Algorithms and Methods for High Precision Computer Simulations of Cyclotrons for Proton Therapy: The Case of SC202

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(Dated: January 17, 2019)

Effective and accurate computer simulations are highly important in accelerator design and production. The most difficult and important task in cyclotron development is magnetic field simulations. It is necessary to achieve the accuracy of the model that is higher than the tolerance for the magnetic field in the real magnet. An accurate model of the magnet and other systems of the cyclotron allows us to perform beam tracking through the whole accelerator from the ion source to extraction. While high accuracy is necessary in the late stages of research and development, high performance of the simulations and ability to swiftly analyze and apply changes to the project play a key role in the early stages of the project. Techniques and algorithms for high accuracy and performance of the magnet simulations have been created and used for the development of the SC202 cyclotron for proton therapy, which is under production by collaboration between JINR (Dubna, Russia) and ASIPP (Hefei, China).

I. INTRODUCTION

Two cyclotrons are planned to be manufactured in China: one will operate in Hefei cyclotron medical center, the other will replace Phasotron in Medico-technical complex JINR Dubna1,2 and will be used to treat cancer with protons. We developed computer programs for cyclotron design and implemented them in MATLAB/Simulink environment3. MATLAB software is widely used in accelerator physics4–6. There are number of MATLAB-based application programs for particle tracking. The “Simple Accelerator Modelling in Matlab” (SAMM)4 code is a set of Matlab routines for modelling beam dynamics in high energy particle accelerators. Accelerator Toolbox (AT) is a collection of tools to model storage rings5. We use MATLAB to create input data sets and to access them via Simulink block diagrams during simulation. We perform thousands of particle tracking simulations in the cyclotron in parallel and analyze and visualize the data in MATLAB.

II. MAGNET DESIGN AND BEAM DYNAMICS SIMULATIONS

3D magnet simulation is the most important part when it comes to the development of an isochronous superconducting cyclotron as it defines particle motion in the accelerator. Magnet modeling goes hand in hand with beam dynamics modeling.

Beam dynamics simulations solve the system of differential equations of particle motion with field maps from FEM (finite element method) codes or field measurements with different initial coordinates and velocities. The fourth-order Runge-Kutta method is usually used to solve the system. Systems of differential equations of motion of charged particles in an electromagnetic field are derived from the Newton-Lorentz equations:

$$\frac{d\vec{V}}{dt} = \frac{q}{m} \sqrt{1 - \frac{V^2}{c^2}} \left\{ \vec{E} + \left[ \vec{V} \times \vec{B} \right] \right\} T_0 - \frac{1}{c^2} \vec{V} \left( \vec{V} \cdot \vec{E} \right),$$

where \( \vec{V} \) is the velocity of a charged particle, \( \vec{E} \) and \( \vec{B} \) are the electric and magnetic fields correspondingly,

$$\begin{align*}
\rho'' - \frac{2\rho'^2}{r} - \rho &= \frac{q}{mcV} \sqrt{r^2 + r'^2 + z'^2} \left( r B_z - z' B_\phi - \phi' \frac{r}{r^2} \rho B_r + \frac{2}{r} \frac{r'}{r^2} B_r + \frac{2}{r} B_r + \frac{2}{r} \frac{r'}{r^2} \right) \\
\zeta'' - \frac{2\zeta'^2}{r} - \zeta &= \frac{q}{mcV} \sqrt{r^2 + r'^2 + z'^2} \left( \rho' B_\phi - r B_r - \frac{r'}{r} \frac{2}{r} \rho B_r + \frac{2}{r} B_r - \frac{r'}{r} \frac{2}{r} \frac{r'}{r^2} \right) \\
t' &= \frac{1}{cB} \left( r^2 + r'^2 + z'^2 \right)^{1/2} = \frac{1}{c} \sqrt{\left( r^2 + r'^2 + z'^2 \right)^{1/2}}.
\end{align*}$$

In cyclotrons, it is most convenient to use the cylindrical coordinate system \((r, \phi, z)\). So the representation of the equations of motion with an independent variable azimuth angle \(\phi\) is widely used in the design of cyclotrons. Simulink block diagrams for tracking particles in electromagnetic fields for these equations of motion were created and used for different cyclotrons7,8. Simulink has a disadvantage: the complexity of the block diagram used to simulate the particle motion through the whole accelerator can increase drastically with the number of accelerator systems (harmonic coils, extraction elements) and beam effects like vacuum losses, space charge effects etc. Therefore, we rewrote Simulink block diagrams used for cyclotron design, including the CYCLOPS-like code, in Matlab code. CYCLOPS program9 is one of the most reliable tools for dynamics analysis in cyclotrons. We implemented a version of CYCLOPS using MATLAB R2018a. The program has an equilibrium orbit search algorithm and performs calculations of orbital (Fig. 1) and betatron frequencies (Fig. 2). The calculation results can be used for the isochronisation of the
magnetic field map. Another possible way to use this program is to take its results as input parameters for 3D beam dynamics simulations. The equilibrium orbit search algorithm requires a 2D magnetic field map (in polar coordinate system) of the cyclotron median plane as an input parameter. The field map is preprocessed and smoothed as described in section 3. To improve performance, the map is accessed via Matlab’s griddedInterpolant class. The equations of motion are solved via an ODE solver (ode45 of MATLAB R2018a) employing the fourth-order Runge-Kutta algorithm. Our implementation allows simultaneous calculation of a large number of particles, which improves performance due to lower number of loops and more efficient use of RAM memory. For \(10^6\) particles, the calculation time was 332 seconds (the calculation was executed in a CPU Intel Core i7-7700k 4,2GHz with 64GB of RAM memory). To achieve necessary accuracy, without decrease in performance, we used a timestep of \(2\pi/720\) s in units of \(\omega_c^{-1}\) (\(\omega_c\) is the cyclotron frequency), so that each turn corresponds to approximately 720 timesteps.

### III. REPRESENTATION OF THE ELECTROMAGNETIC FIELD

When calculating particle trajectories, an electromagnetic field can be specified analytically, in the form of a field map obtained as a result of measurements (2D maps) or as a result of model calculations (3D field maps). The representation in the form of a 3D field map is obviously the most acceptable for calculations of beam dynamics, but maps can be huge when high accuracy is needed.

The major problem of R&D phase of the SC202 project was that 3D simulations of the magnet were very time-consuming and it was difficult to achieve acceptable accuracy of the simulated field. In order to fix this issue, CST studio macros and quick analysis of the magnet field map in MATLAB have been developed. Scripts for producing 3D magnetic field maps in CST studio and for reading them into the Matlab workspace were written. This technique allowed us to increase the number of simulated magnet geometries to over 5000 in half a year. Such fine tuning allowed us to optimize the magnet in a very short time.

Using a 2D field map in the median plane for beam dynamics simulations is a traditional method which is widely used in cyclotron physics. Vertical and other components of the magnetic field at the distance \(z\) from the median plain can be calculated by:

\[
B_r = z\frac{\partial B}{\partial r} + \frac{\partial}{\partial r} \left[ \sum_{n=1}^{\infty} (-1)^n \frac{2n+1}{(2n+1)!} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r} \frac{\partial^2}{\partial \phi^2} \right)^n B \right]
\]

\[
rB_\phi = \frac{\partial}{\partial \phi} \left[ \sum_{n=1}^{\infty} (-1)^n \frac{2n+1}{(2n+1)!} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r} \frac{\partial^2}{\partial \phi^2} \right)^n B \right]
\]

\[
B_z = B + \left[ \sum_{n=1}^{\infty} (-1)^n \frac{2n}{(2n)!} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \right)^n \frac{\partial^2}{\partial \phi^2} B \right]
\]

The expansions are presented for a cylindrical coordinate system, which is most suitable for cyclotrons. A rigorous proof of these expansions is presented in\(^\text{10}\). The paper reviews the expansion to arbitrary order. We used the expansion to 2nd order for heavy-ion beam tracking in the CYTRACK cyclotron, which has been working on track membrane production in Dubna since 2004\(^\text{11}\), however, when developing a superconducting cyclotron for medium energy, such as SC202, it is necessary to study the effects of various nonlinear resonances, therefore we have added an expansion to 4th order in our codes.

It is important to be able to calculate all derivatives for correct beam dynamics simulations during research and development, and especially on the commissioning stage, when...
Figure 3. Derivatives of the magnetic field in the median plane taken without smoothing algorithms.

Figure 4. Derivatives of the magnetic field in the median plane taken with smoothing algorithms.

Real magnetic field will be measured only on the median plane (Fig. 3).
The biggest problem of these calculations is that the derivatives must be taken using the measured or calculated field map, which already contains errors. Special smoothing algorithms were applied in order to obtain smooth and realistic derivatives of the magnetic field on the median plane. In particular, we used a MATLAB function SMOOTHN, that provides a fast, unsupervised and robust discretized spline smoother for data of arbitrary dimension\textsuperscript{12,13}.

Fig. 4 represents the results, that were obtained by combining fitting of the field map with spline surface together with smoothing algorithms.

Due to the symmetrical design of the magnet of the cyclotron (usually four fold symmetry), the magnetic field in the median plane is a periodical function from the azimuth angle. As almost every periodical function it could be represented as a Fourier series. Fourier series are easy to differentiate so all angle derivatives (which is half of all) do not need smoothing mentioned above.

So, we have the following ways to get a 3D map of the magnetic field:

- Straightforward one: we obtain raw 3D field map from the simulation.

- Using Maxwell’s equations on 2D map in median plane (usually measured) and some interpolation with smoothing.

- Same as previous, but this time we apply Fourier analysis.

These approaches were coded in MATLAB and performed on three packages: CST, TOSCA and COMSOL. The developed software creates 3D field maps which can be used for beam dynamic simulations.

IV. ACCELERATING RF SYSTEM DESIGN

It is also important for beam dynamics simulations to use an adequate representation of the accelerating field. We simulated the accelerating RF cavity in CST Studio. Both electric and magnetic fields of the RF cavity from 3D simulations were used in particle tracking from the ion source to the extraction point of the SC202. Scripts for producing 3D field maps in CST Studio and for reading them into the MATLAB workspace were written. The code for accelerating voltage distribution calculation was also created. The voltage value was obtained by integrating the electric field in the median plane of the resonant cavity (Fig. 5).

V. CONCLUSION

Codes for beam dynamics simulations were improved with new algorithms where the magnetic field components outside the median plane are calculated up to fourth order.

Scripts were written for producing 3D magnetic field maps, 3D electric and magnetic field maps from RF cavity simulations in CST Studio and for reading them into the MATLAB workspace. MATLAB, being a matrix-oriented tool, allows us to implement an equilibrium orbit search algorithm for a large number of particles with different energies with a good calculation speed.

High accuracy and high efficiency of simulations will help on the commissioning stage during the shimming of the magnet.

REFERENCES

\textsuperscript{1} G.A. Karamysheva et al., Compact Superconducting Cyclotron SC200 for proton therapy, in \textit{Proceedings of Cyclotrons and Their Applications 2016} (Cyclotrons and Their Applications 2016, Zürich, Switzerland, Sept. 2016) pp. 371–373

\textsuperscript{2} The Medico-technical complex JINR Dubna, http://mtk.jinr.ru

\textsuperscript{3} MATLAB, The MathWorks, Inc., Natick, MA, United States.

\textsuperscript{4} A. Wolski, Simple Accelerator Modelling in Matlab, http://pcwww.liv.ac.uk/~awolski/main_links_computercodes.htm

\textsuperscript{5} A. Terebilo, Accelerator Toolbox for MATLAB, SLAC-PUB-8732, May 2001

\textsuperscript{6} D. Campo et al., Central region and static orbit study for the 300 A MeV superconducting cyclotron - 2007. \textit{Cyclotrons and Their Applications}, pp. 391-393.

\textsuperscript{7} Y. Jongen et al., Compact superconducting cyclotron C400 for hadron therapy, \textit{Nuclear Instruments and Methods}, A 624, A 624, Issue 1, p.47-53, 2010
9. G.A. Karamysheva, S.A. Kostromin., Beam dynamics study in the C235 cyclotron for proton therapy. *PEPAN letters*, 6, 1, 2008.

9. Gordon, M.M., 1984. Computation of closed orbits and basic focusing properties for sector-focused cyclotrons and the design of "cyclops". *Part. Accel.*, 16, pp. 39-62.

10. Hart, T.L. et al., Magnetic Field Expansion Out of a Plane: Application to Inverse Cyclotron Muon Cooling, in *arXiv:1105.2754 [physics.acc-ph]*

11. Yu. N. Denisov, V. V. Kalinichenko, and G. A. Karamysheva, Heavy ions dynamic simulations in CYTRACK cyclotron. *Review of Scientific Instruments* 75, 367 (2004).

12. Garcia D. Robust smoothing of gridded data in one and higher dimensions with missing values. *Computat Statist Data Anal*, 2010; 54: 1167-1178.

13. Garcia D. A fast all-in-one method for automated post-processing of PIV data. *Exp Fluids*, 2011; 50: 1247-1259.