

# DEVELOPMENT OF PteqHI

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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 as well as the internal space charge fields with image effect, the Poisson equation has to be solved taking the boundary conditions into account. In PteqHI a multigrid Poisson solver is used to solve the Poisson equation. This method will be described and compared to multipole expansion method to verify the answer of the Poisson solver.

## PTEQHI

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 as PARMTEQM and it also uses the SCHEFF routine for its space charge calculation, but it uses time as the independent variable and corrects other approximations. Simulations of a set of 11 RFQs, which are similar to the IFMIF designs in terms of final energy, frequency, emittance, beam current, but with changing aperture have revealed some limitations of these original methods. This was one of the reasons to change the way the electric field is calculated along the RFQ to Multigrid Poisson Solver.

## MULTIGRID POISSON SOLVER

A classical reference on Poisson equation solution by grid methods is Hockney [2]. The best modern method is to use multiple grids - the multigrid method - as presented in [3], which includes a good summary of how the multigrid method absorbs and extends the earlier methods. Here only the main ideas are presented. The first concept of the multigrid idea is that an iterative solver such as the Gauss-Seidel solver smoothes the error of an approximation within a few iterations and can therefore be used as a smoother. The second concept is the so called coarse grid principle [3]: If an error is well smoothed it can be approximated on a (much) coarser grid without losing information. The low frequency components of the fine grid are transferred to high frequency components on the coarse grid. The error can be further reduced on the coarser grid with less computational effort, since the number of grid points is reduced. The error  $v_h^m$  of an approximation  $u_h^m$  of the solution  $u$  is defined by

$$v_h^m := u - u_h^m \quad (1)$$

and can generally be expressed by an Fourier expansion

$$v_h^m(\vec{x}) = \sum_{i,j,k=1}^{n-1} \alpha_{i,j,k} \sin(i\pi x) \sin(j\pi y) \sin(k\pi z) \quad (2)$$

The error can not be calculated directly, since the solution  $u$  of the Poisson equation is not known at any time. Therefore it is useful to define the defect or residual of the approximation  $u_h^m$  by

$$d_h^m := f_h - L_h u_h^m. \quad (3)$$

The defect is a measure of how much the Laplacian of a given approximation differs from the source term of the Poisson equation. It can therefore be used to determine the quality of the solver and its ability to converge. The defect equation

$$L_h v_h^m = d_h^m \quad (4)$$

is equivalent to the definition of the error

$$u = u_h^m + v_h^m. \quad (5)$$

## Ingredients of Multigrid Cycles

Generally, a multigrid iteration starts on the finest grid  $\Omega_h$  by applying some smoothing cycles to the approximation  $u_h^m$  to reduce the high frequency error. Then the defect  $d_h^m$  is calculated by equation (3) and restricted to the coarser grid by a restriction schema ( $d_{2h}^m$ ). The equation

$$L_{2h} \tilde{v}_{2h}^m = d_{2h}^m \quad (6)$$

has to be solved on  $\Omega_{2h}$ , where  $L_{2h}$  is the corresponding Laplacian on  $\Omega_{2h}$ . This can be either done recursively with another multigrid approach since equation (6) has the same form than the initial Poisson equation, or by a fast iterative solver. The defect equation (6) does not need to be solved exactly. A suitable approximation  $\tilde{v}_{2h}^m$  will work as well without essential loss of convergence speed [3]. After  $\tilde{v}_{2h}^m$  is computed it will be interpolated to the fine grid  $\tilde{v}_h$  ( $\Omega_h$ ) and the new approximation is found by

$$u_h^{m+1} = u_h^m + \tilde{v}_h^m. \quad (7)$$

Finally, some postsmoothing steps will be performed to  $u_h^{m+1}$ . An example of a multigrid iteration cycle is the W-cycle shown on Figure 1.

## COMPARISON TO MULTIPOLE EXPANSION METHOD

The potential at the end of a cell with a modulation of  $m = 2.3$  for the two different methods is shown in

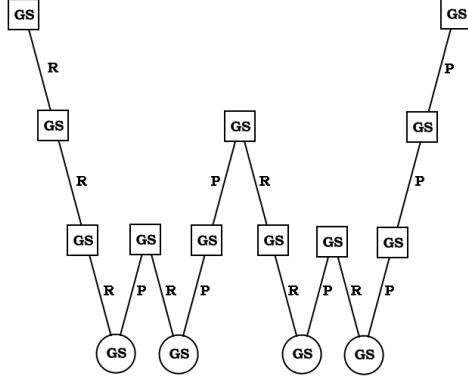


Figure 1: W-cycle.

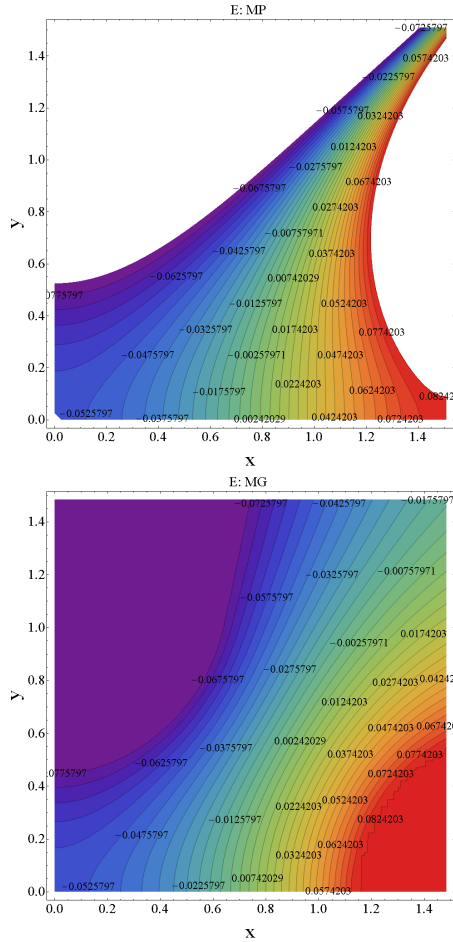


Figure 2: Potential at the end of an accelerating cell: Upper - from multipole expansion method; lower - from Poisson solver method.

Figure 2. Potentials that are greater than the vane voltage have been cut off. Obviously, the shape of the electrodes (white area) of the MP-potential is not even close to the shape of the electrodes. Close to the beam axis the two method give similar potentials, but with increasing

displacement from the beam axis, differences increase as well. In between the electrodes, the potential has to change from plus to minus the vane voltage. For the MP-potential the distance between the electrodes has become very small compared to the actual shape of the electrodes used in the MG-potential (potential from the multigrid Poisson solver), therefore the electric field calculated from the MP-potential will be higher than it actually is. Also the position of the horizontal vane in the MP-potential is too far away from the axes and therefore the corresponding electric field is too low. The absolute value of the electric field at the same

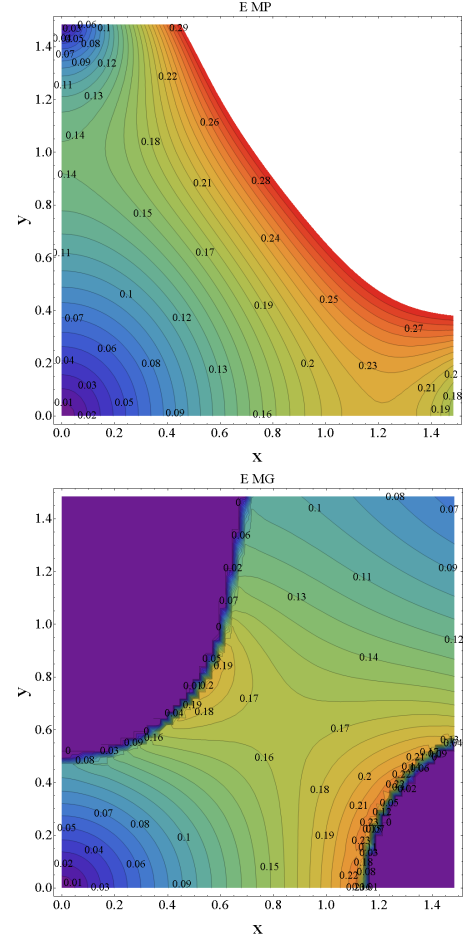


Figure 3: Absolute value of electric field at the end of an accelerating cell: upper - multipole expansion method; lower - Poisson solver method.

position is shown in Figure 3. The maximum electric field is in the region close to the electrodes and is seen to be quite different from the multipole expansion method. At bigger distances away from the beam axis (lower left corner) the MP-field increases to its maximum whereas the MG-field tends to decrease which is reasonable since the vane voltage remains constant and the distance between the electrodes increase.

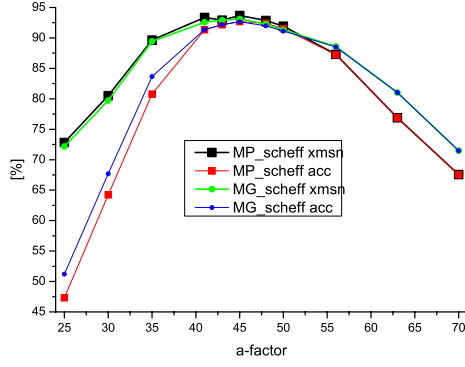


Figure 4: Transmission for the set of 11 RFQs for two different routines for the external field. Xmsn denotes transmission - particles are lost only radially. Acc denotes accelerated particles.

### Influence on Transmission

The influence of the different descriptions of the external field on the transmission on the set of RFQs are shown on Figure 4 for the same space charge routine. The aperture-factor is proportional to the reciprocal value of the aperture at the end of the shaper section. The transmission curves for the multipole expansion method and for the multigrid Poisson solver are very close for the RFQs with a medium and big aperture. Once the aperture has become small enough, the results from the two different method start to deviate from one another with the multigrid Poisson solver giving higher transmission. For the first three large aperture (a-factor 25, 30 and 35) RFQs the fraction of accelerated is higher for the MG cases than for the multipole expansion method. This behavior of the transmission curve fits quite well with the considerations so far. For big apertures, radial losses are not as large an effect, and the multipole expansion method agrees more closely with the Poisson solver. For smaller apertures the effects at the aperture and therefore at the edge of the area of validity of the multipole expansion method become important and the multigrid Poisson solver is a more accurate description of the external field.

## SPACE CHARGE

The multigrid Poisson solver can be used to calculate the effects of space charge as well. The boundary for the mesh is a grounded cylinder with the radius of twice the maximum aperture. Figure 5 shows the transmission curves for the set of RFQs for the space charge routines SCHEFF, PICNIC and the Poisson Solver. The shape of the curves agree quite well, but the absolute values vary a little. SCHEFF gives lower values (3%). PICNIC with two different settings and the multigrid Poisson solver agree very well over the whole curve (better than 1%), but the runtime of the Poisson solver is much shorter.

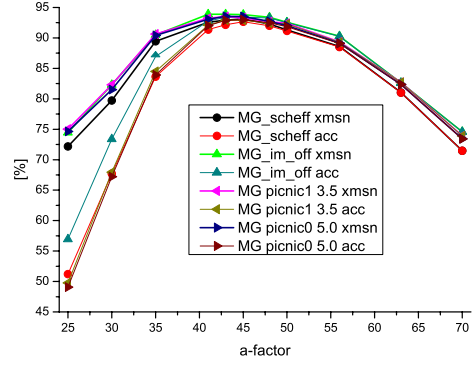


Figure 5: Transmission for the set of 11 RFQs for different space charge routines.

## CONCLUSION

The implemented multigrid Poisson solver shows good agreements to the well known multipole expansion method in the region where the multipole expansion is a good representation of the field. For small apertures particles tend to see wrong fields in the multipole expansion method. For space charge calculations the different routines compare within 3%, with higher transmission for the more accurate models. Further steps will be to use the multigrid Poisson solver to calculate the effect of image charges as well.

## REFERENCES

- [1] R.A. Jameson, "LA-UR-07-0876", Los Alamos National Laboratory
- [2] R.W. Hockney and J.W. Eastwood, "Computer Simulation Using Particles", IOP Publishing Ltd, Bristol and Philadelphia, 1988
- [3] U. Trottenberg and C.W. Oosterlee and A. Schüller, "Multigrid", Academic Press, London, 2001