# DEVELOPMENT OF LARGE SCALE OPTIMIZATION TOOLS FOR BEAM TRACKING CODES*

B. Mustapha# and P. N. Ostroumov
Argonne National Laboratory, 9700 S. Cass Ave, IL 60439, U.S.A.

*Abstract*

Matrix-based beam optics codes such as TRACE-3D are often used for small scale optimizations such as beam matching which involves a limited number of parameters. The limitation of such codes is further amplified for high-intensity and multiple charge state beams as their predictions start to deviate from the more realistic 3D particle tracking codes. For these reasons we have started developing large scale optimization tools for beam tracking codes. The large scale nature comes first from the possibility of optimizing a large number of parameters and second from the minimum number of particles to track especially for space charge dominated beams. The ultimate goal of these developments is not only to optimize the design of an accelerator but also to be able to use a beam dynamics code to operate it once built. A selected set of optimization tools is presented along with specific applications. For most applications, large scale parallel computing will be needed to speed-up the optimization process.

## PARTICLE TRACKING VERSUS TRANSFER MATRIX CODES

In Table 1, we compare the ingredients and capabilities of matrix-based beam optics codes to those of particle-tracking beam dynamics codes.

Table 1: Comparing matrix-based beam optics codes to more detailed 3D beam dynamics codes.

| Code Type | Beam Optics | Beam Dynamics |
|---|---|---|
| Example | Trace-3D [1], … | TRACK [2], IMPACT [3], … |
| Method | Matrix (1st order) | Tracking (all orders) |
| Element model | Hard-edge approximation | 3D model with realistic fringe fields |
| Space charge | Form factor approximation | Solving Poisson equation at every step |
| Output | Centroids, envelopes and emittances | Actual beam particles distribution |
| Use | Preliminary studies | More detailed studies |
| Speed | Fast | Slower |

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# mustapha@phy.anl.gov

It is clear from Table 1 that 3D beam dynamics codes provide more realistic representation of the beam especially for high-intensity beams where the predictions of beam optics codes start to deviate significantly from those of beam dynamics codes. Therefore, it is more appropriate to use beam dynamics codes for the optimization of high-intensity and multiple charge state beams. In addition, it is possible to include information not available from beam optics codes such as beam halo and beam loss in the optimization process.

## TYPICAL OPTIMIZATION PROBLEMS: NATURE AND SCALE

Beam optics codes are often used for fast optimization. Typical problems are beam matching between accelerator sections and finding matched beams for periodic structures. In these cases the number of fit parameters is usually less than 10. To solve the same problems using a beam dynamics code we need to track ~ 1000 particles for statistical significance for ~ 100 iterations which takes few minutes to an hour on a regular PC. This is much slower than matrix-based codes. However, the capability of a beam dynamics could be easily extended to actually tune or retune a whole accelerator section independently from being periodic or not. Such a problem could involve ~ 100 fit parameters and tracking 1E5-1E6 particles may be needed for space charge dominated beams. A larger number of iterations (~ 1000 or more) is usually required for the problem to converge which may take few to several days on a regular PC. Large scale parallel computing will be needed for such applications.

## POTENTIAL APPLICATION: MODEL DRIVEN ACCELERATOR

A potential application of the large scale optimization tools being developed is to be able to use a realistic beam dynamics code for real-time operations of an accelerator system. We refer to this concept as the “Model Driven Accelerator”. The main benefits of realizing this concept are faster automatic tuning and faster recovery after a failure which should improve the availability and reduce the operating budget of the machine. The realization of this concept requires the development of a realistic computer model of the machine. This involves first reducing the gap between the original design and the actual machine by using 3D model for every element and measured field data if needed. Second, tailoring the computer model to the machine by fitting the beam data from diagnostic devices to test and improve the predictability of the model which should reproduce the data. This is better done during the commissioning of the machine. Finally, optimization tools with fast turn-around are needed to support decision making for real-time machine operations.

Clearly more optimization tools are needed for the realization of the model driven accelerator. These optimization needs are different for the three different phases of an accelerator project, namely the design, commissioning and operations. During the design phase, the design parameters are optimized for different design options to produce a robust and cost-effective design. During the commissioning, the computer model needs to be tailored to the actual machine by fitting the data measured at beam diagnostic points. During operations, the computer model is used to retune the machine or to rapidly restore the beam after a failure by fitting element settings for the desired beam conditions.

## DEVELOPED TOOLS AND APPLICATIONS

Most optimization algorithms rely on an analytical expression of the function to be minimized with explicit dependence on the fit parameters. The derivatives of the fit function on the fit parameters are used to guide the optimization process. While it is possible to derive such an explicit expression for matrix-based codes, it is not possible for beam dynamics codes. In this case, the fit function is defined from the statistical beam parameters without explicit dependence on the fit parameters which often results in a slower fit. An optimization algorithm that does not require explicit dependence of the fit function on the fit parameters is needed. The minimization package MINUIT [4] supports this option, so we use it for most of our optimization needs.

The tools presented here are developed for the beam dynamics code TRACK [2] but it should be straightforward to adapt them to IMPACT [3] and other beam dynamics codes.

### *Design of the RIA/FRIB linac*

Most of the tools were developed during the design of the driver linac for the original Rare Isotope Accelerator (RIA) project [5] and later for the Facility for Rare Isotope Beams (FRIB) project [6] which is a smaller scale version of RIA. Both automatic transverse and longitudinal tuning procedures were developed [7, 8].

The automatic tuning procedures are developed to tune a given section of the linac to produce smooth beam dynamics by reducing the fluctuations in the rms beam size along the considered section. For the transverse tuning the fit function is defined as:

$$F = X^0_{rms} + \sum_i \frac{(X^i_{rms} - X^0_{rms})^2}{\varepsilon^2_{X_{rms}}} + Y^0_{rms} + \sum_i \frac{(Y^i_{rms} - Y^0_{rms})^2}{\varepsilon^2_{Y_{rms}}}$$

where $X^0_{rms}$ and $Y^0_{rms}$ are the rms beam sizes at the entrance of the section, the sum index i runs over the focusing periods and $\varepsilon_{Xrms}$ and $\varepsilon_{Yrms}$ are the allowed errors on the rms beam sizes. The fit parameters are the field strengths in focusing elements. This method is general and should produce good results for periodic or non periodic accelerating structures. Applied for a two charge state uranium beam in the low-energy section of the RIA driver linac this method produced the results shown in Figure 1.

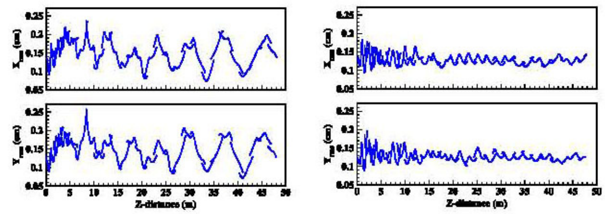

Figure 1: X and Y rms beam sizes before (left) and after (right) applying the automatic transverse tuning procedure. The beam is a two-charge state uranium beam in the low energy section of the RIA/FRIB driver linac.

A similar procedure was developed to smooth the longitudinal envelopes by fitting the RF field phases and amplitudes in accelerating cavities.

Another longitudinal tuning procedure was developed specifically for a multiple charge state beam to minimize its longitudinal emittance right before a stripper [7]. The beam should reach the stripper in the form of an up-right ellipse in the ($\Delta\varphi$, $\Delta W$) plane to minimize the emittance growth from the energy straggling effect in the stripper. This could be realized by matching the beam centroids and Twiss parameters of the different charge state beams. The fit function in this case is:

$$F = \frac{(W_{q0} - W_0)^2}{\varepsilon^2_w} + \sum_{qi} \frac{\Delta W_{qi}^{\,2}}{\varepsilon^2_{\Delta w}} + \sum_{qi} \frac{\Delta\phi_{qi}^{\,2}}{\varepsilon^2_{\Delta\phi}} + \sum_{qi} \frac{\alpha_{qi}^{\,2}}{\varepsilon^2_{\alpha}} + \sum_{qi} \beta_{qi}$$

where $W_0$ is the desired beam energy and $\varepsilon_W$ is the associated error. $\varepsilon_{\Delta W}$, $\varepsilon_{\Delta\varphi}$, and $\varepsilon_\alpha$ are the allowed errors on the relative energy, phase and $\alpha$ shifts of the individual charge state beams from the central beam. The fit parameters in this case are the RF cavities phases and amplitudes in the section up-stream of the stripper. Figure 2 shows the results of the fit for a five charge state uranium beam in the medium energy section of the RIA driver linac. Figure 3 shows how this optimization affected the beam loss in the high energy section of the linac.

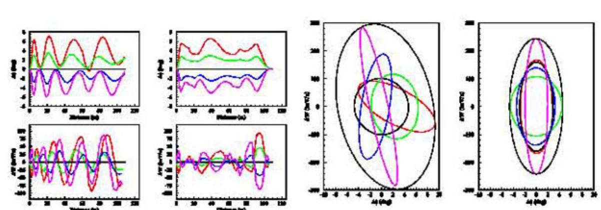

Figure 2: The left 4 plots show the phase and energy oscillations of the five charge states around the central charge state before and after applying the tuning procedure. The right 2 plots show the corresponding beam ellipses on the stripper before and after tuning.

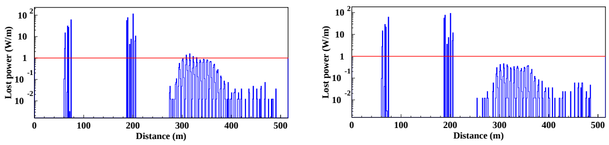


Figure 3: Beam loss in the RIA driver linac before and after applying the longitudinal tuning procedure. The two peaks correspond to the location of the strippers and the scatter loss is in the high energy section which has reduced after fine tuning is applied.

## *Operation of a prototype 2Q-LEBT*

Recently, new optimization tools have been developed to support the operations of the prototype multiple charge state LEBT at Argonne. Figure 4 is a general 3D view of the experimental setup.

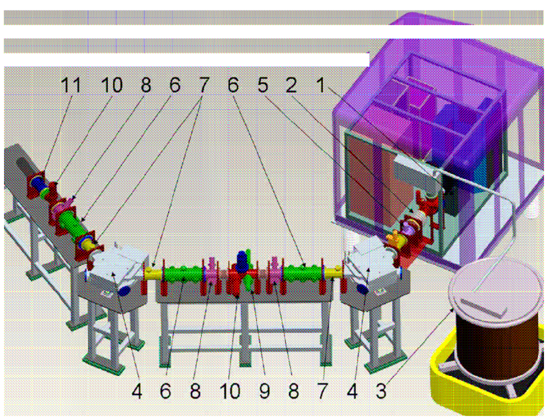


Figure 4: General 3D view of the 2Q-LEBT at Argonne. 1 – All permanent magnet ECRIS on HV platform, 2 – 75-kV Accelerating tube, 3 – Isolation transformer, 4 – 60° Bending magnets, 5 – Einzel lens, 6 – Electrostatic triplets, 7 – Electrostatic steering plates, 8 – Rotating wire scanner, 9 – Horizontal slits, 10 – Faraday cup, 11 – Emittance probe.

Figure 5 shows the measured beam composition after the first magnet. For a realistic beam dynamics simulation, 17 beams (O and Bi) are tracked simultaneously from the ion source through the LEBT with the same composition of Figure 5 but scaled to the measured total current at the source of about 2 mA. We assume the same initial distribution for all beams and a 50 % charge compensation factor in non-electric devices and 0% in electric devices. Realistic 3D models were developed and used for most beam line elements.

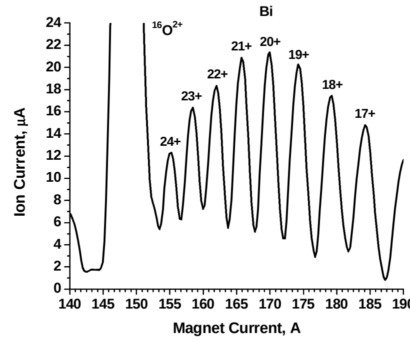


Figure 5: Composition of the Bi-209 beam extracted from the ECR ion source.

In order to tailor the TRACK model to the actual beam line we had first to determine the initial beam parameters at the source. To do so we had to develop a new procedure to fit the beam profiles measured at the middle plane by varying the beam parameters at the source. Figure 6 shows the result of the fit for a two-charge state 75-kV bismuth beam (20+, 21+). The fitted transverse emittances and Twiss parameters at the source are given in Table 2. We notice that despite the axial symmetry of the extraction region, the beam is not axial symmetric. This may be explained by a non symmetric plasma boundary inside the ion source as discussed in [9].

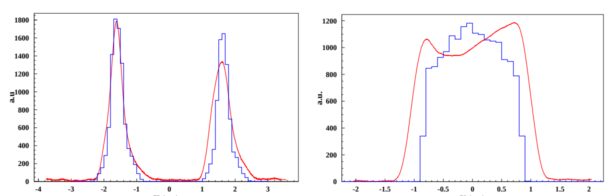

Figure 6: Horizontal (left) and vertical (right) beam profiles. The curves are the measured profiles and the histograms are the result of the TRACK fit.

Table 2: Transverse emittances and Twiss parameters at the source obtained by fitting the measured beam profiles.

| Phase Plane | Tot. norm. ε (mm-mrad) | Twiss α (unitless) | Twiss β (mm/mrad) |
|---|---|---|---|
| (x, x') | 0.309 | -1.00 | 0.230 |
| (y, y') | 0.366 | 1.70 | 0.25 |

Once the initial beam conditions are known, we may use the computer model to find the element settings for the desired operation mode. The main purpose of the prototype 2Q-LEBT is to demonstrate the possibility of accelerating, transporting and combining at least two charge beams at the end of the LEBT for injection to a subsequent RF section. A new fit procedure was developed to produce symmetric beam dynamics between the two bending magnets as this is a necessary condition to recombine the multiple charge state beams. Figure 7 shows the result of a symmetric fit to combine the two charge state bismuth beams (20+, 21+) at 90 kV. The corresponding setting of the triplets is also obtained. Another fit was used to find the setting of the last triplet for a perfect combination at the end of the LEBT where a beam profile monitor and a Pepper-Pot emittance meter are installed. Figure 8 shows the measured beam profiles and Figure 9 shows the Pepper-Pot images at the end of the LEBT. Table 3 shows a comparison of the predicted setting and the actual setting of the triplets. A maximum deviation of 10 % may be explained by the assumption made in the simulation. We notice that the two charge state beams are almost perfectly combined.

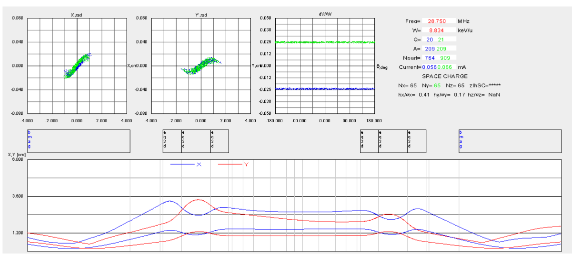

Figure 7: Result of a symmetric fit between the two magnets to recombine the two charge state Bi beams.

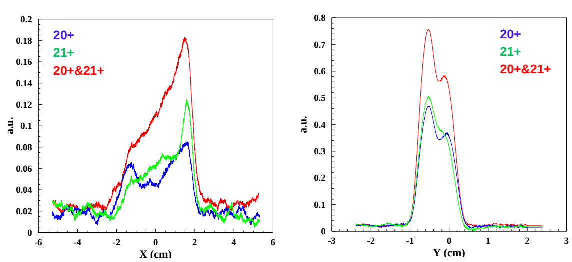


Figure 8: Measured beam profiles at the end of the LEBT for the individual Bi 20+ and 21+ beams and the combined beam.

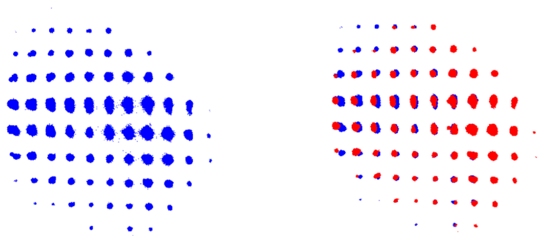

Figure 9: Pepper-Pot images of the combined beam (left) and the individual beams (right). Bi 20+ is in blue and 21+ is in red.

Table 3: Comparison of the quad settings obtained by the TRACK fit and the actual quad settings to combine the two charge state beam.

| Quad. | Fit value (kV) | Set Value (kV) | Diff. (%) |
|---|---|---|---|
| Q1 | 3.312 | 3.299 | 0.4 |
| Q2 | -2.589 | -2.793 | 7.9 |
| Q3 | 1.847 | 1.941 | 5.0 |
| Q4 | 1.794 | 1.922 | 7.1 |
| Q5 | -2.595 | -2.863 | 10. |
| Q6 | 3.372 | 3.373 | 0.1 |
| Q7 | 2.487 | 2.492 | 0.5 |
| Q8 | -3.225 | -3.229 | 0.1 |
| Q9 | 3.743 | 3.431 | 8.3 |

## FUTURE DEVELOPMENTS

The tools developed so far were used only with the serial version of TRACK which is very time consuming. For timely optimizations, large scale parallel computing is required. The parallel version of TRACK is now fully developed and scales reasonably well on very large number of processors [10]. In a future development, we plan to test the existing tools with the parallel version of the code. As a first step we propose to combine parallel tracking with serial optimization. This should be straightforward because the two processes are distinct as the function to minimize is usually evaluated at the end of every tracking iteration. In a further development, we will investigate the use of parallel optimization algorithms such as the Toolkit for Advanced Optimization (TAO) developed at the Mathematics and Computer Science Division at Argonne [11].

Concerning the realization of the concept of the model driven accelerator, more tools are needed to fit the experimental data using a beam dynamics code. Numerical experiments could be used to test the tools before implementation to the real machine by producing detector-like data. For the real machine, interfaces between beam diagnostic devices and the computer model are also required to input calibrated and analyzed data to the code. As a full scale application, we are proposing to realize the concept of the model driven accelerator on the superconducting linac ATLAS at Argonne and eventually on the SNS linac. For such applications, large scale parallel computing is a key to support real-time operations of the machine.

## SUMMARY

For high-intensity beams, it is more appropriate to perform optimization using a beam dynamics code instead of a matrix-based code. Optimization tools are needed not only for the design phase but also to support the commissioning and operations of an accelerator. These optimization needs are different for the different phases of an accelerator project. A realistic computer model could be developed by fitting the experimental data and thus tailoring the model to the actual machine. This is better done during the commissioning phase. Bridging the gap between the design and the actual machine is essential to ensure the continuity between the three phases of a project. To support real-time machine operations, large scale parallel computing will be required.

## REFERENCES

[1] K. R. Crandall, TRACE-3D Manual, Report LA-11054-MS, Los Alamos, 1987.

[2] V.N. Aseev et al., Proceedings of PAC-05 Conference, Knoxville, Tennessee, May 16-20, 2005.

[3] J. Qiang, R. D. Ryne, S. Habib, and V. Decyk, J. Comput. Phys. 163 (2000) 434.

[4] MINUIT – Function Minimization and Error Analysis, CERN Program Library Long Writeup D506.

[5] P. N. Ostroumov, V. N. Aseev, and B. Mustapha. Phys. Rev. ST. Accel. Beams 7, 090101 (2004).

[6] B. Mustapha, P. N. Ostroumov and J. A. Nolen, Proceedings of PAC-07 Conference, Albuquerque, New Mexico, June 25-29, 2007.

[7] B. Mustapha and P. N. Ostroumov, Phys. Rev. ST. Accel. Beams 8, 090101 (2005).

[8] B. Mustapha and P. N. Ostroumov, Proceedings of LINAC-06 Conference, Knoxville, Tennessee, August 21-25, 2006.

[9] P. Spadtke et al., Rev of Sci. Instr. 79, 02B716 (2007).

[10] J. Xu, B. Mustapha, V.N. Aseev and P. N. Ostroumov, presented at this workshop.

[11] S. Benson, L. McInness, J. More, T. Munson and J. Sarich, “TAO User Manual (Revision 1.9)”, Mathematics and Computer Science Division, Argonne National Laboratory, ANL/MCS-TM-242, and at http://www.mcs.anl.gov/tao.