Molecular dynamic simulations with radiation

2009 J. Phys. A: Math. Theor. 42 214030

(http://iopscience.iop.org/1751-8121/42/21/214030)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 214030 (11pp) doi:10.1088/1751-8113/42/21/214030

Molecular dynamic simulations with radiation

J Glosli[1], F Graziani[1], R More[1], M Murillo[2], F Streitz[1] and M Surh[1]

[1] Lawrence Livermore National Laboratory, Livermore, CA 94550, USA
[2] Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Received 15 October 2008, in final form 28 December 2008
Published 8 May 2009
Online at stacks.iop.org/JPhysA/42/214030

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 validations of the models used for describing 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 a first attempt at 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 new technique passes a key test: it relaxes to a blackbody spectrum for a plasma in local thermodynamic equilibrium. This new tool also provides a method for assessing the accuracy of energy and momentum exchange models in hot dense plasmas. As an example, we simulate the evolution of non-equilibrium electron, ion and radiation temperatures for a hydrogen plasma using the new molecular dynamics simulation capability.

PACS number: 52.65.−y, 05.20.Dd

1. Introduction

Matter in the plasma state is found in a wide variety of physical situations including metals, the core of the sun, brown dwarfs, space plasmas, magnetic fusion and inertial confinement fusion (ICF). Plasmas in the high energy density (HED) regime are a very important subset of plasmas and accurate models of HED plasmas require an understanding of matter at extreme conditions. The working definition of high energy density that will be used in this paper is taken from the report 'Frontiers for Discovery in High Energy Density Physics' prepared by

the National Task Force on High Energy Density Physics [1]. High energy density refers to energy densities exceeding 10^{11} J m^{-3}, or equivalently pressures in excess of 1 Mbar.

This paper considers HED plasmas where radiation is a significant factor in energy and momentum transport and affects plasma dynamics through emission, absorption and scattering processes. We call these hot dense radiative (HDR) plasmas. Typically, HDR plasmas have temperatures of a few hundred eV to tens of keV and densities of tens to hundreds of g cm^{-3}. Plasmas occurring in burning inertial confinement fusion (ICF) capsules and the cores of stars are two examples of HDR plasmas. The high temperature and density of HDR plasmas means there is a complex interplay of atomic, radiative and thermonuclear processes that need to be described accurately. The list of properties and processes below conveys a sense of the challenges that must be addressed when HDR matter is investigated

- Multi-species
  – Low Z and high Z ions (p, D, T, He^3, etc).
- Thermonuclear burn
  – Low Z reactants with or without the presence of high Z dopants.
- Atomic processes
  – Bremsstrahlung, photoionization, line absorption, electron impact ionization, etc.
- Radiation field.

The central focus of this paper is the fact that photons interact strongly with the medium. The plasma emits, absorbs and scatters photons. The importance of the radiation field can be qualitatively gauged by examining the radiation pressure. If the temperature is measured in keV and density in grams per cubic centimeter, the ideal-gas radiation and material pressures are given by

$$P_{\mathrm{Rad}}\ (\mathrm{Mbar}) = 45.7\ (T(\mathrm{keV}))^4, \tag{1}$$

$$P(\mathrm{Mbar}) = 965 \left(\frac{Z^* + 1}{A}\right)\ \rho(\mathrm{g\ cm^{-3}})\ T(\mathrm{keV}), \tag{2}$$

where Z^* and A are the ion charge and atomic weight, respectively. Even for densities ρ larger than 1 g cm^{-3}, the radiation pressure exceeds the material pressure for temperatures on the order of several keV. Hence, an accurate treatment of HDR plasmas requires including the effects of radiation. Due to the complexity of the plasma state and the need to make large multi-physics simulations tractable, computational physicists have had to make a variety of assumptions in modeling HDR plasmas in ICF and astrophysical applications. Today's challenge is to validate the assumptions and models in regimes that are difficult to access experimentally.

There has been recent theoretical and experimental work investigating the properties of HDR plasmas. However, different approximations have been proposed for making the theoretical calculations tractable [2], and disagreements between these approximations leave the answers uncertain. Certain questions, such as the effect of the high-frequency quiver-motion of electrons in a radiation field and its effect on electron–ion collision dynamics, remain to be thoroughly studied. In multi-species plasmas with high and low Z constituents, are the current methods of averaging energy exchange rates and stopping powers valid [2]? Are there dense plasma effects associated with the radiation and collision dynamics in HDR plasmas? Addressing these questions theoretically is a challenge especially for HDR plasmas where the low Z constituents are weakly coupled and the high Z constituents are moderately to strongly coupled. When thermonuclear burn is present in HDR plasmas, the burn initiation begins in a strongly coupled regime and rapidly transitions to weakly coupled.

Besides the basic difficulty of accessing regimes typical of HDR plasmas, experimental plasmas typically have strong spatial gradients. The gradients make a challenge for isolating any single process for model validation purposes. Until the National Ignition Facility produces experimental data, direct experimental probes of the densities and temperatures of interest in the hot dense radiative regime are very limited.

An alternative to both the experimental and theoretical methods mentioned above is direct numerical simulation (DNS) based on the molecular dynamics (MD) method. That is, each classical charged particle in the plasma simulation moves under the forces which arise from the other surrounding charged particles. The MD method offers many advantages. Given the accuracy of the force law, this approach is exact (within numerical uncertainties) in that it computes the phase space evolution of the plasma without any approximations. For example, particle–particle correlations are treated without any assumptions as to how strong or short-ranged they may be. Direct numerical simulation of the many-body interactions of plasmas has been performed but unfortunately relies on the collisionless approximation or ignores radiation entirely. For example, particle-in-cell calculations solve the Vlasov equation coupled to the electric and magnetic field present in the plasma but collisions important to HDR are ignored [3]. These calculations are suitable for low-density particle beams or magnetic fusion plasmas. Recent MD simulations have been performed of dense strongly coupled plasmas [4] where collisions are important. However these simulations assume the plasma has Coulomb pair-forces and neglect retardation, magnetic forces and radiation.

Understanding the behavior of HDR plasmas based on their micro-physical foundations using DNS offers many advantages. A DNS capability can validate theoretical and experimental approaches. The direct numerical simulation tool will allow computational physicists involved in modeling ICF and astrophysical plasmas to understand the validity of the approximations that are used in the modeling codes.

In this paper, we describe a new numerical simulation capability that will address a particular piece of the problem: the extension of molecular dynamics to collisional plasmas where radiation is important. For plasmas with temperatures relevant to fusion ignition, e.g., $\geqslant$3 keV, the radiation energy exceeds electron and DT ion kinetic energies and therefore has a significant effect on plasma energy balance and the ignition threshold. The problem we consider here is a fully ionized hydrogen plasma. We perform atomic-scale molecular dynamics simulations including bremsstrahlung emission and inverse-bremsstrahlung absorption of thermal radiation. We use our new molecular dynamics code to study the relaxation of a hydrogen plasma with assigned initial ion, electron and radiation temperatures. We show the time evolution of the temperatures and the photon distribution and compare the results with the results from a radiation-hydrodynamics code where the plasma is assumed to be a fluid in local thermodynamic equilibrium.

2. Radiation processes in HDR plasmas

Since the first studies of the one-component plasma by Brush, Sahlin and Teller [5], classical particle simulations of dense plasmas have concentrated on low temperature conditions. This focus was natural because non-trivial particle pair-correlations are strongest at low temperatures, but also was required because early computers could not handle large numbers of particles (at higher temperatures there are more particles within a screening length). At low temperatures radiation does not play an important role.

Classical OCP simulations assume instantaneous Coulomb interactions between charged particles, neglecting magnetic forces and retardation as well as emission and absorption of radiation. In most cases the simulations are performed for N particles in a simulation box

embedded in an environment modeled by periodic boundary conditions. The technique of periodic continuation leads to rapid convergence of the free energy and other properties with the size of the simulation box. However, the technique of periodic boundary conditions is inconsistent with relativistic causality: it assumes instantaneous correlations between particles separated by large distances ignoring the requirement that these correlations are only established and propagate at speeds less than c. This is an objection, in principle, but the artificial long-range correlations probably have no significant effect on thermodynamic properties in the limit of large N. It is more important that the high-frequency electric field and large energy-density of the radiation is being neglected.

To improve the classical particle simulations, classical electrodynamics offers two straightforward approaches. One can replace the instantaneous Coulomb interaction by the retarded potential (Lienard–Weichert solution) for the electromagnetic field of classical point charges following known trajectories. Alternatively, one can expand the classical EM field in normal modes and solve differential equations for the field amplitude coefficients. Both these methods generate classical solutions of the classical Maxwell equations.

We have written computer codes to explore both these methods. The most interesting aspect concerns the handling of the periodic boundary conditions.

For the Lienard–Weichert method, we sum over a finite number of images, setting aside any difficult question about convergence with the number of images. In the Lienard–Weichert formula the retarded times of the image charges grow with distance and so the simulation must run for a certain length of time before the image-charge location data become available.

For the normal-mode expansion, we find (numerically and analytically) that if the radiation normal modes are defined in the same simulation box used for the particles, also 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 $v \times B$ 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.

These simulations are entirely classical (classical particles and classical electromagnetic field). They necessarily produce an incorrect classical result for the high-frequency electromagnetic field: they 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: it predicts far too much x-ray energy.

It is necessary to include quantum mechanics in the simulation, at least in a semiclassical form, in order that the simulations relax to a Planck distribution for the radiation. At present we accomplish this following Einstein's original discussion of detailed balance: we require that the rates of absorption and emission be respectively proportional to expressions of the functional form

$$\text{Absorption} \sim f(E_{\mathrm{L}}) v_{\mathrm{L}} B n_\nu, \tag{3}$$

$$\text{Emission} \sim f(E_{\mathrm{U}}) v_{\mathrm{U}} B (n_\nu + 1), \tag{4}$$

where $f(E)$ is the electron distribution function for lower and upper states (denoted by subscripts L and U), v_{L}, v_{U} are the approach velocities, B is a coefficient (essentially the 'Einstein B coefficient') which is equal for two processes related by time-reversal and n_ν is the number of photons per normal mode. B depends on the particle and photon energies and is described more fully below. The one-electron states in the classical simulation have specified position and velocity whose apparent accuracy exceeds the uncertainty limit. With this formulation we can expect that our 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 a realistic timescale.

We implement these expressions for absorption/emission rates by a hybrid MD/MC (molecular dynamics/Monte Carlo) algorithm described below. Our method requires approximations that ignore potentially interesting (small) effects. While our algorithm is computationally feasible and does relax to the correct thermal equilibrium, other methods could be developed and we continue to seek better algorithms that might capture other aspects of the (complicated) physics.

3. MC/MD algorithm for radiation

In our approach the radiation field is represented by an isotropic homogeneous photon specific intensity I_ν which is expected to relax to the black-body intensity function B_ν:

$$I_\nu = (2h\nu^3/c^2)\, n_\nu, \tag{5}$$

$$B_\nu(T) = \frac{2h\nu^3}{c^2}\left(\mathrm{e}^{\frac{h\nu}{kT}} - 1\right)^{-1}, \tag{6}$$

in thermal equilibrium. Here the symbol n_ν 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 small contributions from electron–electron or ion–ion collisions.

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

We begin with the Kramers absorption and emission cross-sections σ^{A} and σ^{E}, respectively [6, 7]. Inverse bremsstrahlung absorption is a 3-body reaction (involving electron, ion and photon), so the absorption cross-section has units of cm^5; when multiplied by the spectrum of ambient photons $n_\nu\ \mathrm{d}N/\mathrm{d}h\nu$ (photons/cm^3 eV) and energy integrated it yields a normal cross-section (cm^2). The emission cross-section is a differential cross-section to emit a photon of energy $h\nu$ so its units are cm^2 eV^{-1}; it is multiplied by $(n_\nu + 1)$ to include stimulated emission and integrated over photon energies (up to the electron's initial energy). Explicitly, the cross-sections are given by [7]

$$\frac{\mathrm{d}\sigma^{\mathrm{E}}}{\mathrm{d}h\nu} = \frac{8\pi}{3\sqrt{3}} Z^2\alpha^3 \left(\frac{e^2/a_0}{E_0}\right)\frac{a_0^2}{h\nu} \qquad \sigma^{\mathrm{A}}(E,h\nu) = \frac{8\pi^3}{3\sqrt{3}} Z^2 a_0^5 \left(\frac{e^2/a_0}{h\nu}\right)^3 \frac{e^2/a_0}{E}. \tag{7}$$

In the emission formula, E_0 is the electron kinetic energy, $e^2/a_0 = 27.2$ eV, $a_0 = 0.529$ Å (Bohr radius), $h\nu$ is the energy of the emitted photon, α is the fine structure constant and Z is the nuclear charge. When we multiply the emission differential cross-section by $(1 + n_\nu)$ to account for stimulated emission the rate at which emission occurs is given by

$$\text{Rate} = n_{\text{ion}} \int_{0\leqslant E_0\leqslant h\nu} \frac{2d^3 p_{\mathrm{o}}}{h^3} |v_{\mathrm{o}}| f(E_0) \frac{\mathrm{d}\sigma^E}{\mathrm{d}h\nu} (1 + n_\nu)\,. \tag{8}$$

Here n_{ion} is the ion number density, p_0 and v_0 are the electron momentum and velocity and $f(E_0)$ is the electron distribution function which will be obtained from or sampled by the simulation.

The absorption rate is

$$\text{Rate} = n_{\text{ion}} \int_{\text{all electrons}} \frac{2d^3 p}{h^3} |v| f(E)\sigma^{\mathrm{A}}(E,h\nu) \left(n_\nu \frac{\mathrm{d}N_\nu}{\mathrm{d}h\nu}\right). \tag{9}$$

To verify detailed balance, we note E is related to E_0 by energy conservation, i.e. $E = E_0 + h\nu$. When we compare equations (3) and (9), we see that the coefficient B in equation (3) includes the ion density, radiative cross-section and phase space factors for electrons and photons.

The radiation cross-sections are converted to conditional probabilities when we form the ratio to the Coulomb collision cross-section. The rate of collisions expected from kinetic theory is

$$n_e n_{ion} \langle \sigma_C v \rangle_v, \tag{10}$$

where n_e, n_{ion} are electron and ion number densities, σ_c is the collision cross-section and v is the relative velocity. We have tested this formula in a special MD simulation which ignores long-range pair-forces and only includes the short-range interactions. If we ask this special 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

$$(\mathrm{d}\sigma^E/\mathrm{d}h\nu)\ (n_\nu + 1)\Big/\left(\pi R_B^2\right). \tag{11}$$

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. Typically, we find $R_B \sim 0.5$ Å is satisfactory.

The 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 a radiative process occurs. (The probability of a radiative process is small so this test is rarely passed.) If not, we 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. These tests are based on one or several random numbers; the normalized probability distribution is obtained from the Kramers 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). The energy-change from the average energy to the group-center is an approximation that is less important for larger numbers of photon groups. This approximation has its largest effect for the hardest and softest photons.

What are the strengths and weaknesses of the current approach? First, the method can easily be implemented in any Coulombic MD computer code. Plasmas that would produce blackbody spectra when in equilibrium can be easily simulated using this technique. As far as we are aware, this is the only approach that directly incorporates detailed balance. What are the weaknesses? For dense plasmas, our simulations assume Kramers cross-sections which are appropriate for dilute plasmas where an isolated electron interacting with an isolated ion is accompanied by the emission or absorption of a photon. On the other hand, the MD simulations capture the collective effects of the plasma due to Coulombic interactions and the particle trajectories which produce the radiation reflect this fact. Therefore, our current approach has an inconsistency. However, the x-ray radiation is absorbed or emitted during close collisions at small pair separations and the external plasma environment mainly affects only the rate of these close collisions. Nevertheless this limitation precludes study of dense

plasma changes in the emission/absorption cross-sections. We plan to improve the cross-sections guided by classical calculations (using the above mentioned Lienard–Weichert and normal-mode codes) for few-particle collisions relevant for dense plasmas. In this effort, we expect to encounter special challenges in making 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 simulations we have performed with the algorithm described in section 4 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 A^3 simulation box is not large at $kT < 5$ keV. The algorithm has been added to our larger parallel simulation code and will be used for much larger-size simulations and should give much less numerical noise.

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 the rich dense-plasma 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 blackbody radiation) alters the collision dynamics. For some of these processes considered in isolation there are analytic calculations in the literature [8] 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.

The radiation algorithm described here does not require any specification of a gauge and there is no question of gauge invariance. The quantities which appear in the calculation, the radiation intensity I_ν and the cross-sections are the same in any gauge. (The Lienard–Weichert calculations described above, and the normal-mode calculations, both required choice of an appropriate gauge.)

4. Results and discussion

In order to test the new capability, MD simulations were applied to the three-temperature systems of charged particles and photons in a cubic cell with periodic boundary conditions. The MD was performed with a fully parallel code using a basic leapfrog method [9] with the Coulomb interaction evaluated by an Ewald summation [10, 11]. Because the classical Coulomb many-body problem is unstable for attractive interactions, we employ semi-classical potentials that reduce the Coulomb interaction on short length scales in order to prevent unphysical, deeply-bound states. For the pure Coulomb problem, we tested several forms of the diffractive [12, 13] and Pauli [14, 15] terms for these potentials. The electron–ion equilibration times varied by less than 15% for the various forms of the potential. The similarity is not unexpected, since most semi-classical potentials resemble one another above 10 eV [16]. We report results using the following semi-classical potential [15]:

$$V_{ab}(r) = Z_a Z_b (e^2/r)(1 - \exp(-2\pi r/\Lambda_{ab})) + k_B T \ln 2 \exp\left(-4\pi r^2 \Big/ \Lambda_{ab}^2 \ln 2\right)\delta_{ae}\delta_{be}, \qquad (12)$$

where $\Lambda_{ab} = (h^2/2\pi\mu_{ab}k_B T)^{1/2}$, μ_{ab} is the reduced mass and $T = T_e$ except when a and b are both protons when $T = T_p$. The potentials are temperature (and hence time) dependent. For simulations run to full temperature equilibration, the temperature dependent parameters evolve with time using a smoothed exponential average of the instantaneous MD value. For shorter runs considered in this paper, (during which the temperature did not vary much) we

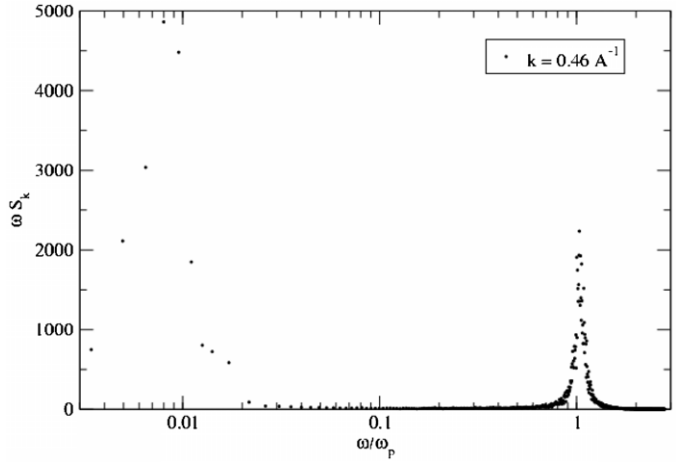

Figure 1. Electron–electron structure factor showing the ion acoustic wave and plasma modes.

held these parameters fixed. In order to test the accuracy of the code, the electron–electron structure factor $S(k, \omega)$ [17] was computed for a dense hydrogen plasma with density $\rho = 1.6 \times 10^{24}$ cm^{-3} and initial proton and electron temperatures of 78.5 eV and 29.8 eV, respectively. Figure 1 shows a representative example of $S(k = k_0, \omega)$ as a function of frequency (in units of the plasma frequency) for the mode $k_0 = 4\pi/L$ where L is the edge of the simulation box. The result is averaged over the three directions (along x, y or z). As expected, the structure factor clearly shows the ion acoustic wave mode near zero frequency and the plasma mode at the electron plasma frequency.

A simulation was performed for a weakly coupled hydrogen plasma with a particle number density of 10^{26} cm^{-3}, initial ion temperature of 20 keV, electron temperature of 10 keV and radiation temperature of 3 keV. The 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 (2). The electron and ion temperatures evolve according to an energy balance relationship. The set of coupled radiation and matter equations used by the multi-group radiation code are

$$\frac{1}{c}\frac{\partial \psi_\nu(t)}{\partial t} = \sigma_\nu B_\nu(T_\mathrm{e}) - \sigma_\nu \psi_\nu(t), \tag{13}$$

$$\frac{\partial \rho c_\mathrm{V} T_\mathrm{e}}{\partial t} = -4\pi \int \mathrm{d}\nu\, \nu_\nu(B_\nu(T_\mathrm{e}) - \psi_\nu(t)) - \Omega_\mathrm{ei}(T_\mathrm{i} - T_\mathrm{e}), \tag{14}$$

$$\frac{\partial \rho C_\mathrm{V} T_\mathrm{i}}{\partial t} = \Omega_\mathrm{ei}(T_\mathrm{i} - T_\mathrm{e}), \tag{15}$$

$$B_\nu(T) = \frac{2h\nu^3}{c^2}\left(\mathrm{e}^{\frac{h\nu}{kT}} - 1\right)^{-1}, \tag{16}$$

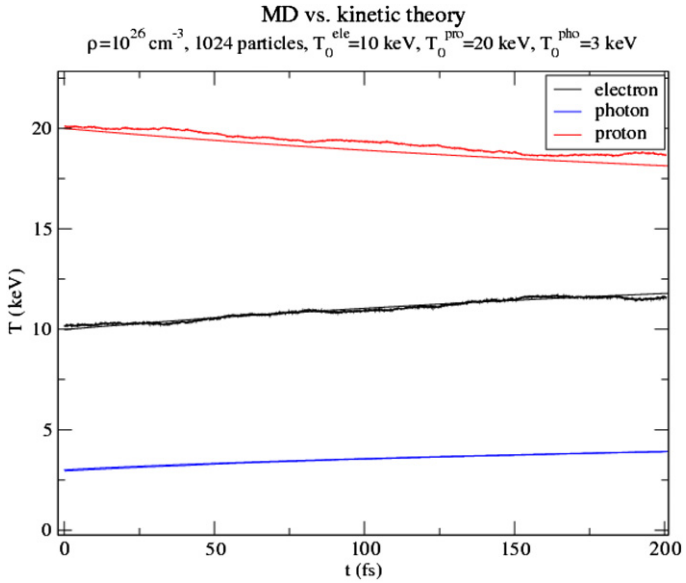

Figure 2. MD and radiation code results for a relaxing non-equilibrium hydrogen plasma. The noisy lines are the MD results.

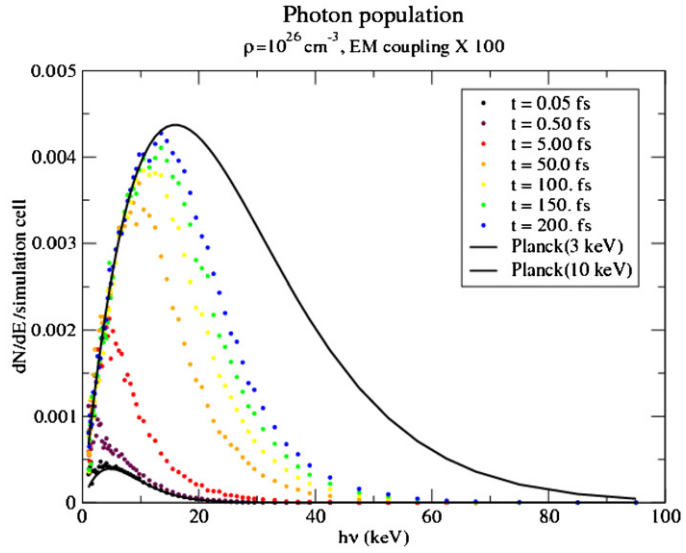

Figure 3. Time snapshots of the radiation specific intensity as a function of photon energy.

where $\psi_\nu(t)$ is the frequency-dependent specific intensity, σ_ν/ρ is the opacity, $c\sigma_\nu$ is the electron-radiation coupling rate, c_V and C_V are the electron and ion specific heats, Ω_{ei} is the electron–ion coupling function and $B_\nu(T)$ is the Planck function.

Figure 2 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 other than that the collisions are Coulombic and the emission and absorption are governed by the Kramers cross-section. For a hydrogen plasma at the specified conditions, the agreement is very good between the early time evolution of the MD suggesting that the multi-group radiation code assumptions of an electron–ion coupling based on Gericke-Murillo–Schlanges [18], and a radiation treatment based on the semi-classical transport equation are adequate for modeling the three temperature equilibration problem for hydrogen at the chosen density and temperature. This is not surprising considering the plasma conditions produce a weakly coupled plasma where MD and multi-group radiation results should agree.

In order to follow the evolution of the radiation field, we enhanced the coupling between photons and electrons by a factor of 100. Figure 3 shows time snap-shots of the evolving specific intensity from a Planckian at 3 keV for the same three temperature equilibration problem. It is important to observe that the low frequency groups are populated earlier as one would expect for an electron-radiation (bremsstrahlung) coupling rate going as $\tau^{-1} \sim 1/\nu^3$.

5. Conclusion

We have described a first attempt at a new numerical simulation capability that addresses a currently unsolved problem: the extension of molecular dynamics to collisional plasmas including emission and absorption of radiation. The new technique relaxes to a blackbody spectrum for a plasma in local thermodynamic equilibrium. This new tool also provides a method for assessing the accuracy of energy and momentum exchange models in hot dense plasmas. We should mention that Monte Carlo sampling methods are used in a wide variety of applications of relevance to this work. In particular particle-in-cell simulations where electron–ion recombination is present use the notion of cross sections and probabilities to identify when an event occurs [19]. Our approach uses a similar philosophy but applied to radiative processes.

Understanding the behavior of HDR plasmas based on their micro-physical foundations using DNS offers many advantages. A DNS capability can validate theoretical and experimental approaches. In addition, such a tool would allow computational physicists involved in modeling ICF and astrophysical plasmas to understand the validity of the approximations that are used in the codes.

In this paper, we performed atomic-scale molecular dynamics simulations of a hot non-equilibrium hydrogen plasma undergoing bremsstrahlung and inverse bremsstrahlung radiative processes. We used the new molecular dynamics capability to study the relaxation of a hydrogen plasma with the initial ion, electron and radiation temperatures out of equilibrium. We showed that the time evolution of the temperatures and the photon distribution compare well with the results of a radiation-hydrodynamics code where the plasma is assumed to be a fluid in local thermodynamic equilibrium.

Acknowledgments

This work is performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 07-ERD-044. We wish to thank an anonymous referee for informing us of the use of Monte Carlo methods in particle-in-cell codes and their application to electron–ion recombination.

References

[1] National Task Force on HED Physics 2004 *Frontiers for Discovery in High Energy Density Physics*
[2] Castor J 2007 *Radiation Hydrodynamics* (Cambridge: Cambridge University Press)
[3] Zwicknagel G, Toepffer C and Reinhard P-G 1999 *Phys. Rep.* **309** 117
[4] Glosli J, Graziani F R, More R, Murillo M, Streitz F, Surh M, Benedict L, Hau-Riege S, Langdon B and London R 2008 *Phys. Rev.* E **78** 025401
Jeon B, Foster M, Colgan J, Csanak G, Kress J, Collins L and Grønbech-Jensen N 2008 *Phys. Rev.* E **78** 036403
Dimonte G and Daligault J 2008 *Phys. Rev. Lett.* **101** 135001
[5] Brush S, Sahlin H and Teller E 1966 *J. Chem. Phys.* **45** 2102
[6] Kramers H A 1923 *Phil. Mag.* **46** 836
[7] More R 1991 Atomic physics of laser-produced plasmas *Handbook of Plasma Physics* vol 3, ed M Rosenbluth, R Sagdeev, A Rubenchik and S Witkowski (Amsterdam: North-Holland) Chapter 2
[8] See, for example, Ichimaru S 1973 *Basic Principles of Plasma Physics* (Reading, MA: Benjamin)
[9] Streitz F, Glosli J and Patel M 2006 *Phys. Rev. Lett.* **96** 225701
[10] Ewald P 1921 *Ann. Phys.* **64** 253
[11] DeLeeuw S, Perram J and Smith E 1980 *Proc. R. Soc.* A **373** 27
[12] Jones C and Murillo M 2007 *High Energy Density Phys.* **3** 379
[13] Dunn T and Broyles A 1967 *Phys. Rev.* **157** 156
[14] Minoo H, Gombert M and Deutsch C 1981 *Phys. Rev.* A **23** 924
[15] Kelbg G 1963 *Ann. Phys.* **12** 219
[16] Filinov A, Golubnychiy V, Bonitz M, Ebeling W and Dufty J 2004 *Phys. Rev.* E **70** 046411
[17] Pschiwul T and Zwicknagel G 2003 *J. Phys. A: Math. Gen.* **36** 6251
[18] Gericke D, Murillo M and Schlanges M 2002 *Phys. Rev.* E **65** 036418
[19] Vahedi V and Surendra M 1995 *Comput. Phys. Commun.* **87** 179