

Mass Spectrometry & Purification Techniques

**Research Article** 

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# Mass Resolution Study in the Cylindrical Ion Trap by Using Three-Point One Block Method

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#### Abstract

Motion equations in cylindrical ion trap (CIT) coupled in *u* and *v* (respective *r* and *z*), and thus, can only be treated as a rough approximation. Hence, studies on cylindrical ion trap (CIT) equations are more complicated and involved. Therefore, a three point one block method (3POBM) of Adams Moulton type is presented to study a cylindrical ion trap (CIT) motion equations. The advantage of the three point one block method (3POBM) is to estimate the approximate solutions directly at three points simultaneously. Numerical results from three point one block method (3POBM) will compare with fifth order Runge-Kutta method (RKM5). The proposed three points one block method has a potential application to solve complicated linear and nonlinear equations of the charge particle confinement in the cylindrical field especially in fine tuning accelerators, and generally speaking, in physics of high energy. The physical properties of the confined ions in the *r* and *z* axises are illustrated and the fractional mass resolutions  $m/\Delta m$  of the confined ions in the first stability region was analyzed by the fifth order Runge-Kutta method (RKM5) and three points one block method (3POBM).

**Keywords:** Cylindrical ion trap; Three point one block method; Fifth order Runge-Kutta method; Lagrange interpolating polynomial; Ion trajectories

#### Introduction

An ion trap mass spectrometer may incorporate a Penning trap [1], Paul trap [2] or the Kingdon trap [3]. The Orbitrap, introduced in 2005, is based on the Kingdon trap [4]. The two most common types of ion traps are the Penning trap and the Paul trap (Quadrupole ion trap) [5-9]. Other types of mass spectrometers may also use a linear Quadrupole ion trap as a selective mass filter.

A Quadrupole ion trap mass analyzer with simplified geometry, the cylindrical ion trap (CIT), was shown to be well-suited to use in miniature mass spectrometers and even mass spectrometer arrays. Experiments with a single miniature CIT showed acceptable resolution and sensitivity, limited by the ion trapping capacity of the miniature device. The CIT has received much attention of a number of research groups because of several merits. The CIT is easier to fabricate than the Paul ion trap which has hyperbolic surfaces [10]. And the relative simplicity and small size of the CIT make it an ideal candidate for miniaturization. With these interests, many groups in, such as Purdue University [11] and Oak Ridge National Laboratory [12] have researched on the applications of the CIT to a miniaturized mass spectrometry.

#### Formulation of Three Point One Block Method

Numerical solutions for ODEs have great importance in scientific computation as they were widely used to model in representing the real world problems such as Quadrupol ion trap with damping force. Many of these problems are of higher order and cannot be solved analytically and hence the use of numerical methods is advocated. There are several methods that can be used to solve the higher order ODEs numerically [13]. Block method for numerical solution of higher order ODEs directly had been proposed by several researchers [13-17]. The general theory of block method for solving first order ODE is given in Fatunla [15]. A two point block methods for solving higher order ODEs directly are described by Majid [14]. In this paper, we shall consider two point one block method for the numerical solution of solving second order ODEs in the form

$$y''=f(x,y,y'), a \le x \le b \tag{1}$$

subject to an initial conditions

$$y(a) = y_0, y'(a) = y'_0$$

in the interval [*a*, *b*]. The proposed two point block method will approximate the solutions at two points simultaneously.

In this section, we have divided the interval [a, b] into a series of blocks with each block containing three points. Three approximate values that are  $y_{n+1}$ ,  $y_{n+2}$  and  $y_{n+3}$  are simultaneously found using the same back values.

The first point of the method will be obtained by integrating Equation (1) once and twice over the interval  $[x_n, x_{n+1}]$ . By integrating Equation (1) once gives:

$$\int_{x_n}^{x_{n+1}} y''(\mathbf{x}) d\mathbf{x} = \int_{x_n}^{x_{n+1}} f(\mathbf{x}, \mathbf{y}, \mathbf{y}') d\mathbf{x} \text{ and}$$

$$y'(\mathbf{x}_{n+1}) - \mathbf{y}'(\mathbf{x}_n) = \int_{x_n}^{x_{n+1}} f(\mathbf{x}, \mathbf{y}, \mathbf{y}') d\mathbf{x}$$
Integrating Equation (1) trained since:
(2)

Integrating Equation (1) twice gives:  $\int_{x_{rel}}^{x_{rel}} \int_{x_{rel}}^{x} \int_{x_{rel}}^{x}$ 

$$\int_{x_n}^{x_n} \int_{x_n}^{x_n} y''(\mathbf{x}) dx dx = \int_{x_n}^{x_n} \int_{x_n}^{x_n} f(\mathbf{x}, \mathbf{y}, \mathbf{y}') dx dx \text{ and}$$

$$y(x_{n+1}) - y(x_n) - hy'(x_n) = \int_{x_n}^{x_{n+1}} (x_{n+1} - x) f(x, y, y') dx \qquad (3)$$

The second point of the method obtain by integrating (1) over the interval  $[x_n, x_{n+2}]$  once and twice will respectively give,

$$y'(x_{n+2}) - y'(x_n) = \int_{x_n}^{x_{n+2}} f(x, y, y') dx$$
(4)

$$y(x_{n+2}) - y(x_n) - 2 hy'(x_n) = \int_{x_n}^{x_{n+2}} (x_{n+2} - x) f(x, y, y') dx$$
 (5)

The same process is applied to derive the third point of the method, integrate (1) over the interval  $[x_n, x_{n+3}]$  once and twice will respectively

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Received May 14, 2017; Accepted May 23, 2017; Published May 29, 2017

Citation: Chaharborj SS, Gheisari Y (2017) Mass Resolution Study in the Cylindrical Ion Trap by Using Three-Point One Block Method. Mass Spectrom Purif Tech 3: 117. doi:10.4172/2469-9861.1000117

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give,

$$y'(x_{n+3}) - y'(x_n) = \int_{x_n}^{x_{n+3}} f(x, y, y') dx$$
(6)

$$y(x_{n+3}) - y(x_n) - 3hy'(x_n) = \int_{x_n}^{x_n} (x_{n+3} - x) f(x, y, y') dx$$
(7)

We can rewrite the (2), (3), (4), (5), (6) and (7) into r point k step Adams Moulton:

$$y'_{n+r} - y'_n = h \sum_{j=0}^{n} \beta_j f_{n+j-k+2}$$
 (8)

$$y_{n+r} - y_n - rhy'_n = h^2 \sum_{j=0}^k \gamma_j f_{n+j-k+2}, r = 1, 2, 3$$
(9)

Figure 1 showed the seven mesh points *i.e.*,  $(x_{n-3}, f_{n-3})$ ,  $(x_{n-2}, f_{n-2})$ ,  $(x_{n-1}, f_{n-1})$ ,  $(x_n, f_n)$ ,  $(x_{n+1}, f_{n+1})$ ,  $(x_{n+2}, f_{n+2})$  and  $(x_{n+3}, f_{n+3})$  involved in the three point one block method. Therefore, we substitute k=6 into Equation (8) and (9) will obtain,

$$h\sum_{j=0}^{6} \beta_{j} f_{n+j-4} = \int_{x_{n}}^{x+r} f(x, y, y') dx, \qquad (10)$$
$$h^{2} \sum_{j=0}^{6} \gamma_{j} f_{n+j-4} = \int_{x_{n}}^{x+r} (x_{n+r} - x) f(x, y, y') dx$$

with r=1, 2, 3. The function  $f(x, y, y^0)$  in (10) will be replaced by Lagrange interpolating polynomial. Lagrange Interpolating is a method of finding an unique polynomial,  $P_n$  which passes through a specified set of points. Define  $x_0$ ,  $x_1$ ,  $x_2$ , ...,  $x_n$  are (n+1) distinct numbers obtained from a function f, then exists a polynomial as follows:

$$p_{n}(x) = \sum_{k=0}^{n} f(x_{k})L_{k}(x)$$
(11)  
Where  $L_{k} = \frac{(x - x_{0})(x - x_{1})...(x - x_{k-1})(x - x_{k+1})...(x - x_{n})}{(x_{k} - x_{0})(x_{k} - x_{1})...(x_{k} - x_{k-1})(x_{k} - x_{k+1})...(x_{k} - x_{n})}$ 

$$\prod_{i=0}^{n} \frac{(x - x_{i})}{(x_{k} - x_{i})} \text{ for each } k = 0, 1, ..., n$$

For the general case when there are n+1 points, the polynomial,  $P_n$  in Equation (11) are *nth*-order. Seven interpolating points involved in three point one block method, we will obtain the lagrange interpolating polynomial,  $P_6$  from Equation (11).

Let 
$$S = \frac{x - x_{n+3}}{h}$$
, replacing  $dx = hds$  gives,  
 $h(\beta_0 f_{n-3} + \beta_1 f_{n-2} + \beta_2 f_{n-1} + \beta_3 f_n + \beta_4 f_n + \beta_4 f_{n+1} + \beta_5 f_{n+2} + \beta_6 f_{n+3} = \int_{-3}^{-3+r} P_6 hds$   
 $h^2(\gamma_0 f_{n-3} + \gamma_1 f_{n-2} + \gamma_2 f_{n-1} + \gamma_3 f_n + \gamma_4 f_n + \gamma_4 f_{n+1} + \gamma_5 f_{n+2} + \gamma_6 f_{n+3} = \int_{-3}^{-3+r} -(s+2)P_6 h^2 ds$ 
(12)

Evaluate these integrals in (12) using MAPLE. The value of the coefficients,  $\beta_i$  and  $\gamma_i$ , *i*=0, 1, 2, ..., 6 can be obtained. The corrector formulae of three point one block method as follows:



$$y'_{n+r} = y'_{n} + h(\beta_{0}f_{n-3} + \beta_{1}f_{n-2} + \beta_{2}f_{n-1} + \beta_{3}f_{n} + \beta_{4}f_{n+1} + \beta_{5}f_{n+2} + \beta_{6}f_{n+3}$$

$$y_{n+r} = y_{n} + hy'_{n} + h^{2}(\gamma_{0}f_{n-3} + \gamma_{1}f_{n-2} + \gamma_{2}f_{n-1} + \gamma_{3}f_{n} + \gamma_{4}f_{n+1} + \gamma_{5}f_{n+2} + \gamma_{6}f_{n+3}$$
(13)

with *r*=1, 2, 3. Where the coefficient  $\beta_i$  and  $\gamma_i$ , *i*=0, 1, 2, 3, 4, 5, 6 shown in Table 1.

Apply the same process to find the predictor formulae of the two point direct method. The method is the combination of predictor of one order less than the corrector. The Euler method will be used only once at the beginning of the code to find the additional points for the starting initial points. The Euler method also will solve the problem directly. Then, the predictor and corrector direct method can be applied until the end of the interval. The sequence of computation involved was *PECE* where *P* and *C* indicate the application of the predictor and corrector formula respectively and *E* indicate the evaluation of the function *f*. The convergence test involved the corrector formulae and it will be iterated to convergence. The iterates are said to have converged when an iterate  $y_{n+2}^{(0)}$  satisfies as follows:

$$\Box y_{n+2}^{(i)} - y_{n+2}^{(i-1)} \Box \le 0.1 \times TOL, i = 1, 2, ...,$$
(14)

where  $y_{n+2}^{(0)}$  is come from predictor formula and "TOL" mean Tolerance. For numerical results has been used *Tol*=10<sup>-10</sup>.

#### Electric Field Inside Cylindrical Ion Trap

In cylindrical ion trap (CIT), the hyperbolic ring electrode [18], as in Paul ion trap, is replaced by a simple cylinder and the two hyperbolic end-cap electrodes are replaced by two planar end-plate electrodes [19]. If opposite pairs of the electrodes have steady potentials  $\Psi_0$  and  $-\Psi_0$  [20], the potential difference applied to the electrodes [18,21] is:

$$\Psi(r, \theta, z) = \sum_{i} \frac{2\Psi_{0}}{m_{i}r_{1}} \frac{J_{0}(m_{i}r)}{m_{i}r_{1}} \frac{ch(m_{i}z)}{(m_{i}z_{1})},$$
(15)  
With

$$\Psi_0 = U_{dc} + V_{ac} \cos(\Omega t) \tag{16}$$

Where  $U_{dc}$  is a direct potential,  $U_{ac}$  is the zero to peak amplitude of the RF voltage, and  $\Omega$  is RF angular frequency [20]. The electric field in a cylindrical coordinate  $(r, z, \theta)$  inside the CIT can be written as follows:

$$(E_{r}, E_{0}, E_{z}) = \begin{bmatrix} \sum_{i} \frac{2\Psi_{0}}{r_{1}} \cdot \frac{J_{0}(m_{i}r)}{J_{1}(m_{i}r_{1})} \cdot \frac{ch(m_{i}z)}{ch(m_{i}z_{1})} \\ 0 \\ -\sum_{i} \frac{2\Psi_{0}}{r_{1}} \cdot \frac{J_{0}(m_{i}r)}{J_{1}(m_{i}r_{1})} \cdot \frac{sh(m_{i}z)}{ch(m_{i}z_{1})} \end{bmatrix}$$
(17)

here,  $\nabla$  is gradient. From Equation (17), the following is retrieved:

$$(E_r, E_0, E_z) = \begin{bmatrix} \sum_{i} \frac{2\Psi_0}{r_1} \cdot \frac{J_0(m_i r)}{J_1(m_i r_1)} \cdot \frac{ch(m_i z)}{ch(m_i z_1)} \\ 0 \\ -\sum_{i} \frac{2\Psi_0}{r_1} \cdot \frac{J_0(m_i r)}{J_1(m_i r_1)} \cdot \frac{sh(m_i z)}{ch(m_i z_1)} \end{bmatrix},$$
(18)

The equation of the motions [8,18,19,22-24] of the ion of mass m and charge e can be written as

$$d^2 u J_1(\lambda_i u) ch(\lambda_i v)$$

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r	i	0	1	2	3	4	5	6
	β	$\frac{67}{2520}$	$\frac{67}{2520}$	$\frac{-2257}{20160}$	$\frac{1027}{2016}$	$\frac{10273}{20160}$	$\frac{271}{6048}$	$\frac{271}{60480}$
1	Yi	$\frac{271}{20160}$	$\frac{271}{20160}$	$\frac{12067}{30240}$	$\frac{12067}{30240}$	$\frac{191}{1152}$	$\frac{253}{120960}$	$\frac{253}{120960}$
	$\boldsymbol{\beta}_i$	$\frac{-1}{126}$	$\frac{-1}{126}$	$\frac{11}{1260}$	$\frac{1621}{1260}$	$\frac{1621}{1260}$	$\frac{-37}{3780}$	$\frac{-37}{3780}$
2	Yi	$\frac{1}{42}$	$\frac{1}{42}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{1890}$
	$\beta_i$	$\frac{271}{20160}$	$\frac{271}{20160}$	$\frac{12067}{30240}$	$\frac{12067}{30240}$	$\frac{-139}{6720}$	$\frac{-139}{6720}$	$\frac{253}{120960}$
3	Y <sub>i</sub>	$\frac{27}{448}$	$\frac{27}{448}$	$\frac{1689}{1120}$	$\frac{1689}{1120}$	$\frac{459}{448}$	$\frac{459}{448}$	$\frac{9}{128}$

Table 1: The coefficients for the corrector formulae of three point one block method.

Methods ↓	X <sub>max</sub>	V <sub>max</sub>
RKM5	0.64	5982.9425
3POBM	0.63	6077.9099

**Table 2:** The values of  $\chi_{max}$  and  $V_{max}$  for the cylindrical ion trap in the first stability region when  $\alpha$ =0 with using RKM5 and three-point one block method (3POBM) when h=0.01 and h=0.05, respectively.



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$$\frac{d^2 u}{d\xi^2} - (\alpha - 2\chi \cos 2\xi) \sum_i \frac{J_1(\lambda_i u)}{J_1(\lambda_i)} \cdot \frac{\operatorname{ch}(\lambda_i v)}{\operatorname{ch}\left(\lambda_i \frac{z_1}{r_1}\right)} = 0,$$
(19)

$$\frac{d^2v}{d\xi^2} - (\alpha - 2\chi\cos 2\xi) \cdot \sum_i \frac{J_0(\lambda_i u)}{J_1(\lambda_i)} \cdot \frac{\operatorname{sh}(\lambda_i v)}{ch\left(\lambda_i \frac{z_1}{r_1}\right)} = 0,$$
(20)

and the following

$$r_{1}^{2} = 2z_{1}^{2}, \ \xi = \frac{\Omega t}{2}, \ m_{i}r_{1} = \lambda_{i}, \ \frac{r}{r_{1}} = u \ \frac{z}{r_{1}} = v, \ \alpha = -8\frac{e}{m} \cdot \frac{U_{dc}}{r_{1}^{2}\Omega^{2}}, \ \chi = -4\frac{e}{m} \cdot \frac{V_{ac}}{r_{1}^{2}\Omega^{2}}$$

Where  $J_0$  and  $J_1$  are the Bessel functions of the first kind of order 0 and order 1, respectively, whereas *ch* is the hyperbolic *cosine* function,  $m_i r$  is the roots of equation  $J_0(m_i r)=0$ ,  $U_{dc}$ , whereas  $V_{ac}$  are the amplitudes and the radio frequency (rf) drive frequency. Equations (19) and (20) are coupled in *u* and *v* (respective *r* and *z*), and thus, can only be treated as a rough approximation [19,23,25-27]. Therefore, studies on CIT equations are more difficult and complex.

#### Implementation of Block Method in Cylindrical Ion Trap Motion Equations

In this section implementation of block method has been done for cylindrical ion trap motion equations. From Equation (13) with Equation (19) and Equation (20), respectively we have, the corrector formulae of the three point one block method as follow:

$$y'_{n+1} = y'_{n} + \frac{h}{60480} - \left(191f_{n-3} + 1608f_{n-2} - 6771f_{n-1} + 37504f_{n-3} + 30819f_{n+1} - 2760f_{n+2} + 271f_{n+3}\right)$$
(21)

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{120960} \left( -191f_{n-3} + 1626f_{n-2} - 7029f_n + 48268f_{n-1} + 20055f_{n+1} - 2502f_{n+2} + 253f_{n+3} \right)$$
(22)

$$y'_{n+2} = y'_{n} + \frac{h}{3780} \left( 5f_{n-3} - 30f_{n-2} + 33f_{n-1} + 1328f_{n} + 4863f_{n+1} + 1398f_{n+2} - 37f_{n+3} \right)$$
(23)

$$y_{n+2} = y_n + 2hy'_n + \frac{h^2}{1890} \left( -5f_{n-3} + 45f_{n-2} - 213f_{n-1} + 1678f_n + 2169f_{n+1} + 105f_{n+2} + f_{n+3} \right)$$
(24)

$$y'_{n+3} = y'_{n} + \frac{h}{2240} \left( -29f_{n-3} + 216f_{n-2} - 729f_{n-1} + 2176f_{n} + 1161f_{n+1} + 3240f_{n+2} + 685f_{n+3} \right)$$
(25)

$$y_{n+3} = y_n + 3hy'_n + \frac{3h^2}{4480} \left( -11f_{n-3} + 90f_{n-2} - 369f_{n-1} + 2252f_n + 3123f_{n+1} + 1530f_{n+2} + 105f_{n+3} \right)$$
(26)

here y=u or y=v with

$$f_{n-3} = (\alpha - 2\chi \cos 2\xi_{n-3}) \sum_{i} \frac{(J_1 \lambda_i u(\xi_{n-3}))}{J_1(\lambda_i)} \cdot \frac{ch(\lambda_i v(\xi_{n-3}))}{ch(\lambda_i \frac{z_1}{r_1})},$$

$$f_{n-2} = (\alpha - 2\chi \cos 2\xi_{n-2}) \sum_{i} \frac{(J_1 \lambda_i u(\xi_{n-2}))}{J_1(\lambda_i)} \cdot \frac{ch(\lambda_i v(\xi_{n-2}))}{ch(\lambda_i \frac{z_1}{r_1})},$$

$$f_{n-1} = (\alpha - 2\chi \cos 2\xi_{n-1}) \sum_{i} \frac{(J_1 \lambda_i u(\xi_{n-1}))}{J_1(\lambda_i)} \cdot \frac{ch(\lambda_i v(\xi_{n-1}))}{ch(\lambda_i \frac{z_1}{r_1})},$$

$$f_n = (\alpha - 2\chi \cos 2\xi_n) \sum_{i} \frac{(J_1 \lambda_i u(\xi_n))}{J_1(\lambda_i)} \cdot \frac{ch(\lambda_i v(\xi_n))}{ch(\lambda_i \frac{z_1}{r_1})},$$

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$$f_{n+1} = (\alpha - 2\chi \cos 2\xi_{n+1}) \sum_{i} \frac{(J_1 \lambda_i u(\xi_{n+1}))}{J_1(\lambda_i)} \cdot \frac{ch(\lambda_i v(\xi_{n+1}))}{ch(\lambda_i \frac{z_1}{r_1})},$$

$$f_{n+2} = (\alpha - 2\chi \cos 2\xi_{n+2}) \sum_{i} \frac{(J_1 \lambda_i u(\xi_{n+2}))}{J_1(\lambda_i)} \cdot \frac{ch(\lambda_i v(\xi_{n+2}))}{ch(\lambda_i \frac{z_1}{r_1})},$$

$$f_{n+3} = (\alpha - 2\chi \cos 2\xi_{n+3}) \sum_{i} \frac{(J_1 \lambda_i u(\xi_{n+3}))}{J_1(\lambda_i)} \cdot \frac{ch(\lambda_i v(\xi_{n+3}))}{ch(\lambda_i \frac{z_1}{r_1})},$$

and

$$\begin{split} f_{n-3} &= -\left(\alpha - 2\chi\cos 2\xi_{n-3}\right) \sum_{i} \frac{\left(J_{0}\lambda_{i}u\left(\xi_{n-3}\right)\right)}{J_{1}(\lambda_{i})} \cdot \frac{sh\left(\lambda_{i}v\left(\xi_{n-3}\right)\right)}{ch\left(\lambda_{i}\frac{z_{1}}{r_{1}}\right)},\\ f_{n-2} &= -\left(\alpha - 2\chi\cos 2\xi_{n-2}\right) \sum_{i} \frac{\left(J_{0}\lambda_{i}u\left(\xi_{n-2}\right)\right)}{J_{1}(\lambda_{i})} \cdot \frac{sh\left(\lambda_{i}v\left(\xi_{n-2}\right)\right)}{ch\left(\lambda_{i}\frac{z_{1}}{r_{1}}\right)},\\ f_{n-1} &= -\left(\alpha - 2\chi\cos 2\xi_{n-1}\right) \sum_{i} \frac{\left(J_{0}\lambda_{i}u\left(\xi_{n-1}\right)\right)}{J_{1}(\lambda_{i})} \cdot \frac{sh\left(\lambda_{i}v\left(\xi_{n-1}\right)\right)}{ch\left(\lambda_{i}\frac{z_{1}}{r_{1}}\right)}, \end{split}$$

$$f_{n} = -\left(\alpha - 2\chi\cos 2\xi_{n}\right)\sum_{i}\frac{\left(J_{0}\lambda_{i}u\left(\xi_{n}\right)\right)}{J_{1}(\lambda_{i})}\cdot\frac{sh\left(\lambda_{i}v\left(\xi_{n}\right)\right)}{ch\left(\lambda_{i}\frac{z_{1}}{r_{1}}\right)}$$
$$f_{n+1} = -\left(\alpha - 2\chi\cos 2\xi_{n+1}\right)\sum_{i}\frac{\left(J_{0}\lambda_{i}u\left(\xi_{n+1}\right)\right)}{J_{1}(\lambda_{i})}\cdot\frac{sh\left(\lambda_{i}v\left(\xi_{n+1}\right)\right)}{ch\left(\lambda_{i}\frac{z_{1}}{r_{1}}\right)},$$

$$f_{n+2} = -\left(\alpha - 2\chi\cos 2\xi_{n+2}\right)\sum_{i} \frac{\left(J_{0}\lambda_{i}u\left(\xi_{n+2}\right)\right)}{J_{1}(\lambda_{i})} \cdot \frac{sh\left(\lambda_{i}v\left(\xi_{n+2}\right)\right)}{ch\left(\lambda_{i}\frac{z_{1}}{r_{1}}\right)},$$

$$f_{n+3} = -\left(\alpha - 2\chi\cos 2\xi_{n+3}\right)\sum_{i} \frac{\left(J_{0}\lambda_{i}u\left(\xi_{n+3}\right)\right)}{J_{1}(\lambda_{i})} \cdot \frac{sh\left(\lambda_{i}v\left(\xi_{n+3}\right)\right)}{ch\left(\lambda_{i}\frac{z_{1}}{r_{1}}\right)},$$
for Equations (10) and (20) are extincted.

for Equations (19) and (20), respectively.

#### Numerical Results

Figures 2a and 2b show the ion trajectories in real time for cylindrical ion trap with  $\alpha$ =0 and  $\chi$ =0.4,  $z_1$ =0.05 and  $r_1 = \sqrt{2}z_1$ , (a): red

color (solid line): RKM5 method using h=0.01 steps, (*b*): black color (dash line): three-point one block method using h=0.05 steps. Figure 3 shows the ion trajectories in u - v plan for cylindrical ion trap with  $\alpha$ =0 and  $\chi$ =0.4,  $z_1$ =0.05 and  $r_1 = \sqrt{2}z_1$ ,(*a*): red color (solid line): RKM5 method using h=0.01 steps, (*b*): black color (dash line): three-point one block method using h=0.1 steps. Figure 4a and 4b show the ion trajectories for cylindrical ion trap in z-z plan for  $\alpha$ =0 and  $\chi$ =0.4,  $z_1$ =0.05 and  $r_1 = \sqrt{2}z_1$ ,(*a*): red color (solid line): RKM5 method using h=0.01 steps. Figure 4a and 4b show the ion trajectories for cylindrical ion trap in z-z plan for  $\alpha$ =0 and  $\chi$ =0.4,  $z_1$ =0.05 and  $r_1 = \sqrt{2}z_1$ ,(*a*): red color (solid line): RKM5 method using h=0.01 steps, (*b*): black color (dash line): three point one block method using h=0.05 steps.

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Numerical examples has been tested for  $t \in [0,60]$  and  $TOL=10^{-10}$ . The results obtained from three point one block method and fifth order Runge-Kutta method are comparable for h=0.05 and h=0.01, respectively. The running steps taken by three-point one block method using h=0.05 and RKM5 using h=0.01 are 601 and 6000, respectively. Therefore, to obtain the comparable results from both method the total number of running steps for RKM5 is around 10 times more than three-point one block method. Hence, the execution time taken by three-point one block method using h=0.05 is less than RKM5 method using h=0.01.

## The effect of three-point one block method on the mass resolution

The resolution of a cylindrical ion trap mass spectrometry [22] in general, is a function of the mechanical accuracy of the hyperboloid of the CIT  $\Delta r_1$ , and the stability performances of the electronics device such as, variations in voltage amplitude  $\Delta V$ , the rf frequency  $\Delta \Omega$  [22,28], which tell us, how accurate is the form of the voltage signal. Here we study the resolution of a cylindrical ion trap with RKM5 and three-point one block methods.

Table 2 shows the values of  $\chi_{max}$  and  $V_{max}$  for the cylindrical ion trap in the first stability region when  $\alpha$ =0 with using RKM5 and three-point one block method when h=0.01 and h=0.05, respectively. The values of  $V_{max}$  has been obtained for <sup>131</sup>Xe with  $\Omega$ =2 $\Pi$  × 1.05 × 10<sup>6</sup> rad/s, U=0 V and  $z_0$ =0.82 cm in the first stability region when  $\alpha$ =0. To derive a useful theoretical formula for the fractional resolution, one has to recall the stability parameters of the impulse excitation for the CIT with RKM5 and three-point one block methods, respectively as follows,

$$\chi_{RKM5} = 4 \frac{e}{m} \times \frac{V_{RKM5}}{r_1^2 \Omega^2},$$
(27)

$$\chi_{3POBM} = 4 \frac{e}{m} \times \frac{V_{3POBM}}{r_1^2 \Omega^2}.$$
(28)

Here "RKM5" and "3POBM" mean fifth order Runge-Kutta method and three-point one block method, respectively. By taking the partial derivatives with respect to the variables of the stability parameters  $\chi_{RKM5}$ for Equation (27) and  $\chi_{3POBM}$  for Equation (28), then the expression of the resolution  $\Delta m$  of the CIT with RKM5 and 3POBM are as follows,

$$\Delta m = \frac{8eV_{RKM5}}{r_1^3 \Omega^2 \chi_{RKM5}} \left| \Delta r_1 \right| + \frac{4e}{r_1^2 \Omega^2 \chi_{RKM5}} \left| \Delta V_{RKM5} \right| + \frac{8eV_{RKM5}}{r_1^2 \Omega^3 \chi_{RKM5}} \left| \Delta \Omega \right|, \tag{29}$$

$$\Delta m = \frac{8eV_{3POBM}}{r_1^3 \Omega^2 \chi_{3POBM}} \left| \Delta r_1 \right| + \frac{4e}{r_1^2 \Omega^2 \chi_{3POBM}} \left| \Delta V_{3POBM} \right| + \frac{8eV_{3POBM}}{r_1^2 \Omega^3 \chi_{3POBM}} \left| \Delta \Omega \right|, \tag{30}$$

Now to find the fractional resolution we have,

$$\frac{m}{\Delta m} = \left\{ \left| \frac{\Delta V_{RKM5}}{V_{RKM5}} \right| + 2 \left| \frac{\Delta \Omega}{\Omega} \right| + 2 \left| \frac{\Delta r_1}{r_1} \right| \right\} - 1, \quad (31)$$

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**Figure 3:** The ion trajectories in *u*-*v* plan for cylindrical ion trap with  $\alpha$ =0 and  $\chi$ =0.4,  $z_1$ =0.05 and  $r_1 = \sqrt{2}z_1$ , (*a*): red color (solid line): RKM5 method using *h*=0.01 steps, (*b*): black color (dash line): three-point one block method using *h*=0.1 steps (color figure just online).









$$\frac{m}{\Delta m} = \left\{ \left| \frac{\Delta V_{3POBM}}{V_{3POBM}} \right| + 2 \left| \frac{\Delta \Omega}{\Omega} \right| + 2 \left| \frac{\Delta r_1}{r_1} \right| \right\} - 1,$$
(32)

here Equation (31) and Equation (32) are the fractional resolutions for CIT with RKM5 and 3POBM, respectively. For the fractional mass resolution we have used the following uncertainties for the voltage, rf frequency and the geometry;  $\Delta V/V=10^{-5}$ ,  $\Delta\Omega/\Omega=10^{-7}$ ,  $\Delta r_1/r_1=3 \times 10^{-4}$ . The fractional resolutions obtained are  $m/\Delta m=1638.806949$ ;1638.380841 for RKM5 and three-point one block methods with using 0.01 and 0.05 steps, respectively. When three-point one block method is applied, the rf only limited voltage is increased by the factor of approximately 1.01587, therefore, we have taken the voltage uncertainties as  $\Delta V_{3POBM} = 1.01587 \times 10^{-5}$ . When these fractional resolutions are considered for the tritium isotope mass m=3.20, then, we have  $\Delta m=0.001952640$  and 0.1953148 for RKM5 and three-point one block methods with using 0.01 and 0.05 steps, respectively. This means that, as the value of  $m/\Delta m$  is decreased, the power of resolution is increased due to increment in  $\Delta m$ . Experimentally, this means that the width of the mass signal spectra is better separated (Figure 5).

#### **Discussion and Conclusion**

We have demonstrated the three points one block method to solve some complicated differential equations concerned the cylindrical ion trap. We can observe to obtain the comparable results from both methods the total number of running steps for RKM5 is around ten times more than three point one block method. When these fractional resolutions are considered for the tritium isotope mass m=3.20, then, we have  $\Delta m=0.001952640$  and 0.1953148 for RKM5 and three point one block methods with using 0.01 and 0.05 steps, respectively. This indicates that as the value of  $m/\Delta m$  decreased, the power of resolution is increased due to increment in  $\Delta m$ . However, it is clear that, at least in the lower mass range the impulse voltage with using the three points one block method is quit suitable than using the RKM5 for the CIT with higher in mass resolution. Apart from numerical result, the method showed a potential application to solve complicated linear and nonlinear equations of the charged particle confinement in the cylindrical field especially in fine tuning accelerators, and generally speaking, in physics of high energy.

#### Acknowledgements

The authors thank the referees for valuable comments and suggestions which improved the presentation of this manuscript.

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