SOLVING COMPLEX BEAMLINE FITTING AND OPTIMIZATION PROBLEMS WITH THE PARTICLE BEAM OPTICS LAB (PBO LAB $^{\text{TM}}$)

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Abstract

A second generation of the Particle Beam Optics Laboratory has been developed with an emphasis on applications to problems in accelerator optimization. The new version of the software incorporates several enhancements that significantly extend the capabilities of the first release of PBO Lab described at EPAC98. Several charged particle optics programs, including TRANSPORT, TURTLE, MARYLIE and TRACE 3-D, are integrated with the new version. Three optimizers have been added as a new PBO Lab Optimization Module. Any optics model input parameter can be included in the set of optimizer variables, and any of the outputs from the computation engines can be used in the formulation of the nonlinear constraints and/or the objective (merit) function. The Optimization Module is described briefly and an application to a typical beamline problem is presented.

1 INTRODUCTION

The PBO Lab family of accelerator related applications was developed to provide advanced software tools for beamline design [1], personnel training [2], and accelerator operations [3]. The basic PBO Lab package provides an easy-to-use intuitive interface for graphically constructing, manipulating and editing computer models of accelerators and beamlines. Interactive tutorials, training aids and expert system features provide an enhanced environment that significantly improves the scientific productivity of both novice and advanced users. Several Application Modules, each of which incorporates TRANSPORT [4], TURTLE [5], DECAY-TURTLE [5], MARYLIE [6] or TRACE 3-D [7], are available and allow users to carry out extensive particle optics studies without any knowledge of the I/O format or syntax for individual codes - the PBO Lab automatically handles the setup of all inputs, the execution of the codes, and the visualization of results.

A new Optimization Module has been developed to extend the capabilities of PBO Lab to address beamline optimization problems that are more complex than can be addressed by the individual Application Module optics codes [4-7]. This paper summarizes key features of the Optimization Module and describes a selected application.

2 OPTIMIZATION MODULE

2.1 Overview

The approach to the development of the Optimization Module follows the basic guidelines that have underpinned the development of all applications for the PBO Lab software [1-3]. Paramount in this approach is that the Optimization Module must be very easy to use and that users need have no knowledge of the detailed I/O required to run individual optimization programs. Optimization problems are set up and executed graphically using intuitive graphic user interface (GUI) components.

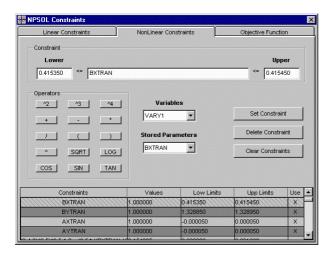
GUI components have been developed and other software elements implemented within the context of the PBO Lab beamline object model for three optimization programs: LSSOL, NPSOL and MINOS. LSSOL [8] is a constrained linear least-squares and quadratic optimization program. NPSOL [9] and MINOS [10] are both constrained nonlinear optimization programs, but the two packages use different approaches and are applied to different types of optimization problems.

Any input parameter to an optics code can be declared as an Optimization Module variable. Output parameters from the optics codes can be defined as store parameters. The store parameters may then be used to formulate the nonlinear constraints and/or merit functions for NPSOL or MINOS. More than one optics code may be included in a problem, and hierarchical problems can be formulated using the fitting/optimization capabilities of the optics codes inside the Optimization Module.

2.2 Setting Up Optimization Problems

The power of the NPSOL and MINOS components of the Optimization Module is the ability to utilize essentially any output from the PBO Lab suite of optics codes to construct nonlinear constraints and merit functions. Figure 1 illustrates two panels of the NPSOL constraint window in the PBO Lab Optimization Module that are used for this purpose.

In the example shown in Figure 1, the four TRANSPORT inputs VARY1-VARY4 have (previously) been defined as optimization variables, and the parameters BXTRAN, AXTRAN, BYTRAN, AYTRAN have been specified as store parameters. These have then been used to formulate four nonlinear constraints and the objective (merit) function for NPSOL. An unlimited number of constraints and merit functions may be defined (and saved) which can easily be turned on (X in the "Use" column) or off. This allows for several different formulations of a problem to be readily defined. The PBO Lab Optimization Module encapsulates a suite of algebraic operators, optics code interfaces, and other I/O requirements to provide an easy-to-use GUI that completely defines the NPSOL problem.



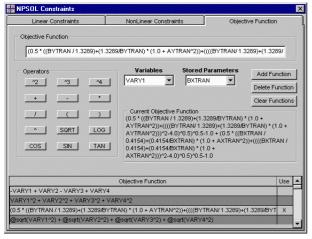


Figure 1: Window panels used to set up the nonlinear constraints (top) and the merit function (bottom).

3 OPTIMIZATION EXAMPLE

The optimization codes NPSOL and MINOS have been used in conjunction with the optics Application Modules

to examine several beamline optimization problems. One representative example using NPSOL with TRANSPORT and TRACE 3-D is described here: a four-quadrupole transfer line matching problem.

3.1 Transfer Line Matching

One common type of transfer line optimization problem involves finding values for four (4) quadrupole strengths that will transport a beam with a given set of initial horizontal and vertical Twiss parameters (β_{xi} , α_{xi} , β_{vi} , α_{vi}) through the transfer line and produce a beam with a specified set of final output Twiss parameters (β_{xf} , α_{xf} , $\beta_{\rm vf}$, $\alpha_{\rm vf}$). There are four constraints to satisfy (given by the final Twiss parameters) and four unknowns to find (the quadrupole strengths), and most optics codes with firstorder matching (or fitting) capabilities can find a solution to this type of problem. However, the solutions are *not* unique. It can be difficult to determine if a solution exists that also meets other criteria (such as the solution with minimum quadrupole power requirement) using the optics codes alone. The PBO Lab Optimization Module was used to explore for such solutions.

The transfer line problem studied is a variation of the linac intertank matching section named "Example B" in reference [7] with the radiofrequency elements removed so that the line has only magnetic elements and drifts. This transfer line is referred to as "Example B – Modified". Figure 2 shows a PBO Lab iconic representation of the transfer line. The four field gradients of quadrupoles labeled QD-1 to QD-4 are adjusted in the optimization.

Table 1 summarizes the characteristics of four known solutions to the transfer line matching problem. The solutions are ranked in the increasing order of the sum of the magnitudes of the quadrupole gradients (Σ |Gradient i|). All four solutions produce the same desired output beam Twiss parameters, but the transverse phase advances (ψ_x and ψ_y) are different for each solution.



Figure 2: The Example B – Modified beamline problem is representative of typical transfer line matching problems.

Table 1: Characteristics of solutions to the four-quadrupole matching problem (Example B – Modified). All gradients are in Tesla/meter and the phase advances (ψ_x and ψ_y) are in radians.

ID	Gradient 1	Gradient 2	Gradient 3	Gradient 4	$\psi_{\rm x}$	$\Psi_{ m v}$	Σ Gradient i
1	- 20.2647	+ 22.4726	- 19.6899	+ 18.3534	0.4728	0.4744	80.7774
2	- 22.4496	+ 36.6889	- 22.6956	+ 26.1708	0.7690	0.4475	108.0011
3	- 23.3109	+ 24.4553	- 39.4066	+ 22.2276	0.5167	0.6428	113.3990
4	- 23.9339	+ 35.9110	- 34.5967	+ 26.3365	0.7355	0.5934	120.7768

3.2 Optimization Results

The NPSOL program in the PBO Lab Optimization Module was used to look for solutions to the four-

quadrupole matching problem. The goal was to determine whether NPSOL could be used to find a particular solution given in Table 1, for example, solution 1 corresponding to the minimum quad excitation. Several different

formulations of the constraints and merit functions were examined. For all of the results described here, the four nonlinear constraints on the Twiss parameters illustrated in the top half of Figure 1 were utilized. In addition, the polarities of the quadrupoles were maintained by imposing bounds $(0, \pm 50 \text{ T/m})$ on the optimization variables.

Four different objective functions were studied. The functions are shown in the lower window of Figure 1, and are referred to here as A, B, C, D, from top to bottom respectively. Functions A and D are essentially identical, when the quadrupole polarity constraints are considered, and are equal to Σ [Gradient i]. Function B is the sum of the squares of the gradients, Σ (Gradient i)². Function C is the sum of the mismatch factors [7] for the two transverse phase planes. It is marked by an "X" in the "Use" column in the lower window of Figure 1, and the complete expression appears in the Current Objective Function panel of that window.

In addition to different merit functions, the utility of including a fifth nonlinear constraint (Σ |Gradient i|<4 G_{max}) was examined. Formulations of the optimization problem

that included this constraint are designated as A+, B+, C+, D+, corresponding to the four objective functions used, while formulations without this additional constraint are denoted by A-, B-, C- and D-.

Table 2 summarizes key optimization results for three different starting values of the quadrupole gradients, corresponding to initial values of Σ |Gradient i| = 66, 106 and 146 T/m, respectively. When the initial gradients are sufficiently "close" to the desired answer, as illustrated by the ± 16.5 T/m case in Table 2, all NPSOL approaches (as well as TRANSPORT and TRACE 3-D) always found the desired solution. However, when the starting gradients were not close, only the NPSOL formulations with the additional constraint (with $G_{\text{max}} = 25 \text{ T/m}$) consistently found the minimum excitation solution. This constraint was clearly more important than the choice of objective function: only NPSOL problem formulations that included this constraint always found the desired solution. (This result was confirmed by additional case studies using other starting gradients not shown in Table 2.)

Table 2: Solutions found by NPSOL, TRANSPORT (TRN) and TRACE 3-D (T3D) for different initial quadrupole gradients (G). For NPSOL, the results for each of eight different problem formulations (see text) are given. TRACE 3-D and TRANSPORT results give the percentage (±2%) of times that each solution was found.

	Initial G:	±16.5	T/m		±26.5	T/m		±36.5	T/m
ID	NPSOL	TRN	T3D	NPSOL	TRN	T3D	NPSOL	TRN	T3D
1	A±,B±,C±,D±	100%	100%	A+,B+,C+,D+	0%	26%	A+,B+,C+,D+	0%	12%
2		0%	0%		100%	6%		0%	24%
3		0%	0%	B-	0%	36%	A-, B-, C-, D-	0%	42%
_ 4		0%	0%	A-, C-, D-	0%	32%		100%	22%

4 SUMMARY

C-language versions of the three optimization codes LSSOL, NPSOL and MINOS have been integrated into an Optimization Module for the PBO Lab software. Inputs to the PBO Lab particle optics codes are used as variables for any of the optimizers, while the outputs provide parameters to formulate nonlinear constraints and merit functions for the NPSOL and MINOS codes. The ease of rapidly setting up and studying various optimizations has proven useful in finding solutions to problems that are not easily addressed with traditional optics codes alone.

REFERENCES

- [1] G. H. Gillespie and B. W. Hill, Nucl. Instr. Meth. B <u>139</u>, 476-480 (1998).
- [2] N. A. Brown, G. H. Gillespie B. W. Hill, M. C. Lampel, H. Martono and J. M. Moore, Proc. 1998 Euro. Particle Accel. Conf., 1183-1185 (1998).
- [3] G. H. Gillespie, B. W. Hill, H. Martono and J. M. Moore, Nucl. Instr. Meth. B <u>161-163</u>, 1168-1173 (2000).
- [4] D. C. Carey, K. L. Brown and F. Rothacker, "Third-Order TRANSPORT with MAD Input - A Computer

- Program for Designing Charged Particle Beam Transport Systems," SLAC-R-530, 316 pp (1998).
- [5] D. C. Carey, "TURTLE with MAD Input (Trace Unlimited Rays Through Lumped Elements), a Computer Program for Simulating Charged Particle Beam Transport Systems, and DECAY-TURTLE Including Decay Calculations," Fermilab-Pub-99/232, 196 pp (1999).
- [6] A. J. Dragt, et al, "MARYLIE 3.0 User's Manual, A Program for Charged Particle Beam Transport Based on Lie Algebraic Methods (draft)," 721 pp (1999).
- [7] K. Crandall and D. Rusthoi, "TRACE 3-D Documentation," LA-UR-97-886, 106 pp (1997).
- [8] P. E. Gill, S. J. Hammarling, W. Murray, M. A. Saunders, M. H. Wright, "User's Guide for LSSOL (Version 1.0): A Fortran Package Constrained Linear Least-Squares and Convex Quadratic Programming," Stanford University Department of Operations Research Report No. SOL 86-1, 38 pp (1986).
- [9] P. E. Gill, W. Murray, M. A. Saunders, M. H. Wright, "User's Guide for NPSOL 5.0: A Fortran Package for Nonlinear Programming," Stanford Univ. Dept. Op. Research, Rpt. SOL 86-2R, 44 pp (1998).
- [10] B. A. Murtagh and M. A. Saunders, "MINOS 5.5 User's Guide," Stanford Univ. Dept. Op. Research, Rpt. SOL 83-20R, 145 pp (1998).