Optimizing ion transport in a multi-reflection time-of-flight mass spectrograph by a modified Nelder–Mead simplex algorithm

Zhengxu Huang[1], Shuxiong Yan[1], and M. Rosenbusch[2]

[1]Jinan University
[2]Institute of Particle and Nuclear Studies (IPNS

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Abstract

RATIONALE: The multi-reflection time-of-flight mass spectrograph (MRTOF-MS) is a complex nonlinear system with dozens of variables that are impossible to determine in theory. Numerical analysis is the only method to determine a solution. Therefore, a numerical simulation is applied with a modified Nelder–Mead simplex (MNMS) algorithm for optimizing voltage configurations. **METHODS**: Ion trajectories for injection and confinement are simulated using the software SIMION 8.1. The goal of optimization is to find a more suitable configuration for the electric field. This task becomes more challenging as the number of variables, the complexity of the objective function, and the accuracy of the variable intervals increase. A simplex search algorithm was used to perform the optimization process. We modified the searching algorithm by incorporating a variable transformation to ensure that the variables have smooth boundaries. Additionally, we introduced a dedicated benchmark to facilitate global searches. **RESULTS**: By iteratively using the MNMS algorithm, a total of eight electrodes have been optimized, resulting in a smaller beam size and more efficient ion transport. **CONCLUSIONS**: The MNMS algorithm is effectively for optimizing nonlinear MRTOF-MS system. It improves the adaptability and globality of the original algorithm, making it applicable for the numerical analysis of complex mass spectrometry systems and problems in engineering.

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S. Yan[1,2], M. Rosenbusch[2*]and Z. Huang[1]**

[1]Institute of Mass Spectrometry and Atmospheric Environment, Jinan University, Guangzhou 510632, China

[2]Wako Nuclear Science Center (WNSC), Institute of Particle and Nuclear Studies (IPNS), High Energy Accelerator Research Organization (KEK), Wako, Saitama 351-0198, Japan

E-mail addresses:*rosmar@post.kek.jp*(M. Rosenbusch *), *hzx126@126.com*(Z.Huang**)

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Key words: Multi-reflection time-of-flight mass spectrograph, numerical analysis, ion transport optimization, modified Nelder–Mead simplex algorithm, constrained nonlinear problem, minimizer solver.

Introduction

The multi-reflection time-of-flight mass spectrograph (MRTOF-MS), first proposed 30 years ago [1], is a fast and precise technique to measure the masses of ions. It has rapidly gained favor at radioactive ion beam (RIB) facilities for high-precision mass measurements of radioactive nuclides, such as CERN-ISOLDE (Switzerland) [2], RIKEN-RIBF(Japan) [3, 4], GSI (Germany) [5], and others (see references in [9]). A new MRTOF-MS for nuclear mass measurements has been constructed at the SLOWRI facility at RIKEN-RIBF [9]. This new structure is described with technical details and features in [6], wherein the design is similar to the previous apparatus reported in Ref[4]. For the initial operation, the voltage configuration previously used for the electrostatic mirrors in the older apparatus has been applied to the new set-up. The potentials described in Ref[4] have been determined through a differential algebra simulation and were optimized with the assumption that the ions start in the center of the MRTOF device.

MRTOF-MS is capable of achieving mass resolving powers exceeding 10^5 and measurement durations on the order of milliseconds [7], enabling a folded ion trajectory for a flight distance typically in the range of a few hundred meters. To achieve optimal performance, it is crucial to properly adjust the distribution of the electric field and inject ions as a focused ion pulse. This means minimizing the uncorrelated (thermal) energy spread, reducing the radial spatial distribution (in the case of concentric systems), and aligning the ion beam with the optical axis of the MRTOF-MS. So, our focus was on optimizing ion transport, which had previously only been achieved through experimentation with scanning voltage settings. But it is a time-consuming process. Therefore, numerical simulations are used, and an algorithm is applied to automatically search for optimized lens voltages that minimize the beam spot size at multiple positions.

The Nelder–Mead simplex (NMS) algorithm, originally published in 1965 by Nelder and Mead [8], is a well-known direct search algorithm for finding local minima. It does not require any information about the derivatives of the function, making it suitable for most common problems in science and engineering. On the other hand, the original Nelder–Mead algorithm is designed to solve unconstrained problems, which means that there are no limitations on the input variables. This can pose a challenge in engineering, as there are always variable constraints to consider, such as upper voltage limits in an ion-optical apparatus. Bound constraints are used to limit the size of each variable, thus excluding solutions that have no physical meaning.

In this study, we modified the NMS algorithm and utilized a variable transformation suggested by Nelder and Mead to automatically enforce constraints within a specific range. Meanwhile, the original local minimum was improved to become a global minimum by the re-check function. We provide a brief description of our apparatus in Section 2 and a numerical simulation setting in Section 3. The searching algorithm, modified with constraints, is introduced in Section 4. The results and discussion of the simulation are presented in Section 5, followed by a summary and an outlook for this auto-search algorithm.

Apparatus

Our implementation of the new MRTOF-MS at the SLOWRI facility uses a suite of radio-frequency (RF) ion traps and three lenses with two pairs of steerers, a pair of electrostatic ion mirrors with a single refocusing

lens (two lenses available), and a long field-free drift region between the mirrors, as shown in Fig. 1. In this work, we primarily focus on the electrodes of the magnified area in Fig. 1, which exert a significant influence on the ion beam during its transfer to the MRTOF-MS, i.e. A1 to A3, and DT1 to DT3. Furthermore, we will focus on the trajectories inside the MRTOF device. Geometric details, functionality, and the timing structure can be reviewed in Refs [4, 6, 9]. The mirrors confine the ions so that they are reflected back and forth and separate by mass with their increasing flight path increasing with time. Electrostatic lenses are used for fine tuning of the transportation and confinement of the ions, more specifically, tuning of the ion pulse profile.

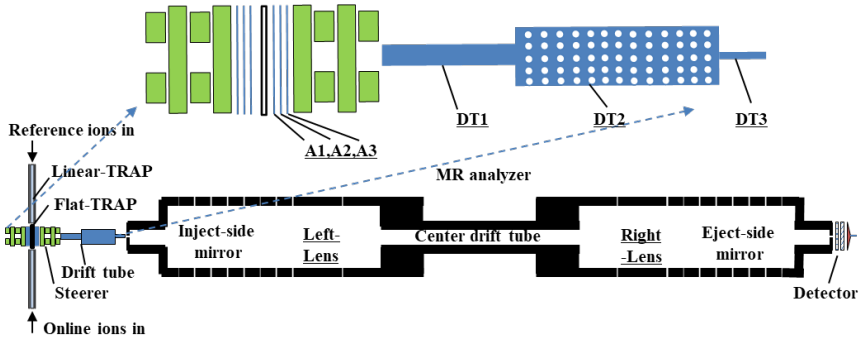

Fig. 1. Schematic of the MRTOF-MS: Ions ejected from the flat trap are accelerated via three thin plates A1, A2 and A3 (each with a 4 mm bore inside), and after passing through a steerer section, ion transport continues through the drift tubes DT1, DT2, and DT3 before reaching the inner of the MRTOF-MS.

The typical measurement cycle proceeds as follows: First, reference and analyte ions accumulate in the linear Paul traps on either side of the flat ion trap (FLT) and are individually transferred to the FLT for a final cooling process. This process takes about 5 ms at a pressure of 10^{-2}~10^{-1} mbar. Ions are orthogonally ejected towards the MRTOF-MS, accelerated by three accelerating lenses (AC), steered by two pairs of steerers (ST), and transported to a system of drift tubes (DT). The tube DT1 is pulsed to adjust the potential energy of the ions due to downstream voltage-supply limitations. However, in the simulation, this is simplified by shifting the whole potential of the MRTOF-MS. Then ions pass through DT2 and DT3. Before injecting ions into the MR analyzer, the voltage applied to the outermost electrode of the injection-side mirror is reduced to allow ions to pass (switching of the end-cap mirror's bias). The ions then reflect between the mirrors for a chosen duration, ensuring that ions with a specific A/q undergo a predetermined number of reflections (where A represents the atomic mass number and $q$represents the electric charge). After the ions have undergone the desired number of reflections and are near the turning point of the injection-side mirror, the voltage applied to the outermost electrode of the ejection-side mirror is reduced to allow the ions to pass. The ions will then travel to the ion detector and generate the stop signals for time-to-digital converter (TDC). While the start signal is the ejection of ions from the FLT. To achieve excellent performance, the electrostatic lenses in-between should be precisely optimized. This will allow the ion pulse to fly close to the optical axis, resulting in a narrow time-of-flight (TOF) focus on the detector.

Simulation setting

3.1. Geometry model.

Numerical simulations are carried out using SIMION 8.1 (Scientific Instrument Services Inc.) [10]. In numerical simulations, it is crucial to accurately construct the geometry model of the MRTOF in order to obtain a realistic trajectory of the ions. Due to limitations in RAM and computing power, the MRTOF model is divided into four separate geometry arrays with varying precision. Our high-resolution SIMION model (with an accuracy up to 0.05 mm grid unit^{-1}) is suitable for predicting ion transmission through medium

and high vacuum systems in mass spectrometry. It also allows for optimizing operational parameters. The structure of the MRTOF model is shown in Fig.2.

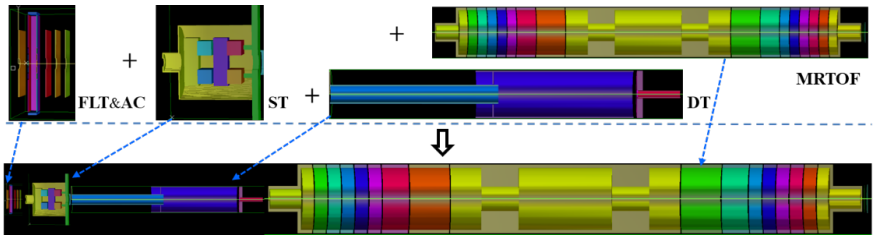

Fig. 2. Geometry model of MRTOF-MS containing four independent geometry arrays. FLT and AC instance (0.05 mm grid unit^{-1}), ST instance (0.2 mm grid unit^{-1}), DT instance (0.25 mm grid unit^{-1}) and MRTOF instance (0.08 mm grid unit^{-1}) are fabricated in various precisions for high performance simulation.

3.2. Programming and initial conditions setting.

The SIMION simulation program is coded to estimate the ions trajectories in the MRTOF model. An algorithm, named NMS simplex algorithm, is applied to control the iterative simulation. It works by repeatedly evaluating different values of the objective function. It starts by evaluating the function at a given starting point and various surrounding points generating by the given step value. The NMS optimization module provided by SIMION requires at least three inputs: a starting point, a step size, and an object function.

The starting point for the optimization process is an essential algorithm parameter that determines the initial searching point. In our simulations, the voltage configuration from the similar device [4] has been used, which provides one feasible parameter. The step size value is another important input parameter that requires careful consideration because it determines the shape of the simplex at startup. Parameter selection of the step size is described in more detail in the subsequent section. The objective of the search is to find the optimal voltage configurations, which entails minimizing the spatial distribution and energy distribution at each test plane in the radial direction while adhering to the voltage value limits. Here, we define the objective function f to be optimized.

f = (α*py_mean + β*pz_mean + γ*vy_mean + η*vz_mean) vy_mean = Stat.array_mean(vy _plane)

vz_mean = Stat.array_mean(vz _plane)

py_mean = Stat.array_mean(py _plane)

pz_mean = Stat.array_mean(pz _plane)

where the py_mean, pz_mean, vy_mean, vz_mean are the average value of radial position and velocity distributions of each test-plane, respectively, α, β, γ, η are coefficients. The 'y' and 'z' present orthogonal components in the radial direction. Stat.array_mean is the averaging operation over an array of numbers, which is available in SIMION's LUA library. Some other parameters can be optionally used to tune performance in simulations, such as maxcalls and minradius, both of which affect when the optimization process stops. In this study, we utilized the default values for both parameters.

In the initialization phase, $^{39}K^{+}$ions are created in the FLT using a Gaussian 3d distribution filling a space larger than the ejection aperture of the trap, so that the maximum possible beam diameter is taken into account. The initial cloud spans over about 1 mm around the center of the trap. The thermal energy distribution of the ion cloud in the trap is set to zero in this test, where the kinetic energy distribution of ions after leaving the trap is defined by the axial position inside the ejection field. Coulomb interactions between the different ions and between ions and image charges on the electrodes are not taken into account as only up to a few ions are transported at the same time in the experiment. The trajectory calculation setting was chosen with the default value. Potential arrays are arranged in a specific order.

As mentioned above, ions must be injected as an excellent ion pulse in order to achieve sustained flight over a long period of time. In the MRTOF setup, eight parameters have been iteratively optimized, including three accelerators, three drift tubes, and two lenses in the MRTOF analyzer.

Optimization method

4.1. Nelder–Mead simplex algorithm with constraints.

The Nelder–Mead simplex algorithm is a straightforward strategy with a small number of function calls, and it produces a fast initial decrease in function values [11] leading to time-efficient performance. The NMS algorithm utilizes the concept of a simplex, which is a special polytope of $N + 1$ vertices in N dimensions of the variable space. It moves the point of worst performance by means of geometrical reflection, expansion, contraction, or reduction [12] (as shown in Fig. 2). Note the following definitions: X_{wst} is the point of worst performance; X_{wsd} is the second-worst performance point; X_{bst} is the point of best performance; and X_{cen} the center of gravity. The possible procedures of the Nelder–Mead downhill simplex algorithm for the two variables case is shown in Fig. 2.

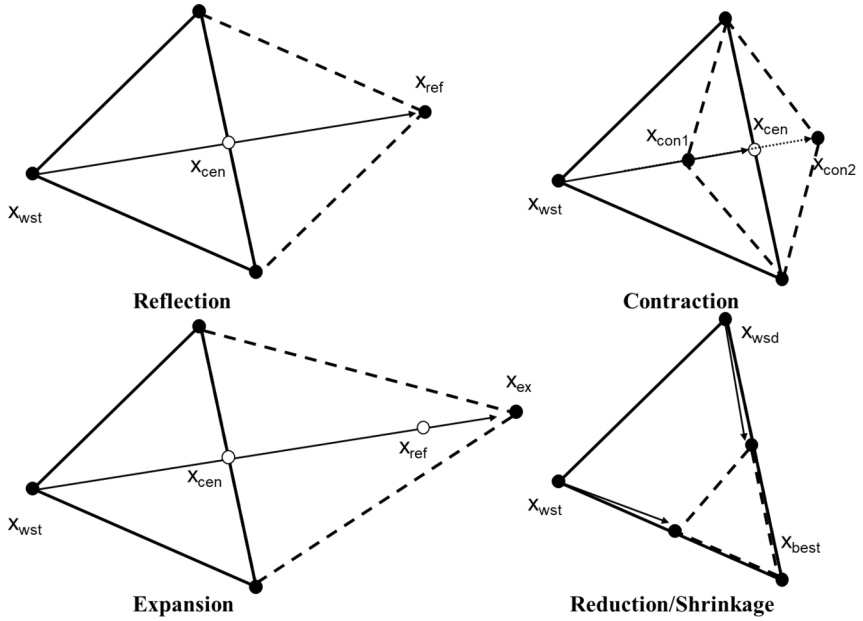

Fig. 3. The image of Nelder–Mead downhill simplex algorithm procedures in two dimensions on a generalized triangle. The modified simplex is shown with a dashed line.

The optimization problem can be written as:

$$\min_x F(x),\ x \in R^n\ ,$$

where $F(x)$ is a scalar function of the variables x, and x is a vector or a matrix with no explicit limitation of the components, where we assume each element is a real number.

The algorithm works by repeatedly evaluating $F(x)$ for different input values x, while replacing the "worst" vertex for producing the largest value for $F(x)$ with a new vertex. A sequence of triangles (in the 2D example) is formed, and the function values at the vertices continuously become smaller. The size of triangles is automatically reduced, and the coordinates of the local minimum point in the vicinity of the initial triangle are found.

For the actual situation of the MRTOF-MS, wherein the variable parameters always have bounds due to high-voltage power supply limitations (or to avoid electric discharges), optimization problems can be rewritten to avoid such parameter values. In order to account for limitations, we aim to solve the following bound-constrained variable optimization problem:

$\min_{x \in R^n} F(x),\ \textit{subject to}\ x_k^l \leq x_k \leq x_k^u,$

where $F\ (x\ )$ is the same scalar functions of the variables$x$, where x_k^l and x_k^u are lower and upper scalar bounds, respectively, and k is the parameter index (in this case one of the voltages).

Although the NMS algorithm is not designed to solve constrained optimization problem in general, it is still a good choice to use this derivative-free algorithm with some modification for the optimum voltage configurations within a given solution space.

Nelder and Mead suggested two ways for handling constraints: (A) transforming the scale of the variables and (B) modifying the function value so that it takes a high positive value in case any constraint is violated[8, 13]. Various constraint handling strategies [14] have been proposed later, like reset the vertices outside the constraints by certain rules.

In our MRTOF situation, for our boundaries, the penalty method frequently gave an unsatisfactory outcome, where the penalty function receives a high merit number for trials outside of the boundaries, and the simplex appears to oscillate around this unfortunate configuration. To improve on such situation, it is a reasonable choice if a proper initial simplex is given [15]. However, this problem can be avoided by defining a periodic function to transform the original variable, whereby the simplex algorithm cannot exceed the boundary for the variables. The variables entering the objective function are replaced by a different value, which is transformed. This leads to a limitation of the space where the simplex algorithm moves. After that, the inverse transform on the initial variable is performed to obtain the original value of the voltage. A typical transforming method [16] is as follows: Let V denote the vector of search variables of size$N$. Let V_i^{ub} and V_i^{lb}denote the upper bound and lower bound on the i -th search variable, respectively, and let denote$x$ the new search variable vector.

We obtain the initial transformed variables from

$$x_i = (\frac{V_i - V_i^{\mathrm{lb}}}{V_i^{\mathrm{ub}} - V_i^{\mathrm{lb}}} \times 2\ -\ 1) + 2\pi$$

And do the inverse transform by:

$$V_i = \frac{\left(V_i^{\mathrm{ub}} - V_i^{\mathrm{lb}}\right) \times (\sin x_i + 1)}{2} + V_i^{\mathrm{lb}}$$

from which follows that$V_i^{\mathrm{lb}} \leq V_i \leq V_i^{\mathrm{ub}}$, since the values of the function$\frac{f(x_i)=(\sin x_i+1)}{2}$ are always inside of the interval 0 ˜ 1 as shown in Fig. 4 and V_i is therefore bound due to the nature of trigonometric functions.

This modified Nelder–Mead simplex (MNMS) algorithm will be utilized as a solver for ion transport optimization problem.

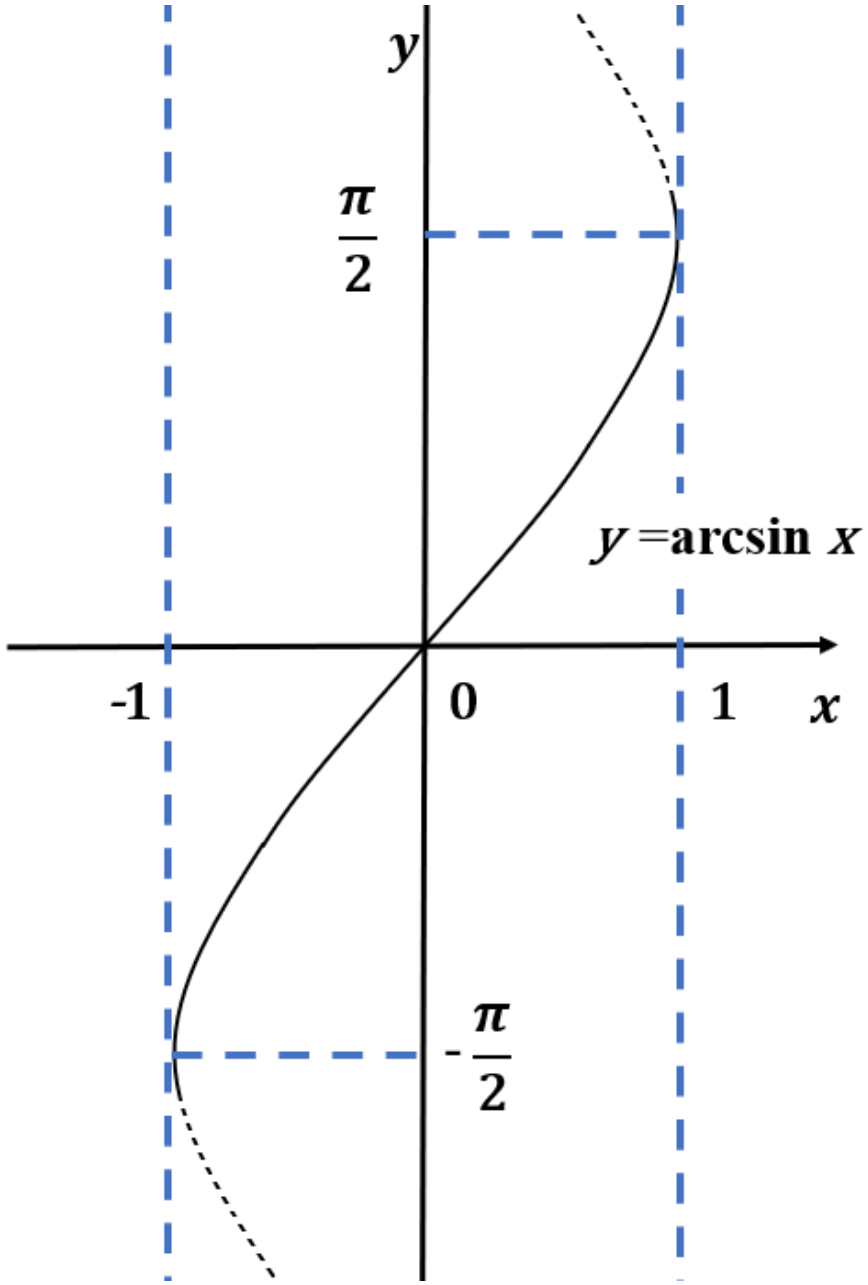

Fig. 4. Schematic of the transformation method to add bound constraints to NMS algorithm

4.2. Routing procedure of optimization.

In order to maximize the performance of the MRTOF-MS, it is crucial that the injection optics provide a well-focused beam. To this end, numerical simulations are employed to track the trajectories of ions from the preparation trap FLT into the MRTOF analyzer. While in the MRTOF system, there are numerous electrodes that can influence the ion motion, an automatic search algorithm can greatly assist in finding the optimal voltage configurations [17, 18]. It should be noted that the NMS algorithm is not an efficient solver for high-dimensional optimization. Arranging the variables into groups and iteratively searching within a realistic interval is a feasible and effective approach. The procedure is outlined graphically in Fig. 5. Eight

variables, including three accelerators (AC), three drift tubes (DT), and two lenses in the MRTOF analyzer (Lens), are grouped according to the laws of electrostatic lenses, e.g., A1 + A2 + A3, A3 + DT1 + DT2 + DT3, DT3 + Left-Lens + Right-Lens, and other combinations like A2 + DT1 + Left-Lens + Right-Lens, or A3 + DT1 + DT3 + Left-Lens + Right-Lens. The voltage configurations are iteratively optimized until the feedback function value is satisfactory.

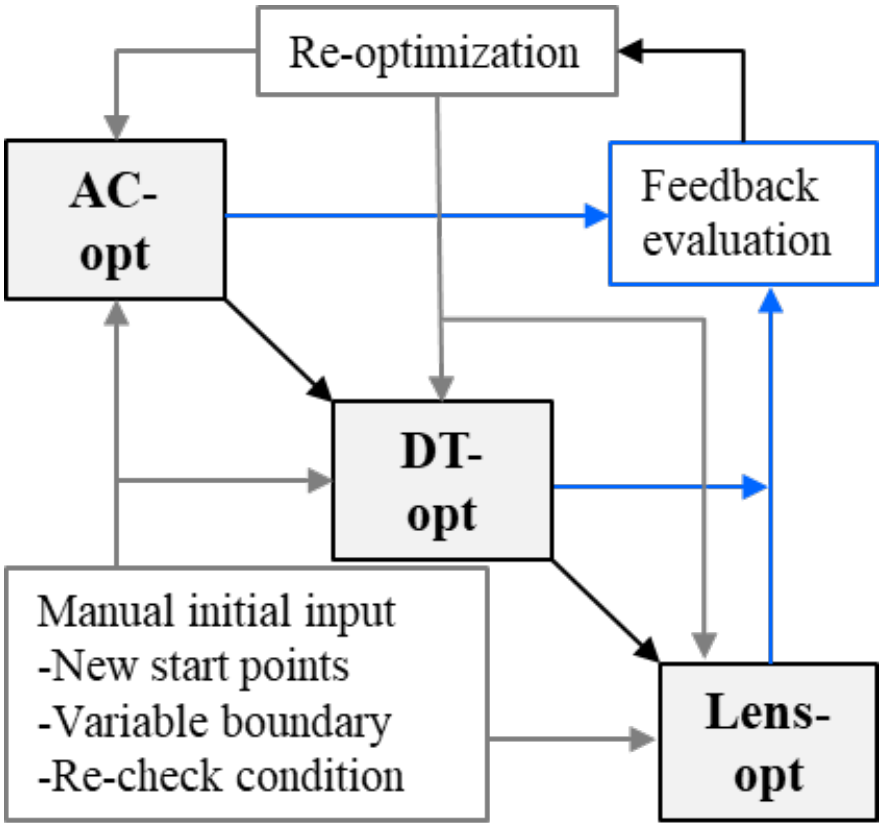

Fig. 5. Iterative loop of optimization work flow, AC (A1-A3), DT (DT1- DT3) and inside-MRTOF electrodes (negative-voltage Lens electrodes) are the variables used in this work. Manual initial input from prior measurements has been used for initialization.

An overview of the object function value changing during a series of optimizing simulations as the iteration number increases is shown in Fig. 6. One noticeable trend in simulation result is that the value of the feedback function consistently decreases with the algorithm performing, especially rapidly at the beginning, while towards the end, the final convergence tends to be slow, as the simplex has already contracted and the function value remains unchanged. This indicates that taking advantage of the efficiency of the earlier optimization could quickly encourage the process. By continuously modifying the electrode potentials from every previous simulation, an acceptable local-minimum voltage configuration in a specific searching area would be obtained.

Fig. 6. Objection function values of various optimizations as functions of the iteration number. (A), (B), and (C) represent three different optimization rounds for different choices of electrodes using subsets as described in the text.

4.3. Global modification of MNMS algorithm

In the MRTOF system, due to the possible roughness of the objective function, demanding high accuracy

for an optimization in a global search space is usually costly. While the NMS algorithm is effective in a local area, it is a challenge to find a reliable global minimum. This also restricts its applicability in broader situations. Thus, adding additional random points to the NMS acts as a double check for the effectiveness of minimum. This re-check validation program is an alternative function that starts manually.

The flowchart of the global MNMS algorithm is shown in Fig. 5. First, the variables are transformed by adding a window with a periodic function. After optimization, they are transformed back to the original domain. It is similar to the processes of the traditional Fourier transform and the inverse Fourier transform. Additional re-checks, which are circled by dotted lines in Fig. 5, are used for global minimum verification. It compares the values of randomly points with the current simplex points to validate the current minimum. If the simplex settles in a local area that is not sufficiently low, the random point will be adopted as a new simplex point, altering the shape of the simplex and subsequently moving it out of the current area. Meanwhile, if it confirms the validity of the simplex after numerous re-checks, we can consider the solution good enough to be accepted.

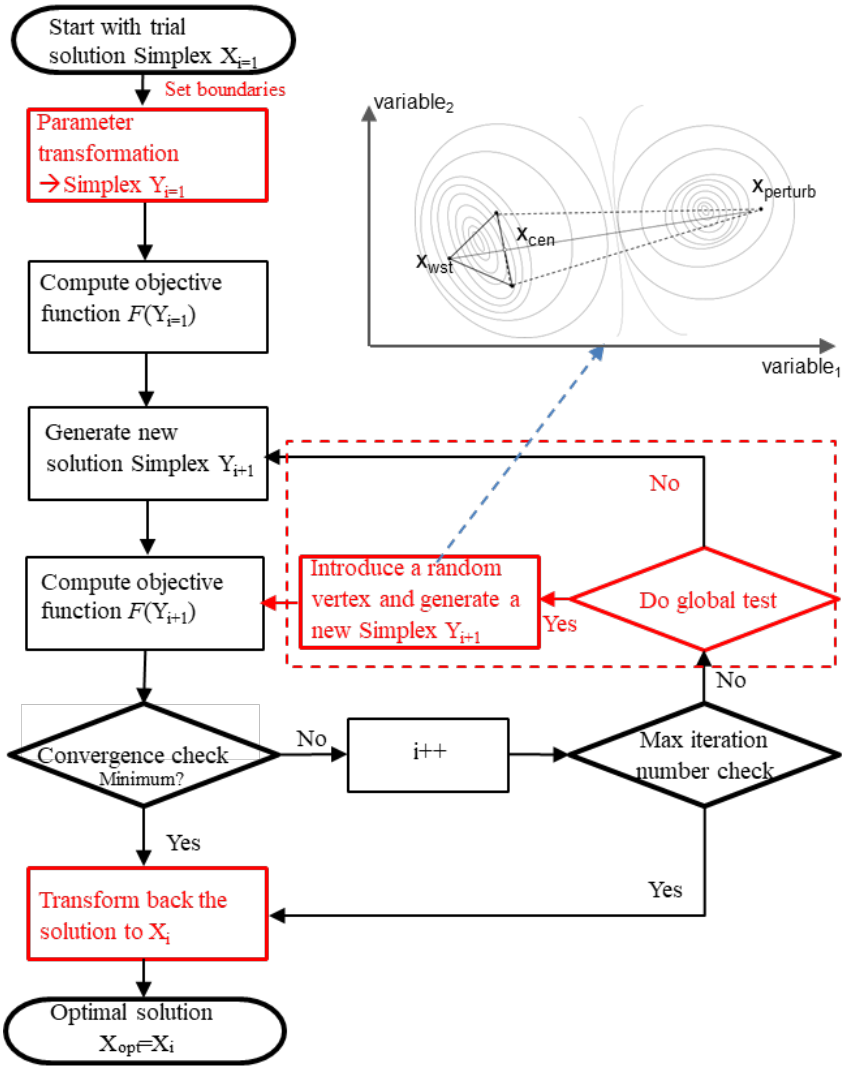

Fig. 7. Flowchart of the MNMS algorithm. Red notes are parts for revision, the blue arrow shows the schematic of the double minimum check, a perturb point is randomly put to adjacent domain.

Fig. 8 shows the changes in function value with the re-checks for the global minimum. After comparing the values of the random points next to the search area with the values of the simplex points numerous times, no superior configuration has been discovered. Thus, we can ensure the validity of the minima. It should be noted that this is not a true global minimum, the globality of the result has not been proven strictly.

Fig. 8. Function value and various electrodes voltages as functions of the iteration number of the algorithm.

4.4. Parameter setting of MNMS algorithm

Correctly setting algorithm parameters is critical as it ensures the correctness of the solutions and the robustness of the optimization procedure. A number of parameters influence the optimization process. To decide the optimal values for these parameters, the performance with different parameter choices was investigated. Four basic algorithm parameters (consisting of coefficients of reflection, expansion, contraction, and shrinkage) that define a complete NMS algorithm are chosen to use the default values. Other optional parameters in simulations, such as maxcalls and minradius, are also set to use the default values. Because the default values of the parameters are suitable for most of the general problems, changing the values did not show much benefit but instead affected algorithm stability.

A problem encountered in this procedure was that the size of the initial simplex had an impact on the speed of convergence and globality of the searching process. The step size is a crucial algorithm parameter that requires careful consideration as it determines the shape of the simplex at startup. Therefore, several simulations are performed to explore the relationship between the step value and the effect of optimizations.

Fig. 9 shows the changes in the searching range in two variable dimensions with the step value increasing from 0.5 to 20. A tendency towards a larger searching area for the two variables was observed as the step value increased until 13, after which an opposite trend was observed. As previously indicated, a variable transformation was introduced to the NMS algorithm. This transformation imposes a periodic change on the variables, making excessively large variable values meaningless. To avoid the optimization result getting trapped in a local minimum prematurely, broad search range for the solution space and a big starting simplex are required. Taking into account the periodicity of the variables, the optimal step value might be selected from 5 to 13. In the following simulation, a step value of 5 is adopted considering the time-consuming of the calculations.

Fig. 9. Distribution in two dimensions under different Step value setting, variable 1 and 4 are first and third drift tube voltages, respectively.

Results and discussion

In this study, we focus on optimizing ion transport in an MRTOF-MS. By utilizing an MNMS algorithm in the simulation analysis, we optimized eight electrodes with significant influence on the transportation of ion beams starting from the flat ion trap. After a series of iterative optimizations, the ion trajectories have been improved, and the objective function value has been reduced from the tens level to 10^{-2}.

In applications, MRTOF works either in straight mode (Fig. 10) for full spectral or in reflection mode (Fig. 11, reflected with 50 laps) for high resolution. The ion trajectory simulation after extraction from the FTL is presented in Figs. 10 and 11. is the optimizations in straight mode, and Fig. 11 is the reflection flight optimizations with 50 laps. The objective of these simulations is to minimize spatial and energy distributions in the radial direction. For each of the figures, the screenshots marked A to D, from top to bottom, show the changes in simulation results during the optimization process. Herein, A1, A2, A3, DT1, DT2, DT3, and two lens electrodes in MRTOF were optimized. Comparing the trajectories of the ions, we can see that constant optimizations produce good results, whether in the full spectral mode or high-resolution mode. The algorithm has apparent optimization effects compared to the initial state. Trajectories become so accordant that they almost overlap in a line. This situation keeps similar in a reflective state. Moreover, in reflection mode, the transmission efficiency also improves. Ion losses before optimization can be clearly observed in Fig. 11(A), where ions are lost due to collision on the lens. While a well-adjusted ion beam appears with

the use of appropriate electrical parameters for optimization and a 100% transmission efficiency is achieved as shown in Figs. 11(B), (C), and (D).

Significant improvements in ion transmission were observed after running the MNMS algorithm, indicating that the new MNMS algorithm is effective in MRTOF simulation. It is quite efficient in quickly finding the optimal solution (within a few hours for each optimization). Moreover, it requires very little storage and information for execution. Because of its simplicity and robustness, it seldom fails in the optimization process.

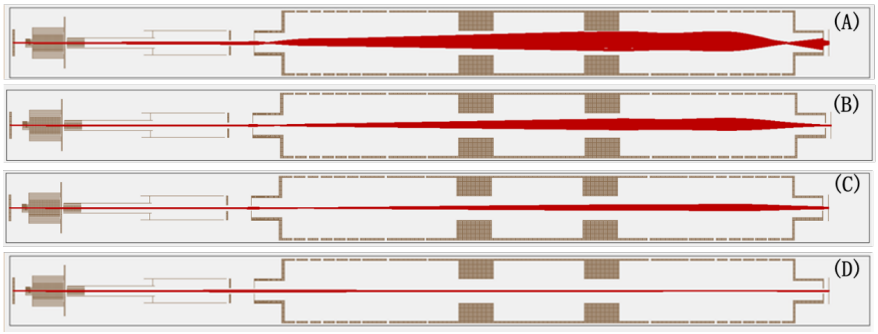

Fig. 10. Section views of ion trajectories ($^{39}K^{+}$) under straight mode. (A) simulation result before optimization, (B), (C), and (D) simulation results using different optimized potentials.

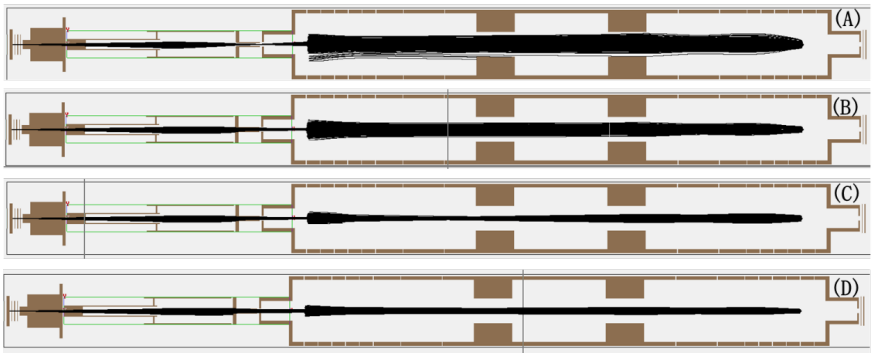

Fig. 11. Section views of ion trajectories ($^{39}K^{+}$) under reflection mode. (A) simulation result before optimization, (B), (C), and (D) simulation results using different optimized potentials.

Conclusion and outlook

In the numerical simulation for mass spectrometry instrumentation, an MNMS algorithm was employed to optimize the voltage configurations of an MRTOF-MS. This algorithm modifies the standard NMS algorithm by incorporating a domain transformation of variables and an additional re-check for optimality. Thus, the MNMS algorithm is effective in solving complex, constrained nonlinear problems and is capable of producing an approximate global optimal solution. Moreover, it is highly efficient in quickly finding the optimal solution and does not require any derivatives of the function. The simulation results demonstrated an improvement in the performance of the MRTOF-MS and confirmed the effectiveness of the method.

Additionally, the MNMS search algorithm is applicable to other numerical simulations for the design and optimization of MS instruments, even in cases where the problems are not smooth or the derivatives are not available. We believe that this improved direct search algorithm has the potential for broader application in various fields.

Acknowledgments

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