Classical Molecular Dynamics Model for Coupled Two-Component Plasmas - Ionization Balance and Time Considerations.

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Classical molecular dynamics (MD) applied to ion and electron systems (TCP) has proven useful for the study of hot and dense non-hydrogenic plasmas. Within the limits of classical mechanics, all charge-charge interactions are accounted for in the particle motion. This makes MD a crucial research tool since it allows the investigation of conditions often inaccessible to other theoretical methods without the use of drastic approximations.

TCP simulations rely on the definition of a soft ion-electron potential which removes Coulomb divergence at short distances.
Non-linear mechanisms driven by the attractive ion-electron potential induce an increase of the electron density around the impurity together with a change of the electron kinetics.
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- Change the deepness of the potential well
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- Change the depthness of the potential well
- Introduce a model to account for ionization and recombination.
Introduction

Objectives

Is it possible to use classical MD to do physics in the hot, dense plasma domain and complement the population kinetics models?
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- Implement in MD a classical model based on collisional ionization and recombination processes.
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- Extend the use of classical molecular dynamics to transient conditions for coupled non-degenerate plasmas.
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- Improve the generation of micro field sequences.
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- Extend the use of classical molecular dynamics to transient conditions for coupled non-degenerate plasmas.
- Improve the generation of micro field sequences
- Make progresses on the MD technique itself.
Modeling

Two-component plasma simulation.

The system inside the simulation box is neutral. Periodic boundary conditions are used and the Newton’s equations are solved using a Velocity-Verlet algorithm.

Electron-electron or ion-ion interactions are taken to be Coulomb:

$$V_{ii,ee} = Z_i^2 e^2 e^{-r/\lambda} / r.$$  

The interactions are screened at a distance $\lambda \simeq s/2$. MD for opposite charges requires a regularized potential at short and large distances:

$$V_{ie}(r) = -Z_i e^2 e^{-r/\lambda} (1 - e^{-r/\delta}) / r.$$  

The regularization distance $\delta$ is associated to the ionization energy of each ion stage:

$$\delta(Z) = -Z_i e^2 / E(Z).$$

$\delta(Z)$ will also play the role of radius of the ion stage $Z$. 
Modeling

Link with quantum data.

\[ V_{ie}(0) \equiv E(Z) = \frac{-Z_i e^2}{\delta(Z)} \]
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Link with quantum data.
Ionization.
Recombination.

Applications
Electron Dynamics.
Ionization balance.
Electric micro fields properties.

Conclusion
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Modeling Ionization.

![Graph showing energy vs. r/(2*a₀)](image)

- **SNN**: Symbol representing a specific point or condition.
- **NN**: Another symbol or point of interest.
- **Z**: Represents another critical point or value in the context of the graph.
Modeling

Ionization.

If $t_1 + t_2 > 0$. 

$Z + 1$ 

$v = 0$ 

$r/(2a_0)$ 

Energy (eV)
Modeling Ionization.
Introduction


Conclusion
Modeling

Ionization.

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Modeling

Recombination.
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Electron Dynamics.

Typical times (for 50eV) :

1. the shortest is the timestep $\sim 0.1\text{as}$
2. electronic average distance crossing time $\sim 0.1\text{fs}$
3. time to populate the electron negative energy states $\sim 0.1\text{ps}$
Applications

Electron Dynamics.

Argon plasma at $N_e = 10^{23} \text{ cm}^{-3}$ and $T_e = 100 \text{ eV}$. A two component neutral plasma is prepared without interactions between ions and electrons. At $t=0$, interactions are switched on with ionization - recombination.
Applications

Electron Dynamics.

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![Graph of probability distribution vs. normalized velocity](image1)

![Graph of total energy distribution vs. energy](image2)
Applications

Electron Dynamics.

Argon plasma at $N_e = 10^{23} \text{cm}^{-3}$ and $T_e = 100 \text{eV}$.
A two component neutral plasma is prepared without interactions between ions and electrons. At $t=0$, interactions are switched on with ionization - recombination.

The time necessary to reach this equilibrium state is of the order of $10^{-13}\text{s}$.
Applications

Ionization balance


$$\Gamma_i = 5., \Gamma_e = 0.11$$
Applications

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\[ \Gamma_i = 0.9, \Gamma_e = 0.06 \]
Applications

Electric micro fields distribution functions.

\[ \vec{E}_{\text{slow}}(t) = \frac{1}{\Delta t} \int_{-\Delta t/2}^{\Delta t/2} \vec{E}_T(t - t') dt'. \]

![Probability vs. E (E_0) graph](#)

Carbon Z=5, N_e = 10^{22} \text{ cm}^{-3}, T_e = 80 \text{ eV}

- Total field
- Holtsmark
- Holtsmark N_e + N_i
- APEX
The numerical approach proposed here, which involves capture and release of electrons by ions, is intended to provide better consistency between the soft potential and the behavior of electrons at short distances. The main objective to implement in MD a classical model based on collisional ionization and recombination processes has been reached. The results presented here validate:
- the choice of an ion-electron potential based on the ionization energies of the various ion stages,
- both the concept of ion-electron collisions and the rules that fix the ionization and recombination mechanisms.

This work is, still, in progress.