Report on changes made to the program [2]

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1 Changes made to the program

- Particles are stored as linked list, it allows to store variable number of particles.

- Structure of the input file. Example with details will be provided in Paragraph 3.

- Program handles two cases: calculation of the stationary electron energy distribution function *eedf* and dynamic change of the *eedf* function during a time. For details concerning initialization of each case look in Section 3.

- Implemented dynamic particle initialization function. For details look in Section 5.1.

2 Electron energy distribution and probability functions

2.1 Normalization of the *eedf*

Normalization is done using equation (3) in [1]. In the final form

$$\int f(\epsilon) \cdot \epsilon^{\frac{1}{2}} \, d\epsilon = 1. \tag{1}$$

In the program normalization of discrete $f(\epsilon_i)$ implemented as

$$f(\epsilon_i) = \frac{f(\epsilon_i)}{\sum\limits_i f(\epsilon_i) \cdot \epsilon_i^{\frac{1}{2}} \cdot \Delta\epsilon}. \tag{2}$$

2.2 Normalization of the electron energy probability function

Function represents the distribution of electrons over energy bins. In the program it is calculated as

$$p(\epsilon_i) = \frac{p(\epsilon_i)}{\sum\limits_i p(\epsilon_i)}. \tag{3}$$

3 Input data example

```
0                   | Simulation mode (0 = stationary, 1 = non-stationary)
1e6                 | Particle initialization expression (e.g., 10^11*t+1e7)
                      In stationary mode skips time dependent part of expression,
                      initializes only constant (e.g., 1e7)
20e-9               | Time of simulation [s]
                      In stationary mode affects iteration number
.1e-9               | Time step [s]
1e3                 | Initial energy of electrons [eV]
50e-3               | Gas pressure [Torr]
7 2                 | Number of collision processes, particle species
1.53e7 2.74e7       | A(b), A(c)
8.84e-10 3.67e-11   | Q(b), Q(c)
"data/N2+B.dat"
```

```
"data/N2C-2.dat"
"data/N2.dat"
"data/N2A3.dat"
"data/N2B3.dat"
"data/N2Bprime3.dat"
"data/N2W3u.dat"
```

4 Stationary case

4.1 Convergence criteria

Since electron energy probability function is normalized $\sum_{i=1}^{N} p(\epsilon_i) = 1$, I chose intuitive convergence criteria:

$$C^t = \sum_{i=1}^{N} |p^t(\epsilon_i) - p^{t-dt}(\epsilon_i)|. \tag{4}$$

Maximum value of C is 1, C is area between plot of electron energy probability functions for two following time steps.

4.2 Results

Average electron energy, total number of electrons, number of electrons with energy below 10 eV and number of electrons with energy 1 keV shown in Figure 1. Normalized electron energy distribution function $f(\epsilon)$ over time shown in Figure 2. Normalized electron energy probability function $f(\epsilon)$ over time shown in Figure 3. Plots for different number of initialized particles that proofs convergence of the solution shown in Figures 4 and 5.
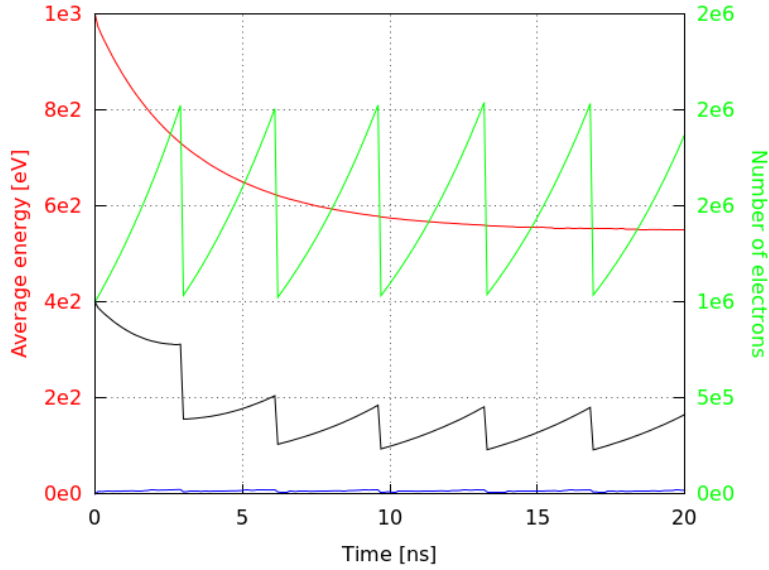

Figure 1: Average electron kinetic energy (red), total number of electrons (green), number of electrons with energy below 10 eV (blue) and number of electrons with energy 1 keV (black).
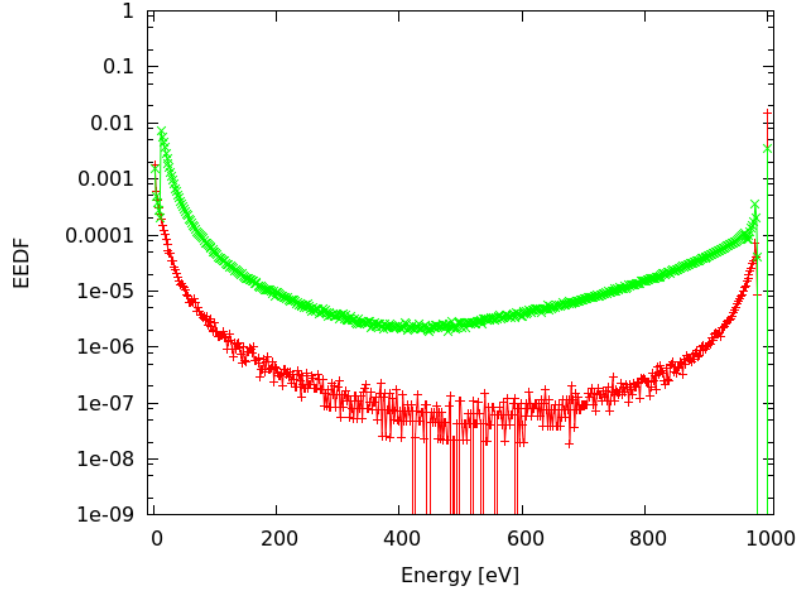
Figure 2: Evolution of normalized *eedf* after first (red) and last (green) time steps.
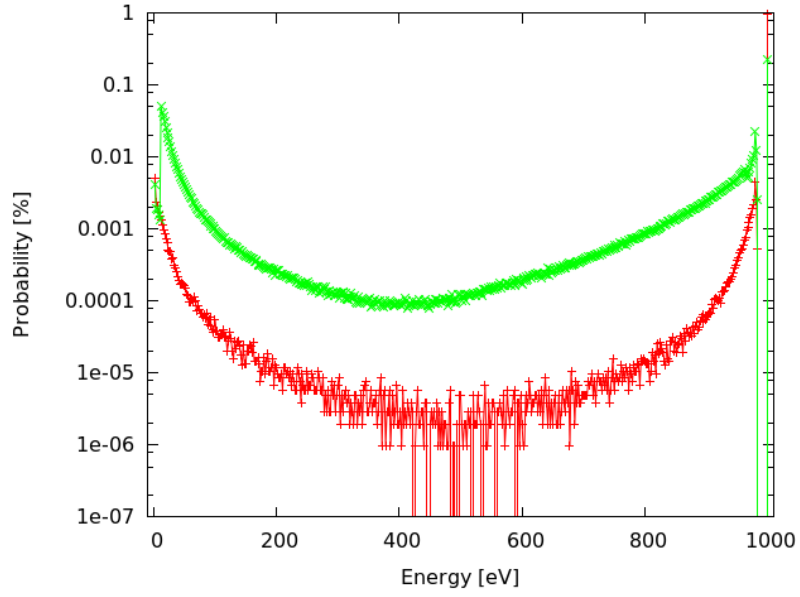

Figure 3: Evolution of the normalized electron probability after first (red) and last (green) time steps. Plot shows distribution of electrons in energy bins in the program.
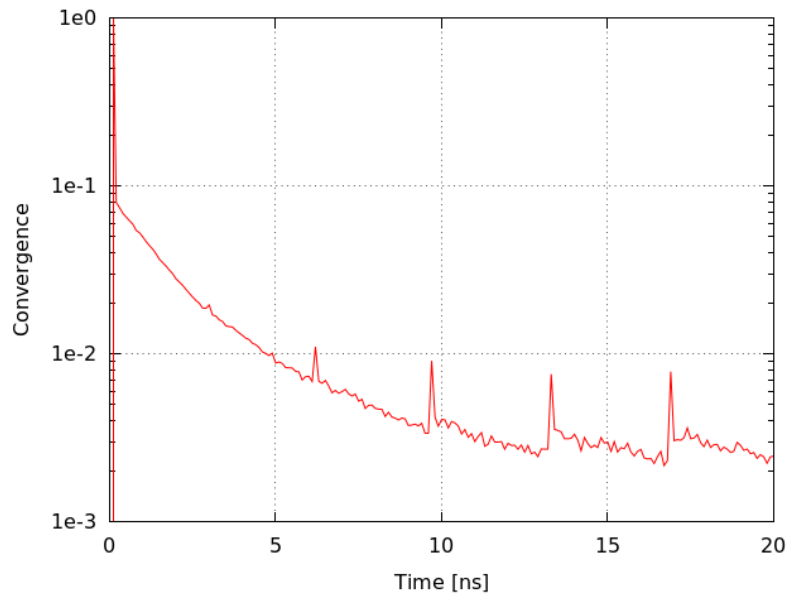
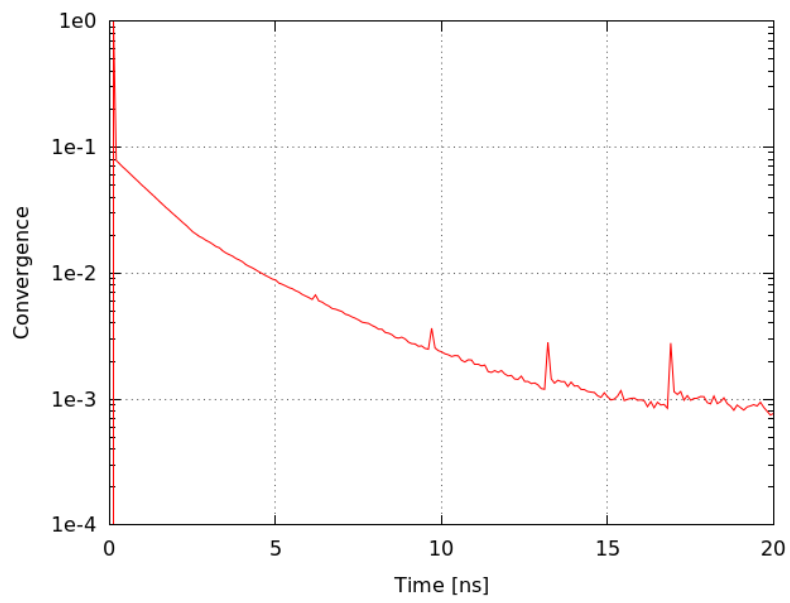Figure 4: Convergence during time for 10^6 particles.

Figure 5: Convergence during time for 10^7 particles.

4

5 Non-stationary case

5.1 Particle initialization function

Particle initialization function $f(t)$ corresponds to number of initialized electrons till corresponding time t. Every time step number of initialized particles is

$$N_{init}^{t} = f(t) - f(t - dt). \tag{5}$$

Derivative of the function $f(t)$ must be non-negative since this feature is not suitable for deletion of particles.

5.2 Input data example for modified program

```
1                    | Simulation mode (0 = stationary, 1 = non-stationary)
1e4+10^20*t^2        | Particle initialization expression (e.g., 10^11*t+1e7)
                       In stationary mode skips time dependent part of expression,
                       initializes only constant (e.g., 1e7)
20e-9                | Time of simulation [s]
                       In stationary mode affects iteration number
.1e-9                | Time step [s]
```
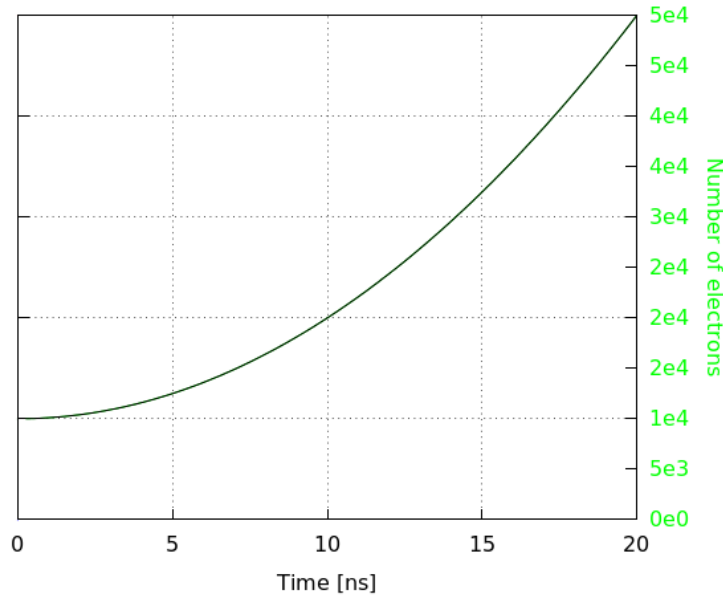
5.3 Results

Figure 6: Total number of electrons. This graph is special case with modified program when collisions doesn't happen, it shows the particle initialization function in work. Note that this plot is the same as expression "$10^4 + 10^{20} \cdot t^2$" in the input data example.

References

[1] Savino Longo. Monte Carlo models of electron and ion transport in non-equilibrium plasmas. 2000.

[2] Tomas Lycken. Monte Carlo Simulation of Electron Beam in Nitrogen. Technical report, 2013.