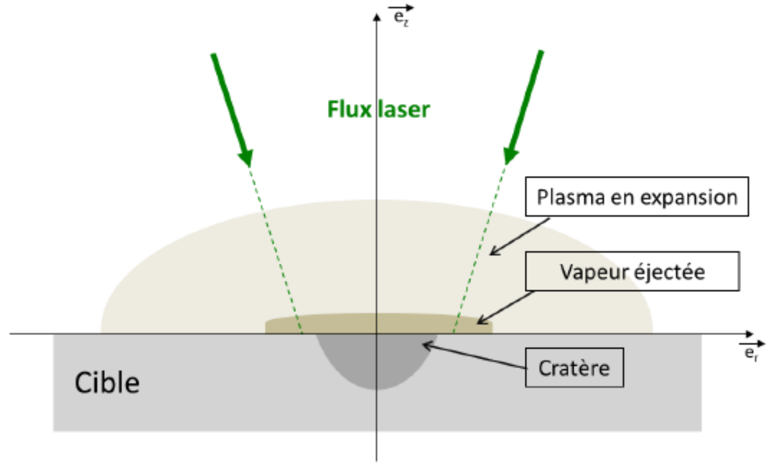
Laser Induced Plasma

Dynamique de la creation d'un plasma d'aluminium induit par laser



Flux laser

Densité de flux laser

$$\varphi_{las}(t) = \varphi_{las}^{max} \exp\left[-\left(2\frac{t-1,2\tau}{\tau}\right)^2\right]$$

Densité de flux maximale :

$$\varphi_{las}^{max} = \frac{4E}{\pi d^2 \tau} = 2.10^{13}\ \mathrm{W\ m^{-2}}$$

Paramètres laser :

Energie : $E = 65\ \mathrm{mJ}$

Longueur d'onde : $\lambda_{las} = 532\ \mathrm{nm}$

Durée de l'impulsion : $\tau = 4\ \mathrm{ns}$.

Diamètre de l'impulsion : $d = 1\ \mathrm{mm}$.

Laser Induced Plasma

Température de la surface de l'échantillon

$$T_S(t) = (T_S^{max} - T_f)\exp\left[-\left(2\frac{t-1,2\tau}{\tau}\right)^2\right] + T_f$$

T_S^{max} Température maximale atteinte par la surface

$T_f \approx 950\ \mathrm{K}$. Température de fusion de l'aluminium

Température des électrons

$$\frac{dT_e}{dt} = \frac{1}{\frac{3}{2}k_B n_e}\left(P_{ee} + \frac{\varphi_{ee}}{Z(t)} - \frac{3}{2}k_B T_e \frac{dn_e}{dt}\right)$$

$\vec{\varphi}_{ee}$ Flux d'évaporation des électrons à la surface.

P_{ee} Terme de production volumique d'énergie au sein du gaz électronique

Température des lourds

$$\frac{dT_A}{dt} = \frac{1}{\frac{3}{2}k_B \sum_{niv}[Al_{niv}]}\left(P_{eA} + \frac{\varphi_{eA}}{Z(t)} - \frac{3}{2}k_B T_A \sum_{niv}\frac{d[Al_{niv}]}{dt} - \sum_{niv}\left\{E_{niv}\frac{d[Al_{niv}]}{dt}\right\}\right)$$

φ_{eA} Flux d'évaporation des lourds

P_{eA} Terme de production volumique d'énergie des lourds

Transport de densités d'espèces (électrons + lourds)

Laser Induced Plasma

L'évaporation (loi de Herz-Knudsen) :

La densité de flux de particules $$\vec{\varphi}_N = \frac{P_{vap}}{\sqrt{2\pi m_A k_B T_S}}\vec{e}_z$$

La densité de flux d'énergie $$\vec{\varphi}_e = \frac{P_{vap}}{\sqrt{2\pi m_A k_B T_S}}2k_B T_S \vec{e}_z$$

Loi des gaz parfaits $$P_{vap} = \left(n_e + [Al_1] + [Al_2] + [Al_1^+]\right) k_B T_S$$

Flux des particules lourdes
et des électrons.

$$\vec{\varphi}_{Al_1} = \vec{\varphi}_N \left(1 - 2f_{evap}\right) \frac{g_1}{g_1 + g_2} \qquad \vec{\varphi}_{Al_2} = \vec{\varphi}_N \left(1 - 2f_{evap}\right) \frac{g_2}{g_1 + g_2}$$

$$\vec{\varphi}_{elec} = \vec{\varphi}_{Al_1^+} = \vec{\varphi}_N f_{evap}$$

Flux d'énergies des lourdes
et des électrons.

$$\varphi_{ee} = \varphi_e f_{evap} \qquad \varphi_{eA} = \varphi_e \left(1 - f_{evap}\right)$$

Laser Induced Plasma

Implementation of source terms and jacobian subroutines plasma chemistry :

- Multi-photon ionization (MPI) $Al_i^{Z_1+} + k\,h\nu_{las} \xrightarrow{k_D} \left(Al_i^{Z_1+}\right)_v \Longrightarrow Al_j^{Z_2+} + (Z_2 - Z_1)e^-$
- Inverse Bremsstrahlung $Al_i^{(Z+)} + e^-(\varepsilon) + h\nu_{las} \rightleftarrows Al_i^{(Z+)} + e^-(\varepsilon')$ $\quad \varepsilon' = \varepsilon + h\nu_{las}$
- Thermal Bremsstrahlung $Al_i^{(Z+)} + e^-(\varepsilon) \rightleftarrows Al_i^{(Z+)} + e^-(\varepsilon') + h\nu$ $\quad \varepsilon' + h\nu = \varepsilon$
- Spontaneous emission $Al_j^{(Z+)} \rightarrow Al_i^{(Z+)} + h\nu$ $\quad h\nu = E_j - E_i$
- Excitation by electronic impact $Al_i^{(Z+)} + e^-(\varepsilon) \xrightarrow{k_D} Al_j^{(Z+)} + e^-(\varepsilon')$ $\quad \varepsilon' = \varepsilon - E_{ji}$
- Ionization by electronic impact $Al_i^{Z+} + e^-(\varepsilon) \xrightarrow{k_D} Al_j^{(Z+1)+} + 2\,e^-\,(\varepsilon')$ $\quad \varepsilon' = \varepsilon - E_{ji}$
- Elastic collisions $Al_i^{(Z+)} + e^-(\varepsilon) \rightleftarrows Al_i^{(Z+)} + e^-(\varepsilon')$ $\quad \varepsilon' \neq \varepsilon$
- Evaporation (Herz-Knudsen law)
- add an ablation method

Laser Induced Plasma

Température des électrons :

$$
\begin{aligned}
\frac{dT_e}{dt} = & \underbrace{\sum_{Z,i,j} \frac{2(kh\nu - \Delta E_{ji})}{3k_B n_e} \left(k_{D,(MPI)} \left[Al_i^{Z+}\right] - k_{I,(MPI)} \left[Al_j^{(Z+1)+}\right] n_e \right)}_{\Theta_e(MPI)} \\
& \underbrace{+ \frac{\varphi_{las}}{\frac{3}{2}k_B} \left(K_{IB}^{e.n}[Al] + \sum_Z \left\{ K_{IB}^{e.i}(Z) \left[Al^{Z+}\right] \right\} \right) \left[1 - \exp\left(-\frac{h\nu_{las}}{k_B T_e} \right) \right]}_{\Theta_e(IB)} \\
& \underbrace{- \frac{32}{3m_e hc^3} \bar{v}_e \frac{e^2}{4\pi\epsilon_0} \left([Al]\bar{\sigma}_{Al} 2k_B T_e^2 + \frac{\pi^2}{3\sqrt{3}k_B} G \frac{e^4}{(4\pi\epsilon_0)^2} \sum_Z Z^2 \left[Al^{Z+}\right] \right)}_{\Theta_e(TB)} \\
& \underbrace{+ \sum_{Z,i,j} \frac{2\Delta E_{ji}}{3k_B} \left\{ k_{I,(EI)} \left[Al_j^{(Z+1)+}\right] n_e - k_{D,(EI)} \left[Al_i^{Z+}\right] \right\}}_{\Theta_e(EI)} \\
& \underbrace{+ \sum_{Z,i,j} \frac{2\Delta E_{ji}}{3k_B} \left(k_{I,(EE)} \left[Al_j^{Z+}\right] - k_{D,(EE)} \left[Al_i^{Z+}\right] \right)}_{\Theta_e(EE)} \\
& \underbrace{+ \frac{m_e}{m_A} \nu_{elas} (T_A - T_e)}_{\Theta_e(EC)} + \underbrace{\frac{2}{3k_B n_e} \frac{\varphi_{ee}}{Z(t)}}_{\Theta_e(\varphi)} \underbrace{- \frac{T_e}{n_e} \frac{dn_e}{dt}}_{\Theta_e(u_1)}
\end{aligned}
$$

Laser Induced Plasma

Température des lourds :

$$
\begin{aligned}
\frac{dT_A}{dt} = & \underbrace{\frac{2}{3k_B\sum\limits_{niv}[Al_{niv}]}\sum_{Z,i,j}\left\{\Delta E_{ji}\left(k_{D,(MPI)}\left[Al_i^{Z+}\right]-k_{I,(MPI)}\left[Al_j^{(Z+1)+}\right]n_e\right)\right\}}_{\Theta_A(MPI)} \\
& \underbrace{-\frac{2n_e}{3k_B\sum\limits_{niv}[Al_{niv}]}\sum_{Z,i,j}\Delta E_{ji}\left\{k_{I,(EI)}\left[Al_j^{(Z+1)+}\right]n_e-k_{D,(EI)}\left[Al_i^{Z+}\right]\right\}}_{\Theta_A(EI)} \\
& \underbrace{-\frac{2n_e}{3k_B\sum\limits_{niv}[Al_{niv}]}\sum_{Z,i,j}\Delta E_{ji}\left(k_{I,(EE)}\left[Al_j^{Z+}\right]-k_{D,(EE)}\left[Al_i^{Z+}\right]\right)}_{\Theta_A(EE)} \\
& \underbrace{-\frac{2}{3k_B\sum\limits_{niv}[Al_{niv}]}\sum_{Z,i,j}\left[Al_j^{Z+}\right]A_{ji}^{*}\Lambda(k_0 Z)\Delta E_{ji}}_{\Theta_A(SE)}\underbrace{-\frac{n_e}{\sum\limits_{niv}[Al_{niv}]}\frac{m_e}{m_A}\nu_{elas}\left(T_A-T_e\right)}_{\Theta_A(EC)} \\
& \underbrace{+\frac{2}{3k_B\sum\limits_{niv}[Al_{niv}]}\frac{\varphi_{eA}}{Z(t)}}_{\Theta_A(\varphi)}\underbrace{-\frac{T_A}{\sum\limits_{niv}[Al_{niv}]}\frac{d\left[Al_{niv}\right]}{dt}}_{\Theta_A(u_1)} \\
& \underbrace{-\frac{2}{3k_B\sum\limits_{niv}[Al_{niv}]}\sum_{niv}\left(E_{niv}\frac{d\left[Al_{niv}\right]}{dt}\right)}_{\Theta_A(u_2)}
\end{aligned}
$$

Laser Induced Plasma

Densité des électrons :

$$\frac{dn_e}{dt} = \underbrace{\sum_j \sum_i \left(k_{D,(MPI)} \left[Al_i^{(Z-1)+} \right] - k_{I,(MPI)} \left[Al_j^{Z+} \right] n_e \right)}_{\Xi_e\ (MPI)}$$
$$+ \underbrace{\sum_j \sum_i \left(k_{D,(EI)} \left[Al_i^{(Z-1)+} \right] - k_{I,(EI)} \left[Al_j^{Z+} \right] n_e \right) n_e}_{\Xi_e\ (EI)} + \underbrace{\frac{\|\vec{\varphi}_N\|}{Z(t)} f_{evap}}_{\Xi_e\ (\varphi)}$$

Laser Induced Plasma

La variation de densité de population de Al

$$
\begin{aligned}
\frac{d\,[Al_1]}{dt} = & \underbrace{\sum_j \left(k_{I,(MPI)}\,[Al_j^+]\,n_e - k_{D,(MPI)}\,[Al_1]\right)}_{\Xi_{Al_1}\,(MPI)} \\
& + \underbrace{\sum_j \left(k_{I,(EI)}\,[Al_j^+]\,n_e - k_{D,(EI)}\,[Al_1]\right) n_e}_{\Xi_{Al_1}\,(EI)} \\
& + \underbrace{\sum_j \left(k_{I,(EE)}\,[Al_j] - k_{D,(EE)}\,[Al_1]\right) n_e}_{\Xi_{Al_1}\,(EE)} \\
& + \underbrace{\sum_j [Al_j]\,A_{j1}^*\Lambda}_{\Xi_{Al_1}\,(SE)} + \underbrace{\frac{\|\vec{\varphi}_N\|}{Z(t)}\,(1-2f_{evap})\,\frac{g_1}{g_1+g_2}}_{\Xi_{Al_1}\,(\varphi)}
\end{aligned}
$$

Laser Induced Plasma

Conditions initiales

Température de la surface : $Ts(0) = 950K$

$Tsmax = 2900K$

Température électrons : $Te : y(2,0) = 950\ K$

Température lourds : $Ta : y(1,0) = 950\ K$

Epaisseur plasma : $e_{plasma}\colon\ y(3,0) = 0\ m$

Densité des particules : loi des gaz parfaits

Paramètres laser :

- Energie : $E = 65$ mJ
- Longueur d'onde : $\lambda_{las} = 532$ nm
- Durée de l'impulsion : τ=4 ns.
- Diamètre de l'impulsion : $d = 1$ mm.

Vecteur d'états:

$Ta : y(1)$

$Te : y(2)$

$e_{plasma}\colon y(3)$

$n_{electrons}\colon y(4)$

Al_i : y(5) … y(47)[43 niveaux]

$Al_i^{+} : y(48) \dots y(89)[42\ niveaux]$

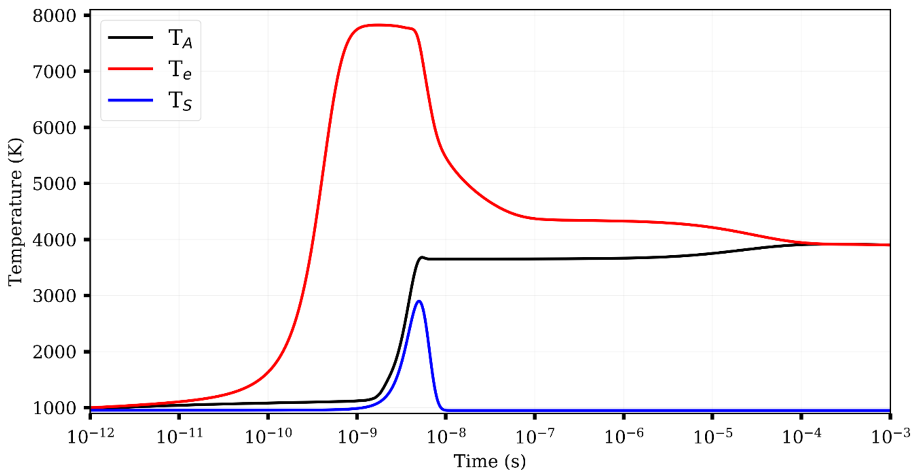
$Al_i^{2+} : y(90) \dots y(110)\ [21\ niveaux]$

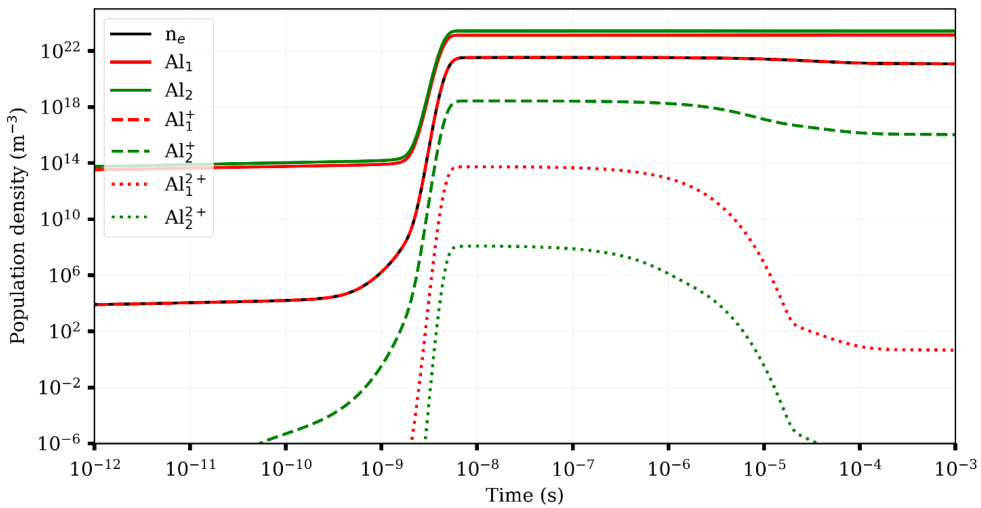
$Al_i^{3+} : y(111)[1\ niveaux]$

Laser Induced Plasma

Températures :
- Plaque [Ts]
- Electrons [Te]
- Gaz [Ta]

Densités :
- Electrons [ne]
- Aluminium [Al*]





Durée du calcul : 5 minutes

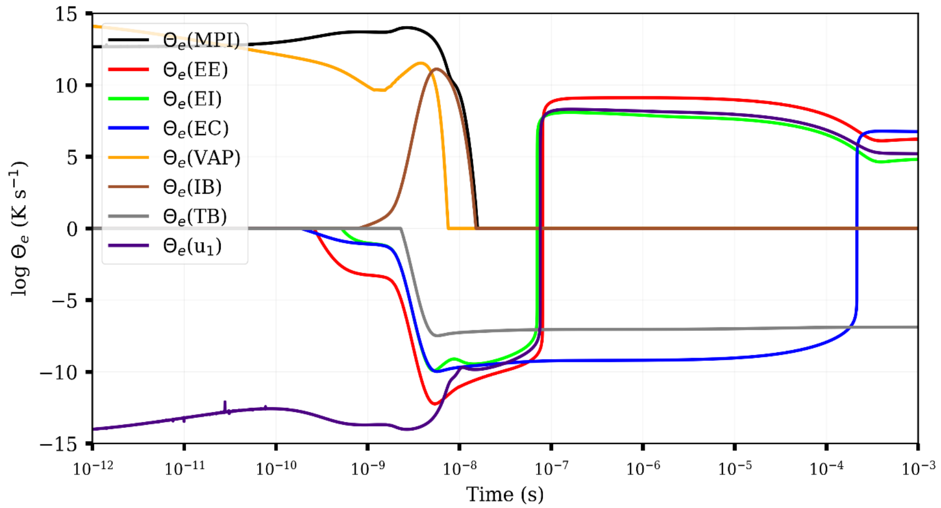
Laser Induced Plasma

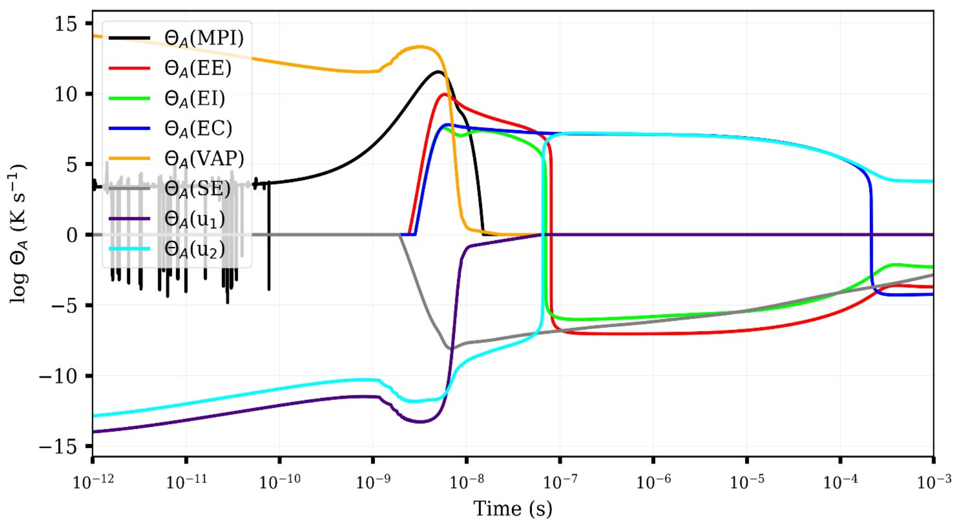
Termes sources Te :

- Ionisation Multi-photonique (MPI)
- Excitation électronique (EE)
- Ionisation électronique (EI)
- Les collisions élastiques (EC)
- Evaporation (VAP)
- Bremsstrahlung inverse (IB)
- Bremsstrahlung Thermique (TB)
- Transport (u1)

Termes sources Ta :

- Ionisation Multi-photonique (MPI)
- Excitation électronique (EE)
- Ionisation électronique (EI)
- Les collisions élastiques (EC)
- Evaporation (VAP)
- Emission spontanée (SE)
- Transport (u1)
- Transport (u2)





Laser Induced Plasma

Conditions initiales

Température de la surface : $Ts(0) = 950K$
$Tsmax = 6700K$

Température électrons : $Te : y(2,0) = 950\ K$

Température lourds : $Ta : y(1,0) = 950\ K$

Epaisseur plasma : $e_{plasma} : y(3,0) = 0\ m$

Densité des particules : loi des gaz parfaits

Paramètres laser :

- Energie : $E = 65$ mJ
- Longueur d'onde : $\lambda_{las} = 532$ nm
- Durée de l'impulsion : $\tau = 4$ ns.
- Diamètre de l'impulsion : $d = 1$ mm.

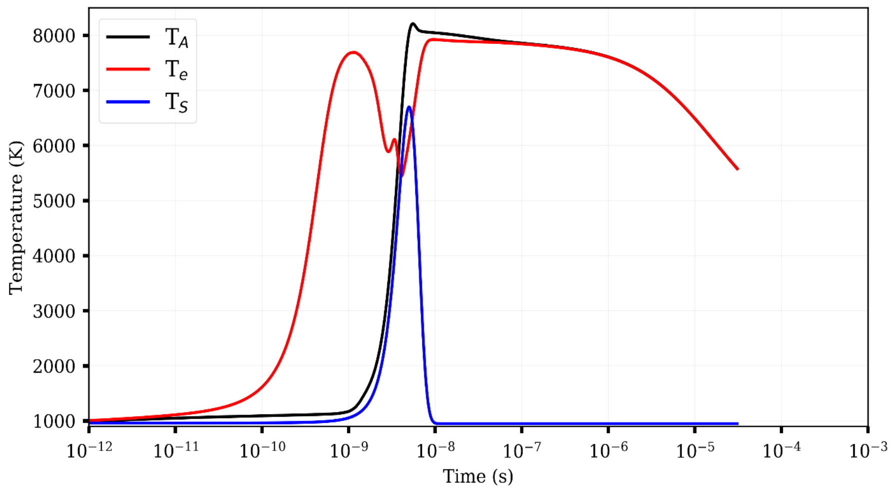
Vecteur d'états:

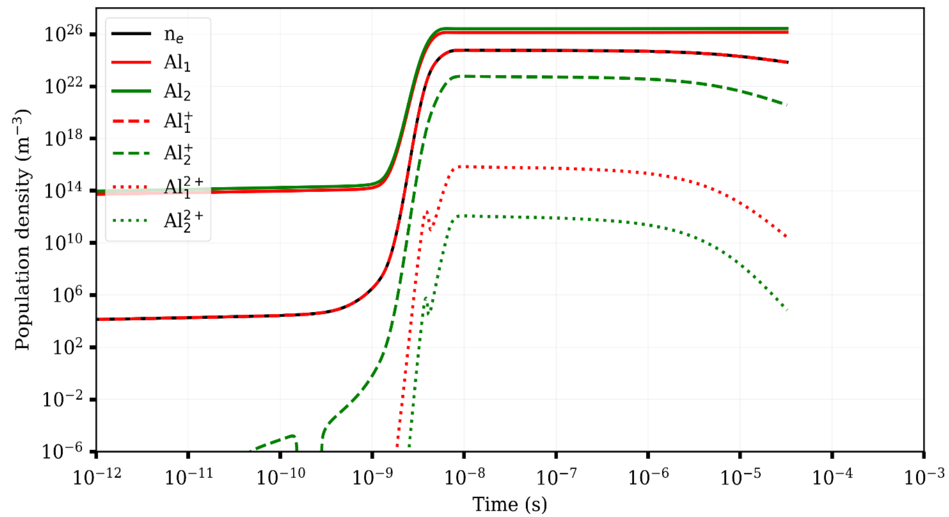
$Ta : y(1)$
$Te : y(2)$
$e_{plasma} : y(3)$
$n_{electrons} : y(4)$
Al_i : y(5) ... y(47)[43 niveaux]
$Al_i^+ : y(48) \dots y(89)[42\ niveaux]$
$Al_i^{2+} : y(90) \dots y(110)\ [21\ niveaux]$
$Al_i^{3+} : y(111)[1\ niveaux]$

Laser Induced Plasma

Températures :
- Plaque [Ts]
- Electrons [Te]
- Gaz [Ta]

Densités :
- Electrons [ne]
- Aluminium [Al*]



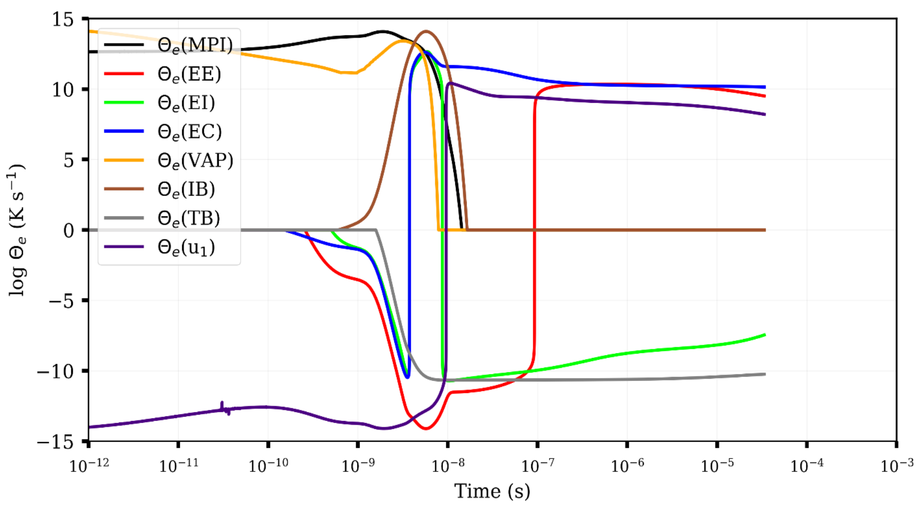


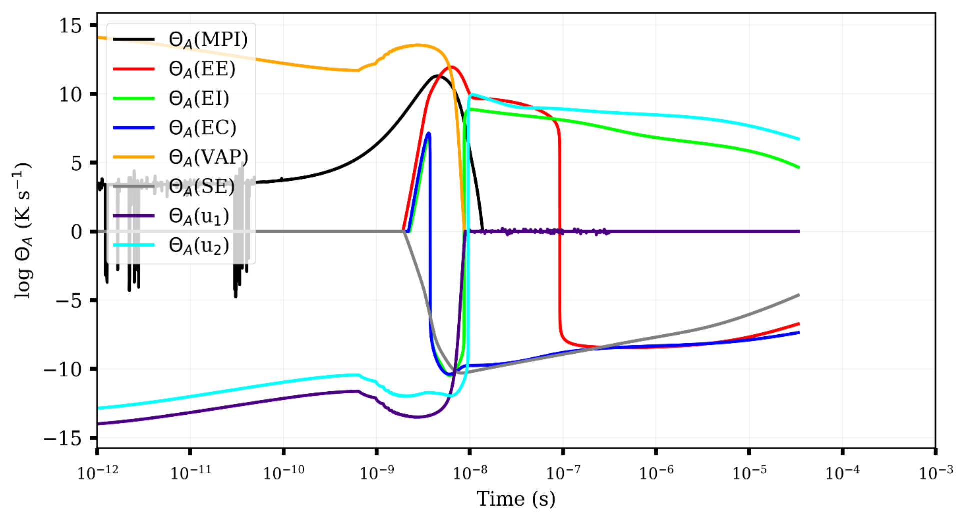
Durée du calcul : 22 minutes

Laser Induced Plasma

Termes sources Te :
- Ionisation Multi-photonique (MPI)
- Excitation électronique (EE)
- Ionisation électronique (EI)
- Les collisions élastiques (EC)
- Evaporation (VAP)
- Bremsstrahlung inverse (IB)
- Bremsstrahlung Thermique (TB)
- Transport (u1)

Termes sources Ta :
- Ionisation Multi-photonique (MPI)
- Excitation électronique (EE)
- Ionisation électronique (EI)
- Les collisions élastiques (EC)
- Evaporation (VAP)
- Emission spontanée (SE)
- Transport (u1)
- Transport (u2)





Two-temperature model

Two-fluid equations

Heavy species

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_h \vec{u}_h) = \dot{\rho}_s$$

$$\frac{\partial \rho_h \vec{u}_h}{\partial t} + \nabla \cdot (\rho_h \vec{u}_h \vec{u}_h) + \nabla p_h = \vec{\mu}_{eh} + n_i e Z_i (\vec{E} + \vec{u}_h \times \vec{B})$$

$$\frac{\partial}{\partial t}\left[\rho_h \left(\varepsilon_h + \frac{1}{2}\vec{u}_h \cdot \vec{u}_h\right)\right] + \nabla \cdot \left[\rho_h \vec{u}_h \left(\varepsilon_h + \frac{1}{2}\vec{u}_h \cdot \vec{u}_h\right)\right] + \nabla \cdot (\vec{u}_h p_h)$$
$$= \vec{u}_h \cdot \vec{\mu}_{eh} - n_i e Z_i \vec{u}_h \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_h \nabla T_h) - \dot{q}_h^{\mathrm{CR}}$$

Electrons

$$\frac{\partial \rho_e}{\partial t} + \nabla \cdot (\rho_e \vec{u}_e) = \dot{\rho}_e$$

$$\frac{\partial \rho_e \vec{u}_e}{\partial t} + \nabla \cdot (\rho_e \vec{u}_e \vec{u}_e) + \nabla p_e = \vec{\mu}_{he} + n_e e (\vec{E} + \vec{u}_e \times \vec{B})$$

$$\frac{\partial}{\partial t}\left[\rho_e \left(\varepsilon_e + \frac{1}{2}\vec{u}_e \cdot \vec{u}_e\right)\right] + \nabla \cdot \left[\rho_e \vec{u}_e \left(\varepsilon_e + \frac{1}{2}\vec{u}_e \cdot \vec{u}_e\right)\right] + \nabla \cdot (\vec{u}_e p_e)$$
$$= \vec{u}_e \cdot \vec{\mu}_{he} - n_e e \vec{u}_e \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_e \nabla T_e) - \dot{q}_e^{\mathrm{CR}}$$

Two-temperature model

Two-fluid equations

Heavy species

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_h \vec{u}_h) = \dot{\rho}_s$$

$$\frac{\partial \rho_h \vec{u}_h}{\partial t} + \nabla \cdot (\rho_h \vec{u}_h \vec{u}_h) + \nabla p_h = \vec{\mu}_{eh} + n_i e Z_i (\vec{E} + \vec{u}_h \times \vec{B})$$

$$\frac{\partial}{\partial t}\left[\rho_h \left(\varepsilon_h + \frac{1}{2}\vec{u}_h \cdot \vec{u}_h\right)\right] + \nabla \cdot \left[\rho_h \vec{u}_h \left(\varepsilon_h + \frac{1}{2}\vec{u}_h \cdot \vec{u}_h\right)\right] + \nabla \cdot (\vec{u}_h p_h)$$
$$= \vec{u}_h \cdot \vec{\mu}_{eh} - n_i e Z_i \vec{u}_h \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_h \nabla T_h) - \dot{q}_h^{\mathrm{CR}}$$

The eigenvalues of the system are : $u_h, u_h + c_h, u_h - c_h$

For perfect gases c_h is the sound speed $c_h = \gamma_h {}^* P_h / \rho_h$

The system is solved with explicit schemes for compressible flows (ECS)

Two-temperature model

Two-fluid equations

Electrons

$$\frac{\partial \rho_e}{\partial t} + \nabla \cdot (\rho_e \vec{u}_e) = \dot{\rho}_e$$

$$\frac{\partial \rho_e \vec{u}_e}{\partial t} + \nabla \cdot (\rho_e \vec{u}_e \vec{u}_e) + \nabla p_e = \vec{\mu}_{he} + n_e e(\vec{E} + \vec{u}_e \times \vec{B})$$

$$\frac{\partial}{\partial t}\left[\rho_e\left(\varepsilon_e + \frac{1}{2}\vec{u}_e \cdot \vec{u}_e\right)\right] + \nabla \cdot \left[\rho_e \vec{u}_e\left(\varepsilon_e + \frac{1}{2}\vec{u}_e \cdot \vec{u}_e\right)\right] + \nabla \cdot (\vec{u}_e p_e)$$
$$= \vec{u}_e \cdot \vec{\mu}_{he} - n_e e \vec{u}_e \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_e \nabla T_e) - \dot{q}_e^{\mathrm{CR}}$$

The eigenvalues of the system are : $u_e, u_e + c_e, u_e - c_e$

c_e is the electrons sound speed $c_e = \gamma_e * P_e / \rho_e$

Consequence of charge neutrality and is valid when considering length scales greater than the Debye length $\quad u_e = u_h$

Laser Induced Plasma

Two-temperature model

Two-fluid equations

Electrons

$$\frac{\partial \rho_e}{\partial t} + \nabla \cdot (\rho_e \vec{u}_e) = \dot{\rho}_e$$

$$\frac{\partial \rho_e \vec{u}_e}{\partial t} + \nabla \cdot (\rho_e \vec{u}_e \vec{u}_e) + \nabla p_e = \vec{\mu}_{he} + n_e e(\vec{E} + \vec{u}_e \times \vec{B})$$

$$\frac{\partial}{\partial t}\left[\rho_e\left(\varepsilon_e + \frac{1}{2}\vec{u}_e \cdot \vec{u}_e\right)\right] + \nabla \cdot \left[\rho_e \vec{u}_e\left(\varepsilon_e + \frac{1}{2}\vec{u}_e \cdot \vec{u}_e\right)\right] + \nabla \cdot (\vec{u}_e p_e)$$
$$= \vec{u}_e \cdot \vec{\mu}_{he} - n_e e \vec{u}_e \cdot \vec{E} - \nabla \cdot (\bar{\kappa}_e \nabla T_e) - \dot{q}_e^{\mathrm{CR}}$$

Electrons thermodynamic properties

$m_e = 9.1 * 10^{-31}$ kg $\qquad W_e = 5.48 * 10^{-7}$ kg/mol

$r_e = 1.5 * 10^{7}$ J/K/Kg $\qquad \gamma_e = 5/3$

$$c_e = \sqrt{\gamma_e r_e T_e}$$

$$T_e \in [300\ K, 10000\ K] \Rightarrow c_e \in [85000 \text{ m/s}, 500000 \text{ m/s}]$$

The low-Mach assumption is verified for electrons equations.
A prediction-correction method for low Mach Flows is used to solved the system (VDS)

Two-temperature model

Two-fluid equations

Heavy species

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_h \vec{u}_h) = \dot{\rho}_s$$

$$\frac{\partial \rho_h \vec{u}_h}{\partial t} + \nabla \cdot (\rho_h \vec{u}_h \vec{u}_h) + \nabla p_h = \vec{\mu}_{eh} + n_i e Z_i (\vec{E} + \vec{u}_h \times \vec{B})$$

$$\frac{\partial}{\partial t}\left[\rho_h \left(\varepsilon_h + \frac{1}{2}\vec{u}_h \cdot \vec{u}_h\right)\right] + \nabla \cdot \left[\rho_h \vec{u}_h \left(\varepsilon_h + \frac{1}{2}\vec{u}_h \cdot \vec{u}_h\right)\right] + \nabla \cdot (\vec{u}_h p_h)$$

$$= \vec{u}_h \cdot \vec{\mu}_{eh} - n_i e Z_i \vec{u}_h \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_h \nabla T_h) - \dot{q}_h^{\mathrm{CR}}$$

Electrons

$$\frac{\partial \rho_e}{\partial t} + \nabla \cdot (\rho_e \vec{u}_e) = \dot{\rho}_e$$

$$\frac{\partial \rho_e \vec{u}_e}{\partial t} + \nabla \cdot (\rho_e \vec{u}_e \vec{u}_e) + \nabla p_e = \vec{\mu}_{he} + n_e e (\vec{E} + \vec{u}_e \times \vec{B})$$

$$\frac{\partial}{\partial t}\left[\rho_e \left(\varepsilon_e + \frac{1}{2}\vec{u}_e \cdot \vec{u}_e\right)\right] + \nabla \cdot \left[\rho_e \vec{u}_e \left(\varepsilon_e + \frac{1}{2}\vec{u}_e \cdot \vec{u}_e\right)\right] + \nabla \cdot (\vec{u}_e p_e)$$

$$= \vec{u}_e \cdot \vec{\mu}_{he} - n_e e \vec{u}_e \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_e \nabla T_e) - \dot{q}_e^{\mathrm{CR}}$$

Two-temperature model

One-fluid equations

$u \approx u_e \approx u_h$ Consequence of charge neutrality and is valid when considering length scales greater than the Debye length

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) + \nabla p = Q\vec{E} + \vec{j}_c \times \vec{B},$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\vec{u} H_\circ) + \nabla p = \vec{j}_c \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_h \nabla T_h) - \nabla \cdot (\bar{\bar{\kappa}}_e \nabla T_e) - \dot{q}_{\mathrm{CR}}$$

$$E = \varepsilon_h + \varepsilon_e + \frac{1}{2}\rho \vec{u} \cdot \vec{u}$$

$$\frac{\partial}{\partial t}\left[\rho_e \left(\varepsilon_e + \frac{1}{2}\vec{u} \cdot \vec{u}\right)\right] + \nabla \cdot \left[\rho_e \left(\varepsilon_e + \frac{1}{2}\vec{u} \cdot \vec{u}\right) \vec{u}\right] + \nabla \cdot (\vec{u} p_e)$$
$$= \vec{u}_{he} \cdot \vec{\mu} - \nabla \cdot \vec{q}_e - \dot{q}_{\mathrm{CR}}$$

The system have 4 eigenvalues : u and 3 complex others values

Laser Induced Plasma

Two-temperature model

One-fluid equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u}\vec{u}) + \nabla p = Q\vec{E} + \vec{j}_c \times \vec{B},$$

$$\frac{\partial \rho_e \vec{u}_e}{\partial t} + \nabla \cdot (\rho_e \vec{u}_e \vec{u}_e) + \nabla p_e = \vec{\mu}_{he} + n_e e(\vec{E} + \vec{u}_e \times \vec{B})$$

$$E = \varepsilon_h + \varepsilon_e + \frac{1}{2}\rho \vec{u} \cdot \vec{u}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\vec{u} H_\circ) + \nabla p = \vec{j}_c \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_h \nabla T_h) - \nabla \cdot (\bar{\bar{\kappa}}_e \nabla T_e) - \dot{q}_{\mathrm{CR}}$$

$$\frac{\partial}{\partial t}\left[\rho_e\left(\varepsilon_e + \frac{1}{2}\vec{u}\cdot\vec{u}\right)\right] + \nabla \cdot \left[\rho_e\left(\varepsilon_e + \frac{1}{2}\vec{u}\cdot\vec{u}\right)\vec{u}\right] + \nabla \cdot (\vec{u} p_e)$$

$$= \vec{u}_{he} \cdot \vec{\mu} - \nabla \cdot \vec{q}_e - \dot{q}_{\mathrm{CR}}$$

The system have 5 eigenvalues : u, $u + c_e$, $u - c_e$, $\dfrac{\sqrt{{Y_e}^2 u^2 + 4c^2} + (Y_e + 2)u}{2}$

$$-\frac{\sqrt{{Y_e}^2 u^2 + 4c^2} + (-Y_e - 2)u}{2}$$

$$\rho * c^2 = P_e(\gamma^h - 1)/(\gamma^e - 1) + P * (\gamma_h - 1) + P_h \qquad \rho_e * c_e^2 = P_e * \gamma^e$$

Laser Induced Plasma

Two-temperature model

One-fluid equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u}\vec{u}) + \nabla p = Q\vec{E} + \vec{j}_c \times \vec{B},$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\vec{u} H_\circ) + \nabla p = \vec{j}_c \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_h \nabla T_h) - \nabla \cdot (\bar{\bar{\kappa}}_e \nabla T_e) - \dot{q}_{\mathrm{CR}}$$

$$E = \varepsilon_h + \varepsilon_e + \frac{1}{2}\rho \vec{u} \cdot \vec{u}$$

$$\frac{\partial}{\partial t}(\rho_e \varepsilon_e) + \nabla \cdot (\rho_e \varepsilon_e \vec{u}) = -p_e \nabla \cdot \vec{u} + \dot{\omega}$$

The eigenvalues of the system are : u, $u + c$,$u - c$

$$\rho * c^2 = P * (\gamma^h - 1) + P_h + P_e * (\gamma^e + 1 - 2 * \gamma^h)/(\gamma^e - 1)$$

$p_e \nabla \cdot \vec{u}$ is in non-conservative form, and may present severe numerical difficulties where the flow gradients are not resolved, degrading solutions at shocks and other discontinuities.

Two-temperature model

One-fluid equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u}\vec{u}) + \nabla p = Q\vec{E} + \vec{j}_c \times \vec{B},$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\vec{u} H_\circ) + \nabla p = \vec{j}_c \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_h \nabla T_h) - \nabla \cdot (\bar{\bar{\kappa}}_e \nabla T_e) - \dot{q}_{\mathrm{CR}} \qquad E = \varepsilon_h + \varepsilon_e + \frac{1}{2}\rho \vec{u} \cdot \vec{u}$$

$$\frac{\partial \rho_e s_e}{\partial t} + \nabla \cdot (\rho_e s_e \vec{u}) = \frac{1}{T_e}(\dot{\omega} - \dot{\rho}_e h_e) + \dot{\rho}_e s_e \qquad s_e \equiv \frac{p_e}{\rho_e^{\gamma_e}} \qquad h_e = \varepsilon_e + p_e/\rho_e$$

The eigenvalues of the system are : u, $u + c$,$u - c$

Two-temperature model

One-fluid equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) + \nabla p = Q\vec{E} + \vec{j}_c \times \vec{B},$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\vec{u} H_\circ) + \nabla p = \vec{j}_c \cdot \vec{E} - \nabla \cdot (\bar{\bar{\kappa}}_h \nabla T_h) - \nabla \cdot (\bar{\bar{\kappa}}_e \nabla T_e) - \dot{q}_{\mathrm{CR}} \qquad E = \varepsilon_h + \varepsilon_e + \frac{1}{2}\rho \vec{u} \cdot \vec{u}$$

$$\frac{\partial \rho_e h_e}{\partial t} + \nabla . (rho_e h_e \overrightarrow{u}) = \frac{dp_e}{dt} + S \qquad h_e = \varepsilon_e + p_e/\rho_e$$

The eigenvalues of the system are : u, $u + c$,$u - c$

Laser Induced Plasma

Plasma Reactor Solver (PRS)

- Implementation of Multi-temperatures EOS (Ts, Tv, Trot, Te)
- Implementation of new species properties (charge, Energy-level …)
- Implementation of ms_electrons
- Implementation of new types of reactions :

  - one-temperature-Arrhenius
  - two-temperature-Arrhenius
  - molecular-excitation
  - molecular-ionization
  - electronic-excitation
  - electronic-ionization
  - electron-ion-recombination
  - dissociative-recombination

```
<!-- reaction 0003    -->
<reaction reversible="no" type="electronic-ionisation" id="0003">
  <equation>AR + e- =] AR+ + 2e-</equation>
  <rateCoeff>
    <Arrhenius type="two-temperatures" >
       <A>4.7850E+09</A>
       <b>0.0</b>
       <E units="K">0.0</E>
       <b_Te>0.735000</b_Te>
       <Ee units="K">183270.00</Ee>
    </Arrhenius>
  </rateCoeff>
  <reactants>AR:1.0 e-:1.0</reactants>
  <products>AR+:1.0 e-:2.0</products>
</reaction>
```

```
<!-- electrons definitions     -->
<electronsData id="electrons_data">

  <!-- electrons e-    -->
  <electrons name="e-">
  </electrons>

</electronsData>
```

```
<!-- species AR+    -->
<species name="AR+">
  <atomArray>Ar:1 </atomArray>
  <charge>1</charge>
  <thermo>
    <MULTIPLE_TEMPERATURES>
      <Energy_level>2.52475000E-18 </Energy_level>
      <Statistical_weight>6.000000000E+00 </Statistical_weight>
      <Quantum_number>0.000000000E+00 </Quantum_number>
      <Angular_momentum>0.000000000E+00 </Angular_momentum>
    </MULTIPLE_TEMPERATURES>
  </thermo>
  <transport model="gas_transport">
    <string title="geometry">linear</string>
    <LJ_welldepth units="K">38.000</LJ_welldepth>
    <LJ_diameter units="A">2.920</LJ_diameter>
    <dipoleMoment units="Debye">0.000</dipoleMoment>
    <polarizability units="A3">0.790</polarizability>
    <rotRelax>280.000</rotRelax>
</transport>
</species>
```

Laser Induced Plasma

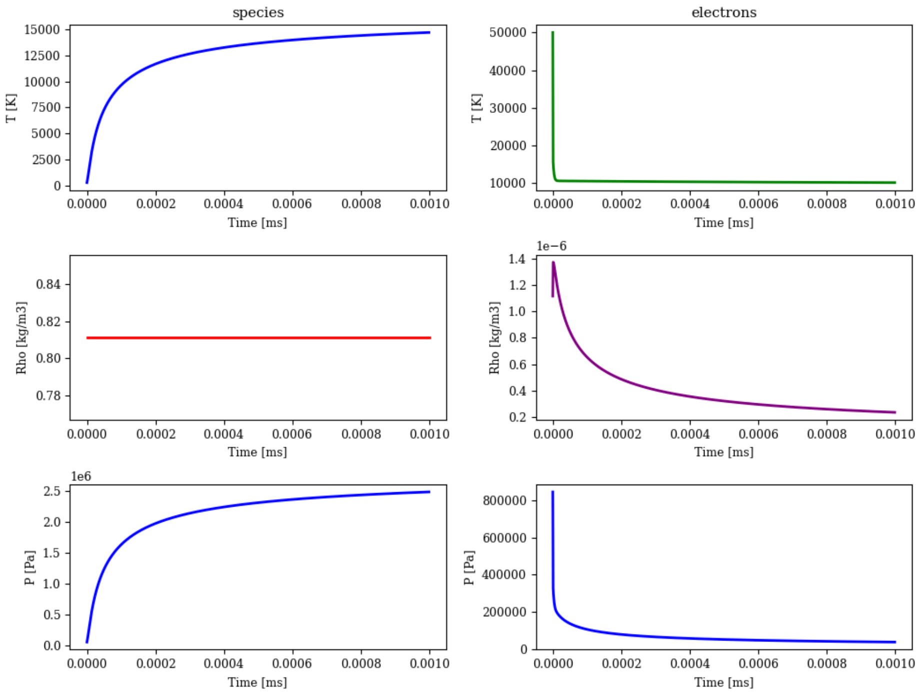
Argon-plasma simulation with PRS

Species : (Ar, Ar*, Ar+, Ar2+, e-)

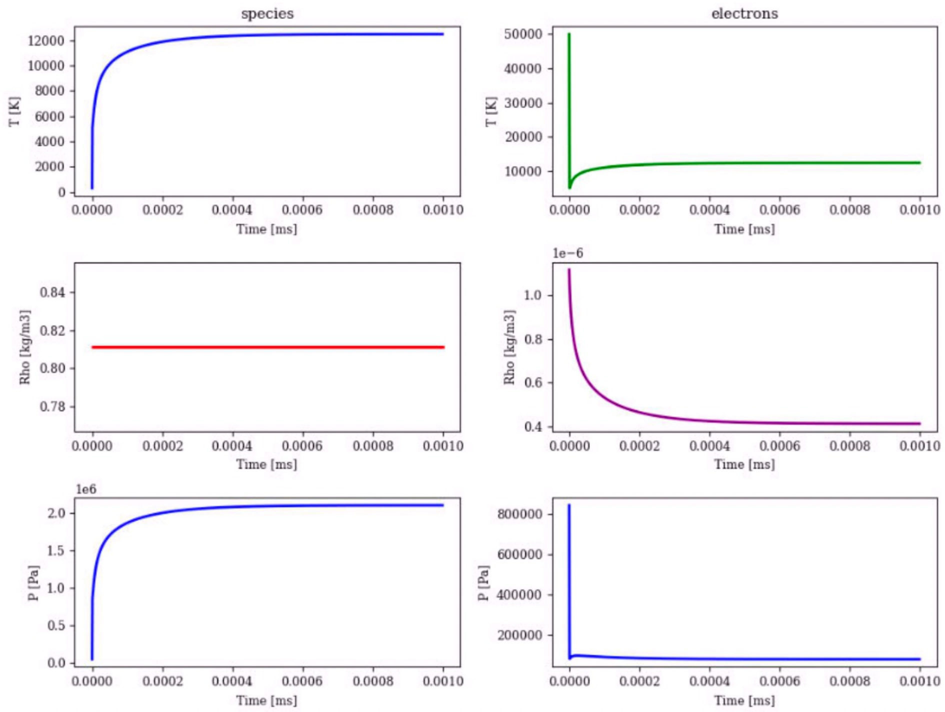
Initial conditions:

- Ar:0.9,Ar+:0.1
- T = 300K
- Te = 50000K
- Electroneutrality

Without elastic collision



With elastic collision



Laser Induced Plasma