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A high-order Boris integrator

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ABSTRACT

This work introduces the high-order Boris-SDC method for integrating the equations of motion for electrically charged particles in electric and magnetic fields. Boris-SDC relies on a combination of the Boris-integrator with spectral deferred corrections (SDC). SDC can be considered as preconditioned Picard iteration to compute the stages of a collocation method. In this interpretation, inverting the preconditioner corresponds to a sweep with a low-order method. In Boris-SDC, the Boris method, a second-order Lorentz force integrator based on velocity-Verlet, is used as a sweeper/preconditioner. The presented method provides a generic way to extend the classical Boris integrator, which is widely used in essentially all particle-based plasma physics simulations involving magnetic fields, to a high-order method. Stability, convergence order and conservation properties of the method are demonstrated for different simulation setups. Boris-SDC reproduces the expected high order of convergence for a single particle and for the center-of-mass of a particle cloud in a Penning trap and shows good long-term energy stability.

1. Introduction

Often when modeling phenomena in plasma physics, for example particle dynamics in fusion vessels or particle accelerators, an externally applied magnetic field is vital to confine the particles in the physical device [1,2]. In many cases, such as instabilities [3] and high-intensity laser plasma interaction [4], the magnetic field even governs the microscopic evolution and drives the phenomena to be studied. Movement of electrically charged particles in electric and magnetic fields is described by the following equations of motion

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathbf{f}(\mathbf{x}, \mathbf{v}) = \alpha \left[\mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t)\right], \tag{1a}$$

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v} \tag{1b}$$

with the particle position $\mathbf{x} \in \mathbb{R}^d$, its velocity $\mathbf{v} \in \mathbb{R}^d$, the magnetic field $\mathbf{B}(\mathbf{x}, t) \in \mathbb{R}^d$, electric field $\mathbf{E}(\mathbf{x}, t) \in \mathbb{R}^d$ and the charge to mass ratio $\alpha \in \mathbb{R}$. In (1a), the well-known Lorentz force $\mathbf{f}$ depends on $\mathbf{x}$ and $\mathbf{v}$ so that a discretizing (1) with a standard velocity-Verlet scheme [5,6] reads

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \Delta t \left(\mathbf{v}_n + \frac{\Delta t}{2}\mathbf{f}(\mathbf{x}_n, \mathbf{v}_n)\right) \tag{2a}$$

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$$\mathbf{v}_{n+1} = \mathbf{v}_n + \frac{\Delta t}{2}\left(\mathbf{f}(\mathbf{x}_n, \mathbf{v}_n) + \mathbf{f}(\mathbf{x}_{n+1}, \mathbf{v}_{n+1})\right), \tag{2b}$$

with an implicit velocity update step (2b). The Boris integration method [6,7] provides a clever way to evaluate (2b) without having to actually solve an implicit system. It has thus become a de-facto standard for the numerical solution of (2) and allows to cheaply integrate the particle trajectory in the presence of electric and magnetic fields.

Being based on the velocity-Verlet scheme, the Boris approach is a second-order method [6]. Whether it is also symplectic is controversial: In [8] it is claimed that it is while [9] claim that it is not, but nevertheless shows excellent long term energy stability due to being phase-space volume preserving. Furthermore, it only requires a single evaluation of the right-hand side **f** per time step, making it a cheap numerical method in terms of computational cost [10]. For these reasons, the Boris method is widely used in many Particle-In-Cell-codes (see e.g. [11]), grid-free methods (e.g. [12]) and Monte-Carlo simulations (e.g. [13]). Several explicit alternatives to the Boris method have been proposed, compare [10] and the references therein. All of them are second-order accurate and apparently no higher-order methods based on the original Boris approach exist. Especially for applications such as trajectory integration in particle accelerators [14], space-weather studies [15], high-intensity laser-plasma interaction [4], and fusion vessel simulations [13,16], where high precision has to be maintained over long physical simulation times, these are desirable, though. In addition, the current development of high-performance computing systems towards high floating point operation rates at stagnating memory data transfer speed favors the use of higher-order methods in essentially all fields of computer simulation [17]. Furthermore, the ability of tuning the order of an integration algorithm adds a new dimension to its parameter space that allows for balancing precision versus runtime.

A number of other high-precision or higher-order methods for (1) have been developed. Examples are methods that use a spatial coordinate instead of time as the independent variable which showed better performance than a fourth-order Runge–Kutta method in beam propagation simulations [18], a quasi-symplectic Trotter-factorization based scheme that builds upon an explicit–implicit mixture of leap-frog, Verlet, exponential differencing and Boris rotations with a sixth-order rotation angle approximation [16] or a Taylor series-based explicit approach with an up to sixth-order replacement for the Boris method using a complex differential operator for the Maxwell fields [19,20]. Essentially, none of these methods are easily tunable for arbitrary order but are formulated for a very specific case. Only the latter, Taylor series-based approach offers this feature but requires a complicated set of appropriate differential operators to be constructed for every order.

In this work, we introduce the high-order *Boris-SDC* integration method for (1), which is a combination of the classical Boris integrator with the spectral deferred corrections method (SDC). The resulting Boris-SDC method retains much of the simplicity of the Boris integrator (in terms of implementation, alas not derivation) while allowing to easily generate a method of essentially arbitrary order. Based on classical defect correction, SDC has originally been introduced for first-order ODEs as an iterative approach for the generic construction of high-order integration schemes using a low-order base propagator (the “sweeper”) such as implicit or explicit Euler for the correction “sweeps” [21]. Several modifications and extensions exist e.g. semi-implicit SDC [22], GMRES-accelerated SDC [23], inexact SDC [24], multi-level SDC [25], SDC based on DIRK methods [26] or the parallel full approximation scheme in space and time (PFASST), a parallel-in-time integrator which exploits the iterative structure of SDC [27]. Recently, SDC has been formulated for second-order problems with the standard Verlet integrator as sweeper [28]. Here, we combine this particular approach with the classical Boris integrator and extend it to a velocity-dependent force of the form (1a).

The derivation of Boris-SDC relies on the interpretation of SDC as a preconditioned Picard iteration for the solution of a collocation problem, see e.g. [23,29]. Collocation methods are based on the integral formulation of an ODE, the approximation of the exact trajectory over a time step by a polynomial and evaluation of the integrals by quadrature. They are a special class of implicit Runge–Kutta methods and, depending on the chosen quadrature nodes, have a number of attractive properties, particularly symplecticness, see e.g. [30,31]. The disadvantage of collocation methods is that they require the solution of a very large, possibly nonlinear system of equations to compute the stages. Picard iteration can be used to solve this system, but often requires a too small time step for convergence. SDC can be considered as a preconditioned Picard iteration, where inverting the preconditioner corresponds to “sweeping” through the quadrature nodes with a low-order method. If sufficiently many sweeps are performed, the advantageous properties of the underlying collocation method are recovered. For e.g. a first-order method such as the implicit Euler as sweeper, SDC formally gains one order per sweep [32], so fixing the number of iterations allows to easily generate a scheme of higher order, up to the order provided by the underlying quadrature. Here, we describe how the classical Boris integrator can be used as a preconditioner to derive an iterative solver for a collocation approximation of (1).

This paper is organized as follows: Section 2 describes collocation methods, briefly discusses their properties and introduces the required notation. In Section 3, we start with spectral deferred corrections based on the velocity-Verlet scheme as base integrator in matrix from. The matrix formulation itself is derived in Appendix A. Concentrating on this rather formal notation, these parts are sufficiently general to also be utilized for force expressions other than the Lorentz force in (1a). In the second part of Section 3 we then specialize the formalism to the case of the Lorentz force as the ODEs right-hand side and derive ready-to-implement expressions for the Boris-SDC method, specifically tailored for problems of the form (1). Section 4 illustrates the properties of Boris-SDC by numerical examples and compares Boris-SDC to the classical Boris integrator. Finally, Section 5 gives a summary and an outlook on possible future directions of research.