Numerical study of space-charge effects and performance evaluation of Coulomb-scaling factors

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The Self-Confining RI Ion Target (SCRIT[1]) facility requires an isobar separator based on a multi-reflection time-of-flight mass spectrometer (MRTOF[2]) that delivers $^{132}Sn^{+}$ at 10^8 ions/s. Previous studies have evaluated the motions of ions inside the MRTOF with space charge using the "Coulomb Scaling Factor (C_{SF})"[3] approximation, which reduces the calculation time to an allowable level. We would like to evaluate whether this approximation can be applied to validating mass separation when the number of ions is high. The validity of the approximation inside the MRTOF must be shown in the multi-reflection motion, but for this study, we limit the motion in free space as a starting point.

In the approximation, all N_{real} real particles are grouped in arbitrary fixed numbers to form N_{pseudo} group, and each group is treated as a pseudo-particle. C_{SF} is defined as N_{real}/N_{pseudo}, and the pseudo-particle's mass M and charge Q become $M = m \times C_{SF}$, $Q = q \times C_{SF}$,where m and q are the mass and charge of the real particles. Note that with $C_{SF} = 1$, all ions are treated as real particles. The Coulomb force acting on i-th pseudo-particle is given by

$$M_i \frac{d^2 \boldsymbol{r}_i}{dt^2} = \sum_{j \neq i}^{N_{pseudo}} \mathrm{k} \frac{Q_i Q_j}{|\boldsymbol{r}_{ij}|^2} \hat{\boldsymbol{r}}_{ij} \,, \tag{1}$$

where k is the Coulomb constant, $\boldsymbol{r}_{ij}$ is the position vector, and $\hat{\boldsymbol{r}}_{ij}$ is the unit vector pointing from Q_j to Q_i. Thus, the computation time can be reduced by a factor of $1/{C_{SF}}^2$.

We have written a 3D Monte-Carlo calculation code in C language for C_{SF} approximation. When the N_{real} and C_{SF} values are entered, it calculates and reflects N_{pseudo} used in it. The equations of motion with Coulomb forces (Eq. (1)) are calculated numerically using the Runge-Kutta method. The code is validated by comparing it with the analytical solution of the two-body problem. Assuming an initial condition in which the two static $^{132}Sn^{+}$ ions and a distance of $r\ (t = 0) = 1$ mm, we investigated how much their distance of $r'\ (t = t')$ would increase over time solely due to Coulomb repulsion (Fig. 1). The result revealed a relative error of 10^{-7}.

The motion of 10^5 real particles was numerically simulated up to 1 μs with a time step of 10 ns using the code. For ease of introduction to the code, the ions were initially stationary and uniformly distributed in a $(2\ \mathrm{mm})^3$ cube. The C_{SF} values were simulated as 1, 10, 10^2, and 10^3. The ion motions were evaluated by determining the standard deviation of position σ, and the difference $\Delta\sigma$ from its initial value (577 µm). The standard error of the σ was determined based on the results of 100 trials.

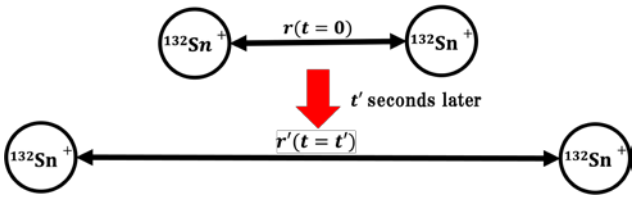

Fig. 1. Evaluation framework for 3D Monte Carlo software; we implemented a test configuration based on a simplified two-body Coulomb system.

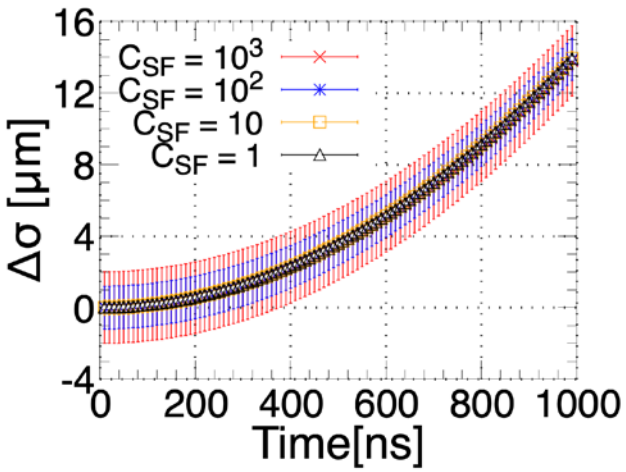

Fig. 2. Change in the standard deviation from the initial state, under a total of 10^5 particles.

The results showed that $\Delta\sigma$ matched within the statistical error range with increasing the C_{SF} (Fig. 2).

In free space, we observed that the use of the C_{SF} does not change the positional distribution. Thus, the usefulness of the C_{SF} in free space was confirmed. As the next step, we aim to evaluate whether the C_{SF} can be applied under multi-reflection. In the future, we will calculate the motion of the multi-reflected ion inside the MRTOF and evaluate the space-charge effects of the ion cloud.

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