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High-accuracy numerical integration of charged particle dynamics based on recurrence formula with symmetric decomposition
漸化的対称分解に基づく荷電粒子運動の高精度数値積分

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An explicit numerical scheme for a charged particle motion in static electromagnetic field is developed. Non-canonical variables are used. The scheme is based on the operator decomposition and preserves symplecticity and time-reversal symmetry. Its accuracy can be improved to arbitrary higher order by the recurrence formula. Numerical examples are presented, with a focus on the trade-off between accuracy improvement and increase of computational cost.

1. Introduction

Charged particle motion is an essence of plasma physics. We often need to calculate its orbit very accurately for a long time period. The numerical scheme we develop here is based on the operator decomposition and the recurrence formula, that were developed separately for quantum Monte Carlo simulation[1, 2] and celestial mechanics[3]. We extend them to non-canonical variables, and obtain an explicit scheme.

In this section, basic idea of the operator decomposition and recurrence formula of [1, 2, 3] is explained briefly. Let us consider a dynamical system $\dot{z} = V[z]$, where z is a state vector and $V[z]$ denotes a vector field. The formal solution is given by $z(t) = \mathrm{e}^{tV[z]}z(0)$. Generally, it is not easy to calculate the exponential operator. For a Hamiltonian system, we have $V[z] = \mathcal{J}\partial_z H[z]$, where $H[z]$ is a Hamiltonian, $z := (q,p)^{\mathrm{T}}$ with q and p being canonical coordinate and momentum, and $\mathcal{J}$ is an anti-symmetric tensor called Poisson tensor. If the Hamiltonian has a separable form $H[z] = H_1[p] + H_2[q]$, $V[z]$ can be decomposed as $V[z] = V_1[p]+V_2[q]$, where $V_1[p]$ and $V_2[q]$ are vector fields generated only by $H_1[p]$ and $H_2[q]$, respectively. A harmonic oscillator has this form.

In numerical computation, we need a formula to evolve $z(t)$ from t_j to $t_{j+1} = t_j + \Delta t$. According to the formal solution, we have $z_{j+1} = \mathrm{e}^{\Delta t V[z(t)]}z_j$, where z_j denotes $z(t_j)$. For the separable Hamiltonian, the exponential operator can be approximated as $\mathrm{e}^{\Delta t(V_1[p]+V_2[q])} = \mathrm{e}^{\Delta t V_1[p]}\mathrm{e}^{\Delta t V_2[q]} + \mathcal{O}(\Delta t^2)$. During the operation of $\mathrm{e}^{\Delta t V_2[q]}$, q does not change. Thus p changes due to a constant vector field $V_2[q_j]$ and we exactly integrate to obtain $p_{j+1} = p_j + \Delta t V_2[q_j]$. Next, during the operation of $\mathrm{e}^{\Delta t V_1[p]}$, p does not change and thus we exactly integrate to obtain $q_{j+1} = q_j + \Delta t V_1[p_{j+1}]$. This gives us the 1st-order explicit scheme "G_1". We can easily prove that the 2nd-order scheme "S_2" is obtained by symmetrizing the operator decomposition as $\mathrm{e}^{\Delta t V} = \mathrm{e}^{\frac{\Delta t}{2}V_1}\mathrm{e}^{\Delta t V_2}\mathrm{e}^{\frac{\Delta t}{2}V_1} + \mathcal{O}(\Delta t^3)$. Further higher-order schemes can be derived by a recurrence formula of the form: $S_{2m}(\Delta t) = S_{2m-2}(p_{m1}\Delta t)\cdots S_{2m-2}(p_{mr}\Delta t)$, where $m = 2, 3, 4, \cdots$ and r is an odd integer. $2m$ becomes the order of the scheme. One of the useful choices is $p_{mj} = k_m$ for $j = 1, 2, 4, 5$ and $p_{m3} = 1 - 4k_m$ for $r = 5$, where $k_m := 1/(4 - 4^{1/2m-1})$.

2. Operator decomposition and recurrence formula for charged particle motion via non-canonical variables

The Hamiltonian of a charged particle in static electromagnetic field is given by $H[\boldsymbol{z}] = (\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{q}))^2/2m + e\phi(\boldsymbol{q})$, where $\boldsymbol{q} = (q^1, q^2, q^3)^{\mathrm{T}}$ and $\boldsymbol{p} = (p_1, p_2, p_3)^{\mathrm{T}}$ are canonical coordinates and momenta, respectively, and $\boldsymbol{z} = (q^1, q^2, q^3, p_1, p_2, p_3)^{\mathrm{T}}$. The mass and the charge are denoted by m and e, respectively, $\boldsymbol{A}$ and ϕ are vector and scalar potentials, respectively.

This Hamiltonian, however, is not separable, and thus the operator decomposition explained above does not seem to give a simple explicit scheme. To resolve it, we adopt non-canonical variables $\boldsymbol{x} = (x, y, z)^{\mathrm{T}}$ and $\boldsymbol{v} = (v_x, v_y, v_z)^{\mathrm{T}}$. Then the Hamiltonian is written in a separable form as $H'[\boldsymbol{z}'] = H'_1[\boldsymbol{v}] + H'_2[\boldsymbol{x}]$ where $\boldsymbol{z}' = (x, y, z, v_x, v_y, v_z)^{\mathrm{T}}$, $H'_1[\boldsymbol{v}] := m\boldsymbol{v}^2/2$ and $H'_2[\boldsymbol{x}] := e\phi(\boldsymbol{x})$.

On the other hand, the Poisson tensor $\mathcal{J}$ transforms to a non-canonical form as $\mathcal{J}' = \mathcal{J}'_1 + \mathcal{J}'_2$ with

$$\mathcal{J}'_1 := \frac{1}{m}\left(\begin{array}{c|c} \mathbf{0} & \mathbf{1} \\ \hline -\mathbf{1} & \mathbf{0} \end{array}\right),$$

$$\mathcal{J}'_2 := \frac{e}{m^2}\left(\begin{array}{c|ccc} \mathbf{0} & & \mathbf{0} & \\ \hline & 0 & B_z & -B_y \\ \mathbf{0} & -B_z & 0 & B_x \\ & B_y & -B_x & 0 \end{array}\right),$$

where $\mathbf{0}$ and $\mathbf{1}$ denote 3×3 zero and unit matrices, respectively.

Then the evolution equation becomes $\dot{\boldsymbol{z}}' = (\mathcal{J}'_1 + \mathcal{J}'_2)\partial_{\boldsymbol{z}'}(H'_1 + H'_2)$. The $\mathcal{J}'_1$ terms allow us a simple explicit integration scheme. In order to obtain a simple explicit scheme for $\mathcal{J}'_2$ terms, we introduce $H'_1 = H'_{1x} + H'_{1y} + H'_{1z}$ with $H'_{1x} := mv_x^2/2$ and so on. Note that $\mathcal{J}'_2\partial_{\boldsymbol{z}'}H'_2$ vanishes. By these expressions, we obtain the following operator decomposition:

$$\begin{aligned}\dot{\boldsymbol{z}}' &= \mathcal{J}'_1\partial_{\boldsymbol{z}'}H'_1 + \mathcal{J}'_1\partial_{\boldsymbol{z}'}H'_2 \\ &\quad + \mathcal{J}'_2\partial_{\boldsymbol{z}'}H'_{1x} + \mathcal{J}'_2\partial_{\boldsymbol{z}'}H'_{1y} + \mathcal{J}'_2\partial_{\boldsymbol{z}'}H'_{1z} \\ &=: V_1[\boldsymbol{z}'] + V_2[\boldsymbol{z}'] + W_x[\boldsymbol{z}'] + W_y[\boldsymbol{z}'] + W_z[\boldsymbol{z}'].\end{aligned}$$

It is easy to see that each term allows us a simple explicit integration scheme. The formal solution gives us the 1st-order scheme G_1 as

$$\boldsymbol{z}'_{j+1} = \mathrm{e}^{\Delta t V_1}\mathrm{e}^{\Delta t V_2}\mathrm{e}^{\Delta t W_x}\mathrm{e}^{\Delta t W_y}\mathrm{e}^{\Delta t W_z}\boldsymbol{z}'_j + \mathcal{O}(\Delta t^2).$$

As explained in Introduction, we obtain the 2nd-order scheme S_2 by symmetrizing the operator decomposition, and higher-order schemes S_n with $n = 2m$ $(m = 2, 3, 4, \cdots)$ by the recurrence formula.

3. Accuracy and computational cost

The scheme developed above has been implemented numerically. As a test, a charged particle orbit in a uniform magnetic field was calculated during 10^4 times the cyclotron period. Then the change of energy was measured by

$$\frac{\langle \Delta E\rangle}{E_0} := \frac{1}{(t_{\mathrm{end}} - t_{\mathrm{start}})E_0}\int_{t_{\mathrm{start}}}^{t_{\mathrm{end}}} |E(t) - E_0|\mathrm{d}t,$$

where E_0 is the initial value of the energy. Generally, $\langle \Delta E\rangle$ decreases and the accuracy improves as Δt is decreased. On the contrary, the computational time for following 10^4 cyclotron period increases as Δt is decreased. If we require that $\langle \Delta E\rangle/E_0$ is less than a critical value, we may have an allowable maximum Δt for each scheme. Since the allowable maximum Δt is different, the computational time to follow 10^4 cyclotron period is different. Then, we may have an optimum scheme to minimize the computational time. Figure 1 shows the CPU time for obtaining $\langle \Delta E\rangle/E_0 \simeq 10^{-6}$. As a reference, the result by the 4th-order Runge-Kutta method is also plotted. We observe that the CPU time is minimum for S_4. The CPU time for S_6 is even shorter than that of 4th-order Runge-Kutta method.

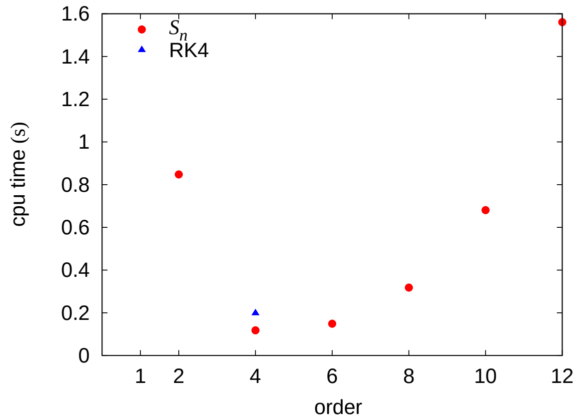

Fig. 1: CPU time for the test problem with the allowable maximum Δt for satisfying $\langle \Delta E\rangle/E_0 \simeq 10^{-6}$ for various orders' schemes (S_n). A result with the 4th-order Runge-Kutta method (RK4) is also plotted for reference. S_4 was the optimum for obtaining the requested accuracy. S_6 was even shorter than RK4.

4. Conclusions

The operator decomposition method was developed for a charged particle motion in static electromagnetic field where non-canonical variables were adopted. The higher-order approximation was obtained by the recurrence formula. The developed scheme was tested by integrating simple cyclotron motion for 10^4 cyclotron period. It was found that the 4th-order scheme was the optimum if we impose a criterion on the relative energy change less than 10^{-6}.

Acknowledgments

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