PteqHI DEVELOPMENT AND CODE COMPARING

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Abstract

For the development of high energy and high duty cycle RFQs accurate particle dynamic simulation tools are important for optimizing designs, especially in high current applications. To describe the external fields in RFQs, the Poisson equation has to be solved taking the boundary conditions into account. In PteqHI this is now done by using a finite difference method on a grid. This method will be described and simulation results will be compared to different RFQ particle dynamic codes.

PTEQHI WITH POISSON SOLVER

PteqHI is a program to simulate particle dynamics in RFQs. It has its roots in PARMTEQ and has continuously been developed and adapted to meet several problems by R. A. Jameson [1]. It describes the external field with the same multipole expansion method than PARMTEQM and it also uses the SCHEFF routine for its space charge calculation, but it uses time as the independent variable. Simulations of a set of 10 RFQs, which are similar to the IFMIF designs in terms of final energy, frequency, emittance, beam current, but with changing aperture have revealed same limitations of these original methods.
This was one of the reason to change the way the electric field is calculated along the RFQ. The new routines solve the Poisson equation directly. This is done by a Solver that uses the finite difference method on a grid.

Generating the grid

The first step is to set up the grid with the boundary conditions figuring out which grid points lie in or on the electrodes. The tip of the electrodes are found using the cell table for the geometry data and interpolating them at each z position using cubic splines. Once the tip position is known the electrode is represented by an arc with a selectable brake out angle. Since the boundary conditions at the electrodes are Dirichlet boundary condition the voltage $\pm\frac{U_0}{2}$ is assigned to the grid points which lie inside the electrodes. In order to describe the surface as smooth as possible the grid points are shifted in such manner that there is always a grid point on the surface. Longitudinal boundary conditions are more difficult to realize, because it cannot be assumed that the structure is symmetric in longitudinal direction. The small changes of the aperture and modulation which disturb the symmetry can be seen in results of the solver. To overcome this problem many cells are combined to a segment and calculated at the same time. Since the segments overlap, the regions with are influenced by the asymmetry are never used for the dynamic calculation.

Transition Region A real RFQ does not start directly with the electrodes, but with a tank wall. So we decided to let the particles start outside the tank wall, where the potential is close to zero. Then they drift through the small gap between the electrodes and the tank wall seeing the rising RF-field. The first segment of the RFQ includes the tank wall, the gap, the radial matching section and the first two regular cells of the RFQ to be able to simulate the effects of the rising RF-field.

Space charge grid The space charge effect is also calculated by solving the Poisson equation which a charge density $\rho \neq 0$. Therefore a second grid is needed which is generated in the same way as the grid for the external field, but with zero potential on the electrodes. By forcing the potential to be equal to zero on the electrodes the image effect is also taken into account directly, since the purpose of the image effect is to make sure that the potential of a conducting surface vanishes. There is also the option to "turn off" the image effect by setting the boundary condition of the grid to a cylinder (e.g., radius m*a) with zero potential on its surface. So the effect of the image charges can be studied.

Poisson solver

For solving the Poisson equation the finite difference method is used. This method is an iterative method where at each iteration step the new value for a grid point is a function of the old value of that point and the values of the neighboring points

$$\varphi_{0,n+1} = F(\varphi_{0,n}, \Sigma_{i=1}^{6} a_i \cdot \varphi_{i,n}, \rho_0), \quad (1)$$

where φ is the potential at the point 0 and ρ_0 is the charge density at that point. Each pair of grid points has a certain distance h_i between them. The a_i are a function of these distances. In general the h_i can vary from one pair of nodes to the next, so that the shifted grid points can be taken into account in order to represent the electrodes correctly without introducing some kind of steps. From one iteration to the next the value at each node converges to the exact answer. The accuracy is limited by the h_i. This basic method is known as the Gauß-Seidel relaxation. For speeding up

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the time the solver needs to converge, a successive overrelaxation (SOR) method can be used. The new value for the node is than calculated as a combination of the old value and the value from the neighboring nodes.

$$\varphi_{0,n+1} = \varphi_{0,n} + \omega\left(\psi - \varphi_{0,n}\right), \tag{2}$$

where ω, ψ are a fixed relaxation parameter and the combination of neighboring nodes. A further improvement in calculation time can be achieved by increasing the relaxation parameter from 1 to its final value. This is called Chebyshev acceleration. For further details see [2] [3].

SIMULATIONS

For studying the influences of the different simulation methods and different simulation programs a set of 12 RFQs was designed with the same design strategy but with different values for the minimum aperture. That leads to a set of RFQs with different performances. Some have an aperture which is too small (cases with a high a-factor) and therefore a bad transmission. Other RFQs have quite big aperture, but a bad ability to catch the beam longitudinally (small a-factor). Overall, RFQs with a high or a low aperture have a bad performance and in the middle there is optimum value for the aperture. The question is, does that optimum depend on the simulation method which has been used?

Figure 1 and 2 show the external field for the synchronous

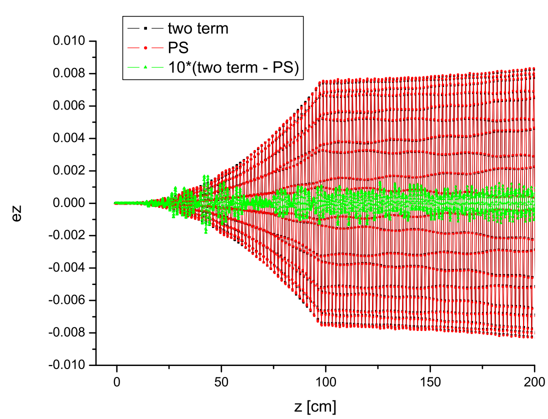

Figure 1: Two Term field and field from the Poisson Solver in the beginning of the RFQ for the synchronous particle. Green curve is 10 times the difference of the two methods.

particle at the beginning and for the entire structure for one of the RFQs with a high transmission. The black curve relates to the field from the two term potential and the red curve to the field found from the Poisson solver. The oscillation comes from the sinusoidal RF. The green curve shows ten times the difference of the other two curves. The differences appear mostly in the beginning of the RFQ and at the end where the amplitude of the field has increased. The major discrepancy is in the region closer to the electrodes where the Two-term-potential assumes a pure quadrupole shape which can differ a lot from the real geometry.

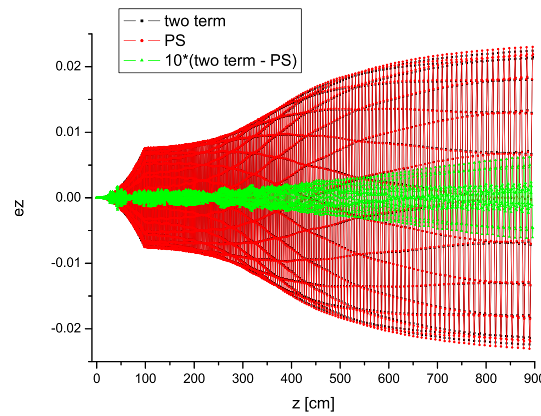

Figure 2: Two Term field and field from the Poisson Solver for the entire RFQ for the synchronous particle. Green curve is 10 times the difference of the two methods.

Space charge and image effect

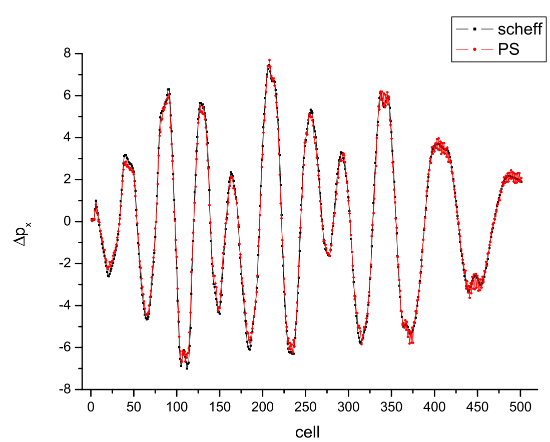

Figure 3: Momentum Δp_x for a specific particle, comparing SCHEFF and Poisson space charge solver with image effect.

The basic routine for space charge calculation in pteqHI as well as PARMTEQM [4] is SCHEFF routine. It is a two dimensional routine assuming cylindric symmetry. So it is normally called once per cell when the shape of the beam is round. There are transformations for a non-cylindrical beam. SCHEFF represents the beam by charged rings and calculates analytically the effect of charged rings on rings. Figure 3 and 4 show the resulting change of the momentum (Δp_x and Δp_z) for a specific particle over the entire RFQ with image effect turned on and figures 5 and 6 with the image effect turned off. The Poisson solver was used to drive the space charge calculation and SCHEFF ran passively to get the corresponding momentums. The basic shape of the curves are very similar, but when the particle has left the center of the beam and the amplitude of the space charge effect increases a difference between the two curves can be seen in any case.

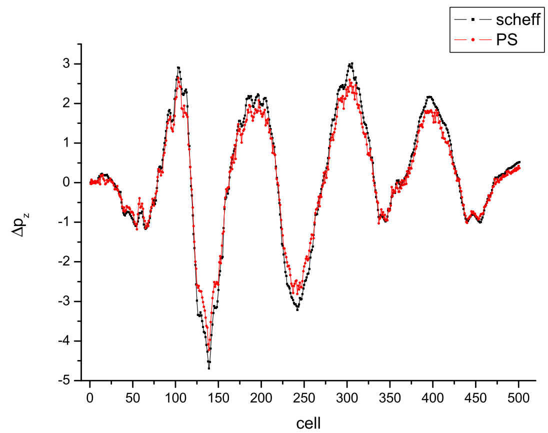

Figure 4: Momentum Δp_z for a specific particle, comparing SCHEFF and Poisson space charge solver with image effect.

In figure 6 it can be seen that the amplitude of the longitudinal momentum change from the Poisson solver with image effect turned off is lower than the with image effect on (Fig. 4). This is due to the fact that the potential was forced to be zero on the cylinder with the radius of $m \cdot a$, but the transverse results are very similar (Figs. 3 and 5).

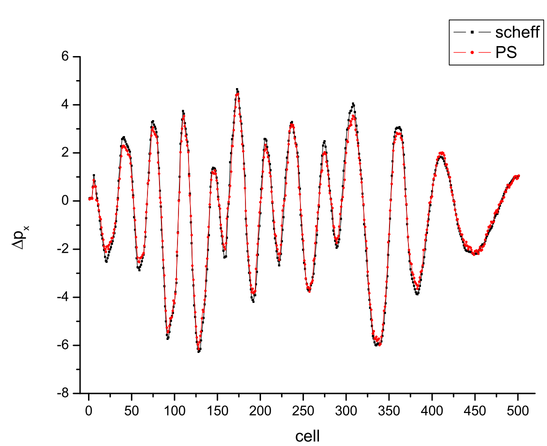

Figure 5: Momentum Δp_x for a specific particle, comparing SCHEFF and Poisson space charge solver with image effect turned off.

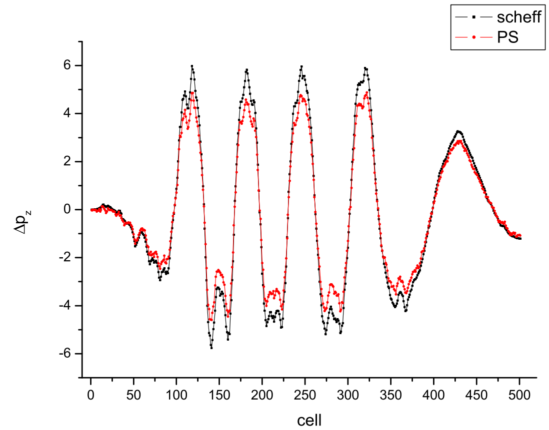

Figure 6: Momentum Δp_z for a specific particle, comparing SCHEFF and Poisson space charge solver with image effect turned off.

Results

Figure 7 and 8 show the transmission and the percentage of accelerated beam for the set of RFQs. All curves have in common, that they have a peak for a certain RFQ. The transmission and the percentage of accelerated beam differ for the RFQs with a small a-factor and therefore with a rather big aperture. Once the aperture is small enough, all particles get accelerated or radically lost. The black curve is the standard pteqHI using the multipole expansion method for the external field and SCHEFF for the space charge routine without the image effect. Its peak is at a a-factor of 41 to 48 and then it falls of in both directions. For the red curve the external field was described using the Poisson solver and SCHEFF was used for the space charge calculation. The curve is similar to the black one with the same peak, but it does not fall off as fast on the right side as the multipole expansion method curve. When the Poisson solver (with image effect turned off) is used for the space charge calculation as well (green curve), the shape of the curve and the position of its optimum change. The peak of the curve is shifted to the left to wider apertures. But the value for the maximum transmission is nearly the same.

This suggests that the treatment of the space charge effect has big influence on the simulation and should therefore be the focus for further studies.

Image charge

As shown above the inclusion of the image charge has an effect on the corresponding change of momentum. In Fig. 9 the effect of the image charge is shown. For a big a-factor the image charge will cause the transmission to drop down (small aperture). For the optimum of the curve the transmission increases with the image charge and on the left hand side it just has a minor effect. The image charge becomes important when particles come close to the

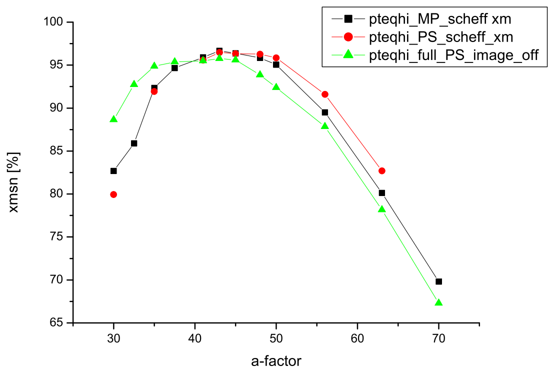

Figure 7: Transmission for the set of RFQs with different simulation methods

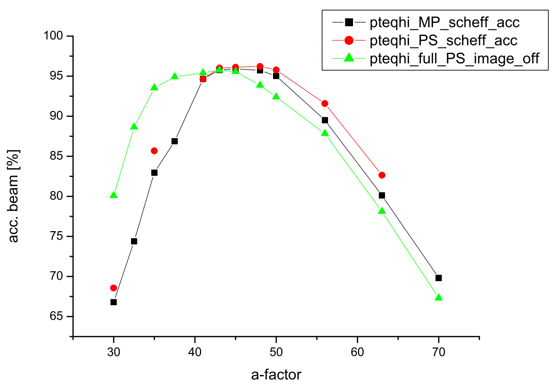

Figure 8: Percentage of accelerated beam for the set of RFQs with different simulation methods

electrodes. This happens more easily when the aperture is small. That can explain, why the transmission drops on the small aperture side. When the aperture is wide enough and the core of the particles stays away from the electrodes the image effect should not make a big difference.

COMPARISON WITH OTHER CODES

Comparing different codes has been a tedious task. One has to make sure, that the different programs simulated the same RFQ with the best match. Some codes start directly with the electrodes while others start the beam inside the tank wall. There were some hidden tricks one needs to know to make the program do what it is supposed to do. Often one must deal with a “black box” with sometimes no support from the coder. That was one major reason for writing an open-source Poisson solver where it is known, what is inside and what decisions have been made.

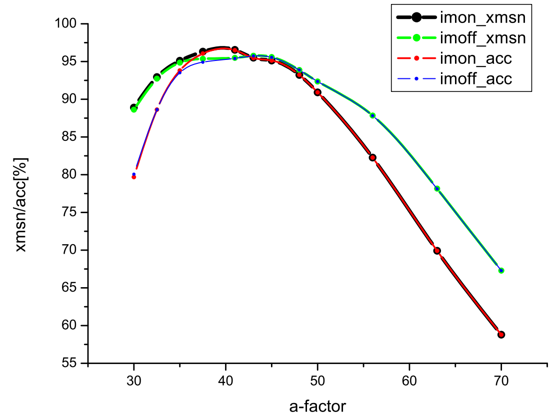

Figure 9: Effect of the image charge on transmission and accelerated particles.

CONCLUSION

For detailed beam dynamic simulation of high current, high power and high energy applications, accurate simulation tools are needed that treat the involved physics correctly and use as few assumptions as possible. One step in that direction has been made by replacing the old multipole expansion method, the SCHEFF routine and the image charge routine with a 3D Poisson solver. It has been shown, what the effects of the routines are and how they change the results of the simulation.

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