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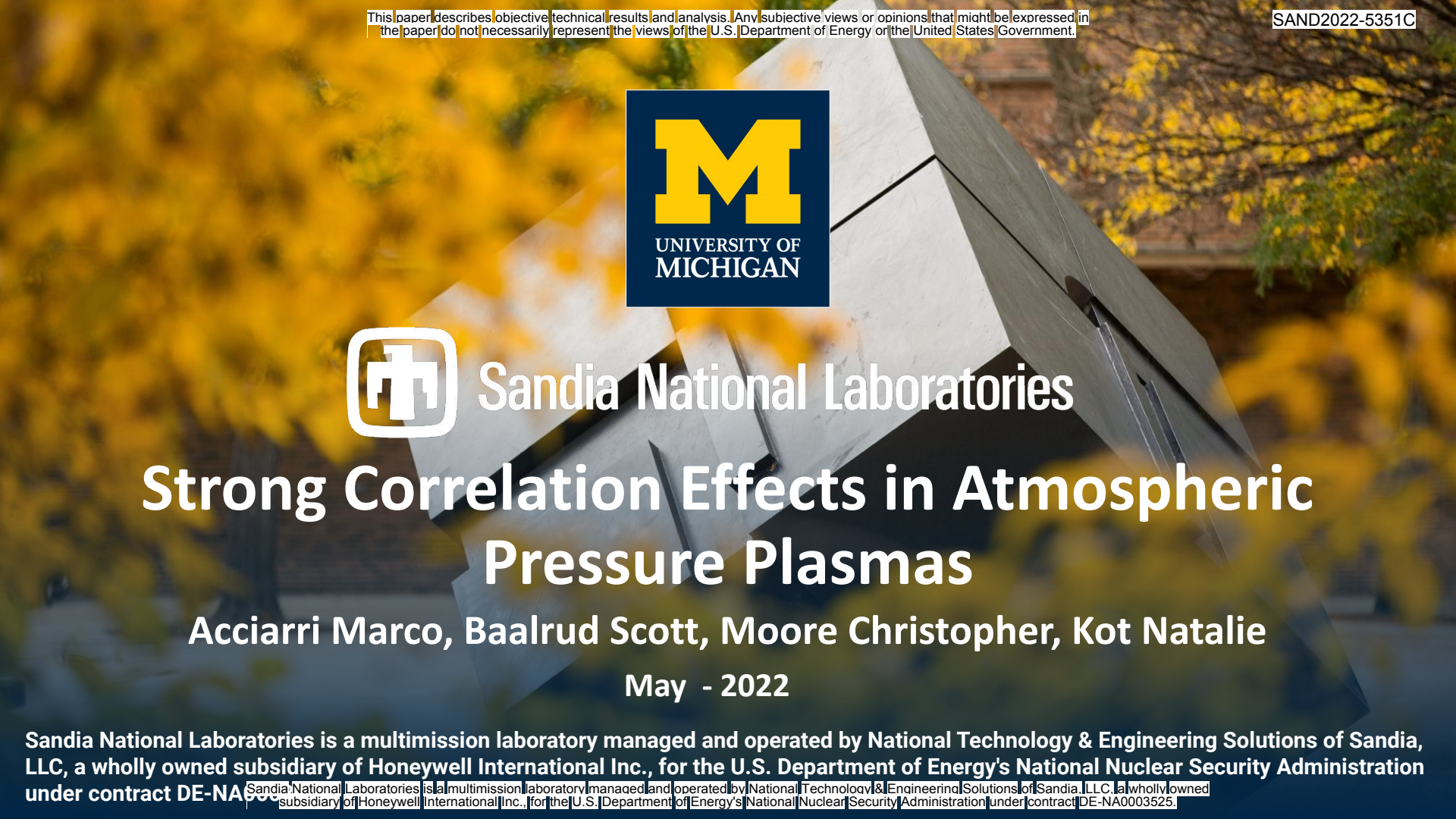

Strong Correlation Effects in Atmospheric Pressure Plasmas

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May - 2022

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Motivation

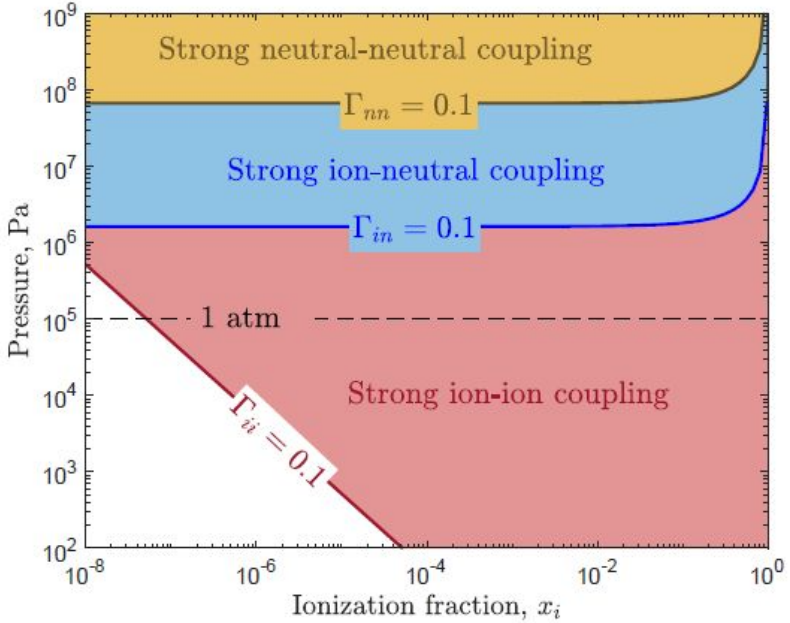
Atmospheric pressure plasmas

- Operational simplicity
- Low running cost (no vacuum system required)
- Highly non-equilibrium plasma state (Te>>Ti) which promotes chemical reactions
- Promising for inactivation of pathogens in medicine, applications in food industry, agriculture, water purification, etc

A key science challenge is to model the main mechanisms involved in the plasma dynamics and transport of reacting species in order to improve the development of plasma sources

Coupling Parameter Space

T = 293 K



Coupling Parameter

$$\Gamma_{ss'} = \frac{\phi_{ss'}(r=a)}{k_B T_{ss'}}$$

Wigner–Seitz radius

$$a = \left(\frac{3}{4\pi n}\right)^{1/3}$$

Coulomb Potential

$$\phi(r) = \frac{q^2}{4\pi\epsilon_0}\frac{1}{r}$$

Charge Induced Dipole

$$\phi_{ind}(r) = -\frac{q^2}{8\pi\epsilon_0}\frac{\alpha_R a_0^3}{r^4}$$

Lennard Jones

$$\phi_{LJ}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

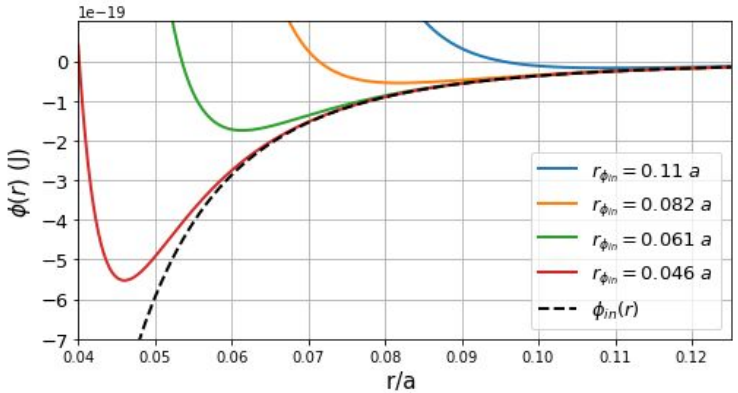
Molecular Dynamics Simulations

- LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator from Sandia National Laboratories).
- Electrons were considered as a non interacting background neutralizing species and were not included in the simulation setup.
- Partially ionized Ar plasma, **T=293 K**, **P = 1 atm**.
- Short (**neutral-neutral**), Medium (**ion - neutral**) and Large (**ion - ion**) range interactions were included..
- 3D periodic box of length ~ 25 a.
- Each simulation was performed by fixing the temperature (NVT stage) and then fixing the total energy (NVE stage). The volume and number of particles remained constant.
- Physical properties were studied in the NVE simulation once the equilibrium was reached.

Ion - Neutral Interactions: Charge Induced Dipole Potential

- Purely attractive potential → Can lead to numerical problems during a MD simulation.
- Need to add a repulsive term in order to avoid that particles get too close to each other.

$$\phi_{ind}(r) = A\left(\frac{B}{r}\right)^{12} - \frac{q^2}{8\pi\epsilon_0}\frac{\alpha_R a_0^3}{r^4}$$

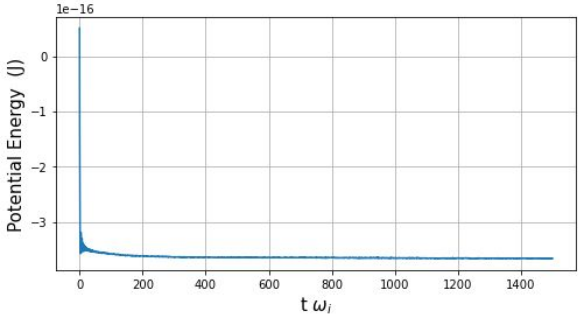


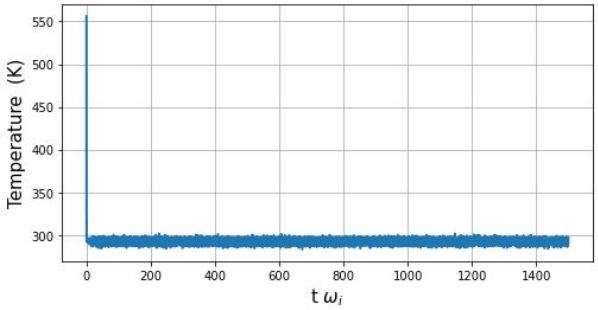
¿ How can we choose the parameters A and B ?

- Too large → May affect the physics of the problem by changing the value of ϕ_{ind} at the average interparticle distance a.
- Too small → huge computational cost associated to the extra requirement on a smaller timestep due to the larger force values at small distances.

MD Simulations: Temperature and Energy evolution

Example of Simulation result, r_φ = 0.11 a

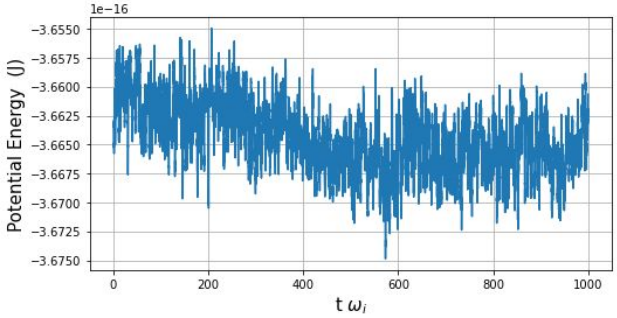


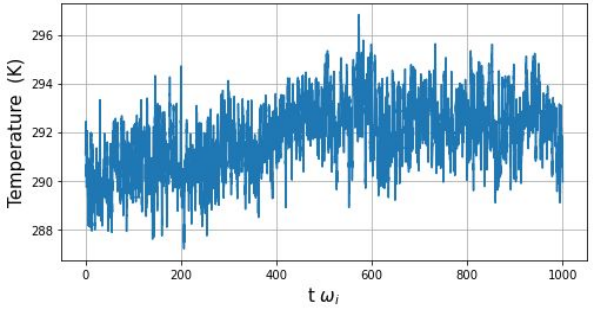


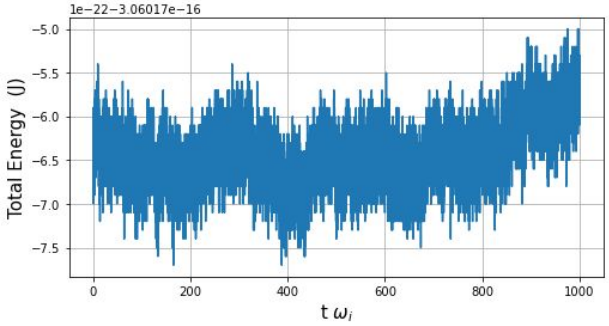
NVT simulation

The temperature was fixed and the Noose Hover algorithm was used to reach the desired room temperature

NVE simulation

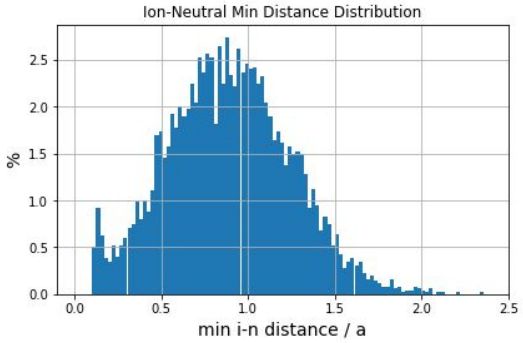


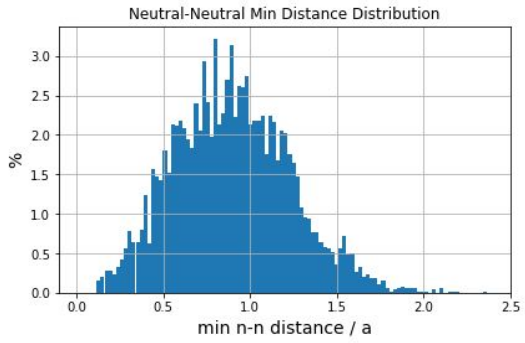


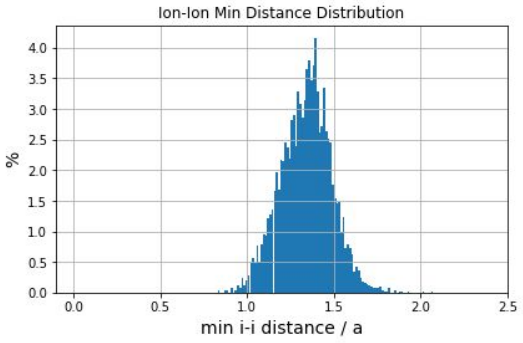


MD Simulations: Results at different r_φ values

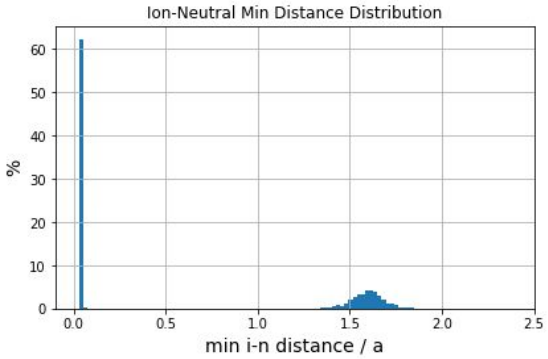
r_φ = 0.133 a

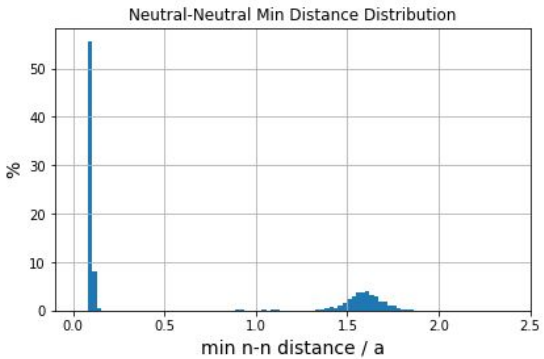


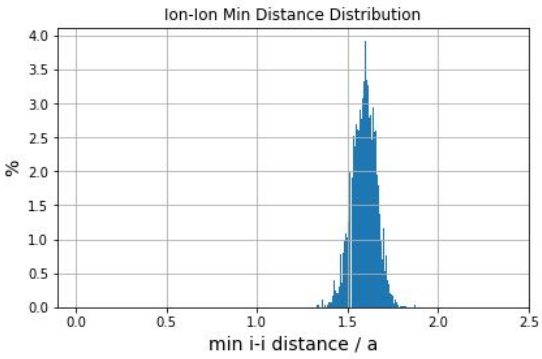




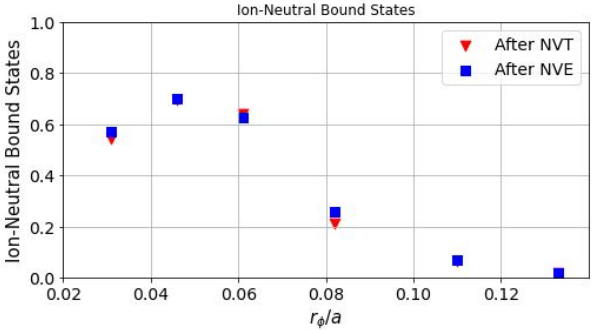
r_φ = 0.046 a

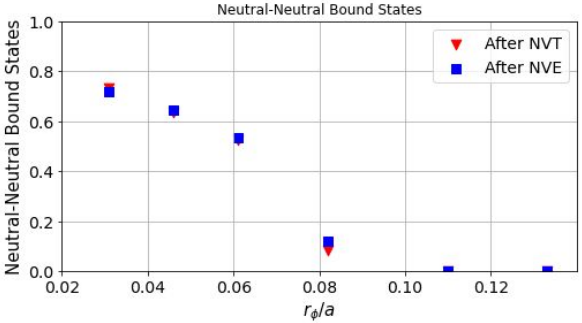






Bounds States Fraction

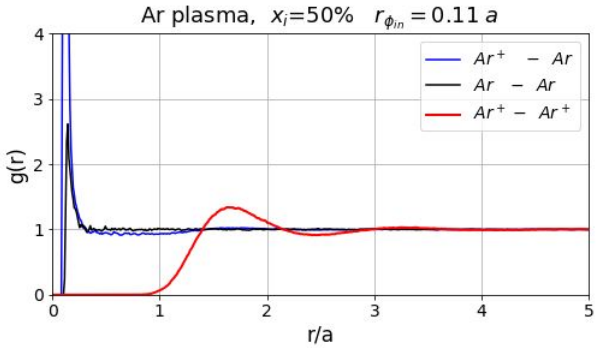


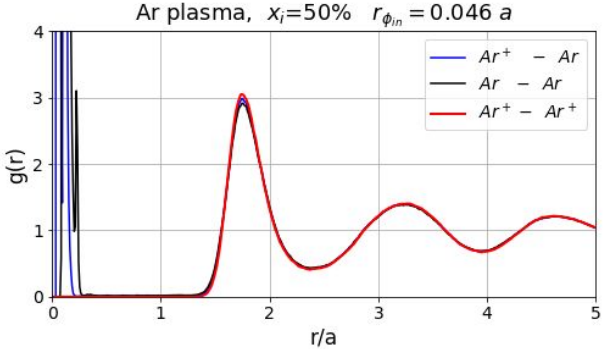


- Bound states fraction increased at smaller $\mathbf{r_\varphi}$ values.
- 3-body recombination process

Radial Distribution Functions for each interaction:

$$g(r) = \frac{N(r)}{4\pi r^2 \Delta_r n_0}$$





MD simulations: Starting with a neutral gas

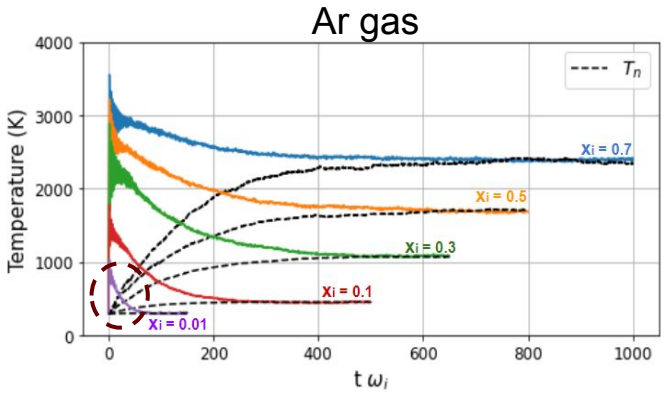
Must improve the simulation in order to have a better physical picture of an experiment !

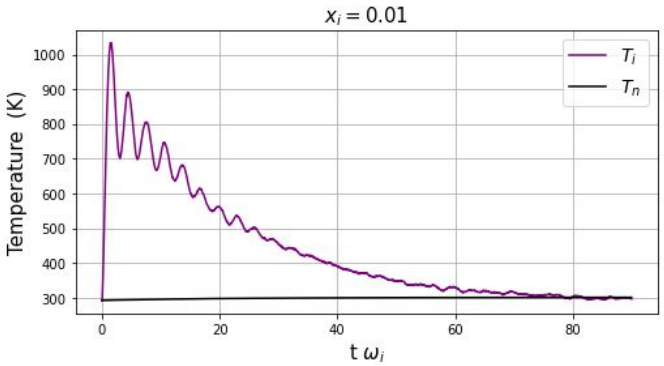
Simulation Setup:

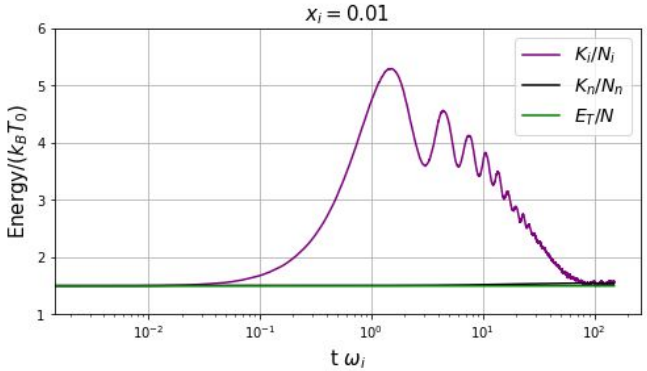
- NVT-NVE simulations for a neutral Ar gas using the LJ potential
- Instant ionization of a fraction of the particles
- NVE simulation including i-n and i-i interactions
- Study the evolution of the temperature after the ionization

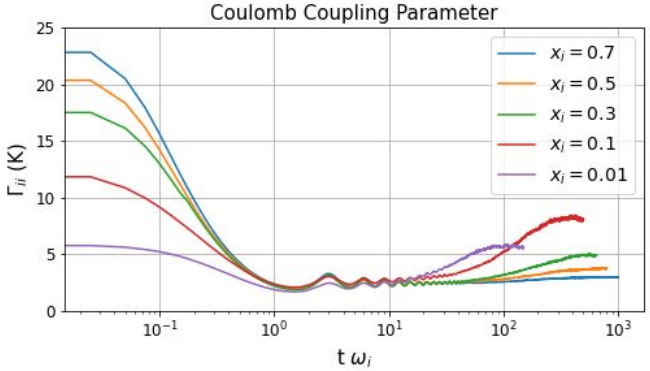
Evolution After a Ionization Pulse

r_φ = 0.133 a









<u>Characteristic regions:</u>

1. Disorder Induced Heating (DIH)
2. Ti fluctuations
3. T relaxation

- Exchange between Ki and PE during the Ti fluctuations

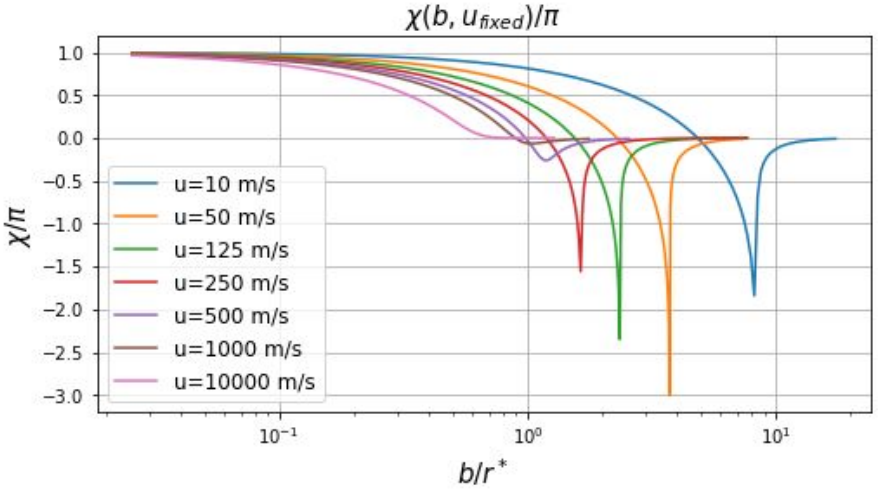
-T_{eq} < T_0 for x_i>0.01

- DIH min(Γii) ~ 2

Ion-Neutral Scattering Angle and Cross Section

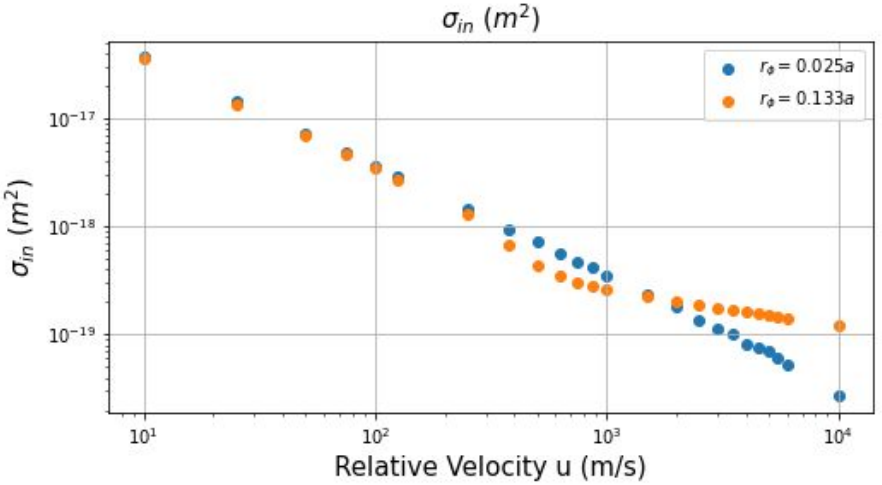
Scattering Angle

$$\chi = \pi - 2b \int_{r_0}^{\infty} \frac{dr/r^2}{\sqrt{1 - \frac{b^2}{r^2} - \frac{2\phi_{in}(r))}{mu^2}}}$$



Cross Section

$$Q_{in}^{(1)} = 2\pi \int_0^{\infty} (1 - cos(\chi))b\ db$$

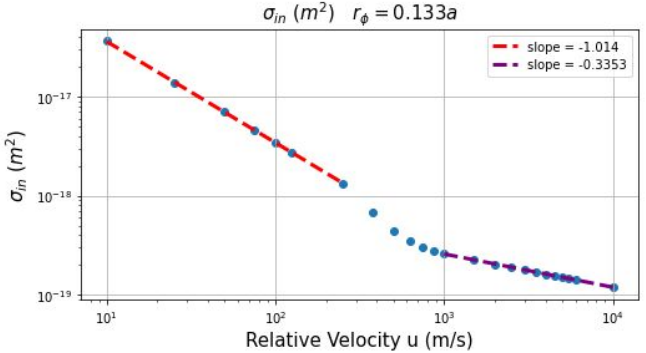


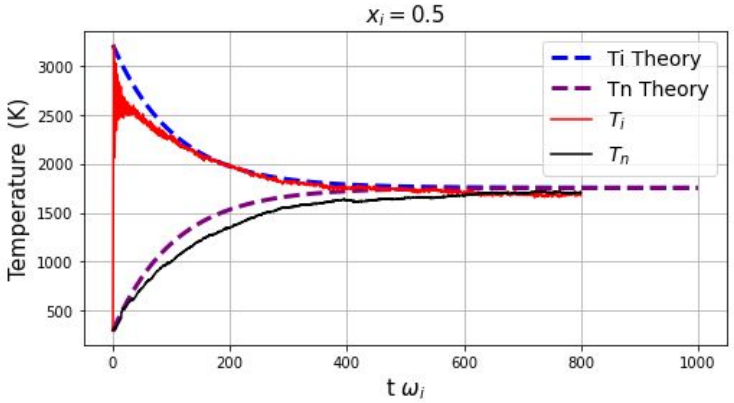
Ion-Neutral Relaxation Time

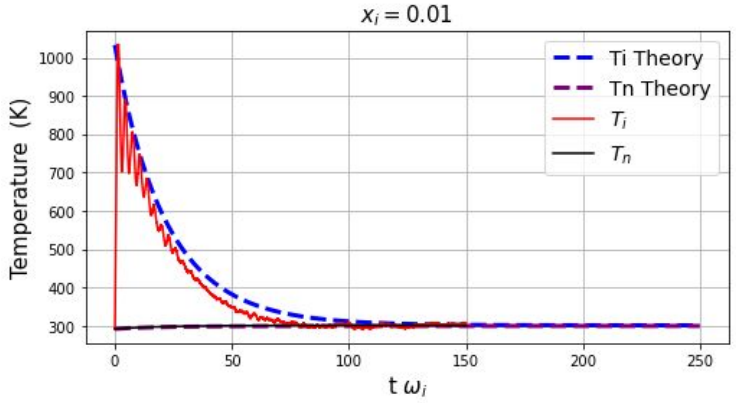
$$\nu_{in} = \frac{4}{3\sqrt{\pi}} n_n \sqrt{\frac{2k_B}{m}} \sqrt{T_i + T_n} \int_0^\infty dg Q_{in}^{(1)}(g) g^5 e^{-g^2}$$

$$\frac{dT_i}{dt} = -\frac{3}{2}\nu_{in}(T_i - T_n)$$

$$\frac{dT_n}{dt} = -\frac{3}{2}\nu_{ni}(T_n - T_i)$$







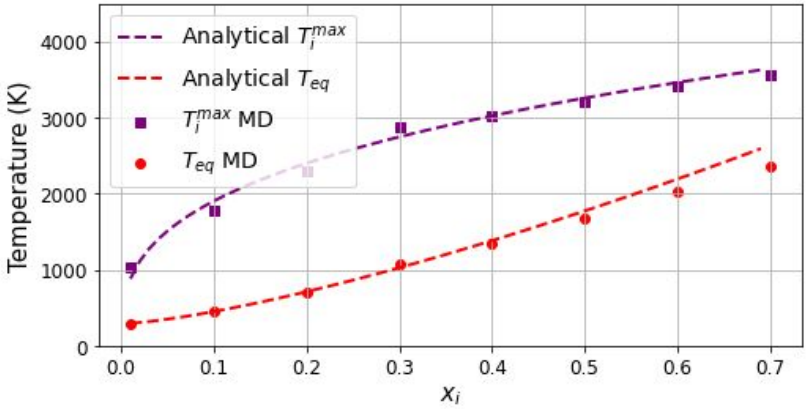
Theory model

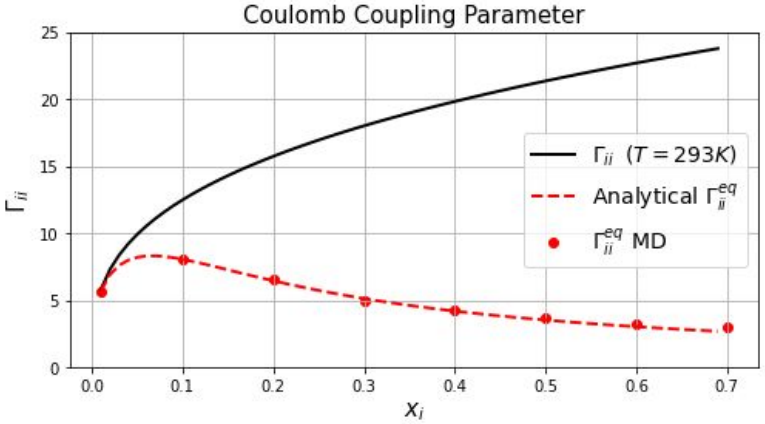
$$T^{eq} = x_i T_i^{max} + (1 - x_i) T_{n,t=0}$$

$$T_i^{max} = \left(\frac{1}{1.91}\right) \frac{Z^2 e^2}{4\pi\epsilon_0 k_B} \left(\frac{4\pi x_i n}{3}\right)^{1/3}$$

$$\Gamma_{min}^{avg}$$

$$\Gamma_{ii}^{eq}(x_i, T^{eq}(x_i))$$

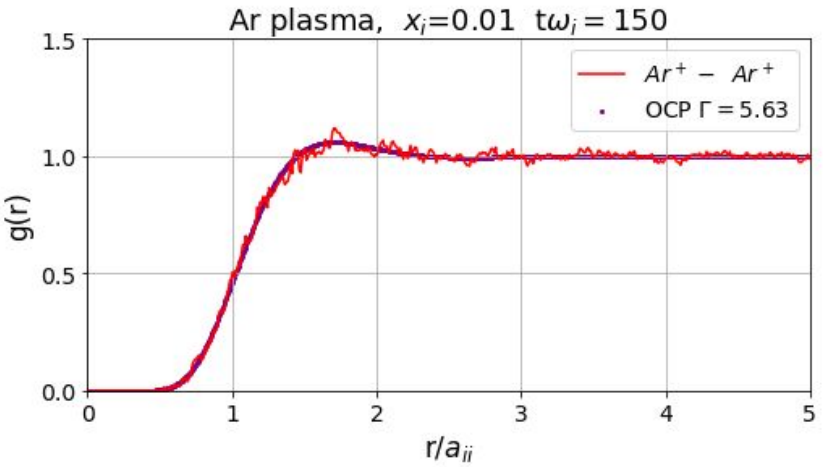


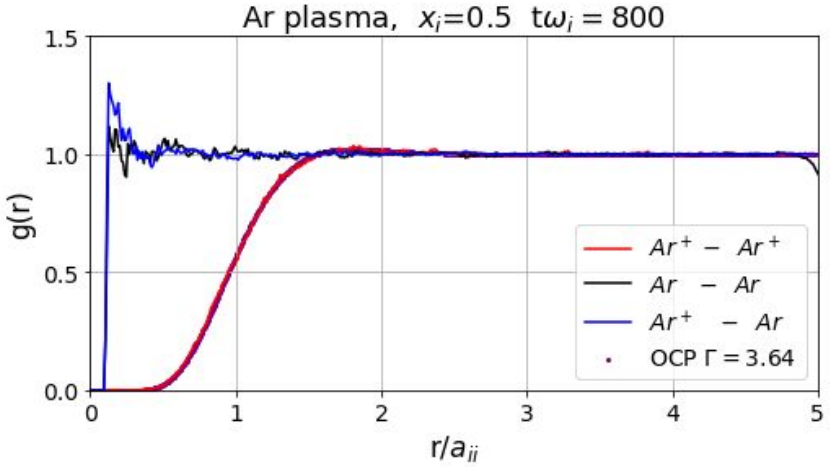


Radial Distribution Function

Change this slide with an animation over time to see how the gr is shifting to the right and at the same time an animation of Ti and Tn on top of each plot (xi =0.01 and xi=0.5)

I need to run an ensemble of this simulations and average the grs to make the animation





Thank you !