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Validation of Space Charge Simulation in a Cyclotron

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Abstract: This note compares the results of space charge simulation that we performed in a cyclotron by using the PIC code `OPAL` and the envelope optics code `TRANSOPTR` respectively.

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1 Comparison

The Particle-In-Cell (PIC) technique has been commonly used in the simulation of charged particle motion in the presence of external and self-induced electromagnetic fields. OPAL [1] is one of the tools that utilize this technique to model charged-particle optics in accelerator structures and beam lines. We validated the simulation of OPAL with space charge force in a cyclotron. This was performed by simulating the evolution of a uniformly-charged sphere of multi-particles under the space charge force, and then comparing with the calculation result of TRANSOPTR [2] which integrates the envelope equation including linear space charge force, rather than using macro-particles. Initially, one million macro-particles are uniformly populated in a sphere of radius equal to $0.2''$. Each particle right starts from its static equilibrium orbit in the median plane, with tangential (i.e. azimuthal) momentum exactly matched with the particle's radial position, while axial (i.e. vertical) momentum assumed to be zero. The first test was using a perfectly isochronous magnetic field of zero flutter. As a result of the isochronism, the whole bunch remains round all the time in the (r, θ) plane, while in the vertical plane the bunch blows up due to the magnetic defocusing. This picture, as shown in Fig. 1, is easily conceivable when the space charge is null. Both OPAL and TRANSOPTR calculations give completely the same result.

When the space charge is switched on, the radial and azimuthal envelopes oscillate periodically with almost an identical frequency, while the vertical envelope blows up significantly faster than the case of zero space charge because of additional defocusing from the space charge. Again, OPAL and TRANSOPTR calculations give very well agreed results. See Fig. 2. This simulation was carried out for a bunch charge of 1.1 nC (i. e. 5 mA protons and 600 keV) in circulation for 6 turns in the cyclotron with no acceleration.

It's worthy to point out that for the TRANSOPTR calculation, the assignment of initial beam is not a trivial thing as TRANSOPTR is using s rather than using time as independent variable like what OPAL does. In our model, the spherical bunch's initial width of $\pm 0.2''$ in the radial direction is totally determined by the initial momentum spread of the particles and the machine's intrinsic dispersion given by as ρ/γ^2, where ρ is the orbital radius of curvature of the reference particle of relativistic factor γ. Besides, the cyclotron aperture is assumed to be sufficiently large so that none of the particles gets lost on the aperture. The run files for the space charge simulations are shown in the Appendix.

The second test simply replaced the isochronous field with a radially-decreasing field so that a vertical focusing is exerted. As a result, the bunch blows up longitudinally because the particles have momentum spread. Radially, the bunch remains round all the time, because every particle just stays on its own equilibrium orbit. Vertically, the envelope displays a periodic oscillation, because particles undergo the magnetic focusing. This is the right picture under zero space charge, revealed by both simulations shown in Fig. 3.

When space charge is turned on, the bunch envelope shows oscillation in each of 3 dimensions. Again, the PIC simulated result agrees well with that of envelope calculation. See Fig. 4.

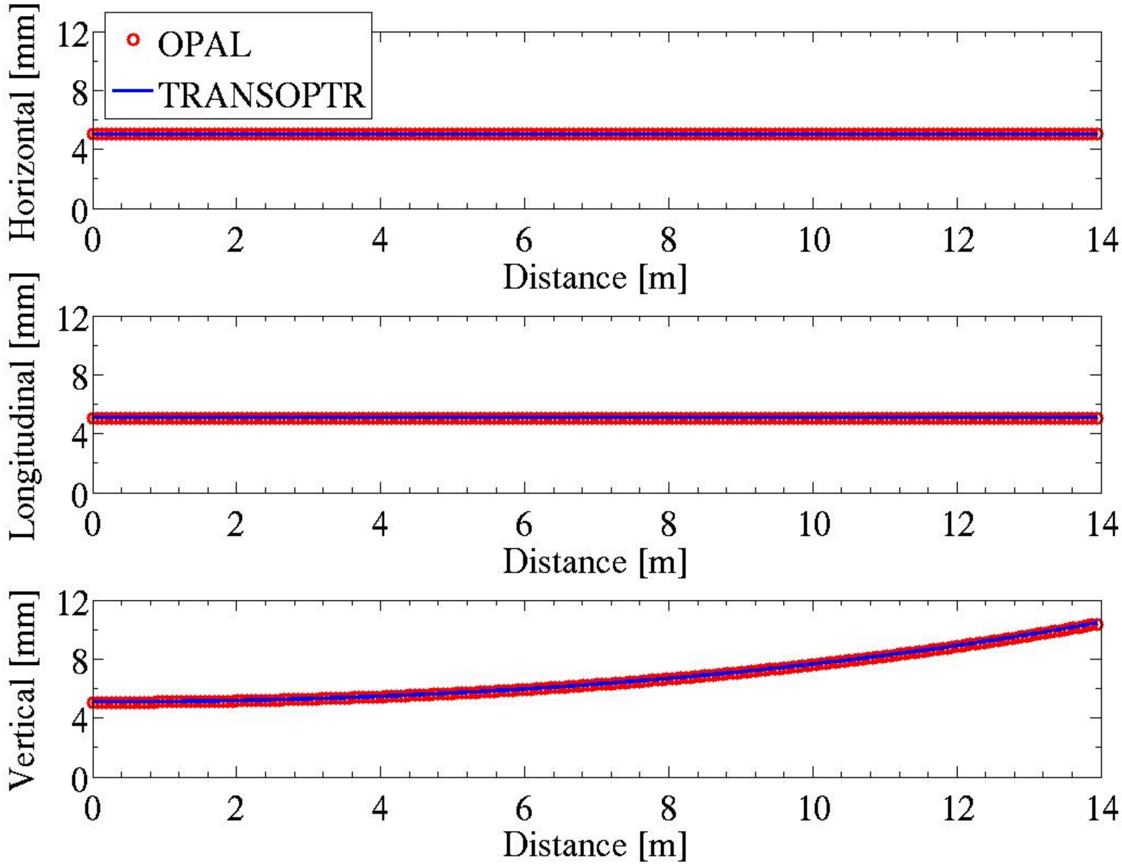

Figure 1: *Evolution of beam envelope (hard-edged) of an initially uniformly-charged sphere of 0.6 MeV protons traveling in an isochronous magnetic field for 6 turns with no acceleration, obtained from the PIC simulation and the envelope calculation respectively. Here the space charge force is turned off.*

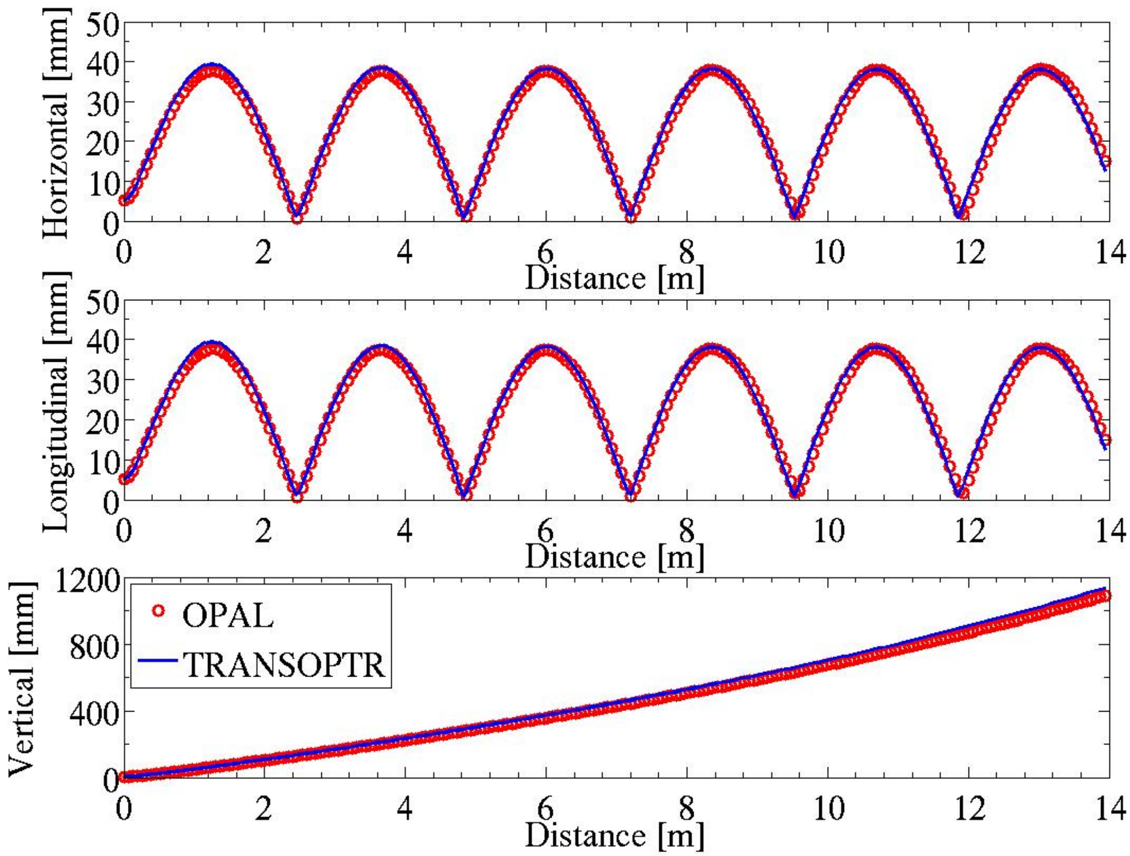

Figure 2: *Evolution of beam envelope (hard-edged) of an initially uniformly-charged sphere of 0.6 MeV and 1.1 nC traveling in an isochronous magnetic field for 6 turns with no acceleration, obtained from the PIC simulation and the envelope calculation respectively. Here the space charge force is switched on.*

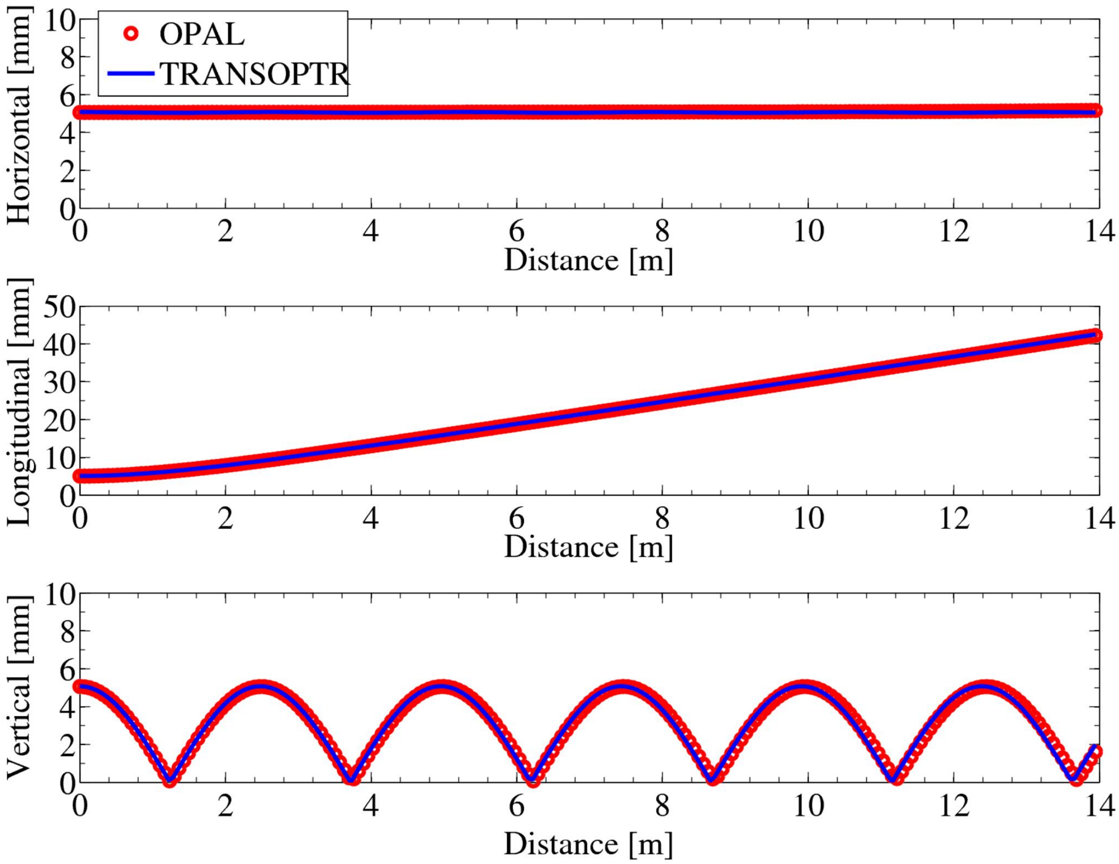

Figure 3: *Evolution of beam envelope (hard-edged) of an initially uniformly-charged sphere of 0.6 MeV protons traveling in a radially-decreasing magnetic field for 6 turns with no acceleration, obtained from the PIC simulation and the envelope calculation respectively. Here the space charge force is turned off.*

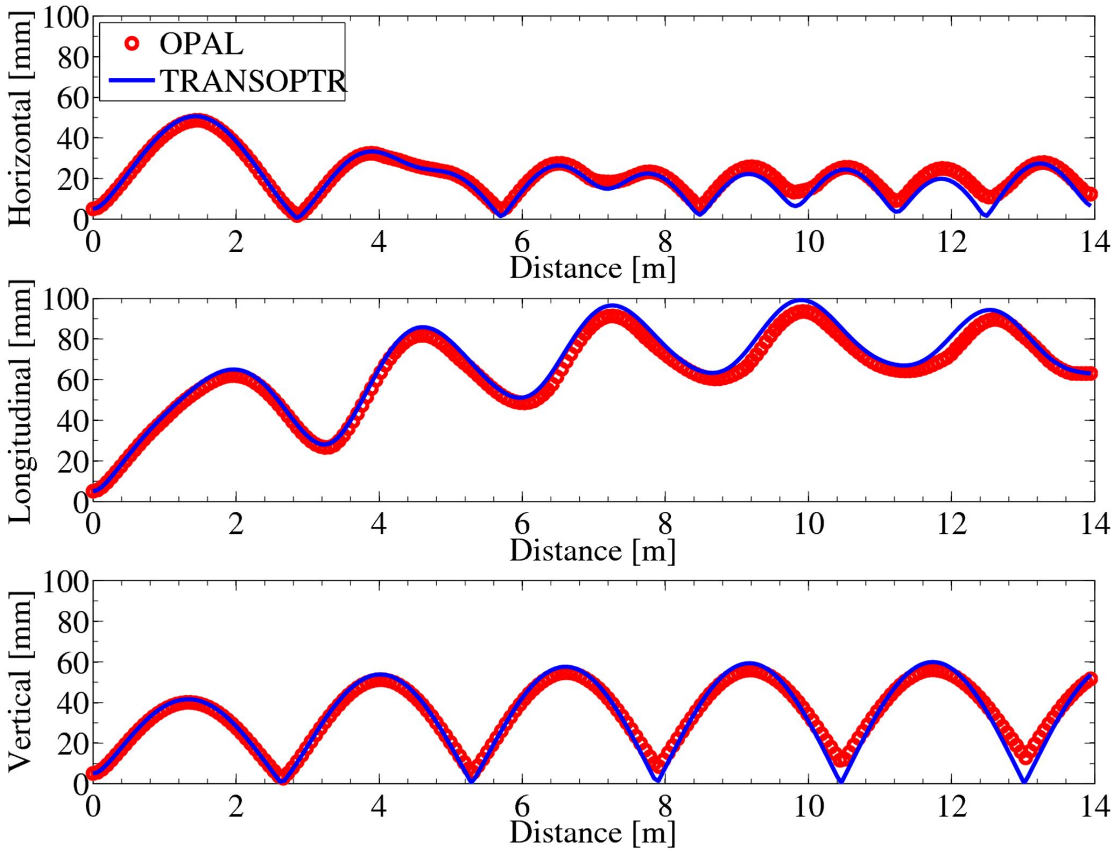

Figure 4: *Evolution of beam envelope (hard-edged) of an initially uniformly-charged sphere of 0.6 MeV and 1.1 nC traveling in a radially-decreasing magnetic field for 6 turns with no acceleration, obtained from the PIC simulation and the envelope calculation respectively. Here the space charge force is switched on.*

2 Appendix

2.1 OPAL Run Files

```
OPTION, ECHO= FALSE;
OPTION, PSDUMPFREQ= 10;
OPTION, PSDUMPLOCALFRAME= TRUE;
TITLE, STRING= "Ring";
Num_of_Turns   = 6;
RK_Steps_per_Turn = 360;
f0=4.611;
NHarm=1.0 ;
frf=f0*NHarm;
Ekin= 0.6e-3;
r0  = 369.882;
pr0 = 0;

gamma=(Ekin+PMASS)/PMASS;
beta=sqrt(1-(1/gamma^2));
gambet=gamma*beta;
P0 = gamma*beta*PMASS;

Ring: CYCLOTRON,
      TYPE=CARBONCYCL,
      SYMMETRY=1.0,
      CYHARMON=NHarm,
      RFFREQ=frf,
      PHIINIT=0,
      RINIT=r0 ,
      PRINIT=pr0,
      MINZ=-5000,
      MAXZ= 5000,
      MINR=   0,
      MAXR=5000,
      FMAPFN="./Create_Bz_Map/Bz_isochronous.dat";

L1:   LINE = (Ring);

Dist1: DISTRIBUTION, DISTRIBUTION=fromfile,
       FNAME="../s2_Create_Initial_Beam_for_OPAL/Particles4OPAL.dat";

Fs1:  FIELDSOLVER, FSTYPE=FFT,
      MX=32, MY=32, MT=32,
```

```
      PARFFTX=true, PARFFTY=true, PARFFTT=false,
      BCFFTX=open, BCFFTY=open, BCFFTT=open;

Beam1: BEAM,
       PARTICLE=PROTON,
       pc=P0,
       BFREQ= f0,
       BCURRENT=5e-3,
       NPART=100001;

SELECT, LINE=L1;

TRACK, LINE= L1,
       BEAM= Beam1,
       MAXSTEPS= RK_Steps_per_Turn * Num_of_Turns,
       STEPSPERTURN= RK_Steps_per_Turn;

RUN,   METHOD = "CYCLOTRON-T",
       BEAM= Beam1,
       FIELDSOLVER= Fs1,
       DISTRIBUTION= Dist1;
ENDTRACK;
STOP;
```

2.2 TRANSOPTR Run Files

2.2.1 Data File

```
0.6  0.  0.  938.272  1.  1.08436E-9
1  5  .1  0.5E-5
0  0.
.0  .0   .2  .0    .2   .013734
 0.3937008 1.  0.3937008 1.  0.3937008  1.   0.  0.3937008
5
 1 2 0.0   3 4 0.0    1 6 0.0   2 6 0.0   5 6 0.0
1
6.      0.   100.   0
1.E-4  20
10 0.0  0.95 10
```

2.2.2 System Subroutine

```
      SUBROUTINE tSYSTEM
      COMMON /BLOC1/ TurnN

      COMMON/MOM/P,BRHO,pMASS,ENERGK,GSQ,ENERGKi,charge,current
      COMMON/PRINT/IPRINT,IQ1,JQ1,IQ2,JQ2,IQ3,JQ3,IQ4,JQ4


      CV  = 2.99792458E8
      E0  = pMASS

      frf  = 4.611
      Harm = 1

      frev = frf/Harm
      Rinf = CV/(2.*3.1415926536 * frev*1.E6)

      GAM = sqrt(GSQ)
      BG  = sqrt(GSQ - 1.)
      BET = BG/GAM

      RHO = Rinf * BET
      Bz   = BRHO/RHO

      NHTurns = int(TurnN * 2)

      RHOin = RHO*100./2.54

      Find  = 1.-GSQ

      call disp_mat(RHOin/gsq, 0.,  0., 0., 0,0)
      call vective(1)
      call TRCYC(RHOin, Find, NHTurns)

      write(26,1003) frf, Rinf,
     &               ENERGKi,
     &               Bz, RHO
     &              ,Find
     &              ,int(TurnN)
 1003 format(/1x,'f_rf = ', F10.6,' MHz'/
     &        1x,'Rinf = ', F10.6,' m'//
     &        1x,'Ekin = ', F10.6,' MeV'/
     &        1x,'Bz   = ', F10.6,' Tesla'/
```

```
     &        1x,'RHO  = ', F10.6,' m'//
     &        1x,'Dipole Field Index = ', F10.6//
     &        1x,'# of Turns to run  = ',I6 )

      return
      end

      subroutine TRCYC(rho, Findex, nhturns)
c Inputs:
c rho = bend radius, in user given unit.
c nhturns= number of half turns
      COMMON/PRINT/IPRINT,IQ1,JQ1,IQ2,JQ2,IQ3,JQ3,IQ4,JQ4
      COMMON/MOM/P,BRHO,PMASS,ENERGK,gsq,ENERGKi,charge,current

      Field_index = Findex
      nsub = 20

      write(6,*) 'Field_index = ',  Field_index
      write(6,*) 'rho = ', rho

      do 999 i=1, nhturns

         do j=1, nsub
            CALL BE(rho, 180./nsub, Field_index, 1,0)
         enddo
         call vective(1)

 999  CONTINUE
      RETURN
      END
```

References

[1] Andreas Adelmann *et al.*, "The OPAL Framework (Object Oriented Parallel Accelerator Library) Version 1.4.0 (compiled March 30, 2016) User's Reference Manual," PSI Report, PSI-PR-08-02.

[2] R. Baartman, "TRANSOPTR: changes since 1984," TRIUMF Beam Physics Note, TRI-BN-16-06, May, 2016.