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Does Boris-SDC conserve phase space volume?

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In this paper we investigate the conservation of phase space volume of the Boris-SDC algorithm. This method provides a generic way to extend the standard, second-order accurate Lorentz force integrator commonly used for charged particles in an electric and magnetic field to a high-order method using spectral deferred corrections. For a single particle in a Penning trap and different frequencies of the electric and magnetic fields, we assess the conservation properties of the method by computing the update matrix of one step of Boris-SDC as well as its determinant. We compare the results to the convergence regions and relate them to energy conservation properties of the method.

1 Introduction

The numerical simulation of the movement of electrically charged particles in an electric and magnetic field is commonly performed using the well-known and widely used Boris scheme [1, 2]. Based on the standard velocity-Verlet scheme for molecular dynamics simulations, this second-order accurate Lorentz force integrator resolves the seemingly implicit velocity dependence in the equations of motion by exploiting the rotational character of the magnetic field contribution. In doing so, it provides a fully explicit, cheap particle pusher and has become the de-facto standard integration method for this kind of problems. Today, the Boris method is applied in essentially all particle-based plasma physics simulations involving magnetic fields, e.g. in laser-plasma physics algorithms as well as space weather and fusion-related simulations.

In [3], we have extended the second-order method to arbitrary orders of accuracy by coupling the Boris approach with spectral deferred corrections (SDC, [4]). SDC can be considered a preconditioned Picard iteration for computing the solution of a collocation method. In this interpretation, inverting the preconditioner corresponds to a sweep with a low-order method. While common implementations make use of implicit or explicit Euler integrators, we employ velocity-Verlet as base sweeper and incorporate the Boris method as solver for the implicit velocity dependency. The order of accuracy of SDC in general and Boris-SDC in particular is controlled by the number and type of collocation nodes used for the discretization of the Picard integral as well as the number of iterations [4].

While it is still disputed whether or not the standard Boris scheme is a symplectic method, it has been shown to conserve phase space volume [5]. In this paper, we investigate this property for Boris-SDC and show that while it does not conserve phase space volume analytically, the deviation can be controlled by the iteration count/the residual. This behavior can also be observed in the energy conservation analysis of Boris-SDC and the results presented here are in line with the findings in [3].

2 Results

For the analysis, we study a single particle in a Penning trap, cf. [6]. Due to the presence of an external magnetic and electric field, the particle is confined to a limited volume and its characteristic properties, such as trajectories in real and phase space, energy conservation, and stability of the integration scheme, can conveniently be analyzed. We assume a constant magnetic field $\mathbf{B} = \mathbf{B}(\omega_B)$ along the z-axis with frequency ω_B and an external electric field $\mathbf{E} = \mathbf{E}(\omega_E)$ with frequency ω_E, which is composed of an ideal quadrupole potential distribution. The equations of motion are then given by

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

with the particle's charge-to-mass ratio α. Since the force is linear in the position and the velocity, k iterations of Boris-SDC on the time interval $[t_n, t_{n+1}]$ can be written as

$$(\mathbf{x}_{n+1}^k, \mathbf{v}_{n+1}^k) = \tilde{\mathbf{P}}_{\mathrm{sdc}}^k(\omega_E, \omega_B, \Delta t) \cdot (\mathbf{x}_n, \mathbf{v}_n) \tag{2}$$

where $\tilde{\mathbf{P}}^k = \tilde{\mathbf{P}}_{\mathrm{sdc}}^k(\omega_E, \omega_B, \Delta t)$ is the update matrix of Boris-SDC, see [3] for the derivation. Following [5], in order to check the conservation of phase space volume, we analyze the determinant of the Jacobian of the one-step map $\psi : (\mathbf{x}_n, \mathbf{v}_n) \to (\mathbf{x}_{n+1}, \mathbf{v}_{n+1})$. In our case, the map is simply the update matrix $\tilde{\mathbf{P}}_{\mathrm{sdc}}^k$ applied to $(\mathbf{x}_n, \mathbf{v}_n)$ so that the Jacobian is the matrix $\tilde{\mathbf{P}}_{\mathrm{sdc}}^k$ itself. Since the construction of this matrix is rather complex, we cannot expect to find a closed form for the determinant,

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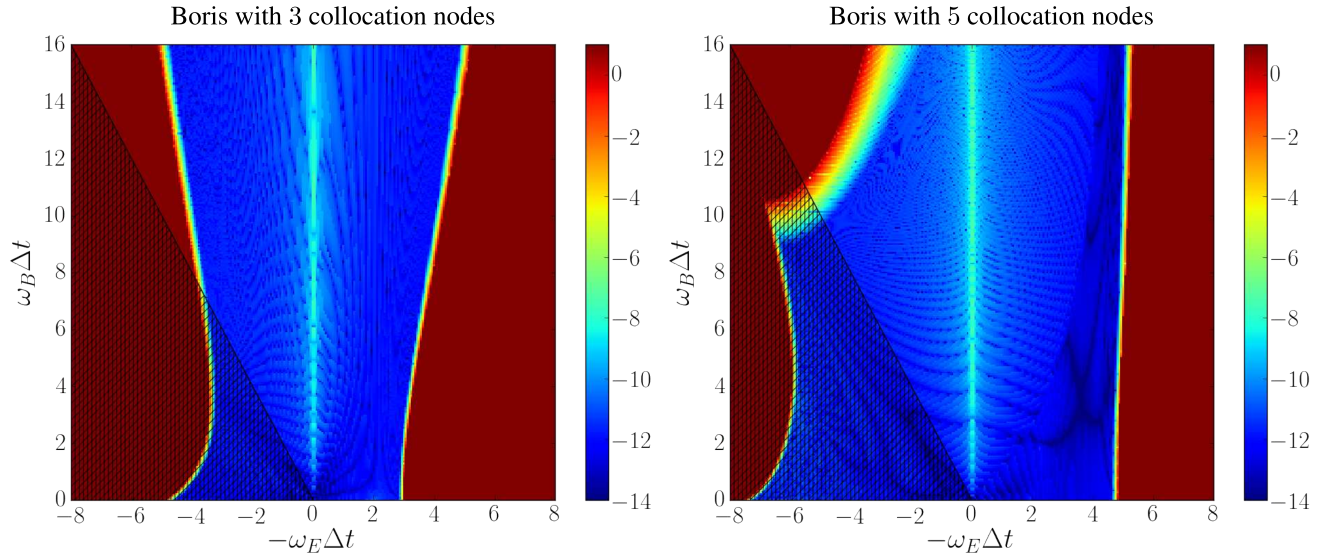

Fig. 1 Analysis of the step-by-step phase space volume conservation of Boris-SDC using the determinate of the update matrix for $M = 3$ and $M = 5$ Gauss-Lobatto nodes. Colors encode $|\det(\tilde{\mathbf{P}}^k_{\mathrm{sdc}}) - 1|$ in $\log 10$, compare (2). The dark gray, hatched regions denote the trap's physical instability region $\omega_B^2 < 4\omega_E^2$ while light gray areas indicate numerical instability. Although showing a different quantity, the figures closely resemble Figures 3 and 9 in [3] analyzing convergence regions of Boris-SDC and energy conservation.

though. We thus compute the determinant numerically and compare the values for different frequencies ω_E and ω_B. For each setup, the number of iterations k for Boris-SDC is chosen such that the residual is below a threshold of 10^{-12}. With this particular iteration number k, we compute $\tilde{\mathbf{P}}^k_{\mathrm{sdc}}$ and evaluate the difference between its determinant and 1, since a conservative scheme would yield a determinant equal to 1, cf. [5]. This procedure is similar to the numerical analysis of the energy conservation properties of Boris-SDC in [3].

In Figure 1, the results for different values of ω_E and ω_B are shown for 3 and 5 collocation nodes. Blue regions correspond to small differences of the determinant to 1 and therefore only minor deviations in the phase space volume, while red colors denote failure to conserve phase space volume. The emerging structure is very similar to the one shown in Figure 9 of [3] and in particular corresponds to the regions where Boris-SDC converges to the collocation solution. The conservation of phase space volume is thus primarily dominated by the convergence properties of the Boris-SDC iteration towards the collocation solution: For parameters ω_E and ω_B, where Boris-SDC converges, phase space volume is conserved with an accuracy corresponding to the residual. Naturally, where Boris-SDC fails to converge, we also see a complete breakdown of conservation.

The analysis presented here confirms, using a different approach, the discussion and results from [3]: The collocation solution is symplectic for a proper choice of quadrature nodes (namely Gauss-Legendre). If the collocation problem were solved with infinite accuracy, the solution therefore would exactly conserve phase space volume. Since Boris-SDC only provides an approximate solution of the collocation problem, it also only approximately conserves phase space volume with errors controlled by the residual. However, as demonstrated in [3], despite not being symplectic, the high accuracy of Boris-SDC results in very small energy errors even for very long integration times.

3 Outlook

An interesting direction for future research would be to test whether Boris-SDC can be accelerated using the multi-level SDC framework [7]. Then, in a second step, it could also be used in the "parallel full approximation scheme in space and time" (PFASST, [8]). Combining Boris-SDC with PFASST could provide a high order parallel-in-time integrator for particle simulations and allow to improve parallel efficiency for large scale runs.

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