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REALISTIC SIMULATION OF THE 76-INCH CYCLOTRON: COMSOL MAGNETIC-FIELD EXPORT INTEGRATED WITH AN OPAL PARTICLE-TRACKING MODEL

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Abstract

Accurate studies of particle behavior in accelerator chambers require precise magnetic field maps with regard to the iron geometry. We generated a realistic magnetic-field map for the 76-inch cyclotron at Crocker Nuclear Lab using COMSOL Multiphysics, then imported it into the OPAL (Object-Oriented Parallel Accelerator Library) software to model particle trajectories. It accurately simulates beam dynamics, provides reliable validation against measured data, and establishes a foundation for future cyclotron optimization and upgrades.

INTRODUCTION

Our facility at UC Davis's Crocker Nuclear Lab (CNL) operates a 76-inch cyclotron, which is based on the design of the Oak Ridge Isochronous Cyclotron (ORIC) and has been operating since 1966. Despite its age and the removal of certain components, such as the valley and harmonic coils, the cyclotron continues operation. Unfortunately, historical data and some detailed documentation for our cyclotron have been lost, which means that although we know how to operate the machine, we know very little about the internal particle dynamics during operations. Scientists used to measure the magnetic field map by using a Hall probe with two-axis statistical analysis [1–3]. Unfortunately, we cannot open the chamber and spend a few weeks measuring the field. In order to get correct data, we have adopted finite element simulation of the magnetic field from COMSOL and use OPAL (Object Oriented Parallel Accelerator Library) [4] to analyze and predict particle behavior inside the machine, which will allow us to effectively analyze and predict particle behavior, including particle trajectories and tunes. This simulation will allow us to optimize performance and potentially plan upgrades without significant operational disruption.

PARTICLE-IN-CELL SIMULATION, OPAL

OPAL is a particle-in-cell (PIC) code for charged particle optics in linear, ring accelerator, cyclotron, etc. It has multiple flavors, such as OPAL-cycl, OPAL-t, and OPAL-map; each can only be applied to specific features. In our work, we used OPAL-cycl to model our structure. The goal of this study is to model particle behavior numerically within the cyclotron and accurately predict beam trajectories, which would result in more effective diagnostics for machine tuning and for planning upgrades.

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OPAL Structure

To model the particle trajectories with OPAL, the system requires the magnetic field in a specific format. Generally, the magnetic field can be expressed by

$$\frac{d\mathbf{p}(t)}{dt} = q\left(c\beta \times \mathbf{B} + \mathbf{E}\right), \tag{1}$$

which comes with rest mass, charge, and Lorentz factor. Our 76-inch cyclotron is designed to be isochronous, and we need to consider that the loss of isochronism due to the relativistic increase in mass limits the energy reach of a classical cyclotron. The momentum p per particle can be denoted in 3D Cartesian coordinates with normalization by $m_0 c$ as:

$$\begin{aligned}\frac{dp_x}{dt} &= \frac{q}{m_0 c}E_x + \frac{q}{\gamma m_0}(p_y B_z - p_z B_y),\\ \frac{dp_y}{dt} &= \frac{q}{m_0 c}E_y + \frac{q}{\gamma m_0}(p_z B_x - p_x B_z),\\ \frac{dp_z}{dt} &= \frac{q}{m_0 c}E_z + \frac{q}{\gamma m_0}(p_x B_y - p_y B_x).\end{aligned} \tag{2}$$

To simplify the model. We start with a single-particle tracking mode. The charged particle is only affected by the electric field E and the magnetic field B, which both are superpositions of external field and self-field.

$$\begin{aligned}\mathbf{E} &= \mathbf{E}_{\text{ext}} + \mathbf{E}_{\text{self}}\\ \mathbf{B} &= \mathbf{B}_{\text{ext}} + \mathbf{B}_{\text{self}}\,.\end{aligned} \tag{3}$$

For given E and B values, we could explicitly calculate each particle with the equation of motion of a charged particle in an electromagnetic field. We could also solve for E_{self} B_{self} numerically as a function of time. With the appropriate Lorentz Transformation L

The modeling capability of OPAL-cycl [5] is solving the Vlasov-Poisson equation system in the cyclotron with an external static magnetic field and fixed-frequency RF field. In modeling a high-intensity isochronous cyclotron, space charge effects should be considered not only in a single bunch but also in the mutual interactions of neighboring multiple bunches in the radial direction [6].

The magnetic field map at the center plane is read from an ASCII file. Instead of Cartesian coordinates, the system required a spherical coordinate frame. In this case, we could only consider two situations: whether the B-Field is at vertical axis $Z = 0$ or $Z \neq 0$

In most cyclotrons, we only measure the median plane B-field ($Z = 0$) by Gaussmeter. The magnetic field outside the median plane needs to be expanded along the Z axis.

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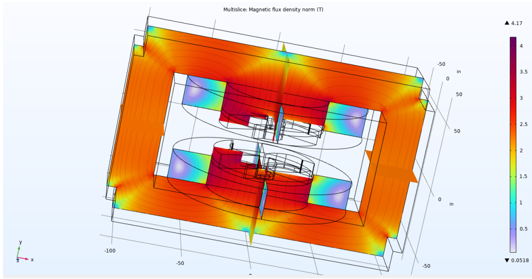

Figure 1: Simulated 3D magnetic field map generated by COMSOL. Blue = low field, red = high field.

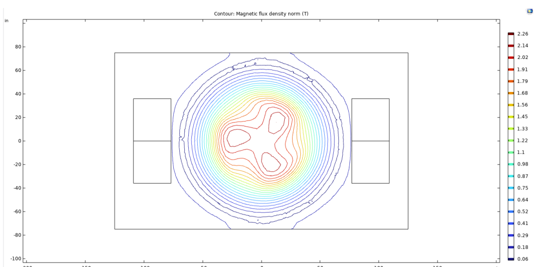

Figure 2: Simulated median-plane B_z map from COMSOL. Blue = minimum 0.0 Tesla , red = maximum 2.2 Tesla

According to the measurement provided by Gordon and Taivassalo [2, 7], we then expressed the field as:

$$B_r(r,\theta,z) = z\frac{\partial B_z}{\partial r} - \frac{1}{6}z^3 C_r, \tag{4}$$

$$B_\theta(r,\theta,z) = \frac{z}{r}\frac{\partial B_z}{\partial \theta} - \frac{1}{6}\frac{z^3}{r}C_\theta, \tag{5}$$

$$B_z(r,\theta,z) = B_z - \frac{1}{2}z^2 C_z \tag{6}$$

where $B_z \equiv B_z(r,\theta,0)$ and the coefficients are derived from the third-order Lagrange interpolation formula:

$$C_r = \frac{\partial^3 B_z}{\partial r^3} + \frac{1}{r}\frac{\partial^2 B_z}{\partial r^2} - \frac{1}{r^2}\frac{\partial B_z}{\partial r} + \frac{1}{r^2}\frac{\partial^3 B_z}{\partial r \partial \theta^2} - \frac{2}{r^3}\frac{\partial^2 B_z}{\partial \theta^2},$$

$$C_\theta = \frac{1}{r}\frac{\partial^2 B_z}{\partial r \partial \theta} + \frac{\partial^3 B_z}{\partial r^2 \partial \theta} + \frac{1}{r^2}\frac{\partial^3 B_z}{\partial \theta^3},$$

$$C_z = \frac{1}{r}\frac{\partial B_z}{\partial r} + \frac{\partial^2 B_z}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 B_z}{\partial \theta^2}\ . \tag{7}$$

In our model, we generated the magnetic field data through COMSOL Multiphysics(Figs. 1 and 2), which is software similar to ANSYS or TOSCA, so that we could realistically simulate the magnetic field with given geometry and physics conditions. We decided to use CARBONCYCL type, which only considers $Z = 0$ case in the OPAL-cycl.

COMSOL can only extract the data through Cartesian coordinates with the magnetic field at the median plane. To satisfy the requirement of OPAL-cycl, we need to transfer the data to spherical coordinates with six parameters at the header of a plain B_z [kG] data file, namely, $r_{\min}$ [mm], Δr [mm], $\theta_{\min}$ [°], $\Delta\theta$ [°], N_θ (total data number in each arc path of azimuthal direction), and N_r (total path number along radial direction). In addition, our trim coils were added through the trim-coil model in OPAL instead of directly modeling it by COMSOL due to calculation limitations.

Field Solver

While generating a particle tracking model, the space charge field can be obtained by a quasi-static approximation. In this approach, the motion of particles becomes non-relativistic in the beam rest frame, where the self-induced magnetic field is partially absent, and the electric field could be solved through the Poisson equation

$$\nabla^2\phi(\mathbf{x}) \quad = \quad -\frac{\rho(\mathbf{x})}{\varepsilon_0} \tag{8}$$

where ϕ and ρ are the electrostatic potential and the spatial charge density in the beam rest frame.

With the boundary condition, the scalar potential can be expressed in Green function,

$$\begin{aligned}\phi(r,\theta,z) \quad = \quad & \int\int\int r'\,dr'\,d\theta'\,dz'\ \rho(r',\theta',z') \\ & \times G(r,r',\theta,\theta',z,z') \end{aligned}\tag{9}$$

describing the contribution of a source charge at a location (r',θ',z') to the observation location(r,θ,z).

To solve the force convolution, we can apply the Fast Fourier Transform (FFT) with zero-padding of the data. The discrete convolutions arise in solving the Poisson equation. The special case of the solution would be the n-th of the brute force convolution equation [8].

$$\begin{aligned}\bar{\phi}_j &= \sum_{k=0}^{K-1}\bar{\rho}_k\bar{G}_{j-k}, \\ \text{with}\quad j &= 0,\ldots,J-1, \\ k &= 0,\ldots,K-1, \\ j-k &= -(K-1),\ldots,J-1,\end{aligned}\tag{10}$$

The relation between the sequences is given by:

$$\bar{G} = \bar{\phi} + \bar{\rho} - 1 \tag{11}$$

where $\bar{G}$ and $\bar{\rho}$ and $\bar{\phi}$ corresponds to the free space Green function, charge density of each particle, and scalar potential. To zero-pad the sequence to become a length, we take sequence elements N larger than or equal to the corresponding $\bar{G}$ elements M. Under the zero-padding condition, the Green's function can be defined periodically.

However, in our simulation, we only consider 2D symmetry model, which is easily simplified to

$$G_m = \begin{cases}\bar{G}_m, & \text{if } m = -(K-1),\ldots,J-1, \\ 0, & \text{if } m = J,\ldots,N-K, \\ G_{m+iN} = G_m, & \text{for } i \text{ integer.}\end{cases}\tag{12}$$

Taking the FFT in the region, $0 \le j \le N-1$ we can solve the formula explicitly. The scalar funciton ϕ become

$$\phi_j := \sum_{n=0}^{K-1}\bar{\rho}_n G_{j-n+iN}, \quad 0 \le j \le N-1. \tag{13}$$

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```
///---------cyclotron configuration---------///
// Definition of 10 trim coils for OPAL-cycl simulation with RMIN and RMAX//


TC1:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=99.949,  RMAX=164.719, BMAX=0.0868, SLPTC=1;
TC2:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=186.055, RMAX=250.825, BMAX=0.0781, SLPTC=1;
TC3:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=272.415, RMAX=337.185, BMAX=0.0747, SLPTC=1;
TC4:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=358.775, RMAX=423.545, BMAX=0.0729, SLPTC=1;
TC5:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=445.135, RMAX=509.905, BMAX=0.0711, SLPTC=1;
TC6:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=531.495, RMAX=596.265, BMAX=0.0694, SLPTC=1;
TC7:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=617.855, RMAX=682.625, BMAX=0.0676, SLPTC=1;
TC8:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=704.015, RMAX=768.785, BMAX=0.0658, SLPTC=1;
TC9:  TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=790.375, RMAX=855.145, BMAX=0.0641, SLPTC=1;
TC10: TRIMCOIL, TYPE="PSI-BFIELD-MIRRORED", RMIN=876.735, RMAX=941.505, BMAX=0.0623, SLPTC=1;


mm: CYCLOTRON, TYPE="CARBONCYCL", CYHARMON=2, PHIINIT=110.0, PRINIT=pr0, RINIT=r0 ,
          SYMMETRY=3.0, RFFREQ=f1, FMAPFN="bfield.dat",
          TRIMCOIL={TC1 TC2 TC3 TC4 TC5 TC6 TC7 TC8 TC9 TC10} , MBTC=14e-3, SLPTC=6.0;
```

Figure 3: Trim coil effect on the magnetic field map. Blue = negative ΔB, red = positive ΔB.

Due to the symmetry of Green's function, we could drop the $j - 1$ term.

APPLICATION

The isochronous cyclotron at UC Davis delivers a proton beam of 67.5 MeV energy at a current up to 0.13 mA, used for the treatment of eye cancer, the of radiation effects, and other research. It contains three sectors and an injector at the center. The beam energy rises from 3 keV to 67.5 MeV before the beam is extracted from the machine.

Trim Coils

Before tune calculation and modeling particle trajectories, we apply trim coils to modify the fixed magnetic field, as shown in Fig. 3. However, since we haven't finished the model, I would like to introduce PSI ring cyclotron simulation as an example. In PSI, the coupling resonance is $V_r = 2V_z$ crossed four times, as the tune calculation shows in Fig. 3, which is due to the large energy losses at the vertical beam. The plot of the trim coil matches with the OPAL simulation conclusion very well.

Particle Tracking Model

Precision particle tracking is the goal of the simulation process. To simplify the model, we start with single-particle tracking and would like to expand into a multi-particle tracking system, which should include the phase space calculation and all tracking position data. The system then solves the array with a field solver to analyze the position. We begin with single-particle tracking, expanding to multi-particle tracking with space charge, seen in Fig. 4.

CONCLUSION

With the finite element simulation we realized that the maximum magnetic field is about 2.0 Tesla, which matches our historical record. According to a measurement done a few years ago, the particle travels approximately 1000 turns in the chamber, and each turn is 44 nanosecond. The simulation from OPAL for a particle to get fully accelerated from 0 to 67.5 MeV is around 44 microsecond, which is the same as 1000 times 44 nanoseconds.

```
OPAL> * *********************** Bunch information in global frame: ***********************
OPAL> * ************** B U N C H *********************************************************
OPAL> * NP                = 2
OPAL> * Qtot              =        0.000 [fC]        Qi    =        0.000 [fC]
OPAL> * Ekin              =       67.500 [MeV]       dEkin =        0.000 [eV]
OPAL> * rmax              = (      0.00000 ,      4.69846 ,      5.00000 ) [mm]
OPAL> * rmin              = (     -1.71010 ,     -0.00000 ,      0.00000 ) [mm]
OPAL> * rms beam size     = (      0.00000 ,      0.00000 ,      0.00000 ) [um]
OPAL> * rms momenta       = (  0.00000e+00 ,  0.00000e+00 ,  0.00000e+00 ) [beta gamma]
OPAL> * mean position     = (     -1.71010 ,      4.69846 ,      5.00000 ) [mm]
OPAL> * mean momenta      = ( -3.62796e-01 , -1.32047e-01 ,  0.00000e+00 ) [beta gamma]
OPAL> * rms emittance     = (  0.00000e+00 ,  0.00000e+00 ,  0.00000e+00 ) (not normalized)
OPAL> * rms correlation   = (         -nan ,         -nan ,         -nan )
OPAL> * hr                = (     79.36508 ,      0.00000 ,     79.36508 ) [um]
OPAL> * dh                =   1.00000e-10 [%]
OPAL> * t                 =        0.000 [fs]        dT    =       61.728 [ps]
OPAL> * spos              =        0.000 [um]
OPAL> * ***********************************************************************************
OPAL>
OPAL> * Beginning of this run is at t = 0 [ns]
OPAL> * The time step is set to dt = 0.061728 [ns]
OPAL> * Single particle trajectory dump frequency is set to 10
OPAL> * The frequency to solve space charge fields is set to 1
OPAL> * The repartition frequency is set to 10
OPAL>
OPAL> * ------------------------- STATIC EQUILIBRIUM ORBIT MODE ----------------------------- *
OPAL> * Instruction: When the total particle number is equal to 2, SEO mode is triggered      *
OPAL> * automatically. This mode does NOT include any RF cavities. The initial distribution   *
OPAL> * file must be specified. In the file the first line is for reference particle and the  *
OPAL> * second line is for off-center particle. The tune is calculated by FFT routines based  *
OPAL> * on these two particles.                                                               *
OPAL> * ---------------- NOTE: SEO MODE ONLY WORKS SERIALLY ON SINGLE NODE ------------------ *
OPAL>
OPAL> * ---------------------- Start tracking ----------------------------------- *
OPAL>
OPAL> * ---------------------- DONE TRACKING PARTICLES ------------------------- *
OPAL> * Final energy of reference particle = 67.5 [MeV]
OPAL> * Total phase space dump number(includes the initial distribution) = 0
OPAL> * One can restart simulation from the last dump step (--restart -1)
OPAL>
OPAL> * **************** The result for tune calculation (NO space charge) ****************** *
OPAL> * Number of tracked turns: 1000
OPAL>
OPAL> * ************************************ nuR ***************************************** *
OPAL>
OPAL> * ===> 72000 data points  Ti=0 Tf= 4.4444e-05 -> T= 71999
OPAL>   0.00075000    19.96    0.001 2
OPAL>   0.00175000    14.40    0.149 6
```

Figure 4: Particle-tracking schematic from OPAL.

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