Optimization of Null Collision Method in Monte Carlo Model

H Akashi(*), K Mizuno, T Yoshinaga

Departmetn of Applied Physics, National Defense Academy, Yokosuka 239-8686 Japan

(*) akashi@nda.ac.jp

Monte Carlo techniques have been developed by many researchers and acknowledged as one of the most useful and exact techniques in simulation methods. A major modification has been done by Skullerud in 1968[1], and introduced so call Null Collison method. Null Collision method decreases computational time significantly, but there is a problem of stochastic choice of free time. To determine the free time τ (=-$\nu^{-1}\ln\xi$, ξ: random number), large enough collision frequency(ν) should be chosen (guess work). Otheriwse a new ν should be chosen again until the condition is satisfied. In 1977, Lin and Bardsley[2] proposed the way to avoid the stochastic choice of free time. They introduced the concept of Null Collision Cross Section, which is no momentum transfer. In present time, many researchers calculating electron properties or other electron-neutral gas collisions using $\nu_{max}=N\{Q_{Real}(\varepsilon_{max})+ Q_{Null}(\varepsilon_{max})\}v=Const.(\gg NQ_{Real}(\varepsilon_{max})\, v)$ to determine the free time. If the ε_{max} is set to several hundreds of eV, almost over all electric field values are covered. This idea simplied the algorithm of Null Collision method. Brennan[3] proposed optimized Null Collision method, but only at low E/N region, and still has a slightly stochastic choice occurence. Recently, Nanbu[4], Horie et al[5] have made minor modification for Null Collision method, but these modifications have been applied on collision determinations or after this procedrues. Since Skullerud had proposed Null Collision method, rarely researchers have mentioned about CPU time. In the present paper, propose a new determination way of free time τ in Null Collision method, and have compared the CPU time to calculate the swarm parameters of severl gases, such as He, Ar, and so on. Fig.1 shows total collision frequency of He, and red line shows proposed method of $\nu_{max}(\varepsilon)$ and green line shows ν_{max} for Lin and Bardley's method. Electron enrgy assumes to vary 10^{-3}~10^{3} [eV], which means wide range electric field could be applied. In He gas, inelastic collision start from 19.5 [eV]. So assuming an electron accelerates from 10^{-3}eV till threshold of metastable state, change of collision frequnecy is less than 10^{2}. And in computer language FORTRAN, single precision real number range is 10^{-38}~10^{38}. Smallest random number ξ would be

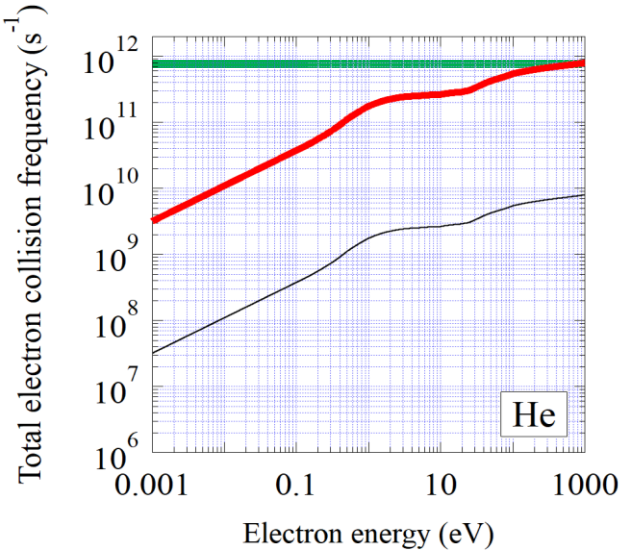

Fig. 1: Proposed total collision frequency used in the present paper for He. Black line: total real collision frequency, Red line: Proposed ν_{max}, Green line: Lin and Bardsley method's ν_{max}

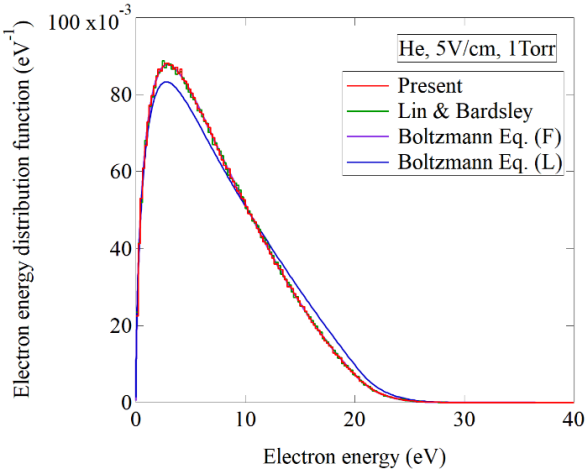

Fig. 2: Electron Energy Distribution Functions in He at E/p_0=5 [V/cm/Torr]

Table 1: Ratio of reduced Computation time (Proposed) / (Lin & Birdsely)

E/p_0 [V/cm/Torr]	He	Ar	N_2	O_2
5	35.7% (2.8)	29.4% (3.4)	21.7% (4.6)	5.4% (18.4)
30	38.5% (2.6)	45.5% (2.2)	35.7% (2.8)	8.2% (12.2)
100	43.5% (2.3)	55.6% (1.8)	50.0% (2.0)	13.5% (7.4)

calculated in 10^{-38} ($\tau=-\nu^{-1}\ln\xi$, $\ln\xi<90$), so $\nu_{max}(\varepsilon)=\nu_{Real}(\varepsilon)$x100 would be large enough to set as a total Null Collision frequency and this conditions are taken into the present calculations. For comparison, Monte Carlo model with Lin and Bardsley's Null Collision method are also calculated with constant ν_{max} ($=\nu_{real}(\varepsilon_{max})$x100) value at $\varepsilon_{max}=10^3$ [eV]. In the case of Ar, O_2, which Q_m values varies significantly in lower energy region, to avoid the stochastic choice of free time, minimum collision frequency $\nu_{min}=10^{10}$ [1/s] is needed to be set. Fig.2 shows the calculated results of Electron Energy Distribution Functions (EEDFs) with results from Boltzmann Equation Analysis. All EEDFs are in good agreement, but the results from 2term expansion Boltzmann Equation Analysis is slightly off. The results of EEDF at other conditions show also in good agreement. Table1 gives Ratio of reduced computational time in Helium and other tested gases. The calculations of swarm parameters have been done in the same conditions in each calculation (initial electron number, E/p_0, simulation time, and so on). The maximum speed up ratio is 18.4 times faster at lower E/p_0 condition in Oxygen. The minimum speed up ratio is 1.8 times faster at higher E/p_0 conditions in Ar. It depends on what kind of collision cross sections using, but proposed method could speed up calculations at least more than 2 times. From the table, it is found that the ratio of reduced computation time is getting higher at low E/p_0 in every gases. As shown in Fig.1, proposed $\nu_{max}(\varepsilon)$ is lower than that of Lin and Bardsley's method in lower energy region, this makes decrease the calculation step of free time until collision. At any E/p_0 computation times become faster than Lin and Bardsley's method, because there are certain number of lower energy electrons, and they consume a lot of computation time. To confirm these speed up in computation time, estimation method have been developed. From the value of product of $\nu_{max}(\varepsilon)$ and EEDF, derive the difference of collision number.The ratio of collision number would relate to ratio of speed up in computation. Fig.3 shows ratio of speed up in computation time. The results show similar tencencies in each gases. So the results of estimation would support the assumption of the proposed method. This method would be helpful to calculate in condition of numerous collisions occurrence, such as atmospheric discharges.

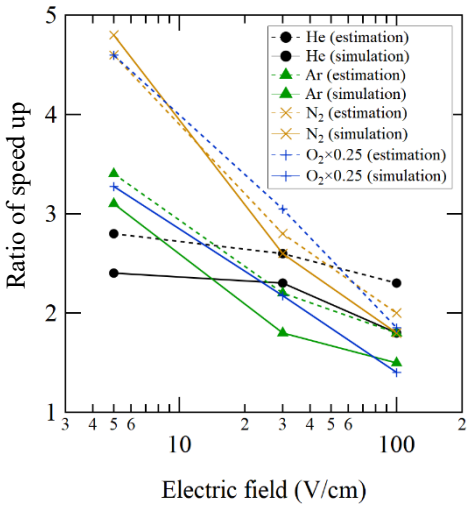

Fig. 3: Ratio of speed up in computation time

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