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New integrator for relativistic equations of motion for charged particles

Takayuki Umeda[1,2], Riku Ozaki[2], Eiichiro Mizoguchi[2]
[1] Information Initiative Center, Hokkaido University, [2] Institute for Space and Earth Environmental Research, Nagoya University
e-mail (speaker): umeda@iic.hokudai.ac.jp

Numerical methods for solving the relativistic motion of charged particles with a higher accuracy is an issue for scientific computing in various fields including plasma physics. The classic fourth-order Runge-Kutta method (RK4) [1] has been used over many years for tracking charged particle motions, although RK4 does not satisfy any conservation law. However, the Boris method [2] has been used over a half century in particle-in-cell plasma simulations because of its property of the energy conservation during the gyro motion, although the Boris method has the second-order accuracy in time.

Recently, a new method for solving relativistic charged particle motions has been developed, which conserves the boosted Lorentz factor during the E-cross-B motion [3]. The new integrator, however, has the second-order accuracy in time and is less accurate than RK4. Then, the new integrator is extended to the fourth-order accuracy in time by combining RK4 [4]. However, it is not easy to implement the new fourth-order integrator into PIC codes, because the new method with RK4 adopted co-located time stepping for position and velocity vectors, which is not compatible with the charge conservation method.

In the present study, the two new relativistic integrators [3,4] are reviewed. Then, a new leap-frog integrator with the fourth-order accuracy in time is developed based on the two integrators, which adopts staggered time-stepping for position and velocity vectors.

The new relativistic particle integrators are developed based on the theoretical solution to the relativistic E-cross-B motion in a constant electromagnetic field. It is known that the theoretical solution falls into three cases depending on the sign of the squared relativistic Lorentz factor for the E-cross-B drift velocity of charged particles [5]. Therefore, the new integrator [4] includes branching statements (IF/CASE) inside a loop involving iterations through particles, which depends on the sign of the squared Lorentz factor for the E-cross-B drift velocity. It is also known, however, that the computational cost of the conditional branching inside a loop is expensive. In the present study, several numerical techniques for the conditional branching inside a loop are implemented based on high-performance computing techniques. A performance comparison of them is also made.

The present numerical experiment shows that (1) a loop processing with IF/ELSE statements costs 1.2 times as expensive as a processing without the conditional branching, if the conditional block is short, (2) a loop processing of conditional branching with multiple streams costs 1.1 times as expensive as a processing without the conditional branching, and (3) a loop processing of conditional branching with complex-type variables costs very expensive.

References

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