Using Bicubic Interpolation of Simion arrays instead of Bilinear Interpolation Greatly Improves Ion Trap Fields Analysis

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INTRODUCTION

The analysis of the fields of ion trap designs as shown by the presenting author at ASMS in 2017 and 2019 provides a deeper insight into the subsequent dynamics of ions in ion traps. In 2019 we showed a method to determine the Fourier-Taylor expansion of a trap modeled in Simion 8.2, by:

$$V(r,\theta) = \frac{V_0}{2}\sum_{n=0}^{\infty} C_n\left({}^{r}/_{r_0}\right)\cos(n\,\theta),$$

Where the C_n are in general functions of ${}^{r}/_{r_0}$, but are given as $({}^{r}/_{r_0})^n$ for pure multipoles. This lends itself to Fourier-Taylor analysis, which is used here. However, the test cases presented in 2019 showed that the accuracy of the analysis yielded results far from machine double precision.

Here we show that the cause of the inaccuracies observed in the 2017 and subsequently the 2019 results were due to the bilinear interpolation method used in Simion. We show that using a bicubic interpolation adequately fixes the inaccuracy.

METHODS

In the poster presented at ASMS2019 we showed that a series of test analyses of the ideal 2D quadrupole potential revealed firstly that our Taylor-Fourier (TF) method correctly determined a quadrupole potential to double precision machine accuracy. However, if the same potential was written into a Simion potential array and the potential interpolation function of Simion was used to feed the analysis, then a comb of harmonic components appeared in the analysis at half the machine accuracy. We have replaced the bilinear interpolation of Simion with a Bicubic interpolation and demonstrate the performance advantages.

Bicubic interpolation on a grid square using the values of the potential on the four corners of the grid square plus the estimated x, y, and mixed partial derivatives at the four corners to solve for the sixteen coefficients a_{ij}.

$$V(x,x) = \sum_{i=0}^{3}\sum_{j=0}^{3} a_{ij}x^i y^j$$

Once the coefficients are found, one can easily interpolate the potential at any point (x,y) in the grid square. The partial derivatives at (x,y), i.e the field components are also easily calculated. For example:

$$\frac{\partial V}{\partial x}(x,y) = \sum_{i=0}^{3}\sum_{j=0}^{3} a_{ij}\; i\; x^{i-1}y^j$$

RESULTS

We test this method on the well known 2D quadrupole potential as shown in fig 1.

$$V(r,\theta) = \frac{V_0}{2}\left({}^{r}/_{r_0}\right)^2 cos(2\theta)$$

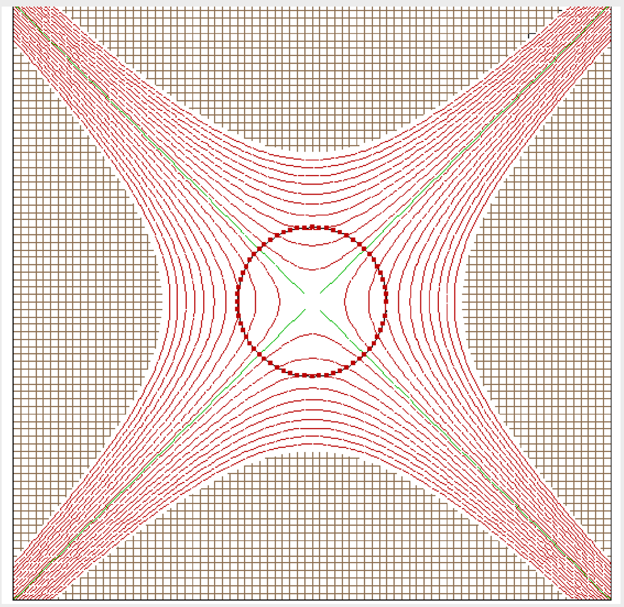

Fig 1: Calculated Quadrupole Fields

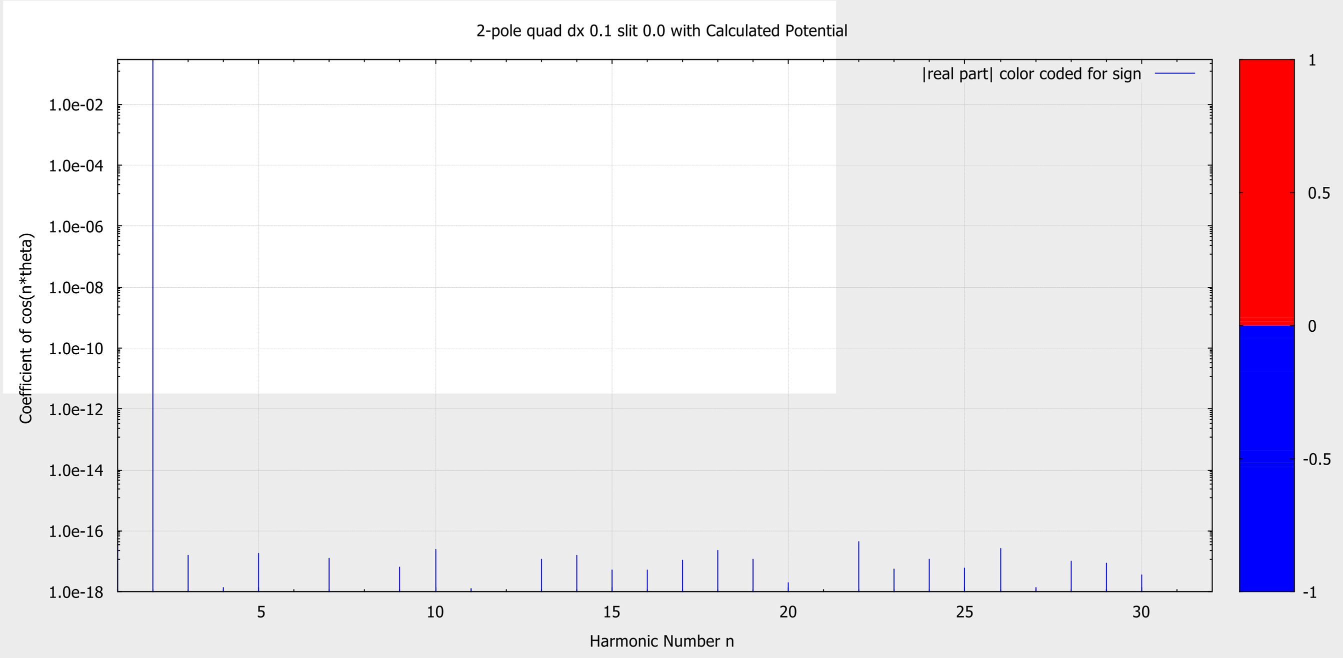

Fig 2a: FFT coefficients of direct calculation

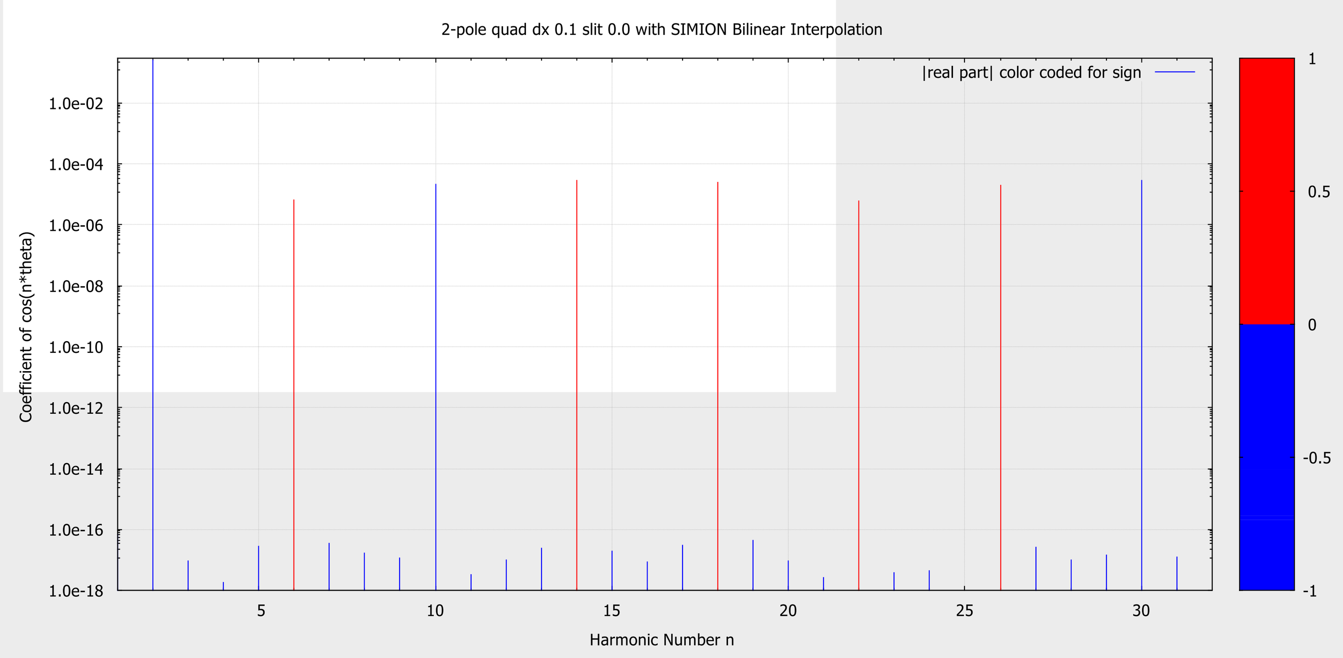

Fig 2b: FFT coefficients of bilinear interpolation

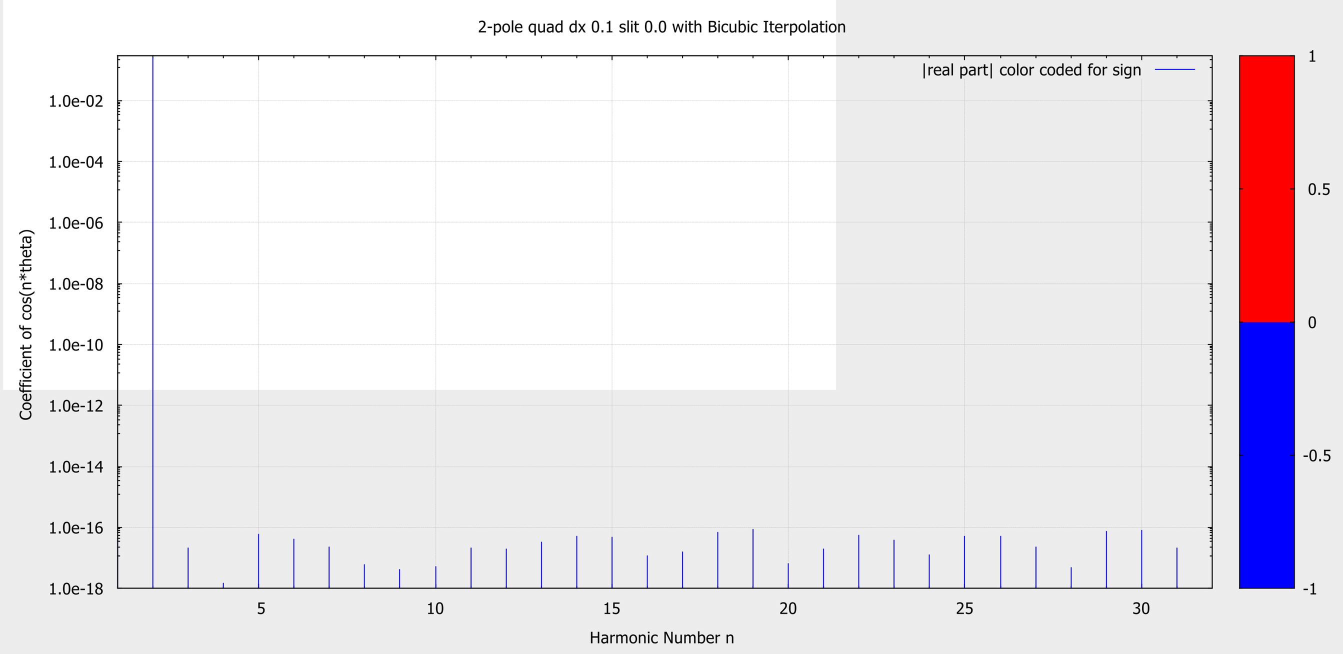

Fig 2c: FFT coefficients of bicubic interpolation

The quadrupole potential is calculated by several methods at 64 points on the circle shown in figure 1. This set of points is analyzed by FFT and the results are shown in:

(Fig. 2a) Direct calculation of the potential

(Fig. 2b) Bilinear interpolation of the potential

(Fig. 2c) Bicubic interpolation of the potential.

CONCLUSION

These results shown in figures 2a through 2c demonstrate the clear advantages of using bicubic interpolation over bilinear interpolation for the purposes of analyzing the potentials. The bicubic interpolation shown in figure 2c is shown to be near the limit of machine accuracy of double precision floating point. While the bilinear interpolation in figure 2b shows anomalous Fourier components greater than ten orders of magnitude above the machine accuracy.

This work identifies and fixes the interpolation accuracy of potentials in Simion for Ion Trap design and analysis.

Future Work

Future work could explore using bicubic interpolation for more accurate trajectory calculations in ion traps.

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