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Particle simulation code for fusion ignition

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ABSTRACT

Inertial fusion ignition phenomena including effects of non-Maxwellian ion velocity distributions are studied by molecular dynamics particle simulation. 10,000 DT ions at a density 100 g/cm^3 and temperature ~10 keV are followed for 10 to 20 ps. The simulations include ion collisions, electron–ion coupling and radiation emission and absorption. Fusion reactions produce energetic alphas and the plasma self-heats to 20–30 keV. It is found that calculations starting from a variety of initial conditions evolve to approach a unique self-heating trajectory which can be called an *ignition attractor*. A calculation starting with 3 keV DT ignites within a few ps after 2 MeV alpha particles are injected and deposit ~300 MJ/g; this demonstrates that fast ions are highly effective for fast ignition of precompressed DT.

1. Introduction

Molecular dynamics (MD) and the Monte Carlo (MC) method can be used to study many-particle systems such as liquids and dense plasmas [1–3]. It is interesting to extend these methods to treat systems in which the particles have internal dynamics (such as transitions between electronic excited states) and/or undergo processes such as chemical or nuclear reactions. As computers increase in speed and memory, particle simulations using increasingly realistic particles and interactions will provide increasingly accurate models which can be diagnosed with precision that rivals plasma experiments. The appeal of such a simulation is that ideally we input only simple and fundamental properties of the particles involved and their interaction forces, and without further assumption the computer works out particle correlations, distribution functions and composite processes.

This paper describes particle simulations of DT fusion ignition in a hot dense plasma at conditions relevant to inertial fusion [4,5,6]. A new computer code named OK calculates ignition histories starting from a variety of initial temperatures and especially ignition driven by fast ions injected into dense DT fuel.

The calculations examine a small volume of DT fuel in the core of an imploded fusion target at an assumed density 100 g/cm^3. The small plasma volume is described by 10,000 DT ions which have an arbitrary velocity distribution. Initial temperatures range from 3 to 10 keV; the radiation begins as a 1 keV black-body field.

The simulation includes the main hot-plasma processes: ion–ion collisions, electron–ion coupling, emission and absorption of radiation and fusion reactions producing energetic alpha particles. The plasma self-heats as fusion alphas deposit energy in electrons and DT ions.

Comparing several simulations with initially hot fuel, it is found that fusion self-heating automatically approaches and follows an *ignition attractor* trajectory, approximately independent of the initial conditions. The attractor trajectory depends on details of the physical model and the target composition and geometry but the existence of an ignition attractor appears to be a general phenomenon independent of those conditions. We calculate ion-driven fast ignition, one strategy for heavy-ion fusion. In this calculation, low-temperature ($T_i^0 = 3$ keV) DT fuel is heated by injection of a burst of energetic alphas and subsequently self-heats to ignition.

The paper is aimed at the basic physics of fusion ignition and does not try to model any specific target experiment. The ultimate purpose is to test kinetic models used in hydrodynamic codes. Hydrodynamic motion and heat conduction are important for a real target but are not included in the MD simulations. The time-duration of high compression is typically something less than 100 ps and the fuel will not ignite if it does not self-heat during this stagnation time. If the heated region is too small, thermal conduction cooling could overcome the fuel self-heating and prevent ignition. If the target does ignite, its temperature and pressure increase rapidly and the hydrodynamic disassembly is accelerated; these well-understood macroscopic phenomena are summarized in the usual rho-R criterion for fusion ignition [4–6].

Specifically, the plasma conditions considered here do not have enough detail about particle and energy loss to the environment outside the hot spot (which has limited ρR) and assume somewhat higher temperatures than are actually achieved, so they do not attempt to describe recent NIF experiments. At the same time the calculation of ignition provoked by ion deposition only has a general similarity to specific target conditions. The important

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point here is that the MD method can offer an independent check of the ignition dynamics in simulations of the complete target implosion and burn performed by the radiation–hydrodynamic codes.

2. Non-Maxwellian ion distribution

Molecular dynamics simulations explore the consequences of a non-Maxwellian ion velocity distribution.

If the plasma temperature rises rapidly, it could be imagined that the diffusion (in energy) of thermal ions to fill the high-energy tail of the ion distribution might be slower than the temperature rise and in this case a non-Maxwellian velocity distribution would be automatically generated and maintained. In fact, we did not yet find a case where this effect is important. Apparently, when fusion reactions add energy to a plasma in the form of fast alpha particles, the alpha energy transfers to the ions slowly enough to permit most ions to relax to a time-dependent Maxwell distribution.

Spatial gradients can cause a non-Maxwellian ion distribution because high energy ("tail") ions have mean free paths $L(E)\sim E^2$ much larger than normal thermal ions. In an inhomogeneous plasma high-energy DT ions are preferentially lost from a hot region to nearby colder plasma, as suggested by Petschek and Henderson [7] and Nishikawa, Takabe and Mima [8]. This effect is expected to occur near an interface between hot and cold fuel caused by Rayleigh–Taylor mixing [9]. Although it could easily be described by MD, this nonlocal effect is not included in the calculations reported here which refer to fusion ignition in homogeneous fuel at large rho-R.

Fusion alphas collide with D or T ions and produce recoil ions with energies up to 30–200 keV $\gg kT_i$. The recoil ions thermalize within a few ps but their fusion reaction cross-sections greatly exceed those of ions having thermal energies. Injected fast ions, either from an external beam heating source or from neighboring parts of the plasma, also can produce recoil ions and make a non-Maxwellian ion population.

MD simulation of fusion ignition faces a practical difficulty because accurate treatment of electron dynamics calls for a very short time-step to resolve electron-ion Coulomb collisions. However it is necessary to follow the plasma evolution for ~10 ps$=10^{-11}$ s to study fusion ignition. On today's computers it is difficult to take more than 10^6 or 10^7 sequential time steps.

In our calculations the electron motion is simplified using a Langevin approximation which permits a time-step ~10^{-17} s. With this approximation, during one time step, each ion experiences many (~100) electron collisions and the momentum transfers from these collisions combine as a random walk. Ion-pair collisions are treated by analytic formulas rather than by numerical integration. Because the plasma composition changes during the calculation, particle lists are updated on every time-step. For computational efficiency, certain processes are subcycled or supercycled (i.e., performed more or less than once per time-step).

The DT ions are described by positions and velocities $\{\boldsymbol{R}_j(t), \boldsymbol{V}_j(t)\}$. At kilovolt temperatures the DT is fully ionized and we assume there are no impurities (except alpha particles). The ion temperature $T_i(t)$ is calculated as 2/3 of the instantaneous average ion kinetic energy. We calculate separate temperatures for D and T ions and find a few percent difference during ignition heating (the D's are hotter).

The code structure resembles other MD particle simulation codes [10]. The plasma is confined in a simulation box which is divided into sub-boxes. DT ions and alphas move with periodic boundary conditions in the large box. Periodic boundary conditions mean the plasma is considered to be embedded in a large volume of plasma having the same density–temperature conditions. The pair-interaction candidates are particles in the same or the 26 adjacent sub-boxes. With this structure, the code calculation time scales with the number of ions N rather than N^2.

For $T \geq 10$ keV, even at a density of 100 g/cm^3, the ion coupling parameter Γ is not large:

$$\Gamma = Z^2 e^2 / R_o kT \leq 0.01 \tag{1}$$

For this reason, equilibrium ion pair-correlations do not have a large effect on fusion plasmas.

Radiation is emitted and absorbed during electron–ion collisions. Isotropic, un-polarized radiation is described by populations of 200 photon frequency groups, logarithmically spaced from 100 eV to 100 keV. The radiation begins with a black-body spectrum ($T_r=1$ keV) but rapidly develops a non-Planck spectrum.

The code follows a variable number of alpha particles produced by DT fusion. The alphas are described by positions and velocities $\boldsymbol{R}_j(t)$, $\boldsymbol{V}_j(t)$ and move through the plasma, subject to periodic boundary conditions. Because the alphas have high velocity compared to thermal ions, their motion is *sub-cycled*: typically 10 alpha time-steps for each main time-step.

Alpha energy loss to electrons, $dE/dt = v_\alpha (dE/dx)_e$ is calculated by the Langevin method. Alpha collisions with DT ions are treated in the same manner as DT collisions by a binary Coulomb collision subroutine. For alpha–ion collisions, the occasional large-angle scattering events can transfer substantial energies to the D or T ions and produce recoil ions with energies of several hundred keV.

When a pair of DT ions enter the small-ball sphere $|\boldsymbol{R}_i - \boldsymbol{R}_j| = R_{sb}$, they are tested for fusion. The DT fusion cross-section is evaluated using the relative kinetic energy E_{rel} and a Monte Carlo test is based on the conditional probability

$$P_{fusion} = \sigma_{DT}(E_{rel}) / \pi R_{sb}^2 \tag{2}$$

This test is used to decide whether a fusion reaction occurs. Because the arriving ion flux is proportional to $\pi {R_{sb}}^2$, the fusion rate obtained from Eq. (2) is independent of the radius chosen for R_{sb}. The number of times/s the test is undertaken is proportional to $\pi {R_{sb}}^2$ so the number of successful outcomes (fusion events) is independent of R_{sb} to a good approximation. (This was verified by numerical experiments.) The fusion cross-sections are taken from the well-known NRL formulary.

Because of Eq. (1), screening corrections to the fusion cross-section for dense or strongly-coupled plasmas are unimportant at the temperatures considered here. The code can also test for DD or TT fusion reactions but these rates are ~100 times smaller than the DT rates, so the tests are normally skipped for code speed.

After each fusion reaction, an alpha particle and neutron are launched in a random direction from the center of mass (CM) of the reacting pair. Neutrons produced in fusion reactions are immediately recorded in detector audit files. We calculate the output neutron velocity distribution, which predicts the neutron time-of-flight spectrum.

3. Code tests and limitations

As the OK code was written, the physical processes were tested to verify that they give reasonable rates and properly obey detailed balance. The results of these tests are briefly summarized:

i) Ion–ion collisions, acting alone, relax an initial non-Maxwellian ion distribution to a Maxwellian in the expected time.
ii) The electron–ion (Langevin) coupling is tested by a special calculation in which the electron temperature is held fixed, ion–ion collisions are suppressed, and the only coupling is the