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High-accuracy particle integrators for particle-in-cell (PIC) simulation

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Particle-in-cell (PIC) simulation is one of the most important research tools in modern plasma physics. In the core part of PIC simulation, the Boris method [1] (a.k.a. the Boris integrator/pusher/solver) has been used for more than a half century. The Boris solver is second-order accurate in time --- its numerical error is proportional to the square of the timestep, $\sim(\Delta t)^2$. Meanwhile, due to ongoing evolution of our computing architecture, there is a growing demand for high-accuracy numerical solvers.

In this contribution, we review our recent efforts in developing high-accuracy particle solvers for PIC simulations. First, we discuss partial subcycling of particle integrators. It was recently proposed to subcycle the Lorentz-force part of the Boris solver [2]. Extending the method to arbitrary subcycle number n, we have successfully derived a vector formula of the subcycled results in a single timestep. Using the formula, we can obtain the result without repeating the same calculation. This led us to propose a family of particle integrators, the *multiple Boris integrators* [3]. In this family, our recommendation is the *quadruple Boris solver* with n=4. There is a connection between the multiple Boris solver and the modified Rodrigues vectors in spacecraft attitude control, because both deal with 3-D rotations.

Upon these developments, we have proposed several improvements to the nonrelativistic Boris solver. Unlike the previous methods, we subcycle the entire Boris procedure, using an n-times smaller timestep ($\Delta t/n$). We have derived a full vector formula for an arbitrary subcycle number n, so that the solver has better second-order accuracy, $\sim(\Delta t/n)^2$. We have also proposed higher-order corrections to the standard Boris method. In addition to the so-called gyrophase correction to the magnetic field [1], we have introduced an anisotropic correction to the electric field. This enables us to solve the equation with fully higher-order accuracy, $\sim(\Delta t/n)^N$ ($N = 2,4,6\ldots$ th order).

Importantly, we find that full subcycling and higher-order correction are compatible with each other. Recognizing this fact, we propose a hybrid solver of these two, to amplify their benefits. We call the new solver *the hyper Boris solvers*, which has two hyperparameters of the subcycling number n and the order of accuracy, N. The n-cycle Nth-order solver has an ultrahigh accuracy of $\sim(\Delta t/n)^N$, as shown in the Figure. Surprisingly, computational cost of the hyper Boris solver remains affordable. Our recommendation is *(n,N) = (2,6)*.

Mathematically, the hyper Boris solver can be applied to any vector equations in the form of $d\boldsymbol{V}/dt = \boldsymbol{A} + \boldsymbol{V}\times\boldsymbol{B}$. We hope that the hyper Boris solver is not only useful for kinetic modeling of plasma processes but also for many other scientific problems.

References:

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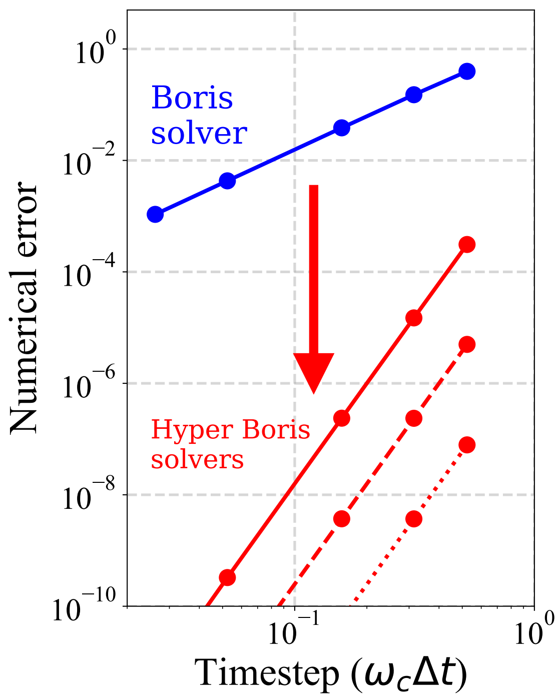

Figure: A scaling relation of numerical errors (vertical axis) as a function of the normalized timestep Δt (horizontal axis) [4]. Numerical errors by the second-order Boris solver [1] (blue line) and by the 6th-order hyper-Boris solvers with *(n,N) = (1,6), (2,6), and (4,6)* (red lines) are presented.