

# Development of a simulation for measuring neutron electric dipole moment

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**Abstract.** The neutron electric dipole moment (nEDM) is sensitive to new physics beyond the standard model and could prove to be a new source of CP violation. Several experiments are being planned worldwide for its high-precision measurement. The nEDM is measured as the ultracold neutron (UCN) spin precession in a storage bottle under homogeneous electric and magnetic fields. In nEDM measurement, the systematic uncertainties are due to the motion of the UCNs, the geometry of the measurement system, and inhomogeneous electric and magnetic fields. Therefore, it is essential to quantitatively understand these effects in order to reduce them. Geant4UCN is an ideal simulation framework because it can compute the UCN trajectory, evaluate the time evolution of the spin precession due to arbitrary electric and magnetic fields, and define the storage geometry flexibly. We checked how accurately Geant4UCN can calculate the spin precession. We found that because of rounding errors, it cannot simulate it accurately enough for nEDM experiments, assuming homogeneous electric and magnetic fields with strengths of 10 kV/cm and 1  $\mu$ T, respectively, and 100 s of storage. In this paper, we report on its discrepancies and describe a solution.

## 1. Introduction

The neutron intrinsic electric dipole moment (nEDM) is sensitive to new physics beyond the standard model (BSM). CP violation, which is equivalent to the violation of invariance under charge conjugation and parity transformations, introduces T violation through the CPT invariance theorem. The existence of an EDM violates T symmetry; therefore, measuring the intrinsic nEDM can allow us to effectively probe the CP violation source. The nEDM in the standard model can arise through second-order  $W$  exchange interactions, whereas those in several BSM theories result from first-order interactions[1]. The standard model predicts an nEDM of  $10^{-31}$  e-cm, which current experimental techniques cannot detect. On the other hand, several BSM models predict a much larger CP violation, which can be close to the experimental bound. For example, supersymmetry (SUSY) predicts the existence of an nEDM from  $10^{-27}$  to  $10^{-28}$  e-cm, whereas the most precise measurement of the nEDM to date yielded  $(0.2 \pm 1.5 \text{ (stat)}) \pm$

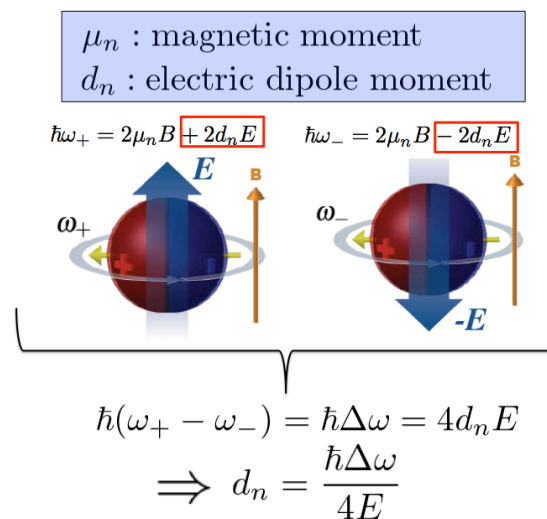


$0.7 \text{ (syst)} \times 10^{-26} \text{ e}\cdot\text{cm}$ [2]. Therefore, by improving the precision of the nEDM by one or two orders of magnitude, we could achieve the range predicted by SUSY.

Ultracold neutrons (UCNs), which are cooled to less than about 300 neV, have the property of being reflected at any angle from material surfaces. The nEDM can be calculated accurately by measuring the spin precession of UCNs stored in a material container. The procedure is described briefly as follows:

- (i) Polarized UCNs are stored in a container in which steady magnetic and electric fields are applied parallel to each other.
- (ii) The spin states, analyzed by the Ramsey method of separated oscillatory fields[1], are measured after a certain time for precession.
- (iii) Repeat (i) and (ii) with an electric field antiparallel to the magnetic field.
- (iv) If an nEDM exists, the spin precession frequency will vary according to whether the electric field is parallel or antiparallel to the magnetic field (see Figure 1). Thus, by subtraction, we extract the nEDM. Ideally, the magnetic field averaged by the UCN must remain constant.

Then, if any process except for the nEDM changing the magnetic field seen by the UCN exists and is not canceled, it causes a systematic uncertainty.



**Figure 1.** Principle of nEDM measurement

A relativistic magnetic field that occurs when a UCN passes through an electric field causes various systematic uncertainties. The relativistic magnetic field due to a net rotation in conjunction with a radial electric field component results in a spin precession frequency shift[2]. Similarly, the relativistic magnetic field connected with a longitudinal magnetic field gradient  $\partial B_z / \partial z$  in a cylindrical trapping material can produce a similar effect[3]. These systematic uncertainties are enhanced when the UCNs are in certain ordered motions; therefore, it is worth studying the mechanism by which ordered UCN motion is diffused. For example, diffuse scattering that occurs when UCNs are reflected at a sidewall strongly inhibits their conservation. Further, a storage cell with a certain geometry is expected to reduce their motion: a cylindrical geometry consisting of a wavy plane should reduce the rotational motion more effectively than

a perfect plane does. Simulation studies are essential to quantitatively understand these effects because they are related to so many factors.

Although there are several simulation toolkits, Geant4UCN[4], based on the Geant4 simulation framework, is particularly good at defining the geometric configuration. For example, an arbitrary geometry can be extracted from CAD data. In addition, it is useful because Geant4 is widely used in particle physics experiments. In those simulations, the trajectory and spin precession are calculated by the Runge–Kutta and adaptive step size methods. We can quantitatively evaluate the suppression of systematic uncertainties by implementing a geometric configuration, a theoretical model for non-specular reflection, and electric and magnetic field distributions in Geant4UCN.

As for other simulations, the two following examples should be shown. The first example is the MATLAB-based simulation used in [5], in which the trajectory is evaluated using the numerical solver for the ordinary differential equation. The reflection points in the geometric configuration are stored from either Geant4UCN or a simple analytic calculation, and the spin precession is computed using the Bloch equation along its trajectory. Another example is the MCUCN used by the PSI collaboration, which is described in reference [6]. In that simulation, the trajectory and spin precession are calculated by a method similar to the calculation in Geant4. By incorporating the geometric configuration into the MCUCN, they calculate the spin tracking.

A Geant4UCN simulation is necessary to calculate a phase of neutron spin with better precision than  $6 \times 10^{-7}$  rad. This is because the nEDM experiments aim for a precision of  $10^{-28}$  e-cm, which corresponds to a  $6 \times 10^{-7}$  rad phase shift from spin precession after 100 s of storage. We checked how accurately the Geant4UCN can calculate the spin precession assuming homogeneous electric and magnetic fields with strengths of 10 kV/cm and  $1\mu\text{T}$ , respectively, and 100 s of storage. In this paper, we report the results. The paper is organized as follows. In Sec.2, we describe how we implemented relativistic spin precession in Geant4 and why the UCN rotational motion enhances the systematic uncertainty of nEDM experiments. In Sec.3, we describe why Geant4 cannot compute the spin precession accurately enough. Then, we describe how to solve these problems. Next, Sec.4 presents a discussion and our future plan. Finally, we summarize the content.

## 2. Systematic uncertainties associated with UCN rotational motion

As mentioned in Sec.1, several systematic uncertainties are enhanced by certain types of UCN motion. In particular, rotational motion is one of the most interesting situations in simulation studies. Accordingly, in this paper we evaluate the relativistic spin precession phase shift associated with UCN rotation.

In this study, we use Geant4UCN. To compute the relativistic spin precession, we incorporated the equation of motion for spin time evolution, the Bargmann–Michel–Telegdi equation, into Geant4UCN, as follows:

$$\frac{d\vec{s}}{dt} = \vec{s} \times \left[ \left( \frac{g_n}{2} - 1 + \frac{1}{\gamma} \right) \vec{B} - \left( \frac{g_n}{2} - 1 \right) \frac{\gamma}{\gamma + 1} (\vec{\beta} \cdot \vec{B}) \vec{\beta} - \left( \frac{g_n}{2} - \frac{\gamma}{\gamma + 1} \right) \vec{\beta} \times \frac{\vec{E}}{c} \right], \quad (1)$$

where  $\vec{s}$  is the UCN spin vector;  $\vec{E}$  and  $\vec{B}$  are the electric and magnetic fields, respectively;  $g_n$  is the  $g$  factor of the neutrons;  $\beta$  denotes the ratio of the UCN velocity to the speed of light; and  $\gamma$  is  $1/\sqrt{1-\beta^2}$ . Assuming the particle velocity is less than 7 m/s, which corresponds to the typical maximum velocity of UCNs, the first term can be regarded as a non-relativistic effect,

the third term can be considered to be relativistic, and the second term is negligible. Note that Geant4UCN has a new release based on Geant4 ver4.9.6, but in this study we used the older code based on ver4.9.2.

When a UCN rotates with an angular velocity in the plane perpendicular to that in which static electric and magnetic fields are applied, a perturbative rotational relativistic magnetic field occurs in the radial direction. Then, the frequency of the UCN spin precession in the  $x - y$  plane,  $\omega_{xy}$ , becomes the following:

$$\omega_{xy} = \omega_0 + \frac{1}{2} \frac{(\omega_{rel})^2}{(\omega_0 \mp |\omega_r|)}, \quad (2)$$

where  $\omega_0$  is the Larmor frequency of the neutrons, and  $\mp|\omega_r|$  represents the angular velocity of counterclockwise/clockwise rotation. Further,  $\omega_{rel}$  is  $-\gamma_n B_v$ , where  $\gamma_n$  and  $B_v$  correspond to the gyromagnetic ratio of neutrons and the third term of (1), respectively. Actually, because of a transverse magnetic field in the experimental facilities, (2) will vary as  $(\omega_{rel})^2 = (\gamma_n |\vec{B}_v|)^2 \rightarrow (\gamma_n |\vec{B}_v + \vec{B}_T|)^2$ , where  $B_T$  is the transverse magnetic field in the experimental facilities. Then, the phase shift of (2), like  $B_v$ , depends on the electric field direction, and a corresponding systematic uncertainty occurs.

Assuming the nEDM is  $10^{-28}$  e-cm and the electric and magnetic field strengths are 10 kV/cm and 1  $\mu$ T, respectively, the expected corresponding phase shift amounts to  $\frac{4 \times 10^{-28} \text{ e-cm} \times 10 \text{ kV/cm} \times 100 \text{ sec} \times 3 \times 10^8 \text{ m/s}}{200 \text{ MeV} \cdot \text{fm}} \simeq 6 \times 10^{-7}$  rad. Therefore, in an nEDM simulation study, we have to calculate a phase of neutron with better precision than this.

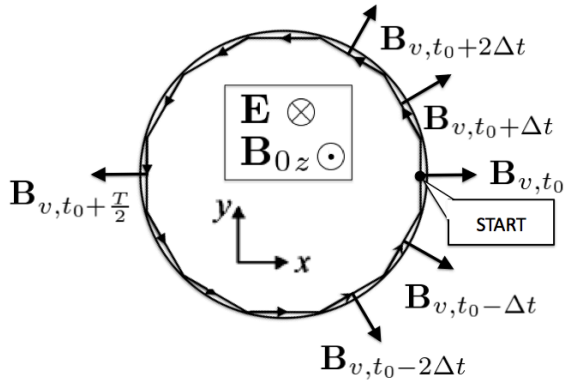
### 3. Test of Geant4UCN

To check whether Geant4UCN simulates UCNs properly, we should compare the analytic solution predicted by (2) with the Geant4UCN simulation result as the UCN rotates in a plane perpendicular to that along which the static electric and magnetic fields are applied. We have done this as follows:

- (i) Neglect the effects of gravity and non-specular reflection so that the UCN can always move in a single plane.
- (ii) Apply static electric and magnetic fields of (0, 0, 1  $\mu$ T) and (0, 0, -10 kV/cm), respectively.
- (iii) Choose a geometry consisting of a cylinder with a 6 cm radius as the simulation geometry. In addition, adopt a coordinate system in which the cylindrical axis lies in the  $z$  direction, which is perpendicular to the plane in which the UCN moves.
- (iv) Throw the UCN from the starting point (5.99 cm, 0, 0), with an initial velocity and unit spin vector of (0, 3 m/s, 0) and (0, 1, 0), respectively. The trajectory that the UCN traces is roughly equivalent to a 54-sided polygon.
- (v) To understand the dependence of the simulation on the step length, perform a simulation study using various initial step lengths: 0.02, 0.03, and 0.04 mm.
- (vi) Compute the phase of the simulation result after a certain time,  $\Phi_{sim}(t)$ , by using the following atan2 function, Four-quadrant inverse tangent:  $\Phi_{sim}(t) = \text{atan2}[\text{spiny}(t), \text{spinx}(t)]$ , where  $\text{spinx}(t)$  and  $\text{spiny}(t)$  denote the UCN spin components in the  $x$  and  $y$  directions, respectively, at a certain time.
- (vii) Compute the phase shift of the analytic solution at a certain time,  $\Phi_{sol}(t)$ , from (2).
- (viii) Evaluate the phase difference between the simulation result and the analytic solution after 0.01 s as follows:  $d\Phi(t) = \Phi_{sim}(t) - \Phi_{sol}(t)$ .

(ix) Repeat procedure (viii) until the simulated time reaches 100 s.

The simulation parameters are listed in Table 1.



**Figure 2.** Schematic view of UCN trajectory trace and time evolution of relativistic magnetic field vector

Rotational Motion	Counterclockwise
Gravity Effect	Neglect
Storage Volume	Cylinder
Cylindrical Radius	6 cm
Cylindrical Axis	(0, 0, 1)
Initial Velocity	(3 m/s, 0, 0)
Electric Field	(0, 0, -10 kV/cm)
Magnetic Field	(0, 0, 1 $\mu$ T)
Starting Position	(0, 5.99 cm, 0)
Initial Unit Spin	(0, 1, 0)
Initial Step Length (mm)	0.02, 0.03, 0.04

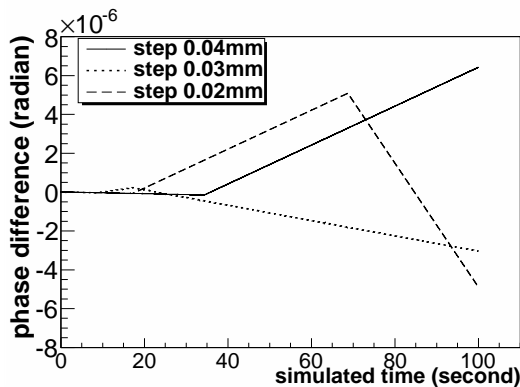
**Table 1.** Profile of simulation study

Figure 2 shows a schematic view of the trajectory the UCN traces in this study. In fact, the UCN traces an  $N$ -sided polygon, not a circle. Its angular velocity therefore varies according to the time, and the relativistic magnetic field differs from the ideal one. However, if the radius is 6 cm and  $N = 54$ , these effects on (2) can be negligible because its phase shift amounts to only  $10^{-10}$ , which corresponds to  $10^{-30}$  e-cm.

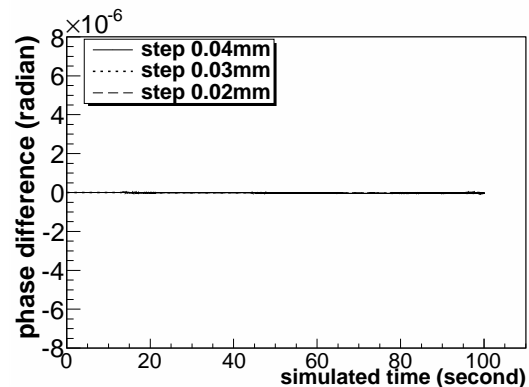
The result obtained from the comparison of the phase differences is shown in Figure 3, where the vertical axis corresponds to the difference between the phase shifts obtained by the simulation and the analytic solution at the simulated time, and the horizontal axis represents the simulated time. The solid, dotted, and broken lines denote the results with minimum step lengths of 0.04, 0.03, and 0.02 mm, respectively. According to Figure 3, the phase differences at 100 s for step sizes of 0.04, 0.03, and 0.02 mm reach about  $6 \times 10^{-6}$ ,  $-2 \times 10^{-6}$ , and  $-4 \times 10^{-6}$  rad, respectively, which correspond to false EDMs of about several  $10^{-28}$  to  $10^{-27}$  e-cm. Considering that nEDM experiments aim to detect values of  $10^{-28}$  e-cm, such a large difference is unacceptable.

We think that the rounding errors of the time variable cause these large differences, because the results shown in Figure 3 actually are not improved even though the step length decreases. In the algorithm using the Runge–Kutta method, a differential time  $\delta t_n$  is calculated as  $\delta s_n / \delta v_n$ , where  $\delta s_n$  and  $\delta v_n$  are the step length and speed, respectively, of the UCN. Thus, if the step length is not divided correctly, a differential step is assigned with an approximate value, namely, the true different time plus a rounding error. These rounding errors accumulate through 100,000,000 steps to the order of 10 ns, which corresponds to several  $10^{-28}$  e-cm. For example, if the time variance due to rounding errors is 10 ns, the resulting false EDM is as follows:  $\omega_0 \times 10^{-8} \text{ s} \times \frac{10^{-28} \text{ e-cm}}{6 \times 10^{-7} \text{ rad}} \sim 3 \times 10^{-28} \text{ e-cm}$ .

We prepared a new simulation that would avoid the rounding errors by extracting the codes relevant to the essential functions and changing the time variable data type from double to long double. The results are shown in Figure 4, where the vertical axis corresponds to the difference between the phase shift obtained by the simulation and the analytic solution at the simulated time, and the horizontal axis represents the simulated time. According to Figure 4, the difference



**Figure 3.** Phase difference between simulation result and analytic solution until 100 s using double time variable for step lengths of 0.02, 0.03, and 0.04 mm



**Figure 4.** Phase difference between simulation result and analytic solution until 100 s using long double time variable for step lengths of 0.02, 0.03, 0.04 mm

at 100 s is about  $2 \times 10^{-8}$ , which corresponds to a false EDM of about less than  $10^{-29}$  e-cm. Consequently, this proves that the difference is suppressed sufficiently.

#### 4. Discussion and future plan

Rounding errors occur regardless of whether Geant4UCN is based on ver4.9.2 or 4.9.6 because they come directly from the Runge–Kutta algorithm. We need to remove the cause of this problem from Geant4 itself so that Geant4UCN can work properly. Because each UCN does not trace the same path, they each suffered from different time rounding errors. Hence, the rounding errors of the time variable could have serious effects on the simulation results. Further, the problem is not related to whether the CPU is 32-bit or 64-bit because the rounding errors were observed when we used a 64-bit CPU. We consulted a Geant4 specialist about the problem that we reported on in this paper. We are now trying to implement the solution he proposed in Geant4UCN.

Non-specular reflection at the sidewalls can suppress the systematic uncertainties, as described in Sec.1. It generally depends on the surface's state, especially on its roughness. If we can develop an nEDM measurement cell consisting of surfaces that can control the non-specular reflection, it will allow us to manage the systematic uncertainty suppression. However, this means that we need to understand the correct dependence on the non-specular reflection. On the other hand, UCNs can be lost when they are bounced off of material surfaces, which increases the statistical uncertainty. The mechanism of UCN loss, particularly at low temperature, i.e., the UCN anomaly, is still being discussed and remains to be determined, even though several models to explain it have been proposed[7][8][9]. By repeating experiments to obtain a more realistic simulation, we need to try to discover a more precise model describing the reactions upon reflection.

#### 5. Summary

In measurement of the nEDM, systematic uncertainties occur because of a relativistic magnetic field arising in conjunction with inhomogeneous electric and magnetic fields. The systematic uncertainties are enhanced when the UCN ensembles exhibit certain ordered motions. Thus, it

is essential to quantitatively understand the effects of diffusing the UCN ordered motion in order to reduce the systematic uncertainties. Geant4UCN is an ideal simulation framework because it can take into account all the essential functions for these effects. Because nEDM experiments aim at detecting values of  $10^{-28}$  e·cm, the simulation study needs to be sufficiently precise.

Rotational motion in inhomogeneous electric and magnetic fields is one of the most interesting situations related to the systematic error enhancement due to certain types of UCN motion. In this situation, a relativistic magnetic field accompanying rotational motion arises, and the UCN spin precession becomes slightly faster. Thus, we can check whether a simulation works properly by comparing the simulation result with the analytic solution for its rotational relativistic magnetic field. Actually, the Geant4 simulation result has rounding errors in the time variable corresponding to a range of several  $10^{-28}$  e·cm to about  $10^{-27}$  e·cm, which is not negligible for nEDM experiments. To avoid this problem, by extracting the set of coding relevant to the essential functions, we prepared an alternative to Geant4UCN that can properly simulate UCNs with errors corresponding to less than  $10^{-29}$  e·cm.

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