Implementation of Splitting-Composition Schemes for the Numerical Study of Charged Particles

Cristian-Constantin Lalescu

Abstract

The correct description of particle transport is important in a huge number of problems encountered by physicists [1, 2, 3], including geophysicists [4] and astrophysicists [5], chemists and engineers. The approximation of non-interacting particles has an extremely wide range of applications, such as the dispersion of pollutants in the atmosphere or in rivers and oceans, the acceleration of charged particles in complex electromagnetic fields in astrophysical systems [5, 6, 7] as well as the estimation of particle loss in magnetic confinement devices. In certain studies, it is interesting to consider the direct description of an ensemble of particle trajectories. The mathematical framework is then quite easy to establish and, considering only classical mechanics (i.e. disregarding quantum and relativistic effects), the evolution of the particles is simply described by Newton's second law [3, 4].

However, this conceptually simple problem proves to require specially constructed numerical schemes for a GOOD solution. For the case of a charged particle moving in an electrostatic field, an elegant method was introduced by Yoshida [8] — the idea of splitting and composition methods. Using this method, explicit and efficient formulas can be found for highly accurate numerical integration schemes (solvers) to be used for the simulation of the particle's trajectory [9]. Recently this method was proven to be applicable to the general case of a charged particle in any complex electromagnetic field by Chin [10]; previous methods required the use of implicit solvers, adding a significant complication to the problem.

In this work these results are brought together, to describe GOOD solvers implemented for the specific task of studying charged particle transport in turbulent electromagnetic fields.

Chapter 1

Composition schemes for charged particles

1.1 The numerical integration of particle trajectories

Generally, the trajectory of a physical particle is very complex (unless the force acting on the particle is simple in some way), in the sense that the solution of the equations of motion cannot be written down explicitely. One approach to obtaining quantitative results about such trajectories is to solve the equations of motion numerically.

Consider the equations that describe the motion of a particle:

$$\begin{cases} \dfrac{dx_i}{dt} = v_i \\ \dfrac{dv_i}{dt} = f_i(x, v, t) \end{cases} \tag{1.1}$$

The simplest numerical scheme that can be used to find a solution for this system of equations is Euler's scheme:

$$\begin{cases} x_i(t + \Delta) = x_i(t) + v_i(t)\Delta \\ v_i(t + \Delta) = v_i(t) + f_i(x(t), v(t), t)\Delta \end{cases} \tag{1.2}$$

Note that this is just a cut off of the Taylor expansion for the solution of (1.1). For small enough time steps Δ this is an acceptable approximation (the derivatives of f can in fact be used to estimate the error). In the following we will rename the pair $y \equiv (x, v)$, and we will rewrite the evolution equation:

$$\frac{dy}{dt} = f(y, t) \tag{1.3}$$

We call an nth order numerical scheme, or solver, any map ξ that gives an estimate of $y(t+\Delta)$, when $y(t)$ is known:

$$\xi(y(t),\Delta) = y(t+\Delta) + O(\Delta^{n+1}) \tag{1.4}$$

Note that the relevant measure of the error is the order of the global error, meaning the error after a relatively large number of timesteps. We call the error generated after one timestep the local error. As we decrease the timestep, the error decreases, but the integration time of applying the solver one time decreases also. Consider the above solver ξ, with timestep Δ and $q\Delta$ (where q is some natural number). Consider a moderate number of timesteps N, such that nonlinear effects can still be neglected:

$$\begin{aligned}\underbrace{\xi\circ\xi\circ\cdots\circ\xi}_{N \text{ times}}(y(t),q\Delta) &= y(t+Nq\Delta) + NO((q\Delta)^{n+1}) \\ &= y(t+Nq\Delta) + Nq^{n+1}O(\Delta^{n+1}) \end{aligned}\tag{1.5}$$

$$\underbrace{\xi\circ\xi\circ\cdots\circ\xi}_{qN \text{ times}}(y(t),\Delta) = y(t+Nq\Delta) + NqO(\Delta^{n+1}) \tag{1.6}$$

Clearly, when the timestep is q times smaller, the global error is q^n times smaller. Here the global order is used to characterize the various solvers.

A classical numerical scheme is the fourth order Runge-Kutta method:

$$k_1 = f(y(t),t) \tag{1.7}$$

$$k_2 = f\left(y(t) + k_1\tfrac{1}{2}\Delta, t+\tfrac{1}{2}\Delta\right) \tag{1.8}$$

$$k_3 = f\left(y(t) + k_2\tfrac{1}{2}\Delta, t+\tfrac{1}{2}\Delta\right) \tag{1.9}$$

$$k_4 = f(y(t)+k_3\Delta, t+\Delta) \tag{1.10}$$

$$\xi_{RK}(y(t),\Delta) = y(t) + \tfrac{1}{6}(k_1+2k_2+2k_3+k_4)\Delta \tag{1.11}$$

However, when dealing with particle trajectories, this scheme is not generally appropiate.

When applying a solver succesively, in order to obtain a trajectory, errors have the tendency to explode when there are nonlinearities present in the equations. No matter how small the local error is, the global error will be very large if the approximated trajectory is long enough.

For a number of particle studies, the interest is to obtain very long trajectories; in fact, specific statistical properties of these very long trajectories ("which are the invariant sets in phase space?", "what is the particles' mean squared displacement?"). For these studies, it becomes crucial to have a strict

control over certain types of errors (the energy must be preserved, invariant sets should be preserved, etc ...).

To this end specially constructed solvers are required, and they are called here "GOOD" solvers; these have certain stability properties, for instance errors in the energy of a particle remain bounded for relatively long times, even for strongly nonlinear equations. One simple example of such a well-behaved solver is the mid-point method, which is in fact a second order implicit Gauss-Runge-Kutta scheme:

$$Y = y(t) + \tfrac{1}{2} f(Y, t + \tfrac{1}{2}\Delta)\Delta \tag{1.12}$$

$$\xi_{iRK2}(y(t), \Delta) = y(t) + f(Y, t + \tfrac{1}{2}\Delta)\Delta \tag{1.13}$$

Note that the implementation of this solver is not trivial, because of the implicit equation that needs to be solved. An entire hierarchy of implicit Gauss Runge Kutta schemes can be formally constructed, and these solvers are well-suited for a number of physical problems. However, as their order increases, their implementation becomes more and more complex because of the implicit equations.

1.2 Splitting and composition schemes

We further concern ourselves with explicit schemes described in [8], that are still well-suited for studying long particle trajectories. Because the construction is quite general, we will change the notation from (x, v) to (x, y).

1.2.1 Construction of composition schemes

Consider the following system of ordinary differential equations:

$$\begin{cases} \dfrac{d}{dt}x = a_x(x, y) + b_x(x, y) \\ \dfrac{d}{dt}y = a_y(x, y) + b_y(x, y) \end{cases} \tag{1.14}$$

Suppose that we can associate a pair of systems of ODEs to (1.14):

$$(I) \begin{cases} \dfrac{d}{dt}x = a_x(x, y) \\ \dfrac{d}{dt}y = a_y(x, y) \end{cases}, \quad (II) \begin{cases} \dfrac{d}{dt}x = b_x(x, y) \\ \dfrac{d}{dt}y = b_y(x, y) \end{cases} \tag{1.15}$$

such that each of these systems has an explicit solution. Formally, if we call $z \equiv (x, y)$, we can define two operators:

$$(I)\frac{d}{dt}z = Az \ , \ (II)\frac{d}{dt}z = Bz \tag{1.16}$$

and the original ODE can be written as

$$\frac{d}{dt}z = (A + B)z \tag{1.17}$$

The formal solution for (1.14) is given by the map $\varphi(z, t) = e^{t(A+B)}z$, in the sense that $z(t) = \varphi(z(0), t)$.

The explicit, exact, solutions for the ODE systems (I) and (II) are $\varphi_x(z, t) = e^{tA}z$ and $\varphi_y(z, t) = e^{tB}z$. This is why the process of finding φ_x and φ_y is called EXPONENTIAL SPLITTING.

A composition method, or scheme, $\varphi^{(\alpha,\beta)}$ in n stages is any map of the form

$$\varphi^{(\alpha,\beta)}(z, t) = \left(\prod_{i=1}^{n} e^{\alpha_i tA}e^{\beta_i tB}\right) z \tag{1.18}$$

This map has an explicit expression, and we can now reduce the problem of integrating the ODE system (1.14) to finding the coefficients α_i and β_i such that formally

$$e^{t(A+B)} = \prod_{i=1}^{n} e^{\alpha_i tA}e^{\beta_i tB} + \epsilon \tag{1.19}$$

where ϵ is small.

The leapfrog method is perhaps the most well-known example of a (second order) composition method:

$$S_2(t) \equiv e^{\frac{1}{2}tA}e^{tB}e^{\frac{1}{2}tA} = e^{t(A+B)+t^3\gamma_3+\cdots} \tag{1.20}$$

In fact, the LF method is symmetric ($S_2(t)S_2(-t) = S_2(-t)S_2(t) = 1$), and it can easily be shown that

$$S_2(t) = e^{t(A+B)+t^3\gamma_3+t^5\gamma_5+t^7\gamma_7+\cdots} \tag{1.21}$$

To find efficient higher order methods, Yoshida [8] applies the Baker-Campbell-Hausdorff formula to a more general symmetric composition:

$$S^{(m)}(t) \equiv S_2(w_m t)\cdots S_2(w_1 t)S_2(w_0 t)S_2(w_1 t)\cdots S_2(w_m t) \tag{1.22}$$

This leads to a more complicated system of algebric equations, that generally has several solutions that can be found numerically (no explicit expressions for the coefficients w).

In practice:

- construct the two maps φ_x and φ_y.
- find the coefficients α and β from the w for any symmetric composition.
- implement the map $\varphi^{(\alpha,\beta)}$. Note that a different map is obtained if the φ_x and φ_y are switched, but the error is of the same order in the timestep.

1.2.2 Splitting for charged particles

Consider the evolution equations for a charged particle:

$$\begin{cases} \dfrac{d}{dt}\mathbf{r} = \mathbf{v} \\ \dfrac{d}{dt}\mathbf{v} = \dfrac{q}{m}(\mathbf{E}(\mathbf{r}) + \mathbf{v} \times \mathbf{B}(\mathbf{r})) \end{cases} \tag{1.23}$$

If the magnetic field is exactly 0 (the case $\mathbf{B} = 0$), then we can directly use the obvious splitting:

$$\varphi^{\mathbf{E}}_{\mathbf{r}}(\mathbf{r}, \mathbf{v}, t) \equiv \begin{cases} \mathbf{r} \to \mathbf{r} + t\mathbf{v} \\ \mathbf{v} \to \mathbf{v} \end{cases} \tag{1.24}$$

$$\varphi^{\mathbf{E}}_{\mathbf{v}}(\mathbf{r}, \mathbf{v}, t) \equiv \begin{cases} \mathbf{r} \to \mathbf{r} \\ \mathbf{v} \to \mathbf{v} + t\dfrac{q}{m}\mathbf{E} \end{cases} \tag{1.25}$$

This is in fact a special case of the splitting for the particles described by a separable hamiltonian $H = T(\mathbf{v}) + V(\mathbf{r})$; composition methods built with these maps will be symplectic [8].

The very useful result presented by Chin in [10] is a splitting for the other two cases:

- ($\mathbf{E} = 0$, $\mathbf{B} \neq 0$)

$$\varphi^{\mathbf{B}}_{\mathbf{r}}(\mathbf{r}, \mathbf{v}, t) \equiv \begin{cases} \mathbf{r} \to \mathbf{r} + t\mathbf{v} \\ \mathbf{v} \to \mathbf{v} \end{cases} \tag{1.26}$$

$$\varphi^{\mathbf{B}}_{\mathbf{v}}(\mathbf{r}, \mathbf{v}, t) \equiv \begin{cases} \mathbf{r} \to \mathbf{r} \\ \mathbf{v} \to \mathbf{v} + \mathbf{v}_b \end{cases} \tag{1.27}$$

with

$$\mathbf{v}_b \equiv \mathbf{b} \times \mathbf{v} \sin\theta + \mathbf{b} \times (\mathbf{b} \times \mathbf{v})(1 - \cos\theta),\ \mathbf{b} \equiv \frac{\mathbf{B}}{|\mathbf{B}|} \text{ and } \theta \equiv -t\frac{q}{m}|\mathbf{B}|$$

- ($\mathbf{E} \neq 0$, $\mathbf{B} \neq 0$)

$$\varphi_{\mathbf{r}}^{\mathbf{EB}}(\mathbf{r}, \mathbf{v}, t) \equiv \begin{cases} \mathbf{r} \to \mathbf{r} + t\mathbf{v} \\ \mathbf{v} \to \mathbf{v} \end{cases} \tag{1.28}$$

$$\varphi_{\mathbf{v}}^{\mathbf{EB}}(\mathbf{r}, \mathbf{v}, t) \equiv \begin{cases} \mathbf{r} \to \mathbf{r} \\ \mathbf{v} \to \mathbf{v} + \mathbf{v}_b + \mathbf{v}_e \end{cases} \tag{1.29}$$

with

$$\mathbf{v}_e \equiv t\left(\mathbf{a} + \frac{1-\cos\theta}{\theta}\mathbf{b}\times\mathbf{a} + \frac{\theta-\sin\theta}{\theta}\mathbf{b}\times(\mathbf{b}\times\mathbf{a})\right) \text{ and } \mathbf{a} \equiv \frac{q}{m}\mathbf{E}$$

Charged particles with drag

We also treat the case of drag force acting on a charged particle additionally to the Lorentz force. This is for the case of a "macroscopic" charged particle moving in a plasma; the plasma (fluid) velocity is $\mathbf{U}$.

$$\begin{cases} \dfrac{d}{dt}\mathbf{r} = \mathbf{v} \\ \dfrac{d}{dt}\mathbf{v} = \dfrac{q}{m}(\mathbf{E}(\mathbf{r}) + \mathbf{v}\times\mathbf{B}(\mathbf{r})) + \mu(\mathbf{U}-\mathbf{v}) \end{cases} \tag{1.30}$$

Note that the splitting in this case is made in three operators: the equation

$$\begin{cases} \dfrac{d}{dt}\mathbf{r} = 0 \\ \dfrac{d}{dt}\mathbf{v} = \mu(\mathbf{U}-\mathbf{v}) \end{cases} \tag{1.31}$$

has the very simple solution

$$\varphi^{\mu}(\mathbf{r}, \mathbf{v}, t) \equiv \begin{cases} \mathbf{r} \to \mathbf{r} \\ \mathbf{v} \to \mathbf{v} + (\mathbf{U}-\mathbf{v})(1-e^{-\mu t}) \end{cases} \tag{1.32}$$

And a second order solver for the equation

$$\frac{d}{dt}z = (A+B+C)z \equiv ((A+B)+C)z \tag{1.33}$$

is an extension of the leapfrog:

$$S_2(t) \equiv e^{\frac{1}{2}tA}e^{\frac{1}{2}tB}e^{tC}e^{\frac{1}{2}tB}e^{\frac{1}{2}tA} \tag{1.34}$$

And this second order solver can be directly used for higher order symmetric compositions.

1.2.3 Magnetic field lines

As a sidenote, we consider the case of a virtual particle, following a magnetic field line (the simplest guyding center approximation). The equation is simply

$$\frac{d}{dt}\mathbf{r} = \mathbf{B} \tag{1.35}$$

One important property of the magnetic field is that it is divergence-free, $\nabla \cdot \mathbf{B} = 0$. This means that this equation generates a volume-preserving flow; which can also be viewed as a topological property of the magnetic field. Volume preservation is a crucial property when studying sets that are invariant to the flow generated by the magnetic field.

One method of constructing a solver that will also be a volume-preserving map is to use exponential splitting. We know that $\mathbf{B} = \nabla \times \mathbf{A}$. This turns the differential equation into

$$\begin{cases} \dfrac{dx}{dt} = \partial_y A_z - \partial_z A_y \\ \dfrac{dy}{dt} = \partial_z A_x - \partial_x A_z \\ \dfrac{dz}{dt} = \partial_x A_y - \partial_y A_x. \end{cases} \tag{1.36}$$

which can be split into the following three sets of hamiltonian equations:

$$\text{(I)} \begin{cases} \dfrac{dx}{dt} = \partial_y A_z \\ \dfrac{dy}{dt} = -\partial_x A_z \\ \dfrac{dz}{dt} = 0 \end{cases} \quad \text{(II)} \begin{cases} \dfrac{dx}{dt} = -\partial_z A_y \\ \dfrac{dy}{dt} = 0 \\ \dfrac{dz}{dt} = \partial_x A_y \end{cases} \quad \text{(III)} \begin{cases} \dfrac{dx}{dt} = 0 \\ \dfrac{dy}{dt} = \partial_z A_x \\ \dfrac{dz}{dt} = -\partial_y A_x \end{cases} \tag{1.37}$$

By applying the midpoint method (the 2nd order implicit Gauss Runge Kutta solver), with a timestep τ, to each of these systems, we obtain the three volume-preserving maps φ_1^τ, φ_2^τ and φ_3^τ. This is because the midpoint method is volume-preserving for 2D systems [9].

So a second order volume-preserving solver for the original system of equations is

$$\varphi^\tau \equiv \varphi_1^{\frac{1}{2}\tau} \varphi_2^{\frac{1}{2}\tau} \varphi_3^\tau \varphi_2^{\frac{1}{2}\tau} \varphi_1^{\frac{1}{2}\tau} \tag{1.38}$$

By constructing standard composition methods from φ, one is able to obtain higher order volume-preserving solvers. Note that the midpoint method is not the exact solution, but it does satisfy the requirement of being volume-preserving.

Chapter 2

Examples and conclusions

We present a quick example, to discuss the efficiency of higher order solvers. Consider an electromagnetic field that is relatively simple, but generates chaotic trajectories for charged particles:

$$\phi = \phi_{xy}\cos x\cos y + \phi_{yz}\cos y\cos z + \phi_{zx}\cos z\cos x,\ \ \mathbf{A} = \begin{pmatrix} A_x\cos y\cos z \\ A_y\cos z\cos x \\ A_z\cos x\cos y \end{pmatrix} \tag{2.1}$$

These potentials generate the following electric and magnetic fields:

$$\mathbf{E} = \begin{pmatrix} \sin x(\phi_{xy}\cos y + \phi_{zx}\cos z) \\ \sin y(\phi_{yz}\cos z + \phi_{xy}\cos x) \\ \sin z(\phi_{zx}\cos x + \phi_{yz}\cos y) \end{pmatrix},\ \ \mathbf{B} = \begin{pmatrix} \cos x(A_y\sin z - A_z\sin y) \\ \cos y(A_z\sin x - A_x\sin z) \\ \cos z(A_x\sin y - A_y\sin x) \end{pmatrix} \tag{2.2}$$

A system of N charged particles in these fields will be studied. The order of the solver is tested by checking the dependency of the global error for the position and momentum on the time-step. Considering the particles indexed by i, their trajectories from $t = 0$ to $t = T$ are computed with a series of decreasing time-steps τ_k, and the approximations of the final position in phase space, $\xi_i^{(k)}(T)$ are obtained. Then, for each particle the following distances in phase space are computed:

$$\varepsilon_i^{(k)} \equiv \left|\left|\xi_i^{(k+1)}(T) - \xi_i^{(k)}(T)\right|\right| \tag{2.3}$$

The composition methods that we use are taken from [9] (where the coefficients are given explicitely). They are:

- CM2 (leap frog)

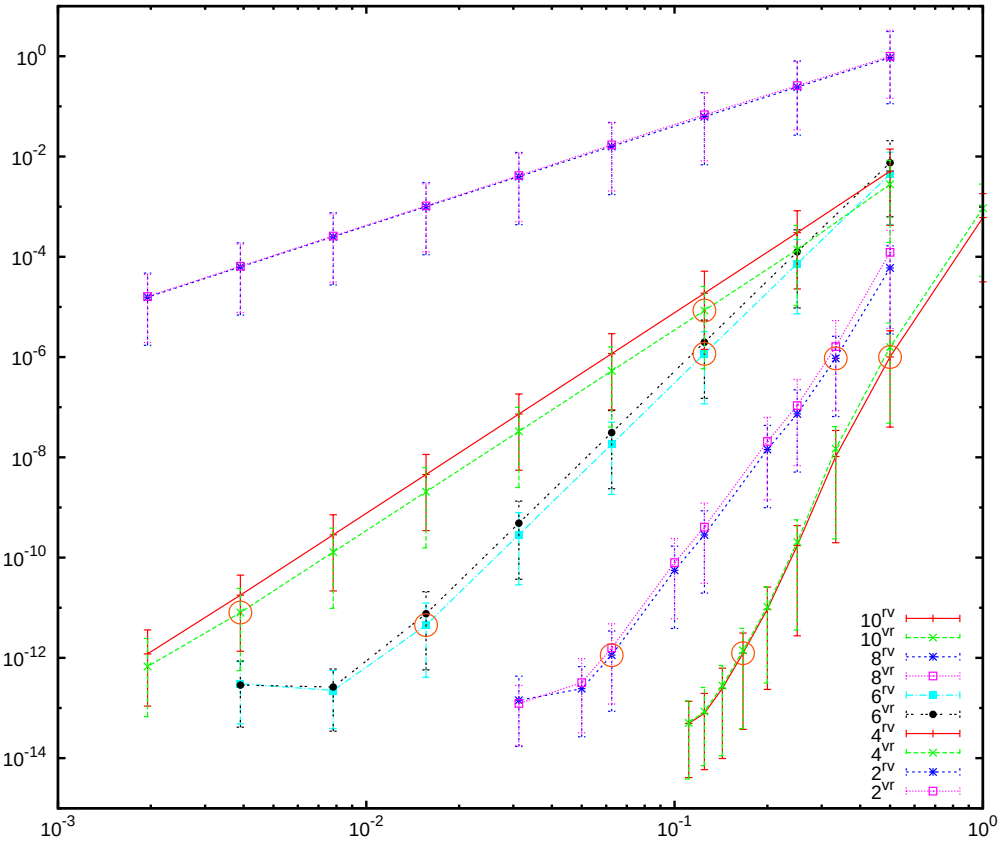

Figure 2.1: Composition methods of various orders. The average distances $\langle \varepsilon_i^{(k)} \rangle$ are plotted against the timesteps τ_k.

- CM4 (Blanes and Moan [11])
- CM6 (Kahan and Li [12])
- CM8 (Kahan and Li [12])
- CM10 (Sofroniou and Spaletta)

In figure 2.1 we also distinguish between "rv" and "vr" methods, depending on whether the base leapfrog of the CM is composed as "halfposition-velocity-halfposition" or "halfvelocity-position-halfvelocity". Some points in figure 2.1 are circled because we use those timesteps in some longer simulations. Note that there are two sets of circled points: some with a fixed error around $10^{-6} - 10^{-5}$, and some with the error around $10^{-12} - 10^{-11}$.

These timesteps are used in longer simulations to look at the energy errors obtained with the different CMs, see figure 2.2. The longer simulations serve

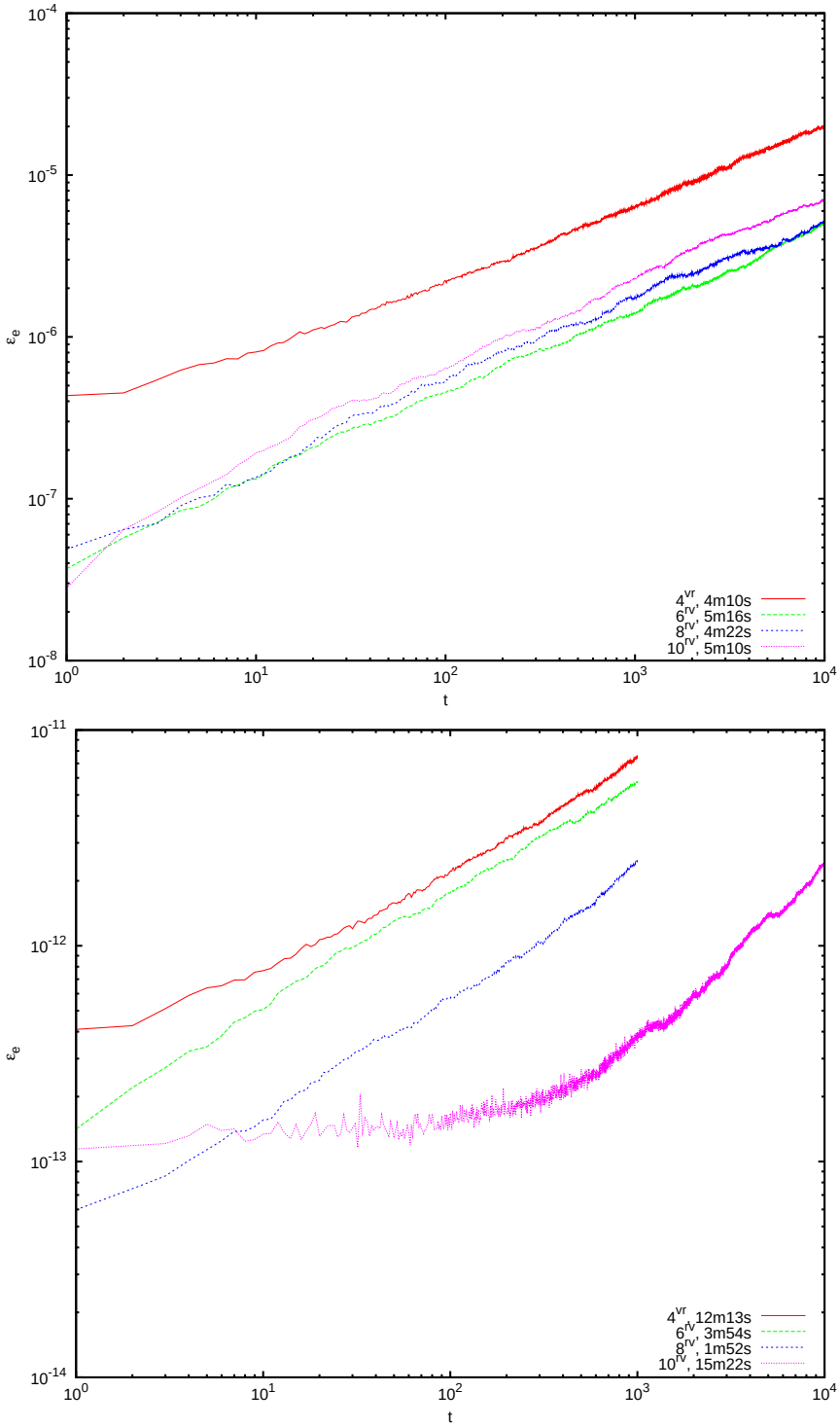

Figure 2.2: Energy errors for composition methods.

to measure the efficiency of the various solvers: it is quite obvious that higher order schemes give better results while keeping computational costs reasonably low (and sometimes they are faster).

These composition methods are not exactly energy preserving, nor symplectic [10]. The energy error seems to grow as the square root of time, but a more careful study should be made before making any conclusion, [13, 14]. When using the classic Runge Kutta scheme the energy error grows linearly with time, and all the errors are generally larger.

The most obvious advantage to using CMs is that they have already been studied and optimized [9], and their implementation is trivial. Once the splitting for a given equation is determined, the high order CMs can be immediately implemented and used with great efficiency. They are particularly well-suited for studies of particle transport, where trajectories over "very long times" are required in order to extract relevant information about the statistics of a particle ensemble. High order solvers also allow for the use of "large" timesteps, thus avoiding as much as possible the accumulation of errors; note that for chaotic trajectories errors can explode very fast if the solver does not have the required stability properties.

To conclude, in this work several results have been gathered to be used in the specific problem of charged particle transport; we have also presented a method meant for the study of magnetic field lines, as it is closely related. The methods have all been implemented and tested, and they will be used in future work for the study of transport in turbulent electromagnetic fields.

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