EFFICIENT TIME INTEGRATION FOR BEAM DYNAMICS SIMULATIONS BASED ON THE MOMENT METHOD*

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Abstract

The moment method model has been proven to be a valuable tool for numerical simulations of charged particle beam transport both in accelerator design studies and in optimization of the operating parameters for an already existing beam line. On the basis of the Vlasov equation which describes a collision-less kinetic approach, the time evolution of such integral quantities like the mean or rms dimensions, the mean or rms kinetic momenta, and the total energy or energy spread for a bunched beam can be described by a set of first order ordinary differential equations (ODEs) under consistent initial conditions. Application of a proper time integrator to such an ODE system enables then to determine the time evolution of all involved ensemble parameters. From the vast amount of available time integration methods different versions have been implemented and evaluated to select a proper one. The computational efficiency in terms of effort and accuracy serves as a selection criterion. Among possible candidates of suited time integrators for the given set of moment equations are the explicit Runge-Kutta (RK) methods, the implicit theta methods, and the linear implicit Rosenbrock methods. Various algorithms have been tested under real-world conditions to select the most suited one for moment method applications.

INTRODUCTION

Numerical simulations of charged particle beam transport can be realized using either discrete individual particles or a continuous charge distribution description. In both cases a discretization process in time and/or space enables to calculate the time evolution of the charge distribution supposed an initial state is given. The underlying computational model has to include all essential physical effects like the external fields along the different beam line elements, the particles self fields and the interaction of the particles with the surrounding materials.

Depending on the operational conditions it is possible to concentrate on dominant effects like wakefields in collimators in the high energy regime or space charge fields in injectors in the low energy regime and to neglect unimportant contributions. Generally, the more physical effects are included in the numerical model, the more expensive it becomes and the more effort has to be applied to solve these problems under the restriction of limited resources. Limitations are imposed on the maximal acceptable simulation time as well as on the available computer storage capacity. In nearly all applications a trade-off between accuracy, simulation time and memory consumption has to be found.

An efficient numerical method for beam dynamics simulations has already been discussed by P. J. Channell in 1983 [1]. Instead of an immediate spatial discretization of the particle distribution, the discrete moments

$$<\mu> = \int_\Omega \mu \; f(\vec{r},\vec{p}) \; \mathrm{d}r^3\mathrm{d}p^3$$

of the distribution function f are used for an approximate description of the particle density distribution. From the numerical point of view it is advantageous to determine the overall position and momentum by the first order raw moments with

$$\mu \in \{x, y, z, p_x, p_y, p_z\}$$

followed by the translatory invariant higher order centralized moments with

$$\mu \in \{(x-<x>)^{l_x} \cdot (y-<y>)^{l_y} \cdot (z-<z>)^{l_z}, \ldots\}$$

which describe the pure shape of the particle distribution function in the underlying six-dimensional phase space Ω. Basically, it is also possible to describe the whole system using raw moments only, but on account of cancellation due to the finite number representation, it is preferable to switch to the centralized versions for higher order moments.

The given notation is based on a Cartesian coordinate system where $\vec{r} = (x, y, z)$ describes the components of a spatial vector, whereas $\vec{p} = (p_x, p_y, p_z)$ specifies the corresponding momentum. The introduced moments can be used to characterize the considered particle distribution at arbitrary time instants.

Starting from the well-known Vlasov equation, a set of ordinary differential equations in the form

$$\begin{aligned}\frac{\partial <\mu>}{c\,\partial t} &= <\mathrm{grad}_{<\vec{r}>}(\mu)> \cdot <\frac{\vec{p}}{\gamma}> \\ &+ <\mathrm{grad}_{<\vec{p}>}(\mu)> \cdot <\frac{\vec{F}}{m_0c^2}> \\ &+ <\mathrm{grad}_{\vec{r}}(\mu) \cdot \frac{\vec{p}}{\gamma}> + <\mathrm{grad}_{\vec{p}}(\mu) \cdot \frac{\vec{F}}{m_0c^2}>\end{aligned}$$

is constructed which allows for further determination of the particle distribution supposed a consistent initial set of moments is provided. Contributions to the differential equations can be grouped into a kinematic part and a kinetic

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part, where the first one represents the fundamental internal feedback and the second one considers the important interaction with the surrounding beam line elements. Space charge forces can be incorporated in this way either.

SIMULATION MODEL

The time integrator evaluation study concentrates on a single rf cavity because all possible contributions to the Lorentz force, the electric field strength as well as the magnetic flux density, are naturally incorporated. Other beam line components like magnetic multipoles are also applicable but due to the fact that they do not include all the conceivable field components they are not considered in this study.

Field Distribution

The field components of the mode which is used for acceleration can be transfered from a separate eigenmode calculation to the beam dynamics simulation avoiding a 3-D field map if one provides merely the longitudinal electric field component along the axis of rotation. This paraxial approach allows to reconstruct the whole field within the cavity on the basis of a polynomial approximation and thus automatically leads to the desired series expansion of the applied forces.

In praxis this series has to be truncated at some order because numerical noise prohibits a further usage. Nevertheless, for moment equations up to order n, forces up to order $n-1$ can be provided. The obtained series expansion can then be incorporated into the specified update equations.

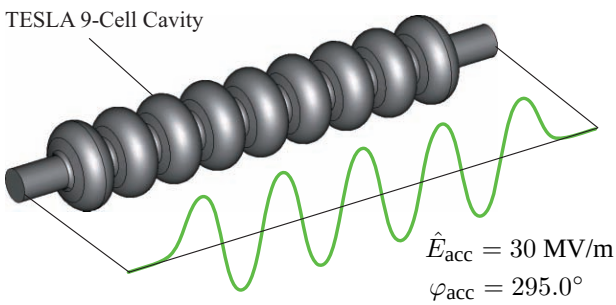

Figure 1: 3-D model of a TESLA 9-cell cavity together with the longitudinal electrical field component of the applied accelerating mode along the axis of rotation.

An overview of the selected simulation model is shown in Fig. 1. In addition to the geometric model, the corresponding longitudinal electrical field component is also displayed. The amplitude and the phase offset measured relatively to the barycenter of the charged particle distribution are further specified.

Particle Distribution

Following roughly the parameters given by the PITZ injector [2], an ideal electron bunch of $Q = -1.0$ nC and kinetic energy $E_{\text{kin}} = 5.0$ MeV is assumed. To properly evaluate the performed beam dynamics simulations based on the moment approach the same situation has been modeled paralelly using the conventional particle tracking code *ASTRA* [3]. The particle distribution is specified to be of Gaussian shape in transversal and of rectangular shape in longitudinal direction according to the data specified in Fig. 2.

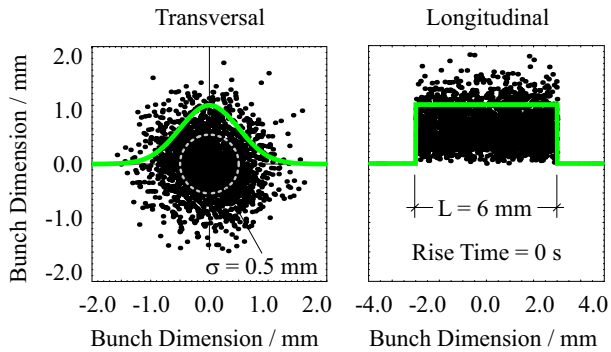

Figure 2: Particle distribution in the transversal and longitudinal direction used as an initial condition for the time integration process.

In the performed simulations, moments up to the fourth order have been considered. All moments constituting the initial particle ensemble have been calculated analytically using the specified distribution function. Since the results of the particle tracking algorithm are intended to serve as a reference, a series of initial bunches consisting of 125000, 250000 and 500000 computational particles has been evaluated.

Because no further improvement between the last two simulations has been observed, the result obtained using the highest amount of particles has been defined as a reference. In Fig. 2, a selection of calculational particles together with the defining distributions functions are shown to get an impression of the initial particle distribution.

TIME INTEGRATION

The time evolution of all moment quantities is governed by the stated fundamental set of differential equations. Because each specified time derivative is generally related to all proposed moments it is convenient to define a comprehensive solution variable y which includes all specified moments in a single mathematical variable. The data can be organized in a way that starting with the 6 first order raw moments the following 21 centralized second order moments are assigned. If required, all higher order moments can be appended successively.

The new time dependent solution variable $y(t)$ consequently represents all moments of the particle distribution function at a time instant t where the initial distribution is characterized by $y(0)$. The whole physical model can then

be written in the standard mathematical form

$$y'(t) = f(t, y(t)) \,, \quad y(t_0) = y_0$$

where y' indicates the time derivative and f summarizes the effects given by the already specified kinematic and kinetic parts. The variable y_0 represents the initial particle distribution.

Runge-Kutta Methods

Following the ideas given in [4, 5], the specified ODEs of first order can be effectively treated using one-step Runge-Kutta type methods. Various methods have been implemented and tested to select a suitable one for the effective time integration of the given differential equation:

Method	Order	Scheme
Crank-Nicolson	2	implicit
RK-Heun	3	explicit
RK-Classic	4	explicit
RK-Fehlberg	4	explicit
Rosenbrock	4	implicit

Once any explicit RK method is implemented, it is possible to switch to a similar method without big efforts. According to the corresponding Butcher tableau, only a few changes in the parameters describing the abscissa values of the applied stages, the weighting coefficients of the stages within the first-order approximations and the final weighting coefficients to determine the higher order solution for each time step are necessary.

All methods except the Rosenbrock method process the nonlinearities by functional iteration. The Rosenbrock type methods introduce a sequence of linearized systems to avoid the solution of nonlinear equations. Applying a symbolic algebra program it is possible to determine the indispensable Jacobian right from the specified moment equations. Due to performance reasons this time dependent derivative matrix is evaluated only at the beginning of each time interval and is supposed to be constant during the evaluation of all subsequent stages thus allowing significant CPU time savings [5].

SIMULATION RESULTS

On the basis of the specified benchmark problem various simulations using the moment method approach have been performed. Important beam dynamics parameter like the kinetic energy, the bunch dimensions and the projected emittances have been compared to the *ASTRA* simulation results. The moment approach, implemented in *V-CODE* [6], has been performed using moments up to the fourth order and a time step ranging from $c \cdot \Delta t = 1.5$ mm to $c \cdot \Delta t = 1.5$ μm. For small time steps one can hardly distinguish between the *V-CODE* and the *ASTRA* results. Hence, to clearly demonstrate the behavior of each implemented time integration method in the following discussion only the difference to the reference solution is shown. Hereby, the solution of the moment approach with the constant time step $c \cdot \Delta t = 1.5$ mm is used.

Kinetic Energy

The kinetic energy of the bunched particle beam increases continuously from the given initial value $E_{\text{kin}} = 5$ MeV to the final value of approximately $E_{\text{kin}} = 20$ MeV. According to Fig. 3, even for the coarse time stepping procedure a rather small relative deviation in the order of 10^{-3} can be observed.

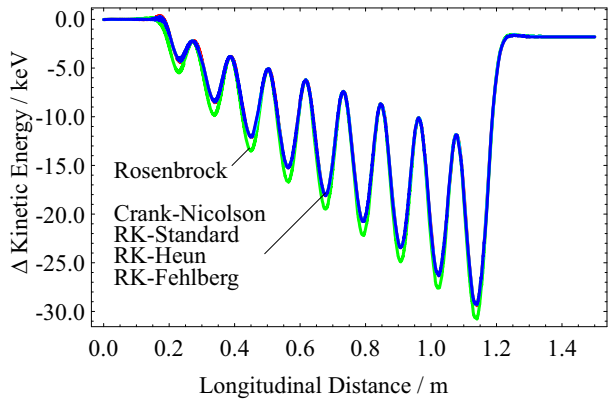

Figure 3: Deviation of the kinetic energy.

Comparing all the implemented integrators one can observe that only the solution given by the Rosenbrock method can be distinguished from the others.

Bunch Dimensions

The numerical simulation of the bunch parameters allows to reveal clearly the individual time integrator capabilities.

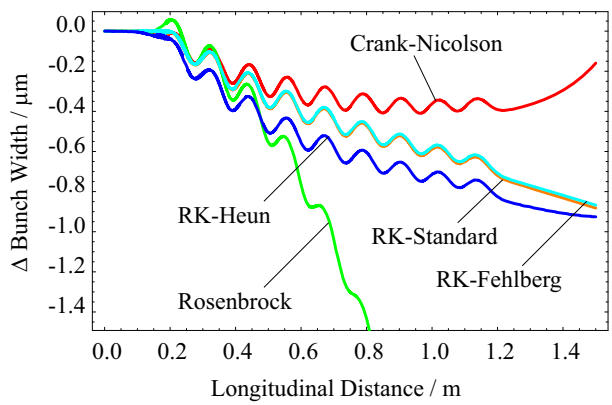

Figure 4: Deviation of the bunch width.

In Fig. 4, one can observe that the second order Crank-Nicolson scheme performs better than the higher order time integrators. Even though all results are acceptable for real-world simulations, a first indication for the decision process can be noticed. On account of the weak coupling be-

tween the transversal and the longitudinal dynamics, the rms-length of the particle distribution behaves differently.

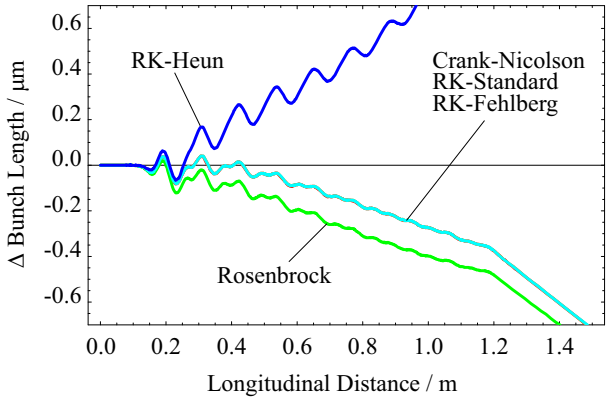

Figure 5: Deviation of the bunch length.

In Fig. 5, the simulation results for the bunch length relatively to the reference solution are displayed. One can observe that nearly all integrators underestimate the bunch length whereas only the Heun method overestimates this parameter for the given time step size.

Transversal and Longitudinal Emittance

A very sensitive parameter for charged particle beam characterization is given by the projected beam emittance

$$\varepsilon_\nu = \sqrt{<r_\nu^2><p_\nu^2> - <r_\nu p_\nu>^2}\,, \quad \nu \in \{x, y, z\}$$

where r_ν and p_ν are the centralized position and momentum vectors, respectively. The sensitivity arises from the subtraction of two nearly identical expressions. It is used as a quality measure for charged particle beams. As it is already accomplished in the previous plots, only the difference to the reference solution is given in Fig. 6 even though the deviation here is in the range of the simulated values.

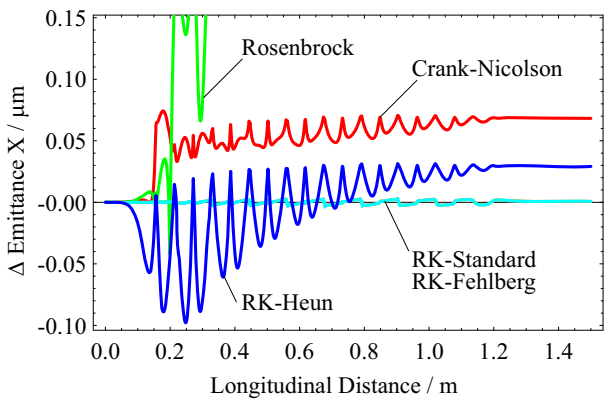

Figure 6: Deviation of the transversal emittance.

Although the results get much better if one uses smaller time steps it can be noticed that only the classical RK-Standard method and the scheme proposed by Fehlberg provide acceptable results even if rather large time steps are chosen.

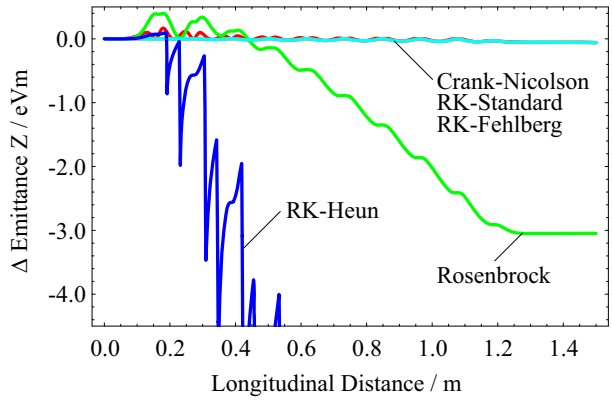

Figure 7: Deviation of the longitudinal emittance.

Taking also the absolute values of the simulation results into account it can be observed, that the longitudinal emittance is simulated more accurately than the transversal one. All integration methods except the Heun and the Rosenbrock methods provide satisfactory results as shown in Fig. 7.

CONCLUSIONS

The implemented time integration schemes given by Heun and Rosenbrock perform worse compared to the Crank-Nicolson, the RK-Standard and the RK-Fehlberg methods. Even though the Crank-Nicolson scheme is able to model accurately the bunch dimensions especially for the transversal emittance calculations, the RK-Standard and RK-Fehlberg methods perform better. Since no clear advantage can be traced between these two numerical schemes and due to the fact that none of them failed in all tests, both methods can be considered as reliable and suitable for time integration based on the moment method.

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