasma hydrodynamic behavior.

For pure hydrogen (or DT) plasmas, the electron-ion Coulomb energy-exchange is faster than radiation processes. Even when multiplied by the small electron-ion mass-ratio m_e/M_i , the Coulomb cross-section exceeds the radiative cross-sections, so the most rapid temperature-equilibration is between electrons and ions. However this is not enough reason to ignore radiation processes.

First, the time-scale of interest is the time-scale for ignition. Just as the Coulomb cross-section exceeds the radiative cross-sections, so the radiation cross-sections greatly

exceed the fusion cross-sections, and therefore radiative phenomena will be well-advanced before fusion self-heating and ignition can occur.

A second reason to include radiation processes is that all real experiments involve plasmas with impurities of various atomic species. The elements present may depend on the specific target but they necessarily have atomic number Z and/or ionization state Z^* much greater than unity. However the radiative rates rise with high powers of Z (or Z^*) and so radiative phenomena are much more important for impure plasmas than for pure-hydrogen (or DT) plasmas.

Given these two reasons, we conclude that some treatment of radiative phenomena is essential to a realistic particle simulation of fusion ignition. Since there is no body of established techniques to perform such a combined simulation (radiation + atomic particle dynamics) we have been compelled to explore various algorithms and approaches, searching for the most appropriate.

This paper considers four methods. The first method applies the Lienard-Weichert solution of Maxwell's equations for a classical particle whose motion is assumed to be known (section 3). The second method expands the electromagnetic field in normal modes (plane-waves in a box with periodic boundary-conditions) and solves the equation for wave amplitudes coupled to the particle motion (section 4). The third method is a hybrid MD/MC (molecular dynamics/Monte Carlo) method which calculates radiation emitted or absorbed by electron-ion pairs during close collisions (section 5). The fourth method is a generalization of the third method to include small clusters of particles emitting radiation during close encounters: one electron simultaneously hitting two ions, two electrons simultaneously hitting one ion, etc.(section 6). This approach is inspired by the Virial expansion method of equilibrium statistical mechanics.

Each of these four approaches has been implemented in test-calculations of various sizes and each offers some insight and poses some difficulties. The present paper is a progress report on this research. We want to evaluate these methods to see whether they can obtain the right answer, whether they are computationally practical, and to see whether they offer the generality and elegance that we always wish to find in a new method of scientific inquiry.

2.) RADIATION IN PARTICLE SIMULATIONS: GENERAL CONSTRAINTS

Our particle simulations are classical but we know that radiation is a quantum phenomenon -- or at least the emission and absorption involve an irreducible minimum of quantum behavior. We must include that minimum but apparently it would be impractical to try to do fully quantum MD simulations. These facts are the fundamental challenge for our research.

As we explore different approaches, we constantly face the difficulty that a complete and rigorous classical solution of Maxwell's equations for the classical many-particle system would give a hopelessly incorrect result: instead of the Planck distribution, it would predict the Rayleigh-Jeans distribution for the radiation intensity. The Rayleigh-Jeans law has far too much energy in high-energy x-rays, and this would completely invalidate the energetics of the simulation. So we *must* force some quantum features onto the classical particle dynamics.

A related technical difficulty for simulations with radiation is caused by the technique of "pseudopotentials" often used to suppress recombination in MD simulations. Classical point-charge electrons and ions, interacting through the Coulomb potential, are unstable with respect to 3-body recombination into deeply bound states not allowed by quantum mechanics. For hydrogen, the lowest allowed boundstate is the 1s groundstate at energy - 13.6 eV; classical mechanics does not recognize this limit. Radiation will increase the recombination problem by adding another type of recombination - unless we limit the classically allowed emission in a way consistent with the quantum theory.

In most MD particle simulations, the 3-body recombination is suppressed by replacing the Coulomb potential by a pseudo-potential that does not support deeply bound states, i.e., by reducing the potential at small distances. If the long-range behavior is unchanged, then many plasma phenomena (screening, plasma waves, Coulomb energy exchange, etc.) are unchanged. Unfortunately the pseudo-potential changes the behavior for collisions with large scattering angles and those collisions are most important for emission or absorption of radiation, especially for high-energy ("hard") photons. In our work, a constant theme has been to search for a way around this difficulty and the algorithm described in section 5 below is one alternative to the pseudopotential method.

The algorithm described in section 5 treats the close collisions by a different method from that used for the main MD simulation. When an electron and an ion approach to within a small distance (typically ~ 0.2 Angstrom) they are treated as a two-body system and their collision is described by matching the current position and velocity to the classical Coulomb-scattering trajectory for the motion of the pair. This solution is used until they again separate. Since this part of the orbit is entirely governed by 2-body forces the 3-body recombination is automatically suppressed. We also can permit emission and absorption of bremsstrahlung radiation during the close collision, controlled by a Monte Carlo algorithm described in section 5, and this leads to a simulation that behaves in an essentially satisfactory manner. However there are questions or difficulties for this method and we discuss them in depth in this paper.

Quite generally, adding radiation to a particle simulation encounters both questions of principle and technical difficulties. We will discuss the difficulties together with the specific methods but give here a short preliminary list:

a.) Stochastic Evolution. The basic quantum nature of emission/absorption appears inconsistent with deterministic molecular dynamics (MD) time-evolution. (That is,

quantum mechanics predicts probabilities for emission, absorption but does not give a deterministic prediction which process occurs in a given encounter.)

b.) Time-scales. The generation of radiation is slow for the electron-proton system, so the simulation must be followed for many time-steps in order to see the appearance of a significant radiation field. Of course the radiative rates rise rapidly with Z and/or they can be artificially increased.

c.) Sampling. The expected number of photons is only comparable to the particle number at high temperatures. In a 1000 \AA^3 simulation box there will only be a few photons at $kT_R \sim 1 \text{ keV}$ and this will make a signal-to-noise problem for our simulations. At temperatures above $\sim 3 \text{ keV}$ this difficulty is greatly reduced.

d.) Fundamental data. We have good approximate rates for radiative processes involving one atom (ion) in a spherically symmetric environment, but do not have corresponding rigorous quantum calculations for non-spherical or multicenter clusters. To analyze emission from such systems we will use classical or hybrid semiclassical methods but would have more confidence in the results if we had rigorous quantum comparison calculations.

Early in this work there was a concern that the technique of simulating a number of particles confined in a computational box would lead to some unrealistic coupling to radiation. For example, if the particles are confined with reflecting boundary conditions by computational box-boundaries, the wall reflections correspond to abrupt accelerations: won't those accelerations cause spurious or unphysical radiation? If the particles are represented by periodic boundary conditions, then when an electron leaves the box on the right wall it is instantaneously re-injected on the left: in effect a sudden (superluminal) jump in position. Does that make some kind of Cerenkov emission? Careful study has shown these problems do not arise if the simulation is performed in a sensible way. For example, even if we used reflecting walls, the abrupt wall-acceleration would occur at a zero of the electromagnetic wave-field and would therefore not couple to radiation. (The periodic boundary-conditions are discussed in sections 3 and 4.)

Throughout this work we must also be alert to the possibility of deeper and more interesting difficulties: it is well-known that classical electrodynamics (and some versions of quantum electrodynamics) lead to divergent results unless the calculations are performed very carefully. In general the divergences affect only the calculation of higher-order processes (pair production, self-interaction, ...). There exists a very satisfactory method, the S-matrix renormalization theory, to remove the divergences, at least for few-particle collision processes. It is not clear today how these methods work out for a statistical ensemble of dense particles continuously interacting with radiation. As we examine the possible methods, we try to point out the possibility of problems with radiation reaction, self-interaction, etc. Divergent integrals do not occur in our work simply because we never consider an infinite number of normal modes; a high-frequency cutoff is artificially imposed by our computational limitations. That this cutoff is sufficient remains to be investigated further. Our simulations make no effort to obtain

results that are covariant or gauge invariant -- as is true for all particle simulations. The radiation algorithm described here does not require any specification of a gauge and there is no specific consideration of gauge invariance. However, the MD algorithms discussed here rely on forces acting on particles which in turn depend on gauge invariant quantities such as electric and magnetic fields.

3.) LIENARD-WEICHERT POTENTIALS

Classical OCP simulations assume instantaneous Coulomb interactions between charged particles.[1] In most cases the simulations are performed for N particles in a simulation box embedded in an environment modelled by periodic boundary conditions. It is known that the technique of periodic continuation leads to rapid convergence of the free energy and other equilibrium properties with the size of the simulation box.[2]

To introduce radiation into such a classical MD particle simulation, classical electrodynamics offers two straightforward approaches. One can replace the instantaneous Coulomb interaction by the retarded potentials (Lienard-Weichert potentials) for the electromagnetic field of classical point charges following known trajectories.[3] Alternatively one can expand the classical EM field in normal modes; Maxwell's equations give differential equations for the field amplitude coefficients (section 4). In this section we discuss the Lienard-Weichert method.

We have written a small code to evolve the motion of a few-particle system replacing the instantaneous Coulomb interaction with forces obtained from the Lienard-Weichert electric and magnetic fields. In doing this we encounter interesting questions to ask about all MD plasma simulations.

A first point is that the usual Coulomb MD simulation neglects the magnetic forces between moving particles. For the ion OCP (One-component plasma) this neglect is clearly justified, but it for simulations of electron motion in hot plasmas the approximation is more debatable. The magnetic forces are of order v/c relative to electrical forces, but this parameter is not small in a fusion ignition plasma. At an electron temperature of 2 keV, already $v_e/c \sim .11$, i.e., the magnetic forces are a 10 % correction.

An interesting fundamental question is that the usual periodic boundary conditions are inconsistent with relativistic causality: these boundary conditions assume instantaneous correlations between particles separated by large distances ignoring the requirement that these correlations can only propagate at speeds less than (and for plasma waves, *much less than*) c .

This is an objection in principle, but it is not clear that the artificial long-range correlations have a significant effect on thermodynamic properties in the limit of large N .

It is probably more important that the strong electric fields and large energy-density of radiation are neglected in the usual simulations.

Using the Planck formula we can calculate the RMS microfield of equilibrium black-body radiation ($T_R =$ radiation temperature):

$$E_{Rad} = 1.2 \cdot 10^{10} \left(\frac{Volt}{cm} \right) \left(\frac{T_R}{keV} \right)^2 \quad (3)$$

At temperatures in the keV range, this electric field exceeds the Coulomb fields of neighbor ions. Of course E_{Rad} is rapidly oscillating and the electron response to a rapidly oscillating field is only a small "quiver motion"

$$\delta v_{rad} \sim eE/(m\omega) \quad (4)$$

This quiver velocity is evidently less than the electron thermal velocity because most of the black-body photons have high frequencies. However since $\langle \omega \rangle \sim T$, δv_{rad} grows proportional to T while the thermal velocity is $\sim \sqrt{T}$. Additional study and verification are probably needed to be sure that the large field of Eq. (3) plays no role in atomic or nuclear processes.

Lienard-Weichert potentials

For calculations by the Lienard-Weichert (LW) method, an electron's position and velocity $\mathbf{r}_p(t)$, $\mathbf{v}_p(t)$ are *assumed to be known*, and we use the LW solution of Maxwell equations for the \mathbf{E} , \mathbf{B} fields generated at a field point \mathbf{r} , t . [3] These fields are simply expressed in terms of the retarded time t_{ret} and retarded distance \mathbf{R}_r defined by:

$$R_r = r - r_p(t_{ret}) \quad R_r = \left| r - r_p(t_{ret}) \right| = c(t - t_{ret}) \quad (5, 6)$$

In this brief summary we use the same notation for vector and scalar distance, e.g., R_r in the line above; the careful reader can easily correct the notation. In the usual Lorentz gauge the fields are obtained from scalar and vector potentials,

$$\phi = \frac{q}{\left(R_r - \frac{\mathbf{v} \cdot \mathbf{R}_r}{c} \right)} = \frac{q}{R} \quad \vec{A} = \frac{q}{c} \frac{\vec{v}}{\left(R_r - \frac{\mathbf{v} \cdot \mathbf{R}_r}{c} \right)} = \frac{q}{c} \frac{\vec{v}}{R} \quad (7, 8)$$

A useful quantity (script \mathcal{R}) is defined by:

$$\mathcal{R} = \left(R_r - \frac{\vec{v} \cdot \vec{R}_r}{c} \right) \quad (9)$$

When appropriately differentiated the potentials give the electric and magnetic fields at the field point r, t :

$$\vec{E} = \frac{q}{R^3} \left(1 - \frac{v^2}{c^2} \right) \left[\vec{R}_r - \frac{\vec{v}}{c} R_r \right] + \frac{q}{R^3 c^2} \vec{R}_r \times \left(\left[\vec{R}_r - \frac{\vec{v}}{c} R_r \right] \times \vec{a} \right) \quad (10)$$

$$\vec{B} = \frac{\vec{R}_r}{R_r} \times \vec{E} \quad (11)$$

Such fields are produced by each particle in the plasma. Each particle is subject to the forces produced by the *other* particles (there is no self-interaction). The formula for the electric field consists of two terms with different dependence on radius. The first term ($\sim 1/R^2$) is a modified Coulomb field while the second term ($\sim 1/R$) is also proportional to the acceleration \mathbf{a} evaluated at the retarded time, and leads to the emission of radiation.

To use the Lienard-Weichert fields in a simulation we save the classical trajectories (histories) $\mathbf{r}_j(t), \mathbf{v}_j(t)$ for each particle. We have this data from each previous time-step, and store the data for $\sim 10^5$ time-steps. When we want to calculate the force on particle j , we search the histories for each other other particle k to find the retarded time for the pair (j,k) . We find time-steps that bracket the retarded time and interpolate. To speed-up the search, it is useful to save a pointer to the previous retarded time; the t_{ret} only increases by about dt during a time-step dt , so the previous value of t_{ret} is a good first guess.

At the beginning of the simulation ($t = 0$) we launch the particles with random positions and velocities sampled from an appropriate Maxwellian. For the first time steps we extrapolate to earlier times ($t < 0$) to find the retarded times and distances; we do this assuming straight-line motion before $t = 0$. Since there is no acceleration at these unphysical times, no radiation is produced. For nearby particles the retarded time is very "recent", i.e., occurs at a time after the end of the last previous time-step. For these cases an extrapolation procedure is needed rather than simple interpolation.

For the LW method, we sum over the N particles in the simulation box and also over a finite number of image charges for each particle, setting aside the difficult question about convergence with the number of images. The retarded times of the image charges grow with distance and so the simulation must run for a certain length of time before image-charge location data becomes available.

We do not start to accumulate data for the thermodynamic averages until the calculation has progressed long enough so that dynamical data (calculated with accelerations) has become available for all particles and their images.

We use electrical forces from the past positions of the image-charges but their current positions are assumed to be exactly correlated with the current positions of the N particles in the simulation box. This is the causality issue. The image charge's past positions affect the motion of the charges in the box after a time-delay of $\Delta t \sim R/c$, but the box particles' current positions instantaneously determine the image particles current positions. The round-trip influence time is then R/c instead of $2R/c$. One might worry that this artificial correlation acts like a "Maxwell Demon" to perturb the entropy of the simulation; deeper study is needed to assuage this concern. This is a question, not just for the Lienard-Weichert simulation but for any particle simulation using periodic boundary conditions. (With pure Coulomb potentials, as is usual in MD simulations, the round-trip influence time is zero!)

The LW potentials give pair-forces between the electrons and ions. In principle the same formulas also predict the EM field throughout the volume of the plasma simulation box. The LW formulas enable us to distinguish emitted radiation from fields attached to the particles (Coulomb + $v \times B$ magnetic fields) but further analysis (more precisely, Fourier analysis) would be required to extract the radiation spectrum.

The LW method has difficulty to describe a pre-existing radiation field, for example in a plasma receiving radiation emitted by a high-temperature source. In order to describe such radiation the simulation would have to carry additional variables such as the amplitudes of the various normal modes of the radiation field. If this were done one might as well use the method of the next section.

The most important defect of the LW method is that it is not quantum mechanical. If we Fourier analyze the LW fields $\mathbf{E}(\mathbf{r}, t)$, $\mathbf{B}(\mathbf{r}, t)$ the best result we can hope for is the basically incorrect Rayleigh-Jeans spectrum. (We did not continue our LW simulations long enough to see this problem.)

For this reason it is a very interesting question whether there is a quantum version of the LW method. Using well-known methods of quantum electrodynamics (Glauber states), one can convert classical field amplitudes into semiclassical quantum fields that are consistent with the specified classical amplitudes.[4, 5] To do this for the LW potentials, it is useful to transform the LW potentials to the Coulomb gauge and we offer here a simple and general formula for this gauge transformation:

$$f(\mathbf{r}, t) = -qc \int_{t_{\text{ret}}(\mathbf{r}, t)}^t \frac{dt'}{|\mathbf{r} - \mathbf{r}_p(t')|} \quad (12)$$

$f(\mathbf{r}, t)$ is the generating function for the gauge transformation. This function f is essentially the potential of a uniformly charged wire running along the spatial trajectory of the electron during its motion from t_{ret} to t . In the Coulomb gauge, the scalar potential is exactly the instantaneous Coulomb potential,

$$\phi(r, t) = \frac{q}{|r - r_p(t)|} \quad (13)$$

and the vector potential is

$$\vec{A}(r, t) = qc \int_{t'=t_{ret}}^{t'=\bar{t}} \frac{\vec{r} - \vec{r}_p(t')}{|r - r_p(t')|^3} dt' + \frac{q}{R} \left(\frac{\vec{v}}{c} - \frac{\vec{R}_r}{R_r} \right) \quad (14)$$

The formulas apply to an electron with an arbitrary (known) trajectory. From Eq. (14) it is easily shown that the transformed potential obeys $\text{div } \vec{A} = 0$, the signature of the Coulomb gauge.

For an electron moving with constant velocity (i.e., $\mathbf{r}_p(t) = \mathbf{v} t$), it is easy to evaluate the integral in Eq. (14). For comparison with the normal-mode method of the next section, we give the Fourier transform of that Coulomb gauge Lienard-Weichert potential (describing motion at constant velocity):

$$A_{Coul}(\vec{k}, t) = 4\pi q \frac{k^2 \vec{v} - (k \cdot v) \vec{k}}{c^2 k^2 - (k \cdot v)^2} e^{-ik \cdot vt} \quad (15)$$

The LW method is clearly an $O(N^2)$ algorithm - we find the force on each particle by a summation over contributions from each other particle - and this limits the number of particles that can be treated. We do not have a generalization of the Ewald summation technique to include retardation and magnetic effects, and have underlined the causality difficulties with such a generalization. Figure 1 shows the simulation results of two electrons and two ions interacting via Coulomb and radiation fields. The sphere represents a unit sphere surrounding the simulation box. The colors denote the magnitude of the normal of the Poynting vector, where blue denotes zero magnitude. The dipole nature of the emission spectrum is clearly seen by the blue shading at the poles. As the electrons move through the system, the blue shading moves around the ball but always in a way such as two poles are always zero.

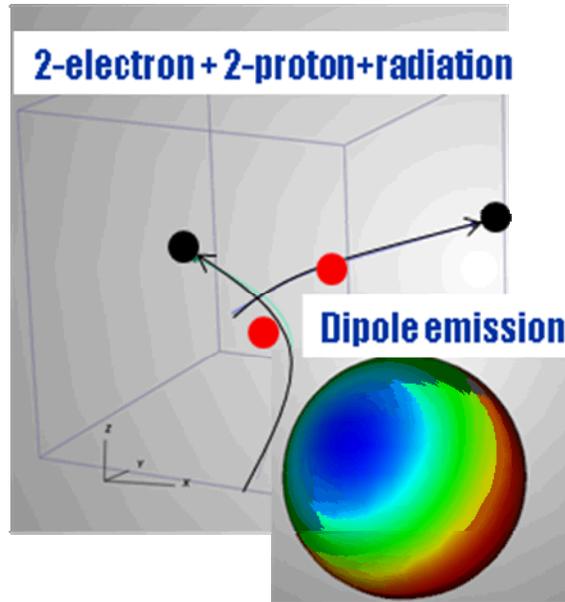


Figure 1: MD plus radiation results for two electrons scattering off of two ions. The sphere represents a unit sphere surrounding the simulation box and the colors refer to the normal component of the Poynting vector.

4.) NORMAL-MODE EXPANSION OF EM FIELD

In the normal-mode method, the classical electromagnetic field is expanded in a set of propagating waves that obey periodic boundary-conditions in some rectangular box. The normal-mode amplitudes change due to absorption and emission by the particles in the simulation box. Since the initial normal-mode amplitudes can be chosen arbitrarily we can simulate plasmas with arbitrary initial radiation spectra with this method.

It is most natural to define these normal modes in the same simulation box used for the particles. The advantage of this choice will be discussed below.

There are *many* normal modes. Our small work-station simulation uses 200 wave-vectors in each spatial direction, i.e., $8 \cdot 10^6$ normal modes. The largest allowed wave-vector k determines the spatial resolution inside the simulation box. The time-step in the simulation should resolve the highest photon frequency ω unless we adopt some method to integrate analytically over short time intervals. For example, with a $(100 \text{ \AA})^3$ box and $8 \cdot 10^6$ normal modes the high-frequency modes have a wavelength of about 1 \AA ($h\nu \sim 10 \text{ keV}$) and the exploratory calculations could be done on a small workstation.

Normal-mode expansion for classical electrodynamics:

It is natural to write the equations for the normal-mode expansion in a notation close to non-relativistic Coulomb-gauge quantum electrodynamics [4, 5]:

$$A(\vec{r}, t) = \sum_{k,\lambda} \hat{e}_{k,\lambda} \left(\frac{2\pi\hbar c^2}{\omega_k V} \right)^{1/2} \left[a_{k,\lambda} e^{i\vec{k}\cdot\vec{r}} + a_{k,\lambda}^+ e^{-i\vec{k}\cdot\vec{r}} \right] \quad (16)$$

$$\frac{\partial A(\vec{r}, t)}{\partial t} = \sum_{k,\lambda} \hat{e}_{k,\lambda} \left(\frac{2\pi\hbar c^2}{\omega_k V} \right)^{1/2} (-i\omega_k) \left[a_{k,\lambda} e^{i\vec{k}\cdot\vec{r}} - a_{k,\lambda}^+ e^{-i\vec{k}\cdot\vec{r}} \right] \quad (17)$$

In this equation, \mathbf{k} denotes a photon wave-vector and $\mathbf{e}_{k\lambda}$ is the polarization vector of the mode defined by \mathbf{k} , λ ($\lambda = 1,2$ identifies the polarization state). The notation

$$C_k = \left(\frac{2\pi\hbar c^2}{\omega_k V} \right)^{1/2} \quad (18)$$

is often used for the coefficient in Eqs. (16,17). In the quantum theory, a and a^+ are field operators but in the classical case they are simply complex numbers; $a_{k\lambda}(t)$ = complex field strength, a^+ is its complex conjugate. V is the volume of the quantization box and $\omega = c k$ is the photon frequency.

This expansion for the vector potential and its derivative applies in the Coulomb (transverse) gauge, expressed by the condition $\mathbf{k} \cdot \mathbf{e}_{k\lambda} = 0$. The functional forms for the vector potential and its derivative already guarantee that the electrical and magnetic fields will satisfy three of the Maxwell equations. The fourth Maxwell equation is satisfied if the field amplitudes $a_{k\lambda}$ obey an equation for the coupling to the particles.

$$i\hbar \frac{\partial a_{k\lambda}}{\partial t} = \hbar\omega a_{k\lambda} - \sum_p \frac{q}{c} C_k (\vec{v}_p \cdot \hat{e}_{k\lambda}) e^{-ik \cdot r_p(t)} \quad (19)$$

From Eq. (18) we can easily derive an equation for the photon number $n_k = a_{k\lambda}^+ a_{k\lambda}$,

$$\hbar\omega \frac{\partial n_{k\lambda}}{\partial t} = q (\vec{v}_p \cdot \hat{e}_{k\lambda}) \frac{i\omega}{c} C_k \left(a_{k,\lambda} e^{ik \cdot r_p(t)} - a_{k,\lambda}^+ e^{-ik \cdot r_p(t)} \right) \quad (20)$$

(The higher-order coupling ($\sim A^2$) is omitted here.) For this normal-mode expansion one has separated transverse and longitudinal contributions to the fields, their energies and to the energy flux. The technical details of the separation are explained in several references (e.g., Kroll [4], Cohen-Tannoudji [5]).

Given the vector potential and its derivatives, the radiation electric and magnetic fields are calculated by

$$E_{k,\lambda} = \hat{e}_{k\lambda} \frac{i\omega}{c} C_k (a_{k,\lambda} e^{ik \cdot r} - a_{k,\lambda}^+ e^{-ik \cdot r}) \quad E = -\frac{1}{c} \frac{\partial A}{\partial t} \quad (21)$$

$$\vec{B}_{k,\lambda} = i\vec{k} \times \hat{e}_{k\lambda} C_k (a_{k,\lambda} e^{ik \cdot r} - a_{k,\lambda}^+ e^{-ik \cdot r}) \quad B = \nabla \times A \quad (22)$$

To these fields must be added the instantaneous Coulomb field between the point charges. Corrections to the instantaneous Coulomb field due to retardation and relativistic distortion of the $1/r^2$ field are obtained through Eq. (21) from Eq. (19). These corrections can be thought of as due to "bound photons" carried by a moving charged particle.

For the case in which there is no coupling to particles, the equation of motion, Eq. (19), for $a_{k\lambda}$ has the simple free-field solution $a_{k\lambda} \sim e^{-i\omega t}$. When there is a coupling, the amplitude changes corresponding to emission and absorption. In the classical theory these are distinguished by the relative phases of the terms in Eq. (19).

Eq. (19) is easily solved for the simplest case of coupling to a particle that moves with constant velocity v . The result agrees with Eq. (15), i.e., the normal-mode method and Lienard-Weichert method contain the same physics.

We can evolve the normal-mode amplitudes using Eq. (19) and then reconstruct the local electric, magnetic fields. This method gives the classical electromagnetic theory in a form closely parallel to nonrelativistic quantum electrodynamics. The particle motion is governed by the total electric and magnetic fields at the location of the particle, so the particles respond to any existing radiation.

A question arises immediately: why do the classical equations (16-22) contain Planck's constant? Examination reveals that Planck's constant is simply a convenient normalization of the field amplitudes $a_{k\lambda}$. If one changes notation by grouping together the product $\sqrt{\hbar} a_{k\lambda}$, it will be found that there's no further appearance of Planck's constant. In the quantum theory the operators a, a^+ cannot be rescaled in this way because they obey the additional equation

$$[a^+, a] = -1 \quad (23)$$

This relation fixes the normalization in the quantum case.

Test-code for the normal-mode method

Our calculations include 8,000,000 normal modes, i.e., *many* normal modes. The spatial resolution is limited by this number. The time-step must be small enough to resolve changes in the particle velocity including high-frequency perturbation by the x-ray photons $v_p(t)$.

The electric and magnetic fields reconstructed from the normal-mode amplitudes, $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$, contain some numerical noise because of the imperfect spatial resolution. Despite this noise it is clear that the results agree with \mathbf{r} -space Lienard-Weichert calculations; in particular, the distortion of the static Coulomb field due to the particle motion, and the magnetic field are found to be essentially the same.

For the normal-mode expansion, we find (both numerically and analytically) that if the radiation normal modes are defined in the same box used for the particles, using periodic boundary conditions, then the fields (near field, emitted radiation) generated by the particle motions move as if in the periodically extended system.

For example, the $O(v^2)$ corrections to the Coulomb potential remain attached to a particle as it exits one side of the simulation box and re-enters the opposite side. It is specially interesting that part of the radiation correction precedes the electron and jumps across the box before the electron itself. The distorted Coulomb field follows when the particle crosses the cell boundary because we use periodic BCs *with the same quantization box* for the radiation as used for the particle simulation. The corrections to Coulomb's law obtained from the normal mode method agree (exactly) with the distortions described by the Lienard-Weichert formulas, when evaluated for the same particle motion.

The normal-mode method automatically includes absorption and emission processes. Absorption occurs because coupling to the high-frequency electric field is contained in the particle equation of motion as well as in the radiation equation.

It might be possible to sample and interpolate for the normal modes, without keeping so many degrees of freedom. It is reasonable to expect an isotropic plasma will create an isotropic radiation spectrum (apart from fluctuations) and that expectation could be forced onto the algorithm with a consequent loss of information about interference effects. We have not yet attempted this type of calculation.

There is an interesting question about self-interaction. In the LW method, all the interactions between particles are explicit pair-interactions (including events in which a photon is emitted, propagates some distance, and then is absorbed later) and our instructions are to never permit self-interaction between the particles. (Interaction of a particle with its periodic image is permitted.) In the normal mode approach, each particle changes the general radiation field which then can interact back with the same particle. Is there a self-interaction? Is it divergent? Why not?

In fact, in the simulations any radiation field generated by a particle leaves the vicinity of that particle at the speed of light, and only returns to interact with the same particle after reflection from the box boundary. It's possible that a simulation with many more normal modes would encounter a difficulty, but our modest simulations do not seem to exhibit any problem from self-interaction.

These simulations are entirely classical (classical particles and a classical electromagnetic field). They necessarily produce an incorrect result for the high-frequency electromagnetic field: they must relax to the Rayleigh-Jeans distribution instead of the Planck distribution for the black-body radiation. The Rayleigh-Jeans law is the classical result, but for fusion plasmas it would be seriously incorrect.

On this point, we have two comments. One is that for the long-wavelength part of the electromagnetic spectrum the Rayleigh-Jeans law is not significantly incorrect. So our ultimate algorithm may use the normal mode equations for this part of the radiation field (although it does not carry a large energy-density in any case).

The second point is the case against trying to develop a quantum version of the normal-mode calculation. A fully-quantum simulation would follow a rapidly-increasing family of copies of the system with different numbers of photons in different photon modes and must permit transitions (including interference) between these copies; a simple estimate of the number of states makes this approach seem impractical. For example, to follow states with 0, 1 and 2 photons each for 10^7 photon modes would require carrying $3^{10 \text{ million}} \sim 10^{3,000,000}$ amplitudes.

Finally there is an important computational question: scaling with the number of particles or size of the system. We imagine comparing systems of constant particle density in large and larger simulation boxes. The number of particles $N_p \sim L^3$, where L is the edge of the box. To obtain a constant spatial resolution (something comparable to the particle separation, for example) the normal mode method requires us to carry more normal modes for the larger box: basically the number of normal modes also scales as L^3 . Since each normal mode must interact with each particle, this is also an N_p^2 algorithm, like the LW method.

5.) BINARY ENCOUNTER EMISSION/ABSORPTION MODEL

At this point it is clear we must include quantum effects in the simulation, at least a semiclassical form, in order that the simulations satisfy the common-sense requirement that they relax toward a Planck spectrum for the radiation.

Apparently the simplest way to accomplish this follows Einstein's original discussion of detailed balance [6]: the probabilities of absorption and emission during a collision are required to be respectively proportional to expressions of the form:

$$\text{absorption} \sim f(E_l) v_l B n_\nu \quad (24)$$

$$\text{emission} \sim f(E_u) v_u B (n_\nu + 1) \quad (25)$$

where $f(E)$ is the electron distribution function for lower and upper electron energy-states (denoted by subscripts l, u); v_l, v_u are the approach velocities; n_ν is the number of photons

per normal mode and B is a coefficient which must be equal for two processes related by time-reversal. We use the symbol B to suggest the Einstein B coefficient (which refers to line transitions) but in our case B is an appropriate average of the bremsstrahlung cross-section and depends on electron and photon energies.

The pair of electron states related by detailed balance have different energies E_u , E_l which differ by the energy $h\nu$ of the photon emitted/absorbed ($E_u - E_l = h\nu$). The one-electron states in the classical simulation have specified position and velocity whose apparent accuracy exceeds the uncertainty limit. With this formulation of the radiative processes we expect that the simulation will drive the two species (electrons, radiation) toward equilibrium with a Maxwell distribution for the electrons and a Planck function for the radiation, and if the coefficient B is approximately correct the relaxation will occur on an realistic time-scale. At equilibrium the rates of emission and absorption will be equal.

We do not have a deterministic algorithm to implement these rates, and instead assume there are probabilities for emission and absorption (during strong collisions). This means we must combine molecular dynamics (a classical and deterministic simulation) with the Monte Carlo method (which uses random numbers to make choices during the simulation) in a semi-quantum simulation.

To obtain a feasible algorithm we implement the Einstein expressions for absorption/emission rates by a hybrid MD/MC (molecular dynamics/Monte Carlo) algorithm described here. Our method requires approximations that ignore potentially interesting (small) effects. While our algorithm does relax to the correct thermal equilibrium, other methods could be considered and we continue to explore other methods that might capture other aspects of the physics.

MC/MD Algorithm

In this approach the radiation field will be represented by an isotropic homogeneous photon spectrum I_ν . In equilibrium I_ν is expected to be the black-body function B_ν :

$$B_\nu = \frac{2h\nu^3}{c^2} n_\nu^0 = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1} \quad (26)$$

Here the symbol n_ν again denotes the number of photons per normal mode of the radiation field. We assume radiation is emitted and/or absorbed in electron-ion collisions and ignore smaller contributions from electron-electron or electron-ion collisions. At present we also ignore Compton scattering although ultimately it must be included.

In this approach we assume the radiation field is isotropic and replace the many normal mode amplitudes by the photon energy-distribution. This means that instead of carrying 10^7 normal modes we carry only ~ 100 photon energy-bin populations. We

make no attempt to represent any spatial variation of the radiation field inside the simulation box, i.e., we are considering electron-photon energy-exchange but not radiative transfer.

The MC algorithm for radiation emission/absorption assigns a conditional probability of emitting/absorbing during each electron-ion collision. We convert existing formulas for bremsstrahlung cross-sections into appropriate conditional probabilities while preserving detailed balance.

We begin with the Kramers' absorption and emission cross-sections.[7] Here we write the cross-sections and show how they are normally used in kinetic theory, i.e., how they generate a number of radiative events dN per volume d^3r , time dt and photon energy range $d(h\nu)$. The notation matches an earlier review article by one of the authors.[8]

Inverse bremsstrahlung absorption is a 3-body reaction (the initial particles are electron, ion and photon), so the absorption cross-section σ^{abs} has units cm^5 . The Kramers form for σ^{abs} is

$$\sigma^{\text{abs}} = \frac{8\pi^3}{3\sqrt{3}} Z^2 a_o^5 \left(\frac{e^2/a_o}{h\nu} \right)^3 \left(\frac{e^2/a_o}{\varepsilon} \right) \quad (27)$$

If σ^{abs} is multiplied by the spectrum of ambient photons $= n_\nu dN/d(h\nu)$ (photons/ cm^3 -eV) and integrated over photon energy it yields a normal cross-section (cm^2) for absorption. In a kinetic theory this cross-section gives the rate of photon absorption events:

$$\frac{dN}{d^3r dt d(h\nu)} = n_I \int \frac{2d^3p}{h^3} |v| f(\varepsilon) \sigma^{\text{abs}} n_\nu \frac{dN_r}{d(h\nu)} \quad (28)$$

Here n_I is the ion number density and $f(\varepsilon)$ is the electron distribution function.

The emission cross-section σ^{emiss} is a differential cross-section to emit a photon of energy $h\nu$ so its units are cm^2/eV .

$$\frac{d\sigma^{\text{emiss}}}{d(h\nu)} = \frac{8\pi}{3\sqrt{3}} Z^2 \alpha^3 \left(\frac{e^2/a_o}{\varepsilon_o} \right) \frac{a_o^2}{h\nu} \quad (29)$$

To obtain the emission rate, σ^{emiss} is multiplied by $(n_\nu + 1)$ to include stimulated emission and integrated over photon energies (up to the electron's initial energy). The rate of emission of photons of energy $h\nu$ is (in kinetic theory)

$$\frac{dN}{d^3r dt d(h\nu)} = n_I \int \frac{2d^3p_o}{h^3} |v_o| f(\varepsilon_o) \frac{d\sigma^{\text{emiss}}}{d(h\nu)} (n_\nu + 1) \quad (30)$$

We must adapt these expressions to the different description used in the MD simulation. In that description the electron distribution function $f(\varepsilon)$ is being sampled

one collision at a time; the factors n_l and $f(\varepsilon)$ are represented by the frequency of attempting the radiation calculation.

The cross-sections become conditional probabilities when we form the ratio to the Coulomb collision cross-section. Analysis of special MD simulations (which did not include pair-interactions) show that the rate of collisions is, as expected from kinetic theory,

$$n_e n_i < \sigma v > \quad (31)$$

where n_e , n_i are electron and ion number densities, σ is the cross-section and v is the relative velocity. For example, if we ask the MD simulation to count the rate at which electrons arrive within a distance R_B of an ion, the MD rate is given by the above formula with $\sigma = \pi R_B^2$ (to about 1 % accuracy).

Given that an electron has arrived within a distance R_B of an ion, we take the conditional probability of emission (of a photon of energy $h\nu$) to be the ratio

$$\frac{\left[\frac{d\sigma}{dh\nu} (n_\nu + 1) \right]}{(\pi R_B^2)} \quad (32)$$

This conditional probability is proportional to $1/R_B^2$ but the dependence on R_B cancels because the rate of arrival of the electrons is proportional to R_B^2 . We have verified that simulations with different values of R_B give similar rates for the radiative events to within the numerical fluctuations.

Our algorithm can now be outlined:

- 1.) When an electron arrives within a distance R_B of an ion, use a random number to decide whether any radiative process occurs. (The probability of a radiative process is small so this test is rarely passed.) If not, proceed with the usual Coulomb collision. The probability is calculated using the current photon populations in the integrated cross-sections.
- 2.) If there is a radiative event, determine whether it is emission or absorption and determine the photon frequency. Emission and absorption do not have equal probabilities (in general) according to Eqs. (24, 25). [It is the time-reversed processes that have equal probabilities.] The determination is based on one or several random numbers; the normalized probability distribution is obtained from the cross-sections by the usual MC cumulative probability.
- 3.) The photons are described by photon frequency groups and the emitted/absorbed photon is assigned the energy at the center of the group (while the photon density of states is an integral over the group). This change of photon energy is an approximation

that has its largest effect for the hardest and softest photons. The electron energy is reduced (or increased) to conserve energy.

This algorithm is installed in the Coulomb molecular dynamics code without changing the Ewald sum used to handle the long-range part of the Coulomb interaction. We select photon energy-groups that put primary emphasis on relatively high-energy photons which are expected to be most important for the energetics. The high-energy photons are emitted and absorbed in relatively strong ("close") collisions and these events are expected to be mainly binary electron-ion collisions not strongly influenced by the neighboring ions. It is likely that a different algorithm could be developed to handle the lower photon energies and this algorithm might not need to make the binary-encounter approximation.

The simulations we have performed with the algorithm described here indeed relax to a photon distribution consistent with a Planck function. The low-energy frequency groups relax much more rapidly than the high-energy photons. Simulations performed on a small workstation have substantial numerical noise because the number of photons in a 1000 \AA^3 simulation box is not large at $kT < 5 \text{ keV}$. The algorithm has been added to our larger parallel simulation code and has been used for larger simulations and which give less numerical noise.

At present the simulations assume the Kramers cross-sections and this is a limitation that precludes study of new effects such as modified emission when an electron simultaneously encounters two nearby ions. We anticipate there should be interference between the emission probabilities and the algorithm described in this section neglects this interference.

The Kramers cross-sections are summed over angular momentum of the incoming electron, although it is evident that the smallest angular momenta are strongly dominant. It would be more accurate to use the L -resolved cross-sections which are given by relatively simple formulas. It would also be possible to improve the accuracy of the Kramers cross-sections by multiplying them by a correction for quantum mechanics (the Gaunt factor), but this is not a large correction for cases where the cross-section is large.

The algorithm described in this section has an important advantage: the close collisions (corresponding to electron-nucleus distance shorter than R_B) are handled as binary collisions and the exact classical Kepler orbits can be used for the Coulomb scattering. These orbits give deflections consistent with the Rutherford cross-section, the same result obtained from a full quantum mechanical solution of the corresponding collision. In this case there is no need for a pseudopotential, which inevitably distorts the large-angle collision cross-section.

The pseudopotential is not needed because the unphysical three-body recombination to negative energy states does not occur in the two-particle classical system. However if we improved the algorithm for motion at $r < R_B$, say by including a microfield from the ambient environment, and if this microfield were allowed to change

during the collision, then we would again have to confront the problem of recombination. At present we omit the possibility of radiative recombination; this phenomenon will enter in future simulations in which each ion is allowed to be coupled to a collisional-radiative kinetic model.

The calculations described here represent one approach to simulating the coupling of particles and radiation but other methods or hybrids need to be explored to evaluate all the many physical processes which are present in such a rich environment. We are especially interested in effects of interference in simultaneous collisions of one electron with two or more ions, interference in collisions of two or more electrons with one ion, interference between subsequent collisions, and processes in which the high-frequency quiver-velocity of electrons (caused by black-body radiation) alters the collision dynamics. For most of these processes considered in isolation there are analytic calculations in the literature but the phenomena interact. It may be difficult to describe all these effects in the same simulation but we plan to improve our algorithms toward that goal.

6.) MULTICENTER EFFECTS

In this section we briefly mention our recent efforts to move to an approximate inclusion of multi-center effects in the emission and absorption of radiation. By multi-center effects we mean the additional emission which occurs when two target ions are close together and one electron simultaneously strikes both, or the additional emission which occurs when two electrons simultaneously strike the same ion. In each case we compare the multiparticle collision with the sum of the the two separate interactions, in the usual spirit of the Virial expansion.

For the multicenter interactions we propose to group together (and allow interference between) the accelerations of the particles involved in the collision. Thus in an electron-electron collision, if we keep the accelerations of both electrons (which are equal and opposite) we find a small result (zero in the dipole approximation).

An expansion in terms of small clusters of near-neighbor particles may seem to be threatened by the long range of the Coulomb interaction, but in fact the situation is more favorable for radiation than for the plasma equation of state. That is because the emission/absorption probabilities are basically proportional to the square of a fourier component of the classical acceleration, i.e., $a(\omega)^2$, and for Coulomb forces this quantity falls off like $1/R^4$, where R is the particle pair-separation. Of course the actual convergence with distance is probably much more rapid because the various regions of the plasma are neutral on the average so positive and negative accelerations by distant charges strongly cancel.

We plan to improve our simulations guided by classical emission calculations (using the Lienard-Weichert or normal-mode methods) for few-particle collisions. In

this effort we expect to encounter special challenges in finding comparison data: we need a quantum or semiclassical emission cross-section for systems that are not spherically symmetric. At a fundamental scientific level these challenges are salient points of interest for this work.

The multicenter calculations predict interference phenomena which have been previously studied using the Born approximation to express the emission/absorption as integrals over the equilibrium pair-correlation functions.[9, 10] Our calculations are effectively non-Born (classical) calculations of the nearest-neighbor part of this interference effect. For specific orientations the interference effects are quite strong but the practical question is what survives averaging over orientations of the local cluster of target particles.

7.) SIMULATIONS USING THE BINARY-ENCOUNTER APPROXIMATION

In order to test the radiation algorithm described in section 6, MD simulations were performed for three-temperature systems of electrons, ions and photons in a cubic simulation box using periodic boundary conditions. The MD was performed with a fully parallel code using a basic leapfrog method [11] with the Coulomb interaction evaluated by an Ewald summation [12, 13].

A simulation was performed for a weakly coupled hydrogen plasma with a particle number density of $10^{26}/\text{cm}^3$, initial ion temperature of 20 keV, electron temperature of 10 keV and radiation temperature of 3 keV. The initial particle distributions were obtained by coupling the two species to separate Langevin thermostats, while the radiation initial conditions were selected from a Planckian distribution. The MD results were compared to a multi-group radiation code which treats the plasma like a fluid and computes the time evolution of electron and ion temperatures for an LTE plasma undergoing emission and absorption due to bremsstrahlung. The radiation field evolves according to the homogeneous and isotropic semi-classical radiation transport equation. The electron and ion temperatures evolve according to an energy balance relationship.

Figure 1 shows the evolution of temperature as a function of time compared to the results coming from the multi-group radiation code. The MD simulation assumes nothing about the plasma properties apart from the Coulomb law; the emission and absorption are governed by the Kramers cross-sections described above. For a hydrogen plasma at the specified conditions, the simulation results are close to the multigroup radiation code.

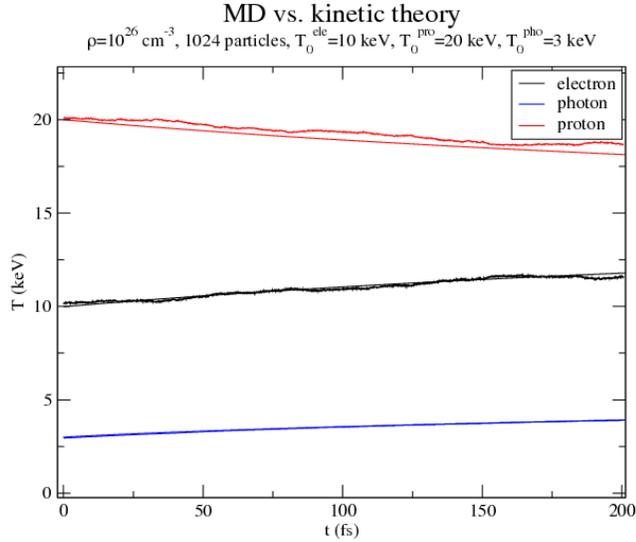


Figure 2: MD and radiation code results for a relaxing non-equilibrium hydrogen plasma. The noisy lines are the MD results.

In order to see the evolution of the radiation field, we enhanced the coupling between photons and electrons by a factor of 100. Figure 2 shows time snapshots of the evolving radiation intensity from a Planckian at 3 keV for the same three temperature equilibration problem. We see that the low frequency groups are populated earlier as expected for an electron-radiation (Bremsstrahlung) coupling rate $\tau^{-1} \sim 1/\nu^3$.

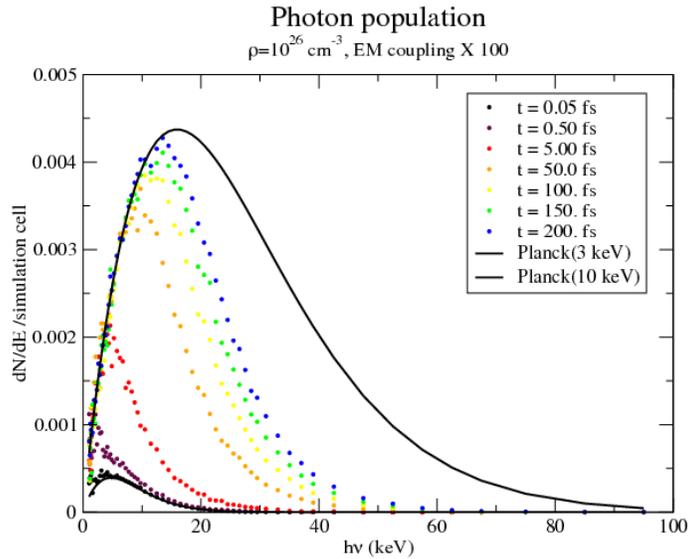


Figure 3: Time snapshots of the radiation specific intensity as a function of photon energy

8.) SUMMARY

The goals of this work are to investigate the effects of impurity ions, fusion products and non-equilibrium kinetic processes in hot plasmas near the threshold for fusion ignition. We will test kinetic-theory models widely used in plasma modeling codes against the fundamental laws of mechanics, electrodynamics, etc. This work is a natural preparation for upcoming fusion ignition experiments that will be performed on the LLNL NIF laser.

The usual atomic-scale particle simulation of plasma consider classical point-charge electrons and ions interacting with instantaneous Coulomb forces. The particles are contained in a simulation box surrounded by periodic images of the instantaneous configuration in the original box. With the development of large parallel computers, this method has come of age and modern simulations involve very large numbers of particles. However realistic simulations must include radiation phenomena

In the work described here, we found it was possible to add a classical EM field to a classical MD particle simulation by two methods: 1.) the Lienard-Weichert solution of the Maxwell equations, or 2.) a normal-mode expansion of classical EM field with a first-order ordinary differential equation for the field amplitudes.

Both methods give retardation, magnetic fields, and low-frequency EM wave effects. In both methods there is an interesting story about the periodic boundary conditions. We wrote codes for both methods and found by both numerical and analytical study of special cases that the Lienard-Weichert and normal-mode solutions agree. This is no surprise because both are (in principle) exact solutions of the classical Maxwell equations; unfortunately *they do not relax to the equilibrium black-body radiation field*. That is because these are classical theories.

We expect that quantum ingredients are always required to calculate the radiation produced by a hot plasma when the photon energy $h\nu$ is greater than or equal to the plasma temperature kT . In this case the classical calculation simply cannot obtain the correct answer. Long ago, Einstein showed what's needed to get a calculation to relax to the Planck spectrum: absorption and emission must be governed by probabilities whose ratio contains the particle distribution and the usual factors $n_\nu, (n_\nu + 1)$.

We have developed a practical strategy to implement this minimum quantum theory at least for radiation from binary electron-ion collisions. The radiation field is represented by an isotropic spectral intensity

$$I_\nu = ch\nu n_\nu dN/dh\nu$$

The emission and absorption probabilities are obtained from Kramers' cross-sections for emission/absorption, scaled to the Coulomb cross-section to make conditional probabilities for emission/absorption during Coulomb collisions. In this work we include electron-ion radiation only, neglecting small contributions from electron-electron

or ion-ion quadrupole emission. At present we also ignore Compton (Thomson) scattering.

We perform MC tests to decide between emission and absorption and to decide the photon frequency. The relative probabilities are obtained from the Kramers cross-sections. Radiation occurs in less than 10^{-3} of the strong collision events (for a hydrogen plasma). Each electron-ion pair gets only one chance to emit or absorb per collision. In this treatment the close collisions are binary (distant particles are neglected during the collision); this approximation is only used for the short time the particles are within a separation like 1/10 of the average distance between particles.

With this approximate method it is possible to do MD simulations including radiative processes. We believe there is a rich variety of microscopic physics to explore using our code: effects of impurities, effects of high-energy particles (e.g., fusion α 's), various types of relaxation to equilibrium, fusion by high-energy knock-on ions, etc.

In this work we have encountered a variety of fundamental questions (we do not repeat the list here) and additional research will be required before all the questions have been thoroughly studied.

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