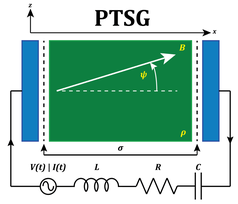
Dynamic evaluation of EEDF with Boltzmann equation solvers in the KGMf*

Janez Krek, Yangyang Fu, John P. Verboncoeur

Michigan State University ({krek,fuyangya,johnv}@msu.edu)

*Work supported by DOE Plasma Science Center grant DE-SC0001939 and MSU Strategic Partnership Grant



Motivation

Global models are widely used to investigate macroscopic parameters in various discharge systems, offering fruitful results with simplicity and high efficiency, while including as many microscopic processes as possible.[1, 2] One common assumption in global models is predefined electron energy distribution function (EEDF), which depends on system variables and might have significant impact on the rate coefficient of electron impact reactions and further on the plasma properties.

The Kinetic Global Model framework (KGMf) is a volume-averaged simulation tool used to explore complicated plasma chemistry in multi-species systems with a goal to find a set of the most influential reactions.[3] The KGMf is currently developed by coupling it with two Boltzmann equation solvers:

- BOLOS[4] (two-term spherical approximation)
- MultiBolt[5] (multi-term spherical approximation)

The KGMf, coupled with Boltzmann equation solver, enables self-consistent evaluation of the EEDF in any given simulation step. A single EEDF evaluation using two-term approximation takes few tens of milliseconds[6], which increases the required computational time in KGMf compared to cases with a fixed EEDF. Implicit integrator in KGMf (`ode` or `bdf` integrators from SciPy library) internally make additional EEDF evaluations when iterating towards solution in the given time step. This adds to total number of calls to EEDF evaluation method.

Dynamic EEDF Evaluation Frequency

- Introduced to lower the total computational time by reducing the number of evaluated EEDFs
- Can be defined in terms of number of integrator steps between EEDF evaluations (Δn) or changes of system variables, such as reduced electric field ($\Delta E/N$), or electron temperature (ΔT_e).
- The condition is defined as, for example for T_e and $\Delta T_{e,thr}$:

$$\frac{|T_e - T_{e,eval}|}{T_{e,eval}} > \Delta T_{e,thr} \tag{1}$$

where T_e is the electron temperature at current time, $T_{e,eval}$ is the electron temperature at last evaluation and $\Delta T_{e,thr}$ is given threshold of temperature, given as input parameter (e.g 0.1 for 10%, 0.4 for 40%).

When the condition is satisfied, the EEDF is evaluated using a coupled Boltzmann equation solver and the updated EEDF is used until the next evaluation.

Results

- The KGMf with coupled Boltzmann equation solver, BOLOS and MultiBolt, was used in a case of high pressure argon gas.
- The electron temperature T_e and the electron density n_e dependence on different EEDF evaluation frequencies was investigated.
- The EEDF evaluation frequency was only dependent on the relative change of the electron temperature ($\Delta T_{e,thr}$), other parameters were kept the same.
- The KGMf simulation parameters were the following: $P_{abs} = 1000$ [W/cm^3], $p = 760$ Torr, $V = 1$ cm^3, $T_g = 300$ K, $t_{end} = 1$ μs.

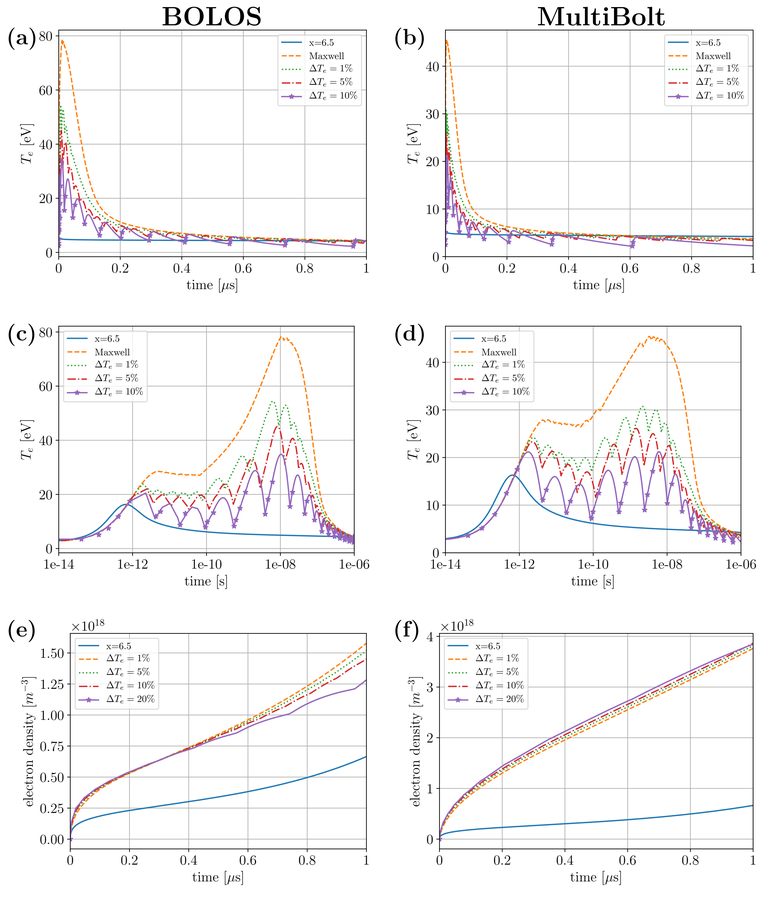


Figure 1: Change of electron temperature and densities using different EEDF evaluation frequencies from BOLOS (left column) and from MultiBolt (right column) with EEDF evaluated on changes of electron temperature T_e.

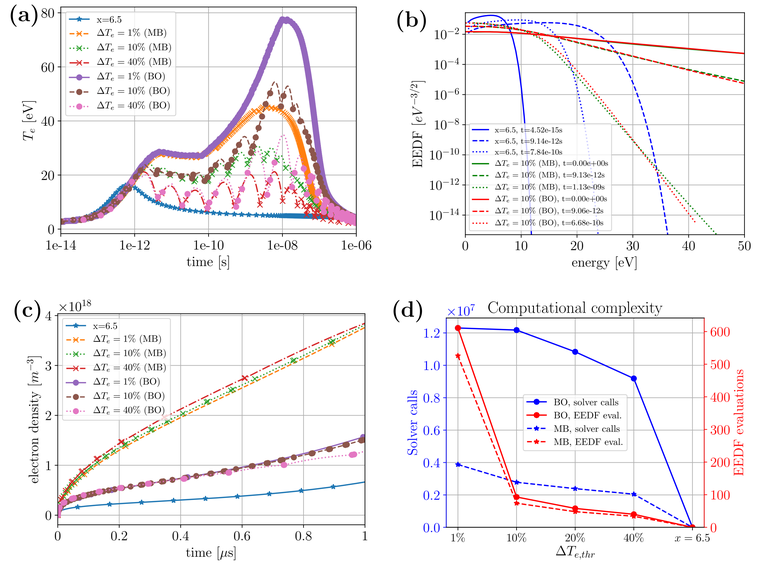


Figure 2: Results comparison for BOLOS (BO) and MultiBolt (MB): electron temperature (a), EEDFs at different times during the simulation (b), electron density (c), and number of solver calls and EEDF evaluations (f) with EEDF evaluated on changes of electron temperature $T_e = \{1, 5, 10, 20, 40\}$%.

Conclusions

- EEDF shows dramatical evolution in early transition regime which result in different electron densities
- comparison between 2- and 8-term approximations (BOLOS and MultiBolt, respectively) show different electron density, but T_e in the same
- total integration time heavily depend on EEDF solver implementation (single- vs. multi-core execution)
- implementation of the dynamic EEDF evaluation frequency is indispensable to preserve the computational advantage of a global model while keeping the results physically accurate

References

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