A dynamic method for charging-up calculations: the case of GEM

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ABSTRACT: The simulation of Micro Pattern Gaseous Detectors (MPGDs) signal response is an important and powerful tool for the design and optimization of such detectors. However, several attempts to exactly simulate the effective gas gain have not been completely successful. Namely, the gain stability over time has not been fully understood. Charging-up of the insulator surfaces have been pointed as one of the responsible for the difference between experimental and Monte Carlo results. This work describes two iterative methods to simulate the charging-up in one MPGD device, the Gas Electron Multiplier (GEM). The first method, which uses a constant step size for avalanches time evolution, is very detailed but slow to compute. The second method instead uses a dynamic step-size that improves the computing time. Good agreement between both methods was achieved. Comparison with experimental results shows that charging-up plays an important role in detectors operation, explaining the time evolution of the gain. However it doesn’t seem to be the only responsible for the difference between measurements and Monte Carlo simulations.

KEYWORDS: Avalanche-induced secondary effects; Detector modelling and simulations II (electric fields, charge transport, multiplication and induction, pulse formation, electron emission, etc); Micropattern gaseous detectors (MSGC, GEM, THGEM, RETHGEM, MHSP, MICROPIC, MICROMEGAS, InGrid, etc); Charge transport and multiplication in gas
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1 Introduction

A considerable amount of work has been done over the last few years to improve the simulations of MPGDs. A full understanding of the micro-physics associated with MPGDs operation is vital for the improvement of such detectors, since some of their behaviours are still not completely understood [1–3].

Some studies report that there is a transient period during which the absolute or total gain, $G_{\text{tot}}$, changes, after voltages are applied and the detector irradiated [4, 5]. $G_{\text{tot}}$ ends up stabilizing after minutes or even hours, depending on the MPGD and the rates of irradiation.

MPGDs were developed to detect radiation, and their main applications are for high energy physics, astrophysics, rare-event searches and medical imaging [6, 7]. The Gas Electron Multiplier (GEM) [8] has been largely used in many of those applications.

The device consists of a thin polyimide (insulator) foil typically 50 $\mu$m thick. The foil is covered on both sides with 5 $\mu$m thick layers of a conductor and etched with an hexagonal pattern of holes. The device operates inside a gas medium and suitable electric potentials are applied between the upper and the lower electrodes of the structure. In this way, a very high electric field is created inside the holes. Electrons created in the drift region by interaction of external radiation, travel...
towards the micro-structure, being focused into the holes and accelerated. They acquire enough energy to ionize atoms/molecules of the gas, creating new ionization. The secondary electrons undergo the same process while inside the hole and a Townsend avalanche is generated.

Neglecting the recombination and attachment processes in the gas, the charges produced during multiplication have two possible destinations: they may be collected by conductor electrodes, both those of the GEM itself or of any other readout setup; or a fraction of them may accumulate in the insulator surfaces. The electronic affinity of the polyimide usually used in these devices is high (1.4 eV [9]). Once electrons are trapped, it is unlikely that they are able to leave the surface. According to [10], the same process happens with positive charges. Simulations considering this process have been done previously, in order to try to reproduce the electron transparency of GEMs [11].

Along this work, we define the effective gain, \( G_{\text{eff}} \), as the number of secondary electrons, for each primary electron, that are collected in an electrode plane located below the GEM, as shown in figure 1b. \( G_{\text{tot}} \) (and also \( G_{\text{eff}} \)) strongly depends on the intensity of the electric field produced in the multiplication region. Charges deposited in the insulator surfaces change locally the electric field, thus modifying the gas gain. This is known as the charging-up effect.

Deposited charges can flow through the insulator surface and insulator bulk under the action of the electric field. Previous studies propose that the positive ions are not captured in insulators surfaces, instead they transfer their charge to intrinsic carriers of the insulator, and the conduction is made by electrons and holes [10]. The time for charges evacuation is of the order of several hours to days, so we did not include this effect in our method, i.e. all deposited charges are considered to remain in the same surface during the whole simulation time. This approach is valid if the charging-up process is much faster than the draining of charges.

In order to study the contribution of the charging-up for \( G_{\text{tot}} \) variations, two methods to simulate the charge accumulation in the detector are presented. We also compare our results with available experimental data.

2 Dimensions and gas parameters

2.1 Geometry

The accumulation of charges in the insulator surface is dependent of the geometry of the GEM. During the simulations, the most common configuration of a single GEM with an hexagonal hole pattern and a pitch of 140 µm was considered. The insulator thickness is 50 µm and the metal electrodes are 5 µm thick. Figure 1a shows the GEM geometry. The corresponding electric field configuration (drift and induction field) is depicted in figure 1b. The holes have a bi-conical shape, the outer diameter is 70 µm, while the narrower part is 50 µm in diameter.

The drift and induction fields (electric fields applied below and above the GEM, respectively) were 0.2 and 0.3 kVcm\(^{-1}\). Taking into account that the computational time strongly depends on \( G_{\text{tot}} \), because a higher number of electrons need to be tracked within the avalanche, a potential of 400 V between electrodes was used for the first simulation test, corresponding to \( G_{\text{tot}} \sim 10^2 \).
2.2 Gas

In order to compare simulation results with our measurements, we simulated a gas mixture of Ar 70% / CO₂ 30%. This is a penning-mixture, due to the presence of the quencher molecule CO₂. Excited argon atoms have energy above the ionization threshold of the quencher molecule, and thus the excitation energy of the argon atom can be transferred to the CO₂ molecule, ionizing it. We used a Penning probability of 0.7 in this simulations based on previous calculations for Ar 70% / CO₂ 30% mixture [2, 12–14].

All simulations were performed considering a temperature of 293 K and a pressure of 760 Torr.

3 Simulation details

3.1 Software platforms

The Monte Carlo calculations involved three programs. Due to the complex shape of the GEM structure, an analytic solution for the electric field cannot be found. To overcome this problem, the electric field is computed with Finite Element Methods (FEM) software, that is used to calculate the electric potential in discrete nodes of a mesh, using boundary conditions. We used ANSYS® to produce potential maps (called generally as field maps), selecting the curved tetrahedral elements as the mesh elements, because they easily fit in sharp curved surfaces present in GEMs.

To simulate the drift and transport properties of electrons and ions in the MPGD gas medium, we used Garfield++ [15]. As input, this software requires the electric field configuration in the MPGD, the gas mixture, temperature, pressure and initial conditions of the primary charges (position and velocity).

The program can read the field maps calculated with ANSYS® and calculate the electric field in any point of the space by interpolation.

A microscopic approach is used to simulate the drift of the charges. This uses Monte-Carlo methods to calculate the probability to occur each type of collision during the drift (elastic, ex-
citation or ionization). The cross sections associated with each collision type are obtained from Magboltz \cite{16, 17}.

Primary electrons start with assigned position $\vec{r}_{\text{start}} = (x_s, y_s, z_s)$ and velocity $\vec{v}_{\text{start}} = (v_{x,s}, v_{y,s}, v_{z,s})$ (generally zero velocity is considered for primary electrons resulting from ionizations), drifting through the gas and producing secondary charges as they pass through the multiplication region. The final position of each secondary charge, $\vec{r}_{\text{end}} = (x_e, y_e, z_e)$ and $G_{\text{tot}}$, are the observables of interest that are recorded for further analysis of the charging-up effect.

### 3.2 Preliminary study

To start our simulations, we randomly distributed $10^4$ primary electrons in the surface of a plane parallel to the GEM, located 100 $\mu$m above the GEM, indicated as the start plane in figure 1a.

In order to determine the number of collected and deposited electrons and ions, the final positions of each electron and ion are analysed:

- Electrons are collected if $z_e < -25 \, \mu$m
- Ions are collected if $z_e > 25 \, \mu$m
- Electrons and ions are deposited in the insulator surface if after the drift $-25 \, \mu$m $\geq z_e \geq 25 \, \mu$m

During the simulation process, to distinguish the situation before and after charging-up, GEMs that have not yet undergone the charging-up effect, i.e. without deposited charges, are called uncharged GEMs. On the contrary, the charged GEMs are those who have already deposited charges in the insulator surfaces.

The deposition distributions of charges (electrons and ions separately) in the insulator, for the uncharged GEM (figure 2a), shows that the charges are not deposited uniformly on the hole surface. In addition, the number of deposited electrons is higher than the number of deposited ions. The diffusion of electrons and ions in gases is different, and since ions are heavier than electrons, they tend to follow the field lines, in the direction of the electrodes. Electrons have a larger diffusion, due to their smaller mass, usually having more probability of ending in the insulator surfaces.

After some avalanches, the distribution of new electrons and ions that reach the insulator tend to compensate each other, due to Coulomb attraction between previously and the new deposited charges (figure 2b). The local variation in the electric field will therefore vanish and a stable configuration is achieved.

In order to simulate the variation of $G_{\text{tot}}$ as avalanches happen, we needed to iteratively include this charge deposition in the field maps computed with ANSYS®. The software does not provide the option to introduce single charges in their exact deposition position in the insulator surface. In addition, this scenario would lead to discontinuities and numerical issues. Instead, we created small slice surfaces in the insulator foil and add the correspondent charge density to each surface. Due to the shape of the deposition, and to computational limitations, we used 24 different slices in the insulator, achieving in this way a good balance between the details of the calculations and the needed computing power. The slices are not regularly distributed, as shown in figure 3, but we try to match the $z$ profile of the charge deposition histograms (figure 2a).
Figure 2. Spatial distribution of charges deposited in the insulator surface of the GEM, before (2a) and after (2b) simulation of some primary avalanches, at $V_{\text{GEM}} = 400$ V.

Figure 3. Unity cell of a GEM, used to calculate the field maps with ANSYS®. 24 slices of different sizes were non regularly distributed due to the charge deposition non uniformity in the insulator surface, shown in figure 2a.

### 3.3 Constant step method

The flow-chart of the first iterative algorithm used to simulate charging-up iterations is depicted in figure 4.

At the first iteration, we compute the electric field map assuming no charges in the insulator surface. Then, we import that field map into Garfield++, simulate a constant step $S_{\text{cons}} = 10^4$ primary avalanches and determine the density charge deposited in each insulator slice surface. A new field map is created, with the contribution of previously deposited charges. The density charge in each slice is calculated taking into account the contribution of both the ions and the electrons ending up in the insulator surface. A new set of $S_{\text{cons}}$ primary avalanches is simulated and the process is repeated iteratively.

It was found that statistical fluctuations in $G_{\text{tot}}$ depends on the number of simulated avalanches per iteration, but the number of deposited charges per avalanche, $D$, exhibits less fluctuations. $S_{\text{cons}}$
= $10^4$ primary electrons was chosen in order to obtain good detail in the time evolution of charging-up. However, this small step implies hundreds of iterations until $G_{tot}$ stabilization, which lead to a very heavy computation.

Since $D$ is the responsible for the local variation in the electric field, we use that observable as our control function for the iterative simulation, i.e. we stop our iterations when function $D$ stabilizes over iterations (corresponding also to $G_{tot}$ stabilization).

### 3.4 Dynamic step method

In order to accelerate the simulation process, we developed an extended method that uses a dynamic step-size, $S_{din}$ (equivalent to $S_{cons}$ in the constant method), in each iteration. $S_{din}$ is the number of simulated primary avalanches, per iteration, being smaller when $D$ changes quickly, i.e., the rate of deposited charges is changing fast, and larger when this quantity is more constant, i.e. the deposition stabilizes. It is important that, for the initial iterations, a small value of $S_{din}$ is used ($\sim 10^4$), for better agreement with the initial behaviour $D$.

To constrain the size of $S_{din}$, we defined that the maximum total charge (considering that ions and electrons contributions cancel out) that can be added to the new field map should be included in the method. The charge that can be added to field maps without significant changes in the electric field depends on the local electric field created by the applied potential to the GEM. Therefore, for different values of $V_{GEM}$, this maximum total charge can be different.

The dynamic method is briefly described in the flow-chart in figure 5.

In the first 5 iterations, the dynamic method is calculated like the constant method. It starts with an uncharged field map of the GEM. Again, in each iteration, we import the field map into Garfield++, simulating, in each iteration, $\sim 10^4$ primary avalanches, which is a good compromise between statistical fluctuations and computational time, and corresponds to the first 5 values of $S_{din}$.

After the first 5 iterations, we apply the algorithm described in figure 5.
1. We first simulate iteration number 6 to get $D_{\text{simu}}$ and the gain, using Garfield++ and the previous Ansys field map.

2. We fit the evolution of $D$ with a first order polynomial, called $F$, as we can see in figure 6b. Then we calculate $D_{\text{fit}}$ for iteration number 6 evaluating the polynomial $F$ at the number of previous simulated avalanches (corresponding to the sum of the previous 5 iterations values of $S_{\text{din}}$) plus the current value of $S_{\text{din}}$, as we can see in equation (3.1).

$$D_{\text{fit}} = F \left( \sum_{\text{iter}=1}^{5} S_{\text{din}}^{\text{iter}} + S_{\text{din}}^{6} \right)$$ (3.1)

3. The algorithm finally compare $D_{\text{simu}}$ with $D_{\text{fit}}$.

For $V_{\text{GEM}} = 400$ V, we defined that $|D_{\text{fit}} - D_{\text{simu}}| \times S_{\text{din}}$ (which corresponds to the difference amount of charge between fitted and simulated calculations, that will be added to the new field map) should not be larger than $C_{\text{lim}} = 2 \times 10^6 \times q_e$, (where $q_e$ is the electron charge). $C_{\text{lim}}$ represents the maximum difference of charges that can be accepted between $D_{\text{fit}}$ and $D_{\text{simu}}$.

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**Figure 5.** Dynamic step method diagram.
$D_{\text{simu}}$, after $S_{\text{din}}$ avalanches. It is an empirical value, based on various attempts, but other values can be used. This assumption ensures that the method does not diverge, due to the introduction of unrealistic changes in the electric field of the new field maps, corresponding to a limitation to the total charge that is added in each new field map.

- If $|D_{\text{fit}} - D_{\text{simu}}| \times S_{\text{din}} > C_{\text{lim}}$, discard the iteration, $S_{\text{din}}$ is reduced to its half, and the iteration number 6 is repeated.
- If $|D_{\text{fit}}D_{\text{simu}}| \times S_{\text{din}} < C_{\text{lim}}$, the iteration is saved, we increase $S_{\text{din}}$ to the double. A new iteration is calculated and the new fit considers only the last 5 valid values of $D$, where the last $D_{\text{simu}}$ is now included in $D$ and $S_{\text{din}}$ is added to the simulated avalanches.

We can see, in figure 6b, that the value of $S_{\text{din}}$ is smaller ($\sim 10^4$) in the first iterations (where $D$ is changing quickly), and became larger ($\sim 10^6$) when the value of $D$ is more stable.

The density charge that is added to each new field map is calculated multiplying the last value of $D_{\text{simu}}$ by the value of $S_{\text{din}}$ used to calculate it. Since $D_{\text{simu}}$ is the number of deposited charges per hole per avalanche, and $S_{\text{din}}$ is the number of simulated avalanches, the result of this multiplication is the number of deposited charges per hole for each iteration.

4 Results

4.1 Comparison between methods

The behaviour of $D$ (the sum of the deposition histograms in figures 2a and 2b), is shown in figures 6a for both methods, as function of the number of avalanches per hole. In figure 6b, we can see in detail the earlier iterations of the dynamic method applied to the calculation of $D$. In particular, the fit applied to the initial 5 iterations is shown.

The agreement between both methods is clear. However, the dynamic step method saves computational resources, using about one tenth of iterations, in the present case.

Figure 7 represents $G_{\text{tot}}$ evolution for the two proposed methods. We observe an increase in $G_{\text{tot}}$, followed by a stabilization plateau, reached in both methods. Due to the previous results, from now on we will only consider the dynamic step method for calculations.

4.2 Charging-up effect in the GEM transmission

Primary electrons produced by incident radiation and drifting towards the GEM holes can be collected in the top electrodes, ending up not producing avalanches. The ratio between the number of primary electrons that enter the holes, producing avalanches and the total number of primary electrons simulated is defined as the electron transmission, shown in figure 8a, for several voltages applied to the GEM electrodes.

The contribution of the charging-up effect in the electron transmission is more important when low voltages ($< 400$ V) are used and negligible when higher electrical potentials are used.

4.3 $G_{\text{eff}}$ with and without charging-up

The dependence of $G_{\text{eff}}$ (the number of secondary electrons collected, for each primary electron) on the voltage applied between electrodes in the GEM detector, is shown in figure 8b. $G_{\text{eff}}$, after charging-up stabilization, is 10–15% higher than the situation without charging-up.
Figure 6. a) Evolution of $D$ for both constant and dynamic methods. b) Detail of the earlier iterations of figure 6a, for the dynamic step method, with representation of the first fit used in the algorithm. Both plots obtained for $V_{GEM} = 400$ V.

Figure 7. Comparison of the $G_{TOT}$, between the constant and dynamic method. Calculated for $V_{GEM} = 400$ V.

4.4 Electric field intensity variation

A 2D representation of the electric field in the GEM hole is shown in figure 9. Each plot is obtained from the calculation of the intensity of the electric field along a plane corresponding to a vertical cross section of the GEM hole, at four different stages of the charging-up process.

We can observe that the biggest change in the electric field occurs near the electrodes. While the intensity of the electric field near the top (negative polarized) electrode decreases, it increases near the center of the hole and the bottom (positive polarized) electrode. The development of an
avalanche inside the hole follows a nearly exponential model. The bigger fraction of secondary
electrons is produced at the exit of the hole, in the last stages of the avalanches. There, the electric
field is higher due to the charging-up effect, and thus, $G_{\text{eff}}$ increases as a result of this process.

4.5 Comparison with experimental results

Experimental measurements were performed at CERN. A single GEM was used. The physical
parameters of the GEM, and the gas mixture used for measurements, corresponds to the simulation
settings described in the section 2.

X-ray photons were used as ionizing radiation, irradiating the detector perpendicularly to the
GEM plane. The use of a collimator (1 mm diameter) allowed to control the photon flux and
regulate the rate of charging up. The GEM structure was housed inside an gas-tight chamber with a
constant gas flowing, and high voltage was applied across the GEM top and bottom electrodes and
to the drift plane, maintaining the readout strips located below the GEM plane at ground potential.

The chamber pressure was maintained at 760 Torr. To calibrate the gain, using the pulse mode,
the rate of primary electrons produced per GEM hole, $N_{\text{pe/hole}}$, was estimated knowing the X-ray
rate, the surface exposed by the collimator and the average of primary electrons produced by each
absorbed X-ray photon. This average, for Ar 70% / CO$_2$ 30%, was estimated analysing the MCA
spectrum, calibrating in pulse mode. The fitting of the photoelectric and escape peaks allows the
calibration of energies of individual channels. Weighting the number of electrons of each individual
channel by its energy, we can estimate the average of primary electrons, per incident photon, from:

$$\sum_i \left( \frac{N_i}{\sum N_i} \times \frac{E_i}{W} \right) \sim 280$$  \hspace{1cm} (4.1)

where $N_i$ is the number of counts and $E_i$ is the energy corresponding to channel $i$ of MCA and
$W$ is the work function of the Ar 70% / CO$_2$ 30% mixture, considering penning transfers, ($W=$
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Figure 9. Evolution of the intensity of the electric field, in a GEM cross section. Computed with ANSYS®. The colorbar refers to the 10-based logarithm of $E$. Only intensities above $40 \text{kV cm}^{-1}$ are colored ($\log_{10} \left(40 \times 10^{3}\right) \sim 4.6$).

26.9 eV [18]), and an average of 280 primary electrons per absorbed X-ray was calculated. $G_{\text{tot}}$ was then measured over the time, in current mode, for a constant irradiation flux. For a more detailed description of the measurement procedure refer to [19].

In order to compare with simulations, the experimental results were translated from the time scale to a charge scale. We experimentally estimate $N_{\text{pe}}/\text{hole}$ and $G_{\text{tot}}$. The value of $N_{\text{pe}}/\text{hole}$ can then be calculated as:

$$N_{\text{pe}}/\text{hole} = 280 \times \frac{r \times t}{S \times \sigma_{\text{holes}}} \quad (4.2)$$

where $r$ is the X-ray absorption rate, $t$ is the time of measurement, $S$ is the collimated surface and $\sigma_{\text{holes}}$ is the surface density of holes. To calculate the total charge available (per hole) for
charging-up, $N_{\text{charge/hole}}$:

$$N_{\text{charge/hole}} = N_{\text{pe/hole}} \times G_{\text{tot}} \times q_e$$  \hspace{1cm} (4.3)

Instead of using the charge scale in $N_{\text{pe/hole}}$ as in figure 6a, we use in $N_{\text{charge/hole}}$ due to the mismatch of the simulated and experimental $G_{\text{tot}}$. Since the gains are different, the same number of $N_{\text{pe/hole}}$ do not correspond to the same $N_{\text{charge/hole}}$. The comparison between experimental and simulated $G_{\text{tot}}$ is shown in figure 10a.

![Figure 10. a) $G_{\text{tot}}$ comparison between measurements (blue squares) and simulated (red triangles) results. Same situation as figure 7 but with $V_{\text{GEM}}$=380 V. b) Same plot as figure 10a but with $G_{\text{tot}}$ normalized. Experimental data taken by Mythra Varun Nemallapudi at RD51 facilities, described in the section 4.5.](image)

Since $G_{\text{tot}}$ doesn’t match between experimental and Monte Carlo calculations, we normalize it, in both cases, to the average value after 0.2 nC (considering the average normalized total gain $\sim 1$ in the plateau region, for simulated and experimental data), as shown in figure 10b. The Monte Carlo reproduces the functional evolution of $G_{\text{tot}}$.

The mismatch between simulated and experimental $G_{\text{tot}}$ may be explained by several factors:

- **Mobility of the charges**, in the insulator surfaces and bulk, not considered in the simulations, is responsible for draining deposited charges, changing the electric field;

- **FEM discontinuities** resulting in numerical issues and wrong calculations of the electric field. Other software tools, like neBEM [20], are being developed and can be used in the near future, to reduce this issues.

- **Electronegative impurities** (not considered in simulations) in the gas may trap charges through attachment processes.

- **Fabrication imperfections** may be introduced in the shape of the electrodes and holes of the GEM, having strong impact in the electric field and experimental results.
5 Conclusion and future work

In this work we have developed two iterative methods for the simulation of the insulator surface charging-up in GEMs, allowing a better understanding of their response.

Both methods agree between each other. However, the dynamic step method saves computational resources. The Monte Carlo functional time behaviour of the gain as the GEM is irradiated reproduces the measured one. However, the absolute scale still does not agree.

Primary electrons transmission is affected by the charging-up at lower voltages, but for higher voltages, used in regular applications, it does not play an important role.

Future work will include the application of the presented charging-up simulation methods to other MPGDs (THGEM) and the study of new geometries and detectors that could take advantages of this effect or minimize it.

The simulation of the mobility of deposited charges in the insulator surfaces and bulk can contribute to obtain more precise values. The use of other software tools for electric field calculations, like neBEM, can also be important to get agreement between simulated and measured gain values.

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