AN ACCURATE AND EFFICIENT NUMERICAL INTEGRATOR FOR PAIR-WISE INTERACTION

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Abstract

We are developing a new numerical integrator based on Picard iteration method for Coulomb collisions. The aim is to achieve a given prescribed accuracy most efficiently. The integrator is designed to have adaptive time stepping, variable order, and dense output. It also has an automatic selection of the order and the time step. We show that with a good estimation of the radius of convergence of the expansion, we can obtain the optimal time step size. We also show how the optimal order of the integration is chosen to maintain the required accuracy. For efficiency, particles are distributed over time bins and propagated accordingly.

INTRODUCTION

Many numerical integrators exist to solve the ordinary differential equations (ODEs) of the n-body problem. The goal of any numerical integrator is to achieve a given prescribed accuracy most efficiently. The main parameters controlled to accomplish this goal are the time step size and the order of the integration. Accuracy is usually attained by using either a very small time step size or a very high order, and both parameters are kept fixed during the simulation. Hence, the available integrators face efficiency challenges while trying to maintain accuracy.

Aiming to achieve both accuracy and efficiency, we developed our numerical integrator to be adaptive, variable order and with dense output. The integrator is proposed to deal with the electrostatic n-body problem. It is based on Picard iteration method combined with differential algebra (DA) [1]. The DA is a powerful tool to deal with ODEs since its structure is based on truncated power series algebra (TPSA) with well defined basic and analytic operations [2]. It has been proven that numerical methods based on Picard iteration can be competitive when implemented with the advanced differential algebra [3]. Here, we present features of our integrator that enable accomplishing accuracy and efficiency with some examples.

THE NUMERICAL INTEGRATOR

Our Picard-based numerical integrator is adaptive, variable order with dense output. Adaptive variable order means that it uses a time step that is as large as possible while varying the order. This allows to maintain efficiency by reducing the order when a small time step is required, and to attain accuracy by increasing the order if a large time step is allowed. This adaptivity was shown to be the most efficient way to achieve the required accuracy [4]. Time stepping is performed using time bins where each particle is propagated with the appropriate time step size. Particles' time step sizes are automatically selected to increase efficiency. The dense output generated by the integrator is important for computations efficiency of time stepping, especially in the very high accuracy regime in certain applications.

System of Equations

Our integrator deals with a system of ODEs (1) that we derived from a net Coulomb force of all the particles in the system. For particle i, there are six differential equations, three for position derivatives, and three for momentum derivatives. Therefore, for N particles, we have $6N$ ODEs to be integrated. Particles can be non-relativistic as well as relativistic.

$$\frac{d\hat{Y}_i}{d\hat{t}} = \left(\frac{dx_i}{d\hat{t}}, \frac{dy_i}{d\hat{t}}, \frac{dz_i}{d\hat{t}}, \frac{d\hat{p}_{x_i}}{d\hat{t}}, \frac{d\hat{p}_{y_i}}{d\hat{t}}, \frac{d\hat{p}_{z_i}}{d\hat{t}}\right) \tag{1}$$

where:

$$\frac{dx_i}{d\hat{t}} = \hat{v}_{x_i} = \frac{\hat{p}_{x_i}}{\sqrt{f_i^2 + \hat{p}_{x_i}^2 + \hat{p}_{y_i}^2 + \hat{p}_{z_i}^2}},$$

$$\frac{d\hat{p}_{x_i}}{d\hat{t}} = \frac{q\, n_i}{mc^2}\left[\frac{q}{4\pi\epsilon_0}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{n_j\,(x_i - x_j)}{\gamma\left[(x_i-x_j)^2+(y_i-y_j)^2+\gamma^2(z_i-z_j)^2\right]^{3/2}}\right],$$

$\frac{dy_i}{d\hat{t}}$ and $\frac{dz_i}{d\hat{t}}$ have the same form as $\frac{dx_i}{d\hat{t}}$. $\frac{d\hat{p}_{y_i}}{d\hat{t}}$ and $\frac{d\hat{p}_{z_i}}{d\hat{t}}$ are similar to $\frac{d\hat{p}_{x_i}}{d\hat{t}}$.

$$\hat{\mathbf{p}} = \frac{\mathbf{p}}{mc}, \quad \hat{t} = tc, \quad f_i = \frac{m_i}{m}, \quad n_i = \frac{q_i}{q}, \quad i = 1, 2, \ldots, N$$

m = mass of particle, q = charge of particle, and c = speed of light.

In case there is an external field (electric and/or magnetic), the components of $\frac{q\,n_i}{mc^2}(\mathbf{E} + c\mathbf{v}\times\mathbf{B})$ will be added to the the respectful components of the momentum derivatives $\frac{d\hat{\mathbf{p}}}{d\hat{t}}$.

Optimal Time Step Size and Optimal Order

Á. Jobra and M. Zou presented two main requirements for the optimal selection of the time step size and the order [5]. The integrator must have a truncation error of the order of a given prescribed accuracy, and it should use the minimum total number of arithmetic operations. In order to meet these requirements, [5] provided a theorem for the optimal selection of the time step size h and the order p up to which Taylor series has to be computed. According to the

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theorem, when the error ε goes to zero, the most efficient step size in the computational sense will be:

$$h = \frac{\rho}{e^2} \tag{2}$$

where ρ is the radius of convergence of the power series. In (2), h does not depend on the accuracy, but once h is selected, the optimal order p that guarantees the required precision is:

$$p = -\frac{1}{2}\ln(\frac{\varepsilon}{M}) - 1 \tag{3}$$

Here M is a positive constant which depends on ρ and the coefficients of the power series $x^{[j]}$ as $M \approx |x^{[j]}|\rho^j$.

Radius of Convergence Each function of the $6N$ ODEs is expanded as a polynomial of time up to some order using Picard iterations. Each function has its own radius of convergence ρ (the distance of the nearest root on the complex plane to the origin). ρ can be different for each particle at each time step. Since the optimal time step size h depends on ρ in (2), we need to calculate the radius of convergence (i.e. we need to find the roots of each polynomial). However, performing such computations will be inefficient for systems with large number of particles or for polynomials of high orders. Therefore, we need to find a good estimation of ρ using the coefficients of the functions expansions.

There are many mathematical theories on the estimation of the upper and lower bounds of a polynomial roots using its coefficients (lower bound = radius of convergence). After testing some of these theories [6–9], we concluded that Lagrange method gives the best estimation of the radius of convergence for the purpose of our research.

Lagrange's lower bound for a polynomial with complex coefficients:

$$P(z) = \sum_{i=0}^{N} a_i z^i$$

is given by the inverse of the sum of the two largest numbers of the set $\left\{\left|\frac{a_i}{a_0}\right|^{1/i}\right\}, (i = 1, \cdots, N)$ [8,9].

Time Stepping

At each time step, we begin Picard iterations for our system of equations and expand each function in (1) as a polynomial of time. For each particle i, we estimate the radius of convergence ρ_i from its polynomials using Lagrange method. The optimal time step size h_i is calculated using (2). The iterations continue until each particle reaches its optimal order p_i that satisfies (3). Then, particles are distributed over a number of bins according to their current time in order to be propagated. We use two types of time bins: bins of equal time widths, and bins of equal number of particles. We propagate particles in the first bin with the appropriate time step size. In later time steps, Picard iterations are performed again only for particles that were not propagated in the previous time step. The advantage of binning will become clear when parallelizing the code to be faster and more efficient.

EXAMPLES

The integrator is implemented using COSY INFINITY software [10]. The following examples are done with uniform distributions within cm dimensions. We used accuracies $\varepsilon = 10^{-7}$ and $\varepsilon = 10^{-16}$. Particles are all protons with high energy of 14 TeV, or low energy of 1 MeV. Some runs were done with time bins of equal time widths and the others were with time bins of equal number of particles.

Non-Relativistic Protons

We used 1000 non-relativisic protons with a uniform initial distribution. The final distributions are almost the same when using bins of equal number of particles and bins of equal time widths (Fig.1). For runs with the same type of bins but with different accuracies, the required orders of the particles varied. Low accuracy did not need orders higher than 2. The higher accuracy of 10^{-16} required orders between 3 and 4.

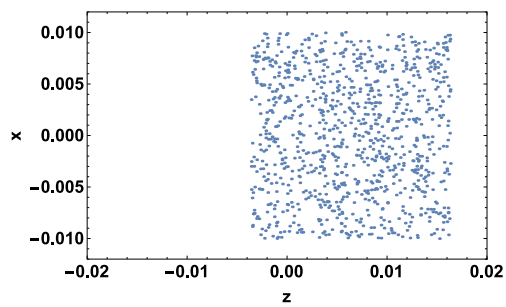

Figure 1: The final distribution using bins of equal time widths for the non-relativistic protons.

The time step sizes did not depend on the accuracies (as (2) implied) and the results are the same for both accuracies. For Bins of equal time widths, a histograms of the time step sizes used in the total run is shown in Fig.2, and a histogram of the calculated time steps of a specific particle is shown in Fig.3 where it was propagated 199 times. For bins with equal number of particles, the time step sizes during the run are shown in Fig.4, and the calculated time steps of the same specific proton are shown in Fig.5, where it was propagated 509 times.

Relativistic Protons

The interactions of 100 relativistic protons with energy of 14 TeV required low order of 2 or less for both accuracies with both types of bins. The time step sizes used in the total run for bins of equal time widths (Fig. 6) are larger (hence, the number of time steps is less and the total run time is faster) than for bins of equal number of particles (Fig.7).

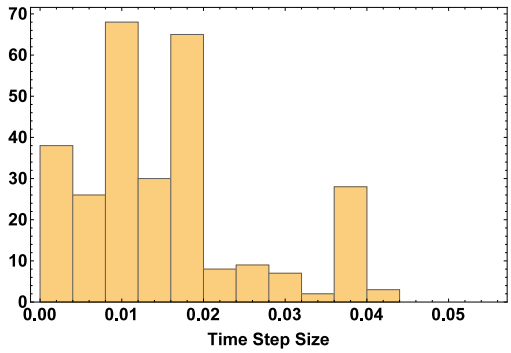

Figure 2: A histogram of the time step sizes used by the integrator at all steps when bins are of equal time widths for the non-relativistic protons.

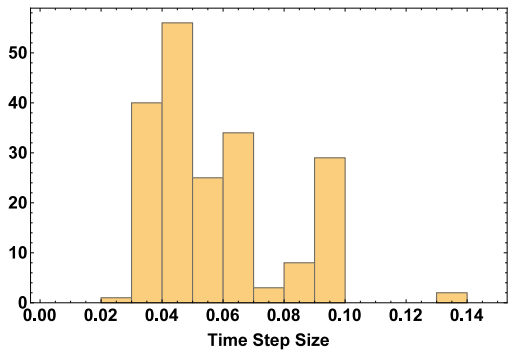

Figure 3: The calculated time step sizes of a proton when bins are of equal time widths.

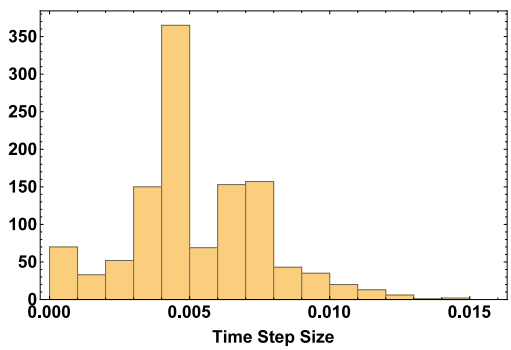

Figure 4: A histogram of the time step sizes used the non-relativistic protons at all steps when bins are of equal number of particles.

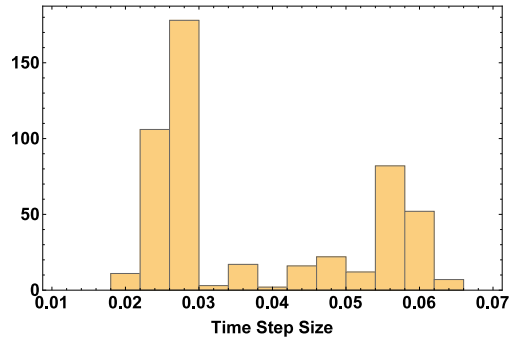

Figure 5: A histogram of the estimated time step sizes for a specific proton when bins are of equal number of particles.

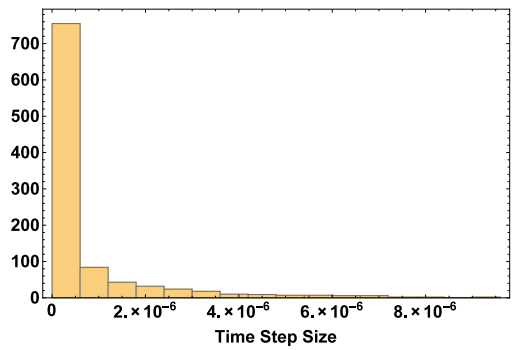

Figure 6: The total run time step sizes histogram for relativistic protons when bins are of equal time widths.

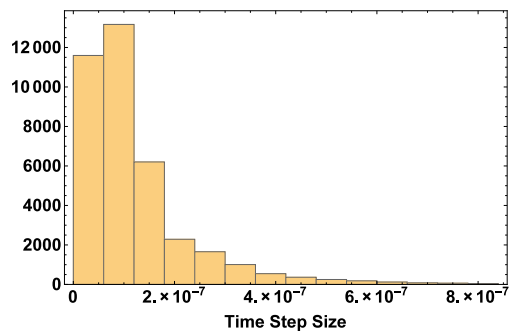

Figure 7: Time step sizes histogram of the whole run for relativistic protons when bins are of equal number of particles.

CONCLUSION

Our Picard-based integrator for pair-wise interactions is equipped with adaptivity, variable order and dense output. It is proposed to overcome efficiency challenges faced by other available integrators. We showed how we can accomplish this goal using optimal selections of the order and time step size, while time stepping is performed using time bins. Our results are as expected based on theorems from [5] where the optimal time step size depends on the initial configuration of the particles, and the optimal order guarantees our required accuracy. We used two different types of time bins. Our runs show that using time bins of equal time widths are faster than using time bins of equal number of particles. As a future work, the integrator can be parallalized to be more efficient when handling large number of particles.

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