PBO Lab™ 2.2
(Particle Beam Optics Laboratory)
User Manual Supplement:
Optimization Module

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PBO Lab 2.2 User Manual Supplement: Optimization Module

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Included with this supplement are the following documents, reproduced and distributed as part of a license agreement between G. H. Gillespie Associates, Inc. and the Board of Trustees of the Leland Stanford Junior University ("STANFORD"):

Appendix A: "NPSOL User's Guide"

User's Guide for NPSOL (Version 4.0), by Philip E. Gill, Walter Murray, Michael A. Saunders and Margaret H Wright.
Department of Operations Research Stanford University Technical Report SOL 86-2, January 1986.
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Appendix B: "MINOS User's Guide"

MINOS 5.4 User's Guide, by Bruce A. Murtagh and Michael A. Saunders.
Department of Operations Research Stanford University Technical Report SOL 83-20R, December 1986, Revised Jan 1987, Mar 1993, Feb 1995.
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Appendix C: "LSSOL User's Guide"

User's Guide for LSSOL (Version 1.0), by Philip E. Gill, Sven J. Hammarling, Walter Murray, Michael A. Saunders and Margaret H Wright.
Department of Operations Research Stanford University Technical Report SOL 86-1, January 1986.
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NPSOL is a sophisticated nonlinear, constrained, optimization program developed at Stanford University's System Optimization Laboratory. It uses a sequential quadratic programming (SQP) algorithm that evaluates the gradient of the objective function, and the Jacobian of the constraint functions, to determine which variables should be varied next in the search, and then treats the problem as a least squares optimization locally. Constraints are satisfied first, and then the code determines if an optimal (locally minimal) solution has been achieved. NPSOL is designed to work on problems in which the variables are tightly connected through linear and nonlinear constraints, e.g. in which the matrices dealt with are dense.

MINOS is designed to solve large-scale optimization problems that can include linear and nonlinear constraints. A system of methods and algorithms are harmoniously combined to address small and large problems in four main problem areas: linear programming, unconstrained optimization, linearly constrained optimization, and nonlinearly constrained optimization. Advanced versions of several classical optimization algorithms are included: the simplex method, a quas-Newtonian method, the reduced-gradient method, and a projected Lagragian method.

Table of Contents

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1. Optimization Tool Module

The Optimization Tool Module for the Particle Beam Optics Laboratory combines three optimization programs: LSSOL, NPSOL and MINOS with a variety of charged particle optics and accelerator simulation codes, all within a single intuitive graphic user interface. This combination yields an advanced analysis and design tool that offers users the ability to significantly improve the optimization process by providing an environment to easily formulate beamline optimization tasks, and to solve problems in an intuitive way.

The Optimization Tool Module for the Particle Beam Optics Laboratory provides three optimization engines, integrated with PBO Lab Application Modules for charged particle optics and accelerator simulations.

LSSOL is a constrained linear least-squares and quadratic optimization program. The NPSOL and MINOS programs are both constrained nonlinear optimization programs.

An optimization problem is specified in terms of variables, constraints and stored output parameters. There are three types of constraints: linear, nonlinear and the objective function. The optimization engine attempts to find values for the variables that will satisfy the constraints.

Optimization problems are defined in terms of user specified variables, constraints and stored output parameters.

Optimization variables are selected from beamline element parameters. Linear constraints are defined in terms of these Optimization Variables. The objective function and nonlinear constraints are defined in terms of variables and stored output parameters. Stored output parameters, from PBO Lab Application Modules (TRANSPORT and TRACE 3-D) are selected by the user and computed by the respective simulation codes.

Optimization variables and stored output parameters are selected in the beamline model and used to define Optimization Constraints.

The Optimization Tool allows optimization problems to be defined over multiple beamline Model Documents and supports aliasing beamline elements between Documents. Multiple beamlines may share (Alias) individual elements or entire beamline segments. The Optimization Tool can also be used in combination with the fitting/matching capabilities of individual Application Modules to perform a hierarchal optimization problem.

Optimization problems can be defined over multiple beamline Model Documents and beamline elements can be shared between Documents.

The Optimization Tool can also be used for hierarchal optimization using the native fitting/matching capabilities of individual Application Modules.

Multiple Model Mode

The Optimization Tool supports the specification of an Optimization Problem that can share (Alias) beamline elements between multiple beamline models in separate Document Windows. This Multiple Model Mode is selected with a user preference as illustrated in Figure 1. To use the Optimization Tool Module, the PBO Lab Preference for Application Type must be set to Multiple Model Mode. This is the default setting when the Optimization Tool Module is installed. Figure 2 illustrates the Optimizer Problem Window that is opened when the PBO Lab application is launched in the Multiple Model Mode.

To use the Optimization Tool Module, the PBO Lab Preference for Application Type must be set to Multiple Model Mode.

If the PBO Lab Application Type Preference is set to Single Model Mode then the Optimizer Problem Window will not be opened and the standard Document Window will be opened. When you change the Application Type Preference, PBO Lab must be restarted in order for the change to take effect. Refer to the *PBO Lab Preferences* Section in the *Analysis Tools* Chapter of the *PBO Lab User Manual* for a description of the Application Type Preference.

PBO Lab must be restarted in order for changes in the Application Type Preference to take effect.

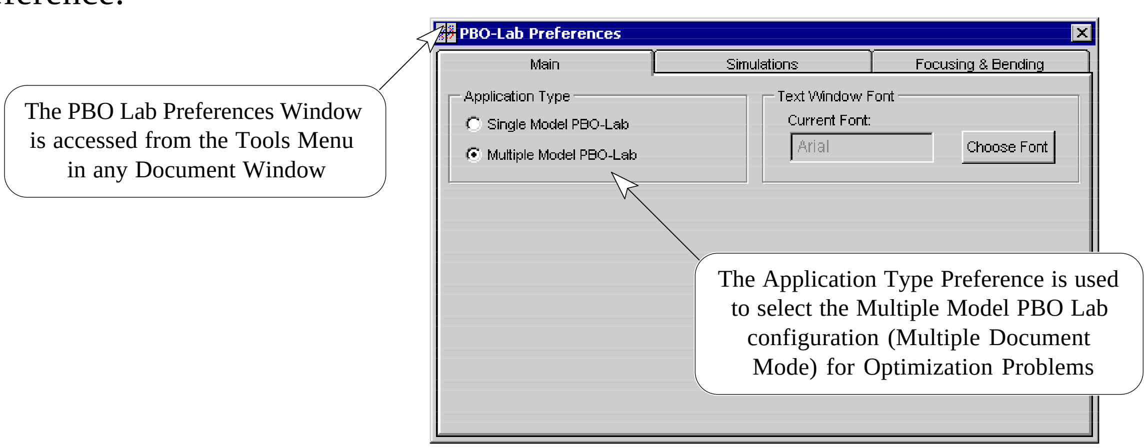

Figure 1. Application Type Preference - Single and Multiple Document Modes.

The Single Model Application Type (Single Document Mode), is the standard configuration for PBO Lab when the Optimization Tool is not installed. The Multiple Model Application Type (Multiple Document Mode) modifies the user interface so that a persistent link can be maintained between multiple Document Windows, allowing beamline elements to be shared (Aliased) between separate beamlines. The Optimizer Problem Window, shown in Figure 2, contains a list of any beamline Model Documents that are linked in the Optimizer Problem. Double-click a model in the Problem Window to open the corresponding beamline Model Document Window.

The Single Model Application Type is the standard configuration when the Optimization Tool is not installed, since most problems do not require multiple beamline Model Documents with shared (Aliased) beamline elements.

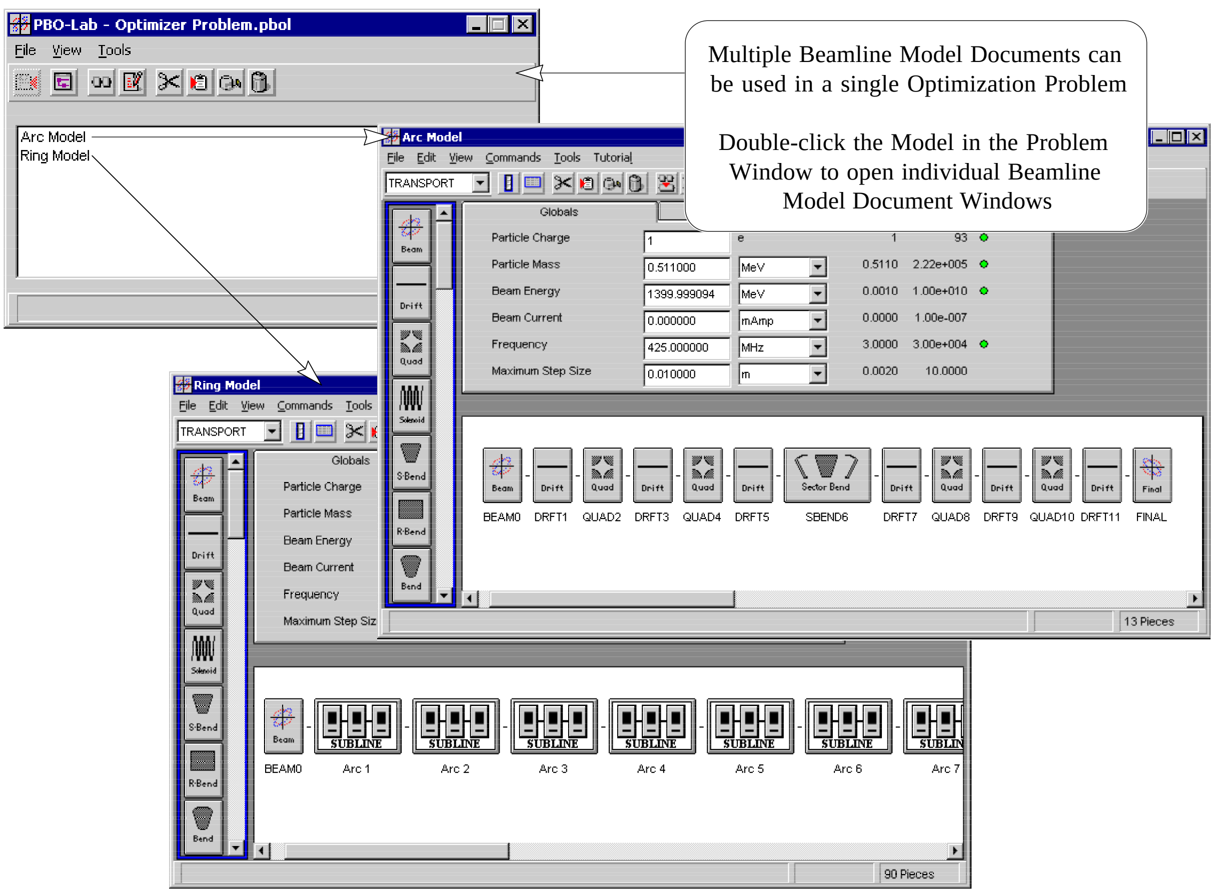

Figure 2. Optimizer Problem Window and Corresponding Document Windows.

The user interface for individual beamline Model Document Windows is the same for both the Single and Multiple Document configurations and is described in the main *PBO Lab User Manual*. However, the Optimizer Problem Window, which is used in the Multiple Document Mode is described in this Supplement.

The Document Windows user interface is the same for both the Single and Multiple Document configurations and is described in the main PBO Lab User Manual.

Optimizer Problem Window

The Optimizer Problem Window is provided when PBO Lab is setup in the Multiple Model Mode. The Multiple Model (Document) Mode is required to run optimization problems, even for problems with single beamline Model Document. The Optimizer Problem Window, shown in Figure 3, is used to execute the Optimization Tool, examine Optimization Variables, Stored Parameters and Constraints, as well as providing a means to define a single Optimization Problem across multiple beamline models.

The Optimizer Problem Window is used to organize multiple beamline Document Windows for a single Optimization Problem. Document Windows are used to graphically construct beamlines, modify input parameters, select optimization variables and Stored Output Parameters.

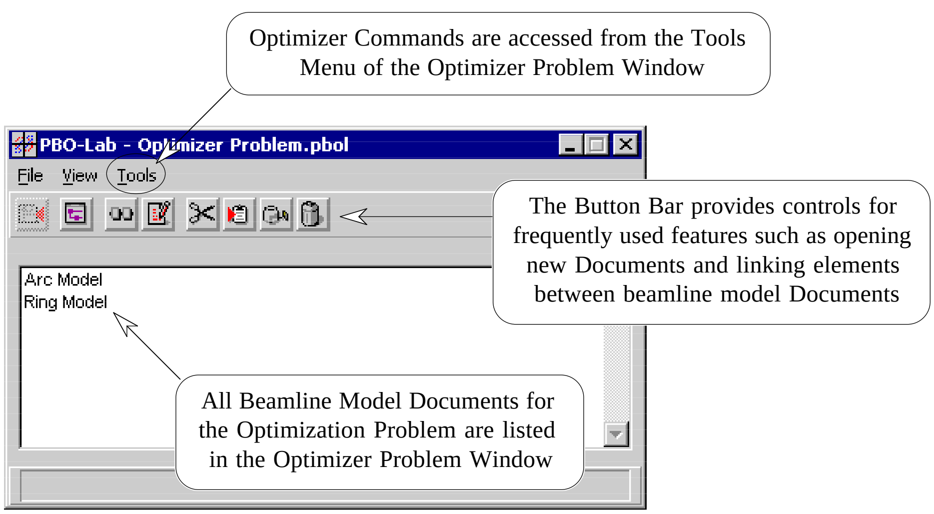

Figure 3. Optimizer Problem Window.

Individual Document Windows, created and accessed from the Problem Window are used to graphically construct beamlines, modify input parameters, select Optimization Variables and define application-specific Stored Output Parameters. The Problem Window contains a Menu Bar, Button Bar and a scrolling list of beamline Model Documents for the Optimizer Problem.

Optimization Engines

The PBO Lab Optimization Module includes three optimization programs: LSSOL, NPSOL and MINOS. LSSOL is a constrained linear least-squares and quadratic optimization program. NPSOL and MINOS are both constrained nonlinear optimization programs, but the two packages use different approaches and are applied to different types of optimization problems. LSSOL and NPSOL are a collection of FORTRAN subroutines developed as a Systems Optimization Laboratory (SOL) by the Department of Operations Research at Stanford University. MINOS is also a FORTRAN code developed at Stanford University. LSSOL finds the solution for a purely quadratic objective function, with linear constraints. NPSOL uses a sequential quadratic programming (SQP) algorithm to address more complicated nonlinear problems. The SQP algorithm evaluates the gradient of the objective (Merit) function, and the Jacobian of the constraint functions, to determine which of the variables should be varied next in the search, and then treats the problem as a least squares optimization locally. Constraints are satisfied first, and then the code determines if an optimal (locally minimal) solution has been achieved. MINOS was developed to solve nonlinear optimization problems which use very large sparse matrices in the representation of the problem to be solved.

The PBO Lab Optimization Module includes three different optimization programs: LSSOL, NPSOL and MINOS.

MINOS addresses problems that can be formulated in slightly more general terms than available in NPSOL.

C-language versions of all three optimization engines have been integrated into the PBO Lab graphic user interface and underlying beamline object model. Any input parameter to a PBO Lab Application Module (TRANSPORT, TURTLE, TRACE 3D or MARYLIE) can be selected as an optimization variable. Stored diagnostic output parameters from the different computational programs are used to formulate the nonlinear constraints and/or merit (objective) function for optimization.

Inputs to PBO Lab Application Modules are used as variables for any of the optimizers, while the outputs provide parameters to formulate nonlinear constraints and merit functions for optimization.

Optimization problems are completely defined using the PBO Lab graphic user interface. Although the optimization programs are complex, the input requirements for each are seamlessly integrated with the different PBO Lab Application Modules in a single easy-to-use graphic interface.

Diagnostic output from the different computational programs is dynamically shared with the different optimization engines and optimization variables are automatically updated in the beamline model during the optimization process. No user written functions (FUNCON, FUNOBJ) are required to define an optimization problem. PBO Lab provides graphic user interface windows for defining the Optimization Objective (merit) function and Optimizer Constraint functions. Optimization Variables and Stored Output Parameters are easily selected in the PBO Lab graphic beamline representation, the same way fitting variables and constraints are specified for the different computational programs.

There are no user written functions required to define an optimization problem in PBO Lab. Graphic user interface windows are provided for specifying the Optimization Objective function and Constraint functions. Optimization Variables and Stored Output Parameters are easily selected in the PBO Lab graphical beamline representation.

Optimization problem setup is similar for each of the optimization programs. Although each has a separate window for specifying objective and constraint functions, these windows are very similar in terms of the user interface.

Setting up a problem for different optimization engines is easy. Optimization Variables and Stored Output Parameters are setup in the beamline model and are independent of the optimization program selection.

Each Optimization program has a corresponding sub-menu in the Tools Menu and in the View Menu of the Optimizer Problem Window. The Tools sub-menus contain the commands to Run a particular optimization program. Each sub-menu also contains a Constrains command that is used to open the Optimization Constraints Window for each of the Optimization programs. The NPSOL and MINOS sub-menus also contain commands to access Watch Setup Windows that are used to select Watch Values from among the Optimization Variables and constraints. These selections will be displayed dynamically in a Watch Window during the optimization process.

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2. *Optimizer Menus & Controls*

In the Multiple Document Mode, the user is provided with a Optimizer Problem Window that contains the *File*, *View* and *Tool* Menus as illustrated in Figure 4. The File Menu is similar to the File Menu in the Document Windows for the Single Document Mode. There are standard commands for opening, closing and saving Optimizer Problem files. An Optimizer Problem may contain multiple beamline Model Documents, but is saved as a single PBO Lab file. The View Menu has commands for opening the optimizer output files in Text Editor Windows for each of the optimization engines. The Optimizer Submenus in the Tools Menu contain commands to run Optimization Problems and commands that access user interface windows for Optimization Constraints and variables, application-specific stored output parameters and for specifying variable order and optimizer options. Submenus are provided for each of the optimization engines in the Tools Menu. These commands are described in the Optimizer Commands Section of this Supplement.

In the Multiple Document Mode, the user is provided with a Optimizer Problem Window that contains the File, View and Tool Menus for the Optimizer.

The Optimizer Tools Menu contains commands to set up and run Optimization Problems using any of the optimization engines.

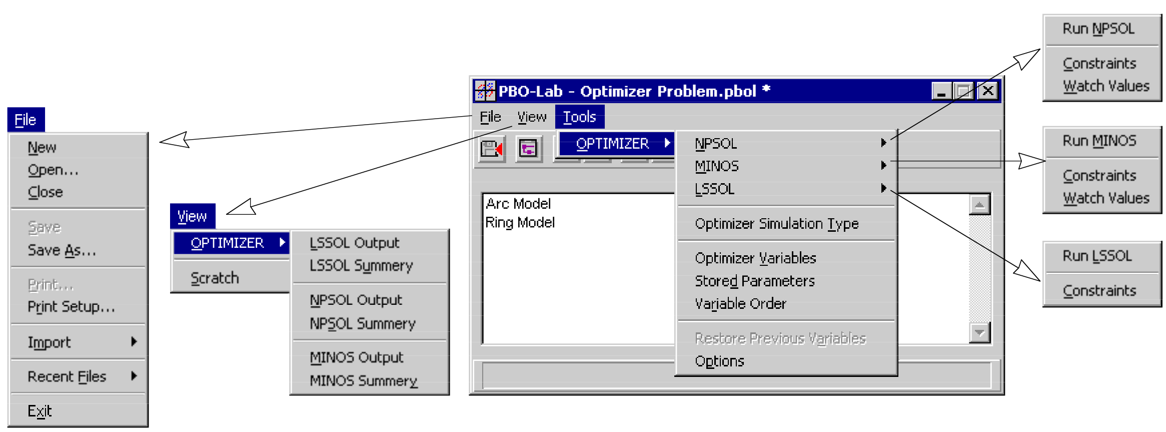
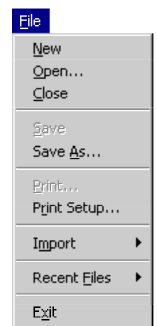


Figure 4. Menus in the Optimizer Problem Window.

Optimizer File Menu

The commands in the File Menu of the Optimizer Problem Window are to create *New* Optimizer Problems, *Open* existing Problems, *Close* the current Problem Window and *Save* the current Optimizer Problem. These commands do not refer to beamline Model Documents in the Optimizer Problem. For example, the *New* command will create and open a new untitled Optimizer Problem Window. In order to create a new beamline Model Document Window in the current Optimizer Problem Window, use the Button Bar in the Problem Window. Refer to the Optimizer Button Bar Section in this Chapter.

The File Menu of the Optimizer Problem Window has commands to create New Optimizer Problems, Open existing Problems, Close the current Problem Window and Save the current Optimizer Problem.



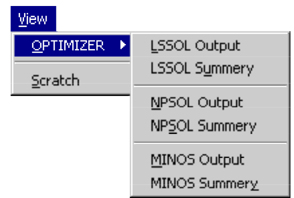
The *Print* and *Print Setup* commands are standard File Menu commands that are identical to the File commands in the Document Window. The *Import* and *Recent Files* Submenus are also identical to the commands in the File Menu of the Document Window. Refer to the *Menu Bar* Section in the *User Interface* Chapter of the main *PBO Lab User Manual* for a description of these commands.

The last command in the File menu of the Problem Window is *Exit*, which is used to close all application windows and quit the PBO Lab application.

Optimizer View Menu

The commands in the View Menu of the Optimizer Problem Window are used to open the native output and summary files produced by each of the optimization engines. There are preferences that can be set in the Optimizer Options Window that will cause these files to be opened automatically after executing the optimizer. Refer to the *Optimizer Options* Section in this Chapter. The View commands do not execute optimization, they simply allow output files previously generated to be viewed in PBO Lab Text Edit Windows.

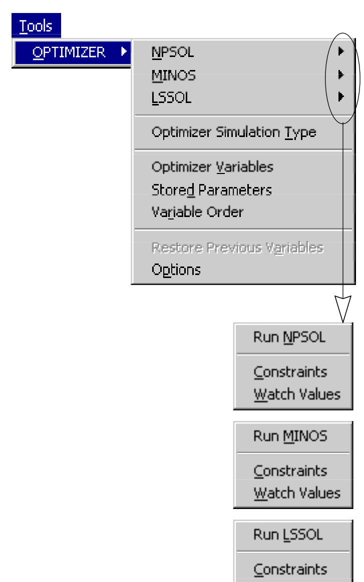
The View Menu is used to open the native output files produced by the different optimizer engines.



Optimizer Tools Menu

The commands in the *Tools* Menu of the Optimizer Problem Window are used to setup and run Optimization Problems using any of the optimization engines. There are also commands to access user interface windows that list Optimization Constraints and variables, application-specific stored output parameters and allow specification of variable order and optimizer options.

The commands in the Tools Menu of the Optimizer Problem Window are used to setup and run Optimization Problems. Submenus are provided for each of the optimizer engines.



The Tools Menu is divided into four groups of commands. The first group contains the main execution submenus for each of the optimizer engines. The *Run...* commands in each submenu are used to start the optimization process using the selected engine. The NPSOL and MINOS submenus also have commands for opening Optimizer Constraint Windows and Watch Value Setup Windows. The LSSOL submenu contains a command for accessing the LSSOL Constraints Windows but does not provide a Watch Values Setup command.

The second command group in the Tools Menu has one command that is used to access the Optics Calculation Options Window.

Optics Calculation Options Window

The third group of commands in the Tools Menu provides access to dynamic list windows for user specified Optimization Variables and application-specific Stored Output Parameters. As well as a command for opening the Variable Order Window. Unlike Optimization Constraints, which are specific to each optimization engine, the Optimization Variables and Stored Output Parameters are selected in the beamline Model Document(s) and are not specific to a particular optimization engine. The list windows for Optimization Variables and Stored Output Parameters provide a convenient list of all the variables and stored parameters that have been selected in the beamline model document(s). Double-clicking an entry in a list window will open the Piece Window in the beamline model for that selection.

Optimization Variables List Window

Stored Output Parameters List Window

Variable Order Window

The last command group in the Tools Menu has two commands. The *Restore Previous Variables* command is used to restore Optimization Variables in the beamline model to previous values (values prior to the last optimization process). The last command in the Tools Menu opens the Optimizer Options Window. This window contains three tab panels (one for each of the optimizer engines) containing native optimization options as well as some PBO Lab user interface Preferences.

Restore Previous Variables Command

Optimizer Options Window

Optimizer Button Bar

The Button Bar of the Optimizer Problem Window provides controls for a variety of problem setup features as illustrated in Figure 5. The first button saves the Optimization Problem file. One or more beamline Model Documents from other Optimization Problem files can be added to the current Optimizer Problem with the second button. New Model Documents can be added to the Optimization Problem with the third button and may be renamed with the fourth button. Cut, Copy and Paste buttons allow Model Documents to be moved between Optimization Problem files and the Delete button removes a Model Document from the Optimization Problem.

The Button Bar of the Optimizer Problem Window provides controls for a variety of problem setup features.

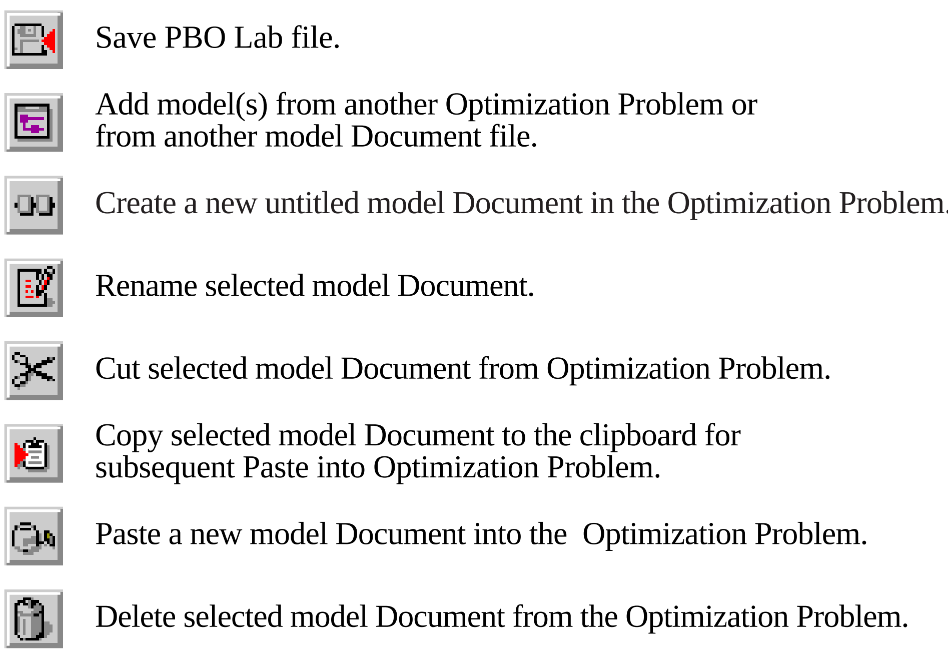


Figure 5. Optimizer Problem Window Button Bar Controls.

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3. Optimization Variables

Optimization Variables are selected in Special Parameter Settings Windows as illustrated in Figure 6.

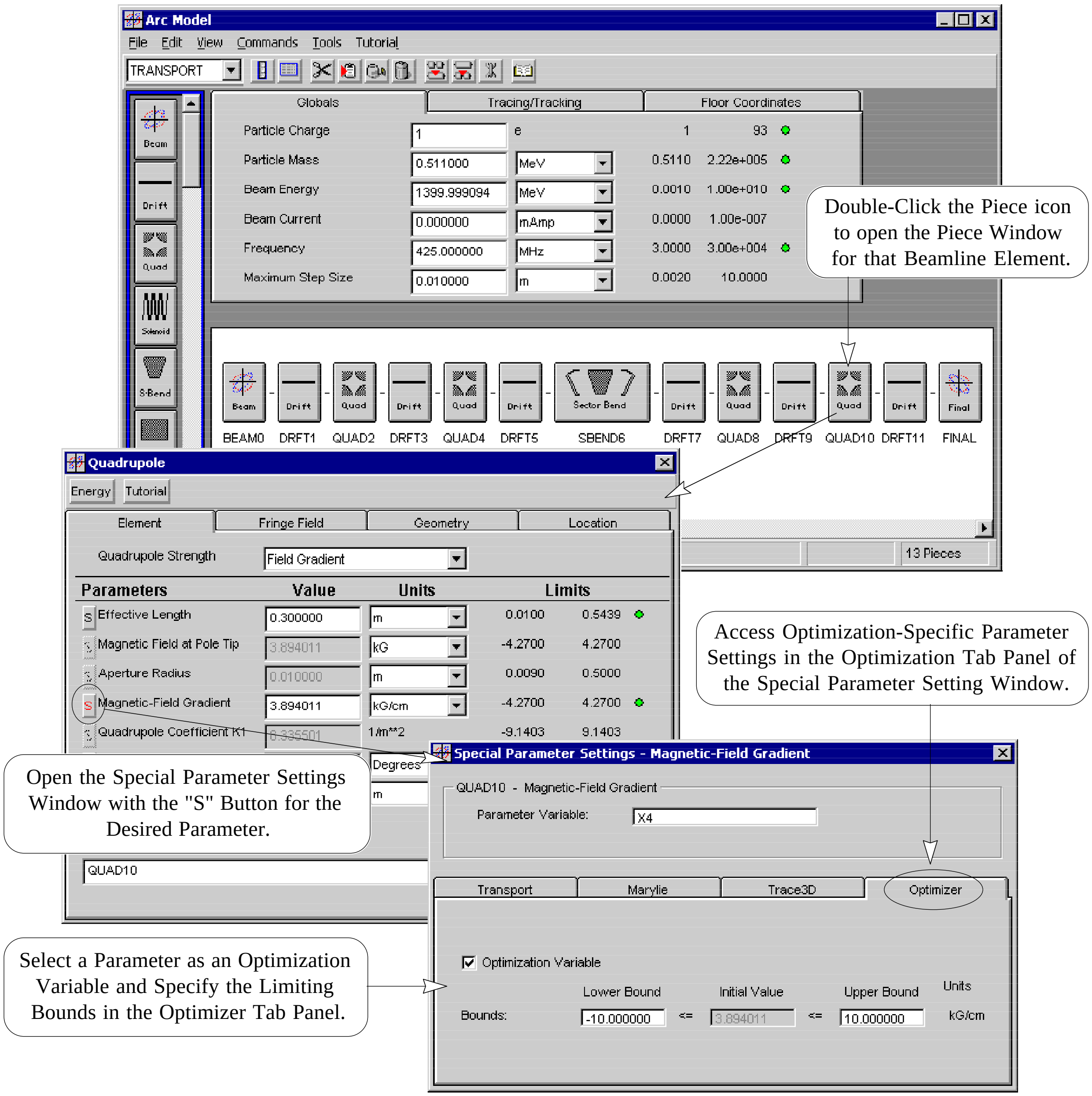

Figure 6. User Interface for Selecting Optimization Variables.

The user interface for selecting Optimization Variables is the same as that used to select fitting variables for the different Application Modules. Input parameters for beamline elements are accessed by double-clicking Piece icons in the beamline model of Document Windows. Figure 6 illustrates opening a Quadrupole Piece Window and selecting the Magnetic-Field Gradient Parameter as an Optimizer Variable.

The user interface for selecting Optimization Variables is the same as that used to select fitting variables for the different Application Modules.

Applicable parameters have Special "S" buttons that are used to access Special Parameter Settings Windows. An example of a Special Parameter Settings Window is shown in Figure 6. The "S-Windows" have tab panels that provide access to application-specific options for installed Application Modules and Tools. The tab panel for the Optimization Tool is shown in Figure 6. It provides a check box that is used to toggle the selection of the parameter as an Optimization Variable, and has inputs for specifying limiting bounds on the variable. The initial value for the variable is specified directly in the Piece Window.

Optimization Variables are selected in the Special Parameter Settings Windows for beamline model Pieces.

Double-click an icon in the beamline model to open a Piece Window and press the "S" button to the right of the desired parameter in the Piece Window. This will open the corresponding Special Parameter Settings Window ("S-Window") for that parameter. Select the *Optimizer* tab panel in the S-Window and click on the *Optimizer Variable* check box. The *Optimizer* tab panel is also used to specify the lower and upper limits that the optimizer will use as bounds for the variable. At the top of the S-Window is a Symbolic Parameter Name field that will automatically be assigned when the Optimizer Variable check box is selected. You may enter your own symbolic name for the Optimizer Variable in this field, but the variable must be named.

Optimization Variables must be named at the top of the S-Window. A Symbolic Parameter Name will be automatically assigned when the Optimizer Variable check box is selected or you may enter your own name.

Variables List Window

The Tools menu provides a command for opening the Variables List Window, illustrated in Figure 7, which lists all of the Optimization Variables for the entire Optimization Problem.

The Tools menu provides a command for opening the Optimization Variables List Window.

All of the Optimization Variables selected over all the beamline models in an Optimization Problem are displayed in the Variables List Window. Double-clicking an entry in the List Window will open the Piece Window for that selection as illustrated in Figure 7. This provides quick access to all of the Optimization Variables specified for beamline and across multiple beamline models as well.

For Optimization Problems with multiple beamline models, the Variables List Window includes all Variables from all of the beamline Model Documents included in the Optimizer Problem Window.

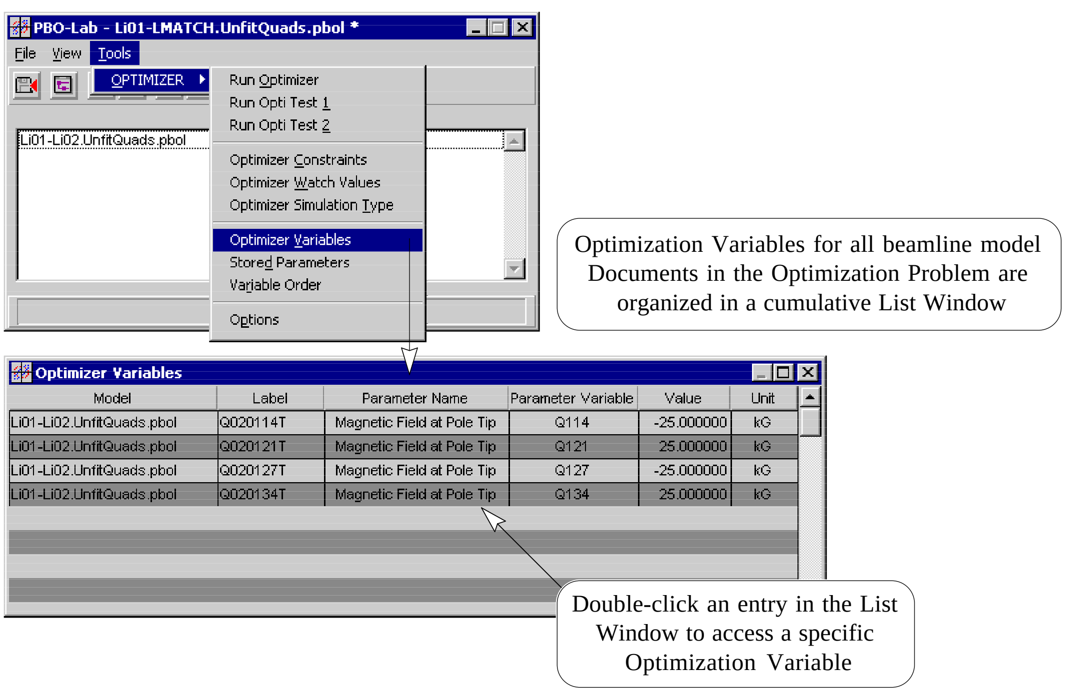

Figure 7. Optimization Variables List Window.

Variable Order Window

The Variable Order Window, illustrated in Figure 8, is accessed from the Tools Menu and is used to change the order that will be used to setup the Optimizer native inputs. Variables are listed by the order in which they are selected, but this order may be changed in the Variable Order Window.

The Tools menu provides a command for opening the Optimizer Variable Order Window.

The Variable Order Window can be used to change the order in which Variables are specified for the Optimization engine. It may be desirable in some cases to start the problem with a different variable order. Refer to the *User's Guide for NPSOL* for a description of variable order.

The Variable Order Window can be used to change the order in which Variables are specified for the Optimization engine.

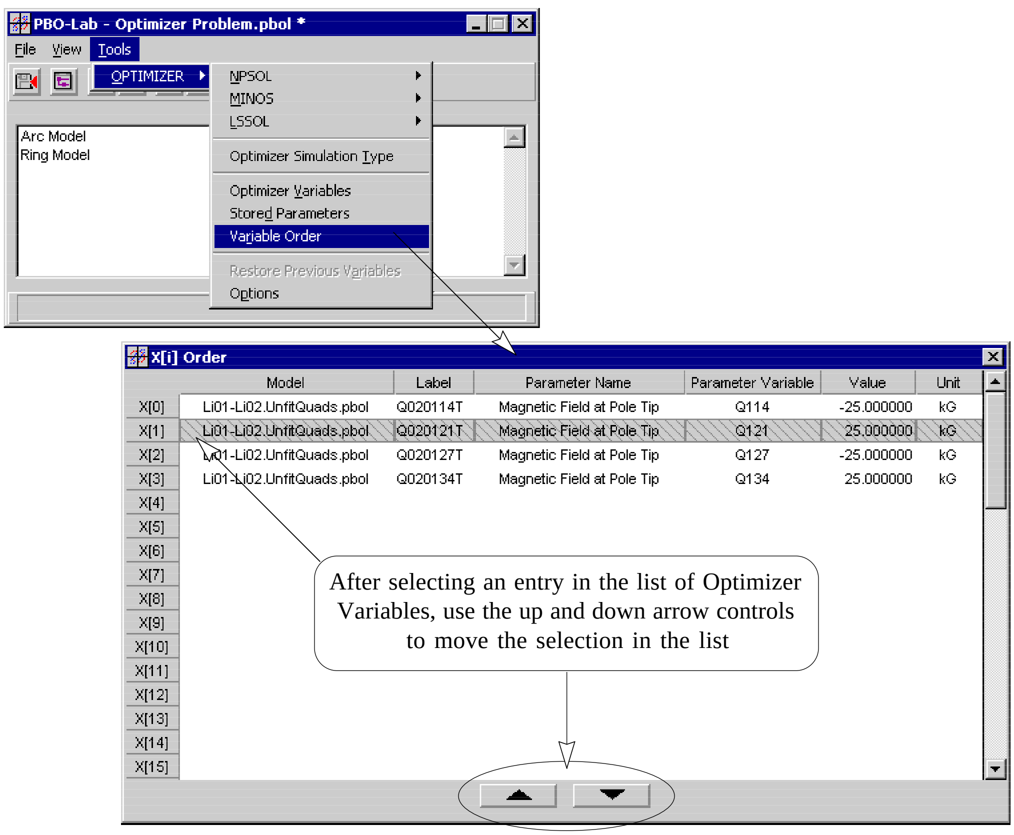

Figure 8. Changing the Order of Optimization Variables.

4. Stored Output Parameters

Stored Output Parameters are application-specific diagnostic output results that are defined with a user-specified name and can be used in the definition of algebraic expressions for Nonlinear Constraints and the Optimization Objective Function.

Stored Parameters are specified at specific locations in the beamline model(s) using a Marker or Final Piece.

Both Linear and Nonlinear Constraints, as well as the Optimization Objective Function are defined as algebraic expressions of user specified Optimization Variables and application-specific Stored Output Parameters. The Optimizer Tool can use application-specific Stored Parameters for the definition of Nonlinear Constraint Expressions and for defining the Objective Function. However, Linear Constraints can only be specified in terms of Optimization Variables selected from beamline model parameters, not in terms of application-specific Stored Output Parameters.

The Optimizer Tool can use application-specific Stored Output Parameters for the definition of Nonlinear Constraint Expressions and for defining the Objective Function.

Stored Parameters are specified at specific locations in the beamline model(s) using a Marker or Final Piece as illustrated in Figure 9. Marker Pieces are inserted into the beamline model by dragging the Piece icon from the Palette Bar to the location in the beamline where the value of a Stored Output Parameter should be collected (TRANSPORT). A Final Piece may also be used for this purpose, since it is a special case of the Marker Piece that is typically used at the end of a beamline model (TRANSPORT and TRACE 3D).

Stored Output Parameters are specified at specific locations in the beamline model(s) using Marker or Final Pieces.

Information regarding the Marker Piece can be found in the main *PBO Lab User Manual*. Individual Application Module *Manual Supplements* contain additional information regarding the Marker Piece and the specification of Stored Parameters for each Module.

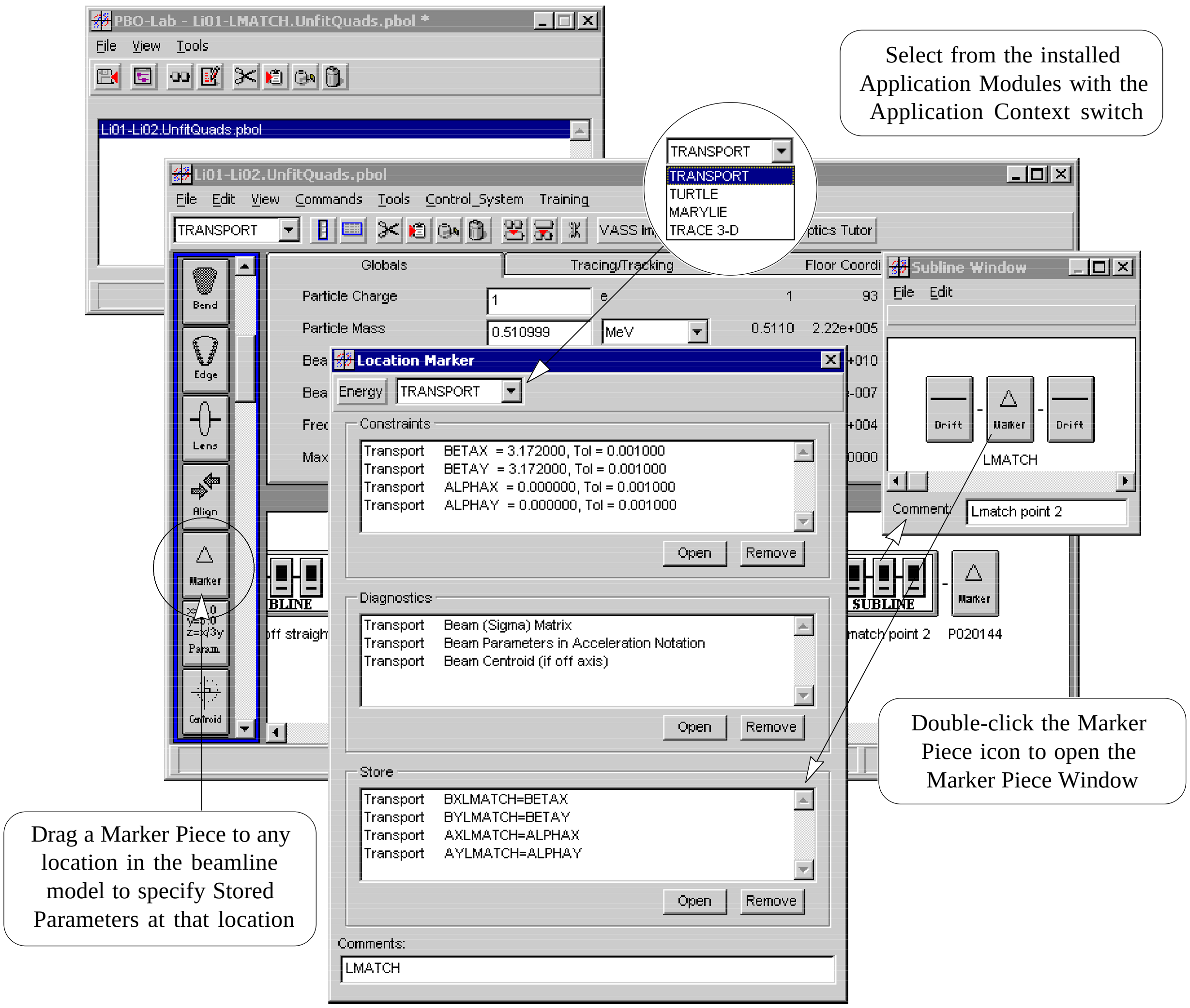

Figure 9. Marker and Final Piece Windows.

The Marker and Final Piece Windows are application-independent. They have an *Application Context* switch that is used to open the appropriate application-specific user interface window for Constraints, Diagnostics or Stored Parameters. There are three panels in the Marker (and Final) Piece Windows. The *Open* buttons in the three panels will open the application-specific user interface window for the current setting of the Application Context switch.

The Application Context switch in the Marker Piece Window is used to open the appropriate application-specific user interface window for TRANSPORT Stored Parameters.

For example, when the Application Context is set for the TRANSPORT Application Module, then the *Open* button in the Stored Parameters panel will open the application-specific Transport Stored Parameters Window as illustrated in Figure 10.

The scrolling lists in each of the three panels of the Marker Piece Window display all selections, independent of the Application Context, and individual selections may be deleted with the *Remove* buttons without changing the Application Context switch or opening the application-specific user interface window.

The Marker and Final Pieces are used to specify location-specific Constraints, Diagnostics and Stored Parameters for individual Application Modules.

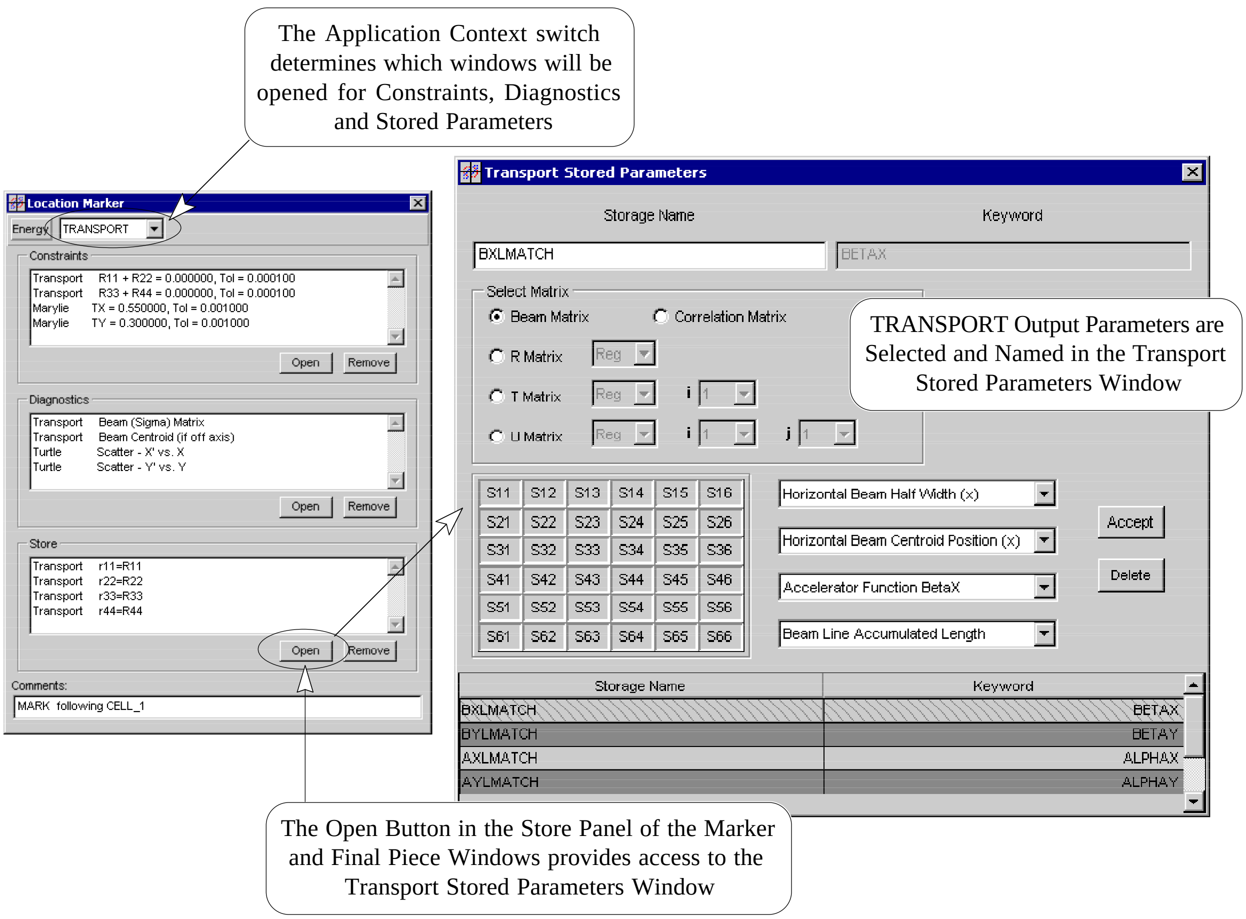

Figure 10. Application-Specific Windows Accessed from Marker Pieces.

The Constraints panel and Diagnostics panel of the Marker and Final Piece Windows are used for application-specific Fitting Constraints and Output Diagnostics. The Output Diagnostics are used to specify various application-specific output data at the location of the Marker in the beamline model and are not required for optimization. The Constraints are also application-specific and are only required for the specification of a hierarchical Optimization Problem in which local application-specific fitting is combined with higher level optimization.

Application-specific Fitting Constraints and Diagnostics are not required to define an Optimization Problem.

Application-specific Constraints are not the same as Optimization Constraints. However, a hierarchical Optimization Problem can be formulated in which local application-specific fitting constraints are combined with the higher level optimization constraints used by the Optimization Tool.

The Stored Parameters panel in the Marker Piece Window is used with the Optimizer Tool to define application-specific Stored Output Parameters that will be used in the definition of the Optimization Objective Function and for use in Nonlinear Optimization Constraints. Stored Parameters are selected and defined by a symbolic name which can then be used in algebraic expressions of the Objective Function and Nonlinear Constraints. The values for these application-specific Output Parameters are calculated by the Application Module and collected at the location of the Marker (or Final) Piece in the beamline model. The different types of Stored Output Parameters that may chosen are dependent on the selected Application Module.

Stored Parameters are selected and defined by a symbolic name which can then be used in algebraic expressions of the Objective Function and Nonlinear Constraints.

TRANSPORT Stored Parameters

The TRANSPORT Application Module supports a variety of Stored Output Parameters that are listed in Table 1. The user interface for selecting TRANSPORT Stored Output Parameters is user friendly and does not require specific knowledge of all the TRANSPORT keywords for storage parameters.

Table 1. TRANSPORT Stored Output Parameters.

Correlation Matrix (i,j =1,6)	**Keyword**
Beam Correlation Matrix Element	C ij

Beam Matrix (i,j =1,6)	**Keyword**
Reduced Sigma Matrix Element	S ij

Transfer Matrices (i,j,k,l =1,6)	**Keyword**
1st-Order Transfer Matrix Element	R ij
2nd-Order Transfer Matrix Element	T ijk
3rd-Order Transfer Matrix Element	U ijkl

Transfer Matrices (i,j,k,l =1,6)	**Keyword**
1st-Order Auxiliary Matrix	RA ij
2nd-Order Auxiliary Matrix	TA ijk
3rd-Order Auxiliary Matrix	UA ijkl

Beam Centroids	**Keyword**
Horizontal Beam Centroid Position	XC
Horizontal Beam Centroid Angle	XPC
Vertical Beam Centroid Position	YC
Vertical Beam Centroid Angle	YPC
Longitudinal Beam Centroid Position	DLC
Longitudinal Beam Centroid Angle	DELC

Beam Envelopes	**Keyword**
Horizontal Beam Half Width	XBEAM
Horizontal Beam Half Angle	XPBEAM
Vertical Beam Half Width	YBEAM
Vertical Beam Half Angle	YPBEAM
Longitudinal Beam Half Width	LBEAM
Longitudinal Beam Half Angle	DELBEAM

Floor Coordinates	**Keyword**
Beamline Accumulated Length	L
Floor Coordinate X Value	XFLOOR
Floor Coordinate Y Value	YFLOOR
Floor Coordinate Z Value	ZFLOOR
View Reference Trajectory Angle	YAW
Reference Trajectory Horz. Angle	PITCH
Net Rotation Angle about Trajectory	ROLL
Elevation	ELEVATION

Lattice Functions	**Keyword**
Accelerator Function BetaX	BETAX
Accelerator Function AlphaX	ALPHAX
Accelerator Function BetaY	BETAY
Accelerator Function AlphaY	ALPHAY
Accelerator Function EtaX	ETAX
Accelerator Function DeltaX	DETAX
Accelerator Function EtaY	ETAY
Accelerator Function DeltaY	DETAY

Figure 11 illustrates the different controls and pop ups in the Transport Stored Parameters Window. All of the selections listed in Table 1 can be made from the various controls and pop ups in the Transport Stored Parameters Window, without having to know the TRANSPORT keywords.

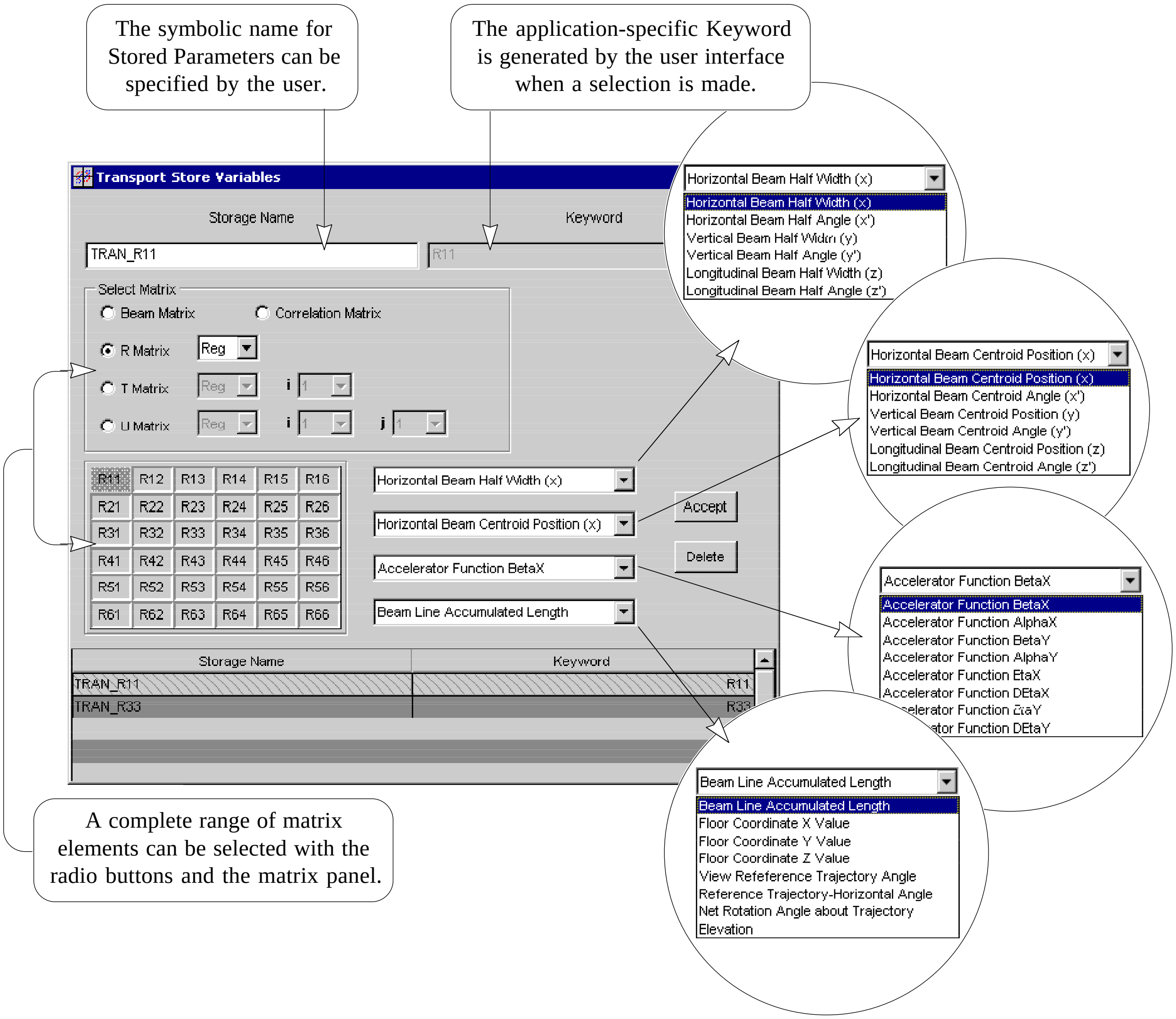

Figure 11. TRANSPORT Stored Output Parameters Window.

Refer to the *TRANSPORT Documentation* for a technical description of the TRANSPORT Output Parameters. The *PBO Lab User Manual Supplement for the TRANSPORT Application Module* also describes the selection of location-specific Stored Output Parameters in the *Marker Piece* Section.

TRACE 3D Stored Output Parameters

Specifying Stored Output Parameters for the TRACE 3D Application Module is similar to selecting TRANSPORT Stored Parameters, except TRACE 3D only supports diagnostic outputs at the end of a beamline model. To define Stored Parameters for TRACE 3D, a Final Piece must be placed at the end of the beamline in the Model Document Window. Double-clicking the Final Piece in the beamline will open the Final Piece Window as illustrated in Figure 12.

The Final Piece is used at the end of a beamline model to specify Stored Output Parameters for the TRACE 3D Application Module.

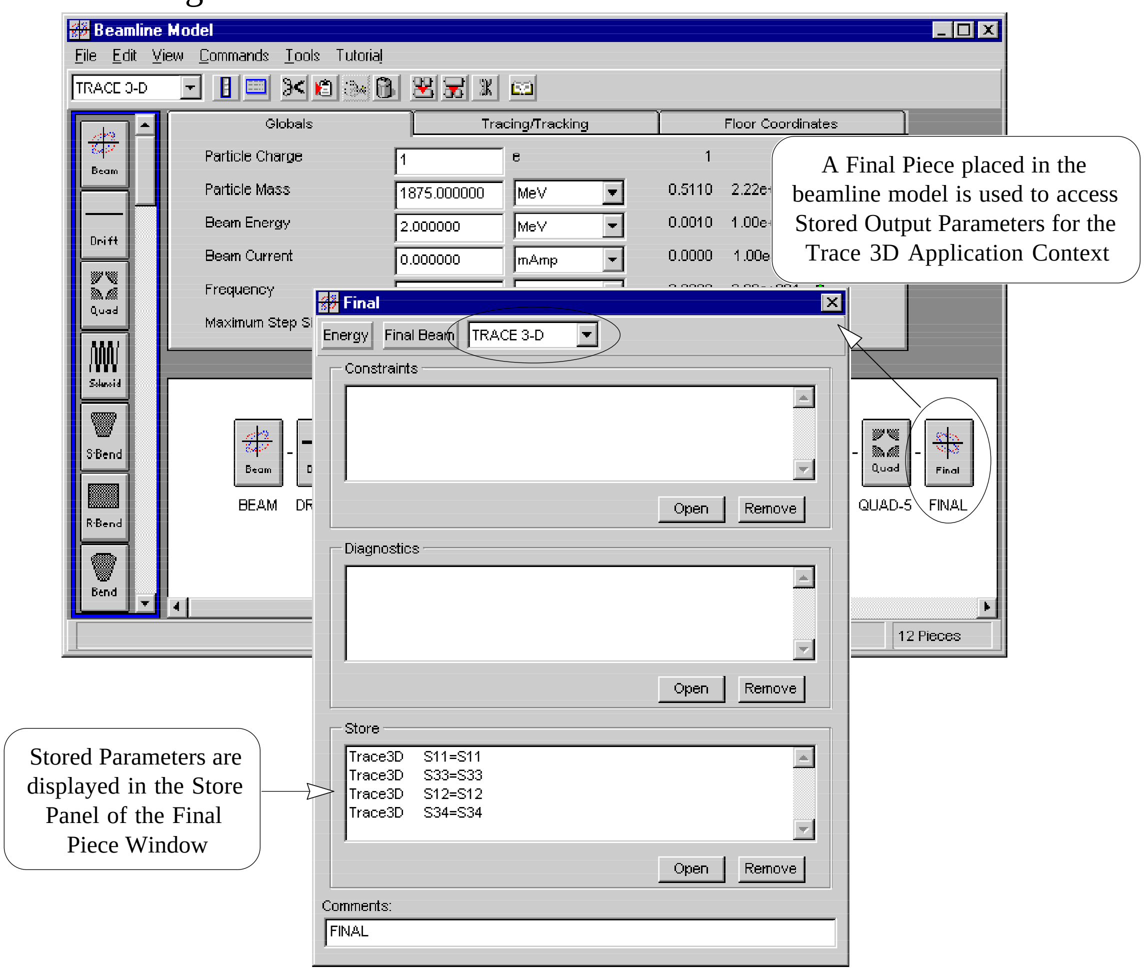

Figure 12. Using the Final Piece to specify TRACE 3D Stored Parameters.

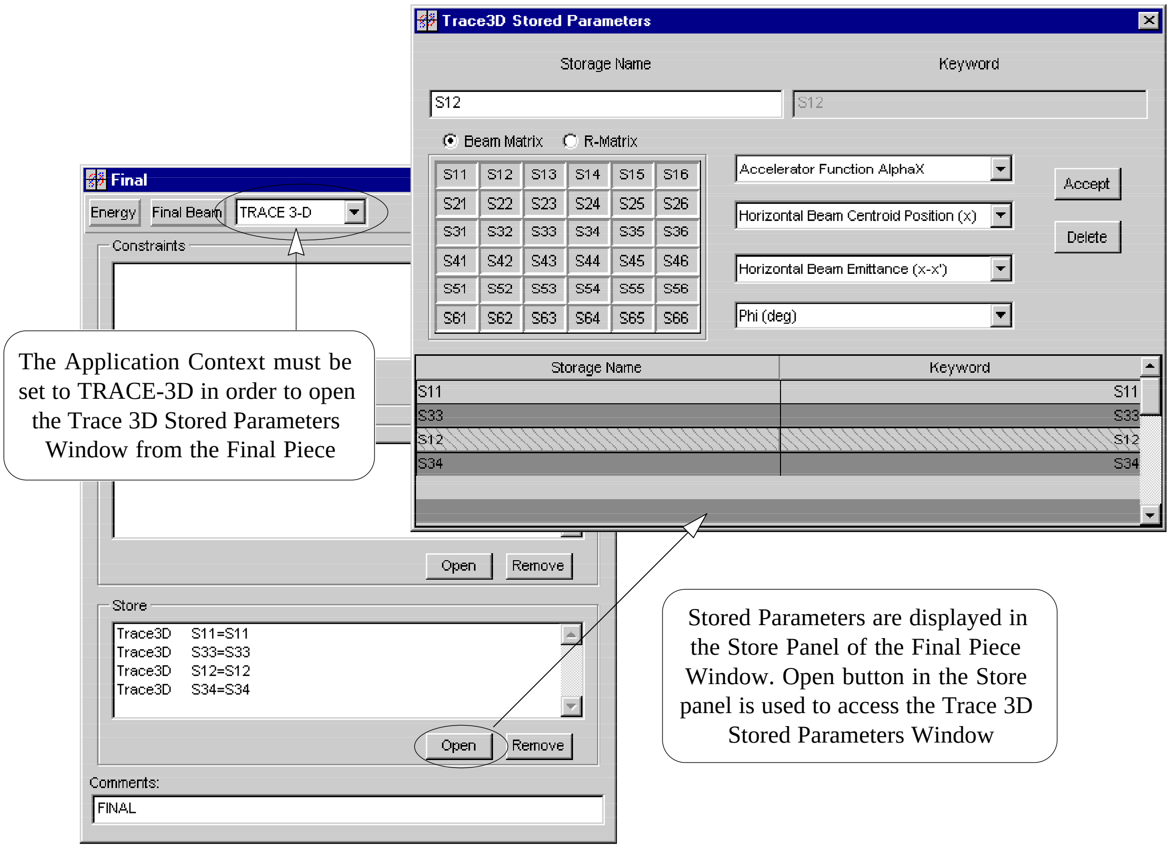

Figure 13. Opening the Trace 3D Stored Output Parameters Window.

The PBO Lab Final Piece is actually a special case of the Marker Piece and double-clicking it will open the same type of Piece Window as the Marker Piece (Figure 10). Refer to the *PBO Lab User Manual Supplement for the TRACE 3D Application Module* for a more detailed description of using the Final Piece to specify Trace 3D Matching Types (Constraints), Diagnostics and Stored Output Parameters. Figure 13 illustrates opening the TRACE 3D Stored Parameters Window from a Final Piece that has been placed at the end of the beamline model. Note that Application Context must be set to TRACE 3D in the Final Piece Window in order to open the Trace 3D Stored Output Parameters Window.

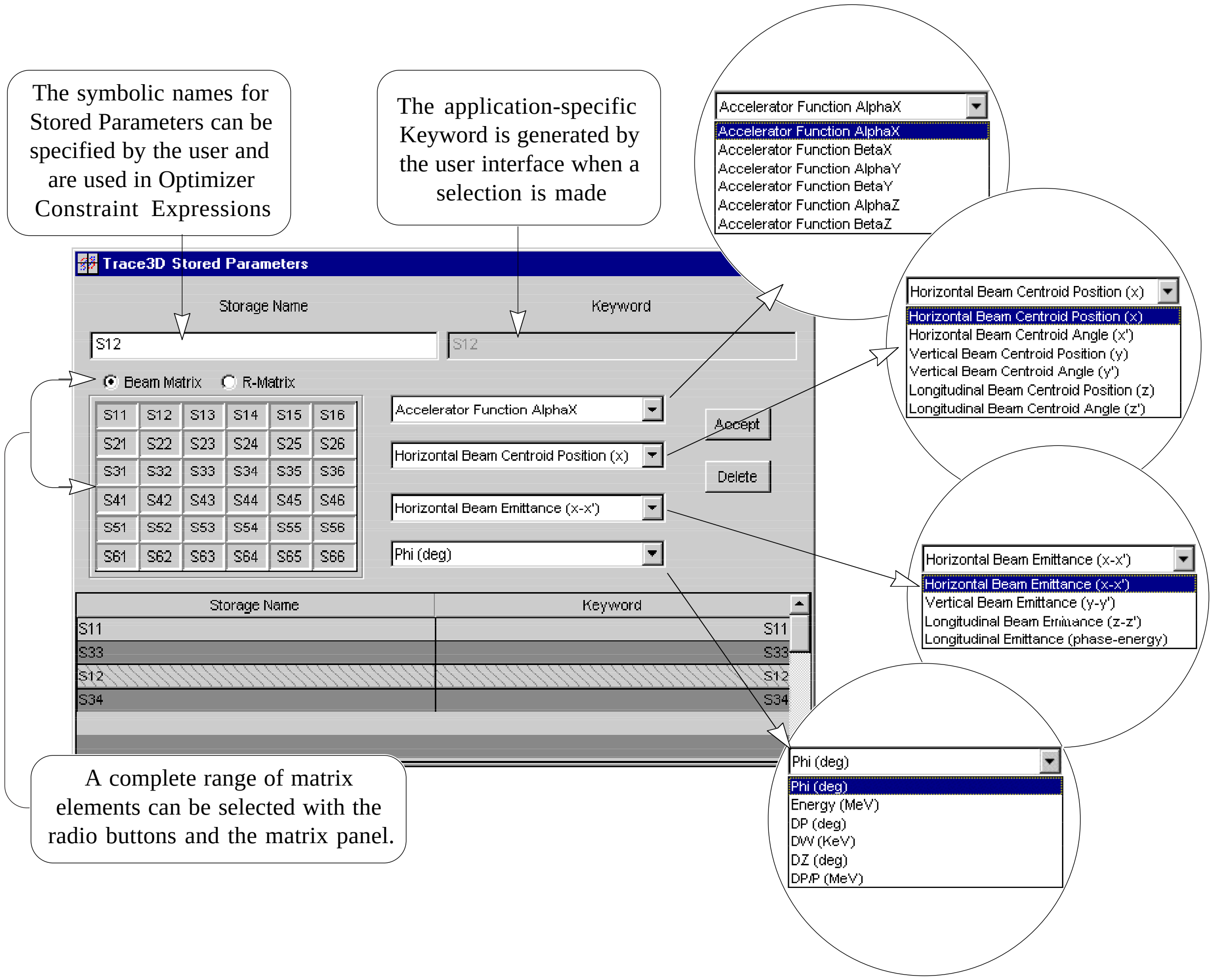

Figure 14. Specification of TRACE 3D Stored Output Parameters.

The user interface for selecting Stored Output Parameters is user friendly and does not require in depth knowledge of the TRACE 3D code. Figure 14 illustrates the different controls and pop ups in the Stored Parameters Window for the TRACE 3D Application Module. All of the selections that are listed in Table 2 can be made from the various controls and pop ups in the Trace3D Stored Parameters Window, without having to know all the TRACE 3D keywords.

Table 2 on the following page list all of the TRACE 3D keywords for Stored Output Parameters.

Table 2. TRACE 3D Stored Output Parameters.

Transfer Matrix (i,j,k,l =1,6)	**Keyword**
1st-Order Transfer (R) Matrix Element	Rij

Beam Centroids	**Keyword**
Horizontal Beam Centroid Position x	beamc(1)
Horizontal Beam Centroid Angle x’	beamc(2)
Vertical Beam Centroid Position y	beamc(3)
Vertical Beam Centroid Angle y’	beamc(4)
Longitudinal Beam Centroid Position z	beamc(5)
Longitudinal Beam Centroid Angle z’	beamc(6)

Beam Emittance	**Keyword**
Horizontal Beam Emittance (x-x’)	emito(1)
Vertical Beam Emittance (y-y’)	emito(1)
Long. Emittance (Phase Energy)	emito(3)
Longitudinal Beam Emittance (z-z’)	Ez

Beam Matrix (i,j =1,6)	**Keyword**
Reduced Sigma Matrix Element	Sij

Longitudinal Parameters	**Keyword**
Phi (deg)	Phi
Energy (MeV)	Energy
DP (deg)	DP
DW	DW
DZ (KeV)	DZ
DP/P (MeV)	DP/P

Lattice Functions	**Keyword**
Accelerator Function AlphaX	beamo(1)
Accelerator Function BetaX	beamo(2)
Accelerator Function AlphaY	beamo(3)
Accelerator Function BetaY	beamo(4)
Accelerator Function AlphaX	beamo(5)
Accelerator Function BetaX	beamo(6)

Stored Parameters List Window

The *Tools* Menu in the Optimizer Problem Window provides a command for opening the *Stored Parameters List Window* which lists all of the stored diagnostic output parameters for the entire Optimization Problem. This List Window is similar to the Optimizer Variable List Window described previously. The Stored Parameters List Window, illustrated in Figure 15, includes all Stored Parameters for all of the beamline Model Documents in the Optimization Problem. The window includes columns for the beamline Model name, the Application Module (optics simulation code), the Piece Label and the symbolic name (Storage Name), as well as the application-specific keyword for each Stored Parameter.

The Optimizer Stored Parameters List Window contains entries for all beamline Model Documents in the Optimization Problem. TRANSPORT Stored Parameters for a single Beamline Model Document are accessed from the TRANSPORT List Windows Submenu in individual Document Windows.

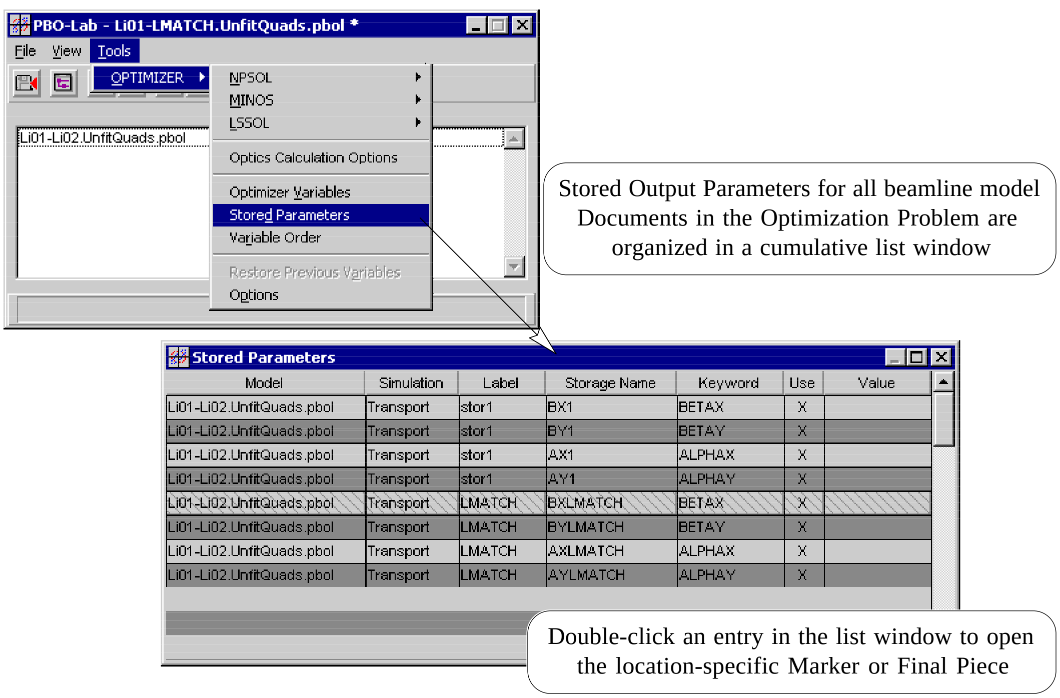

Figure 15. Application-Specific Stored Output Parameters List Window.

Double-clicking an entry in the List Window will open the corresponding Marker Piece Window for that parameter. The *Use* column in the list window allows Stored Parameters to be disabled without actually removing them. Clicking in the *Use* column of a Stored Parameter will toggle that entry on and off. The Value field in the Stored Parameters List Window will contain values after the corresponding optics code (Application Module) is executed, otherwise the Value fields will be empty.

5. *Optimization Constraints*

Optimization Constraints are defined separately for each of the Optimization Engines (NPSOL, LSSOL and MINOS). The Optimization Constraints Windows are opened from the Optimizer Submenus of the Tools Menu in the Optimizer Problem Window as illustrated in Figure 16. The Optimization Constraints Windows are identical for NPSOL and MINOS. These windows provide tab panels for Linear and Nonlinear Constraints, as well as a tab panel for specifying the Optimization Objective Function.

Optimization Constraints are specified in the Optimization Constraints Window, which is opened from the Tools Menu in the Optimizer Problem Window.

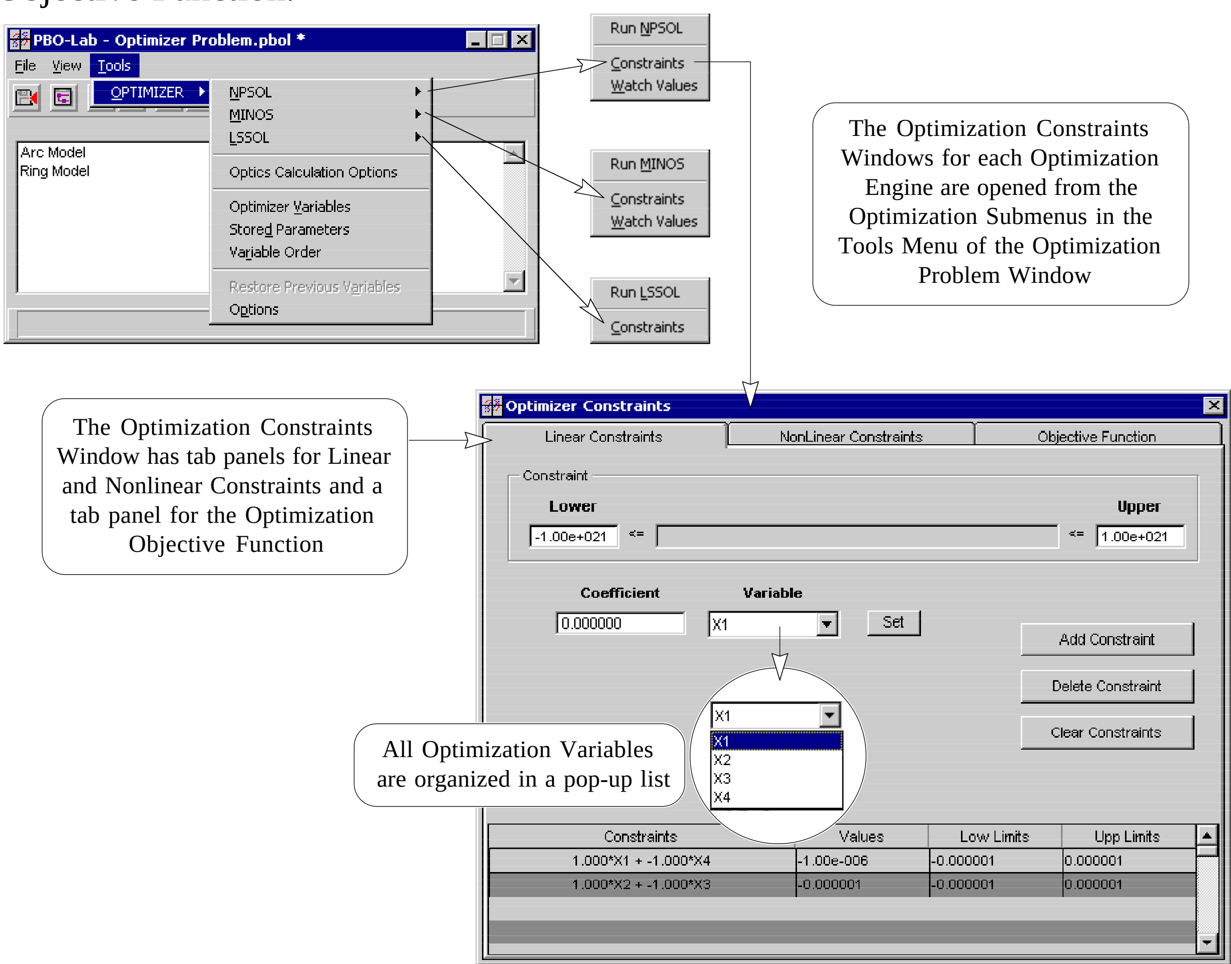

Figure 16. Opening Optimization Constraints Windows.

NPSOL and MINOS Constraints

The Optimization Constraints Windows are used to define constraints in terms of Optimization Variables and Stored Output Parameters. User specified Optimization Variables and Stored Output Parameters are organized in pop-up lists to simplify the definition of constraint algebraic expressions.

The Optimization Constraints Windows are used to define constraint expressions in terms of Optimization Variables and Stored Output Parameters.

By definition, Linear Constraints can only be defined in terms of Optimization Variables. However, Nonlinear Constraints and the Objective Function can be defined with Optimization Variables and Storage Parameters. All Constraints include lower and upper bounds. The Nonlinear Constraint tab panel and the Objective Function tab panel also include a convenient Operators panel, which contains a variety of mathematical operators and functions that can be used in defining constraint expressions. Figure 17 illustrates the main features of the Nonlinear Constraints tab panels for NPSOL. The MINOS Nonlinear Constraints tab panel is identical to the NPSOL example shown in Figure 17, but is accessed from the *Constraints* command in the MINOS Optimizer Submenu of the *Tools* Menu in the Optimization Problem Window.

A Convenient Operators panel provides a variety of mathematical operators and functions for defining algebraic constraint expressions.

A Constraint Expression can be typed directly into the Constraint field at the top of the window, or the pop ups and operators can be used to construct the expression. Defaults are provided for the lower and upper bound values based on an option in the Optimizer Options Window. The *Add Constraint* button is used to accept a Constraint Expression and add it to the list at the bottom of the window. A constraint expression can be removed from the list by selecting it with the mouse and pressing the *Delete Constraint* button. All constraints can be deleted at once using the *Clear Constraints* button.

Constraint Expressions can be typed in directly, or the pop ups and operators can be used to construct expressions.

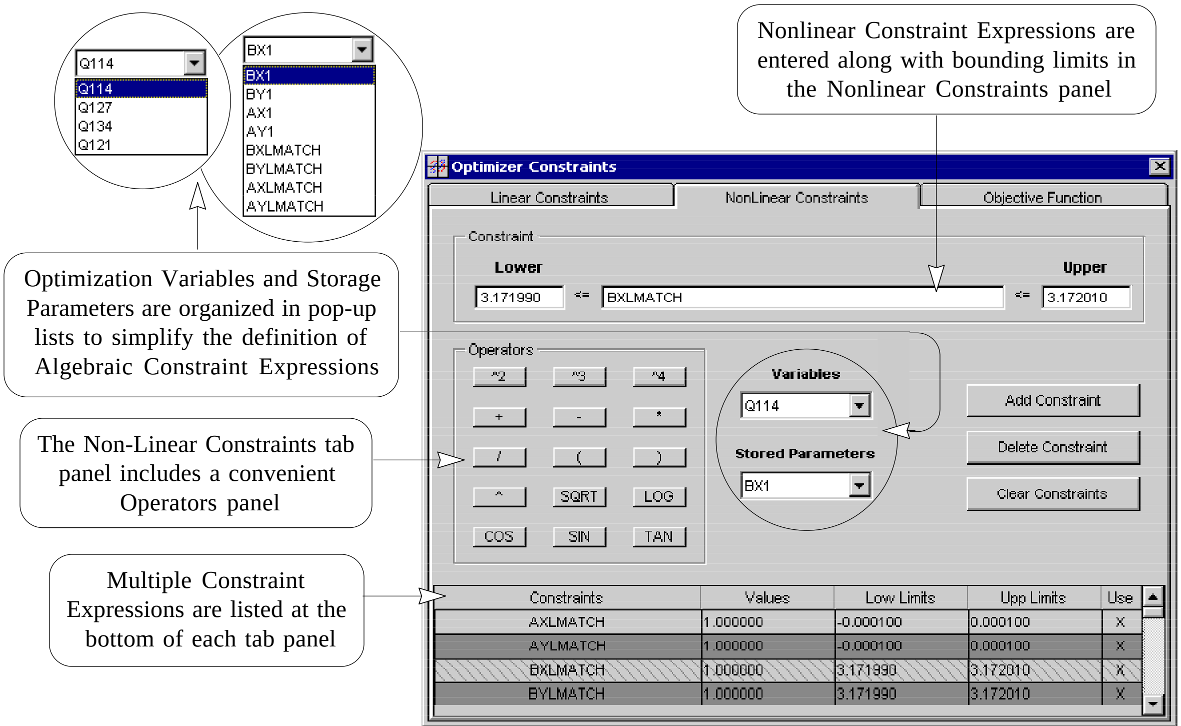

Figure 17. Nonlinear Constraints tab panel for NPSOL.

The Optimization Objective Functions for NPSOL and MINOS are defined in the Objective Function tab panel of their respective Optimization Constraints Windows. Figure 18 shows the Objective Function tab panel from the NPSOL Constraints Window. The MINOS Objective Function tab panel is identical to the NPSOL example shown in Figure 18, but is accessed from the Constraints command in the MINOS Optimizer Submenu of the Tools Menu in the Optimization Problem Window.

The Objective Function is defined in terms of Optimization Variables and Stored Parameters in the Objective Function tab panel of the Constraints Window.

An algebraic expression of the Objective Function in terms of Optimization Variables and Stored Parameters is entered in the text field at the top of the tab panel. The Objective Function tab panel includes an Operators panel and pop-up lists for user specified Optimization Variables and Stored Parameters. Button controls are provided to *Set* and *Clear* the Objective Function with the current Objective Function displayed at the bottom of the tab panel.

The Objective Function tab panel includes an Operators panel and pop-up lists for user specified Optimization Variables and Stored Parameters.

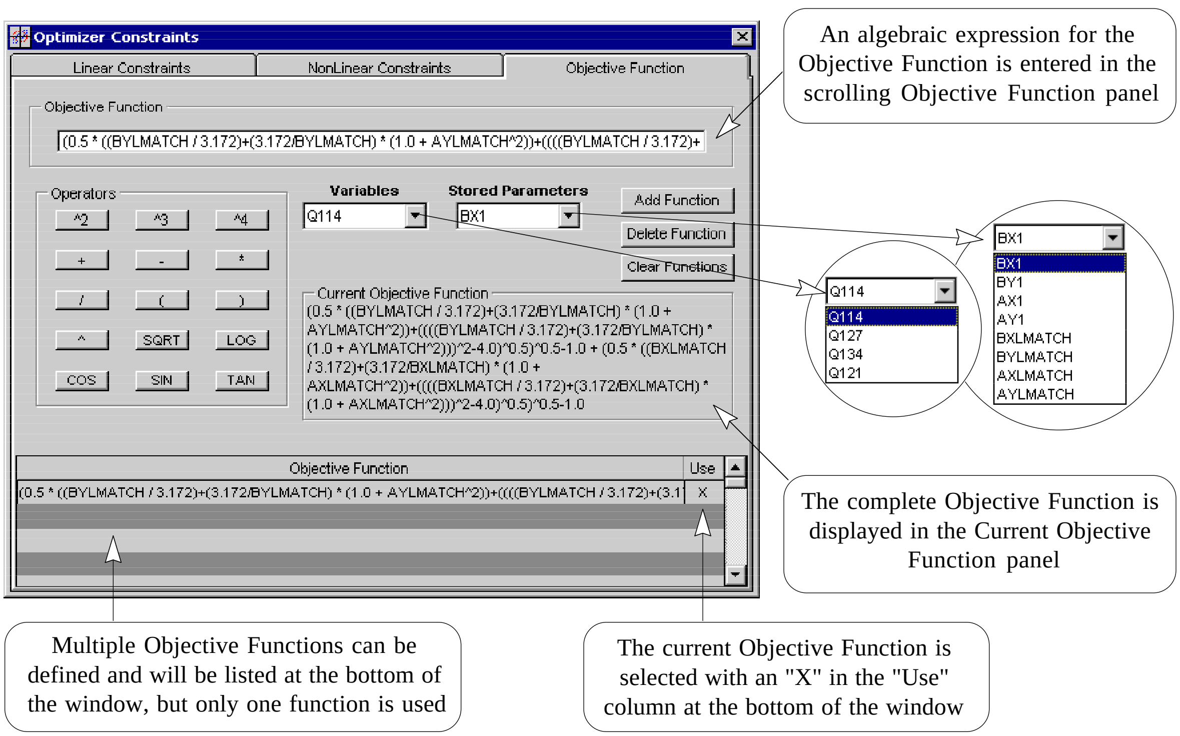

Figure 18. Objective Function tab panel for NPSOL.

LSSOL Constraints

LSSOL is a constrained linear least-squares and quadratic optimization program. Unlike the other two optimization engines (NPSOL and MINOS), LSSOL does not use Output Storage Parameters captured from the various optics codes (Application Modules) in the PBO Lab environment. Constraint expressions for LSSOL are linear and therefore can not contain Output Storage Parameters.

LSSOL does not utilize Output Storage Parameters from PBO Lab Application Modules to specify Optimization Constraints.

The LSSOL Optimization Constraint Window is used to specify constraint expressions in terms of selected Optimization Variables in a beamline model. User specified Optimization Variables are organized in a pop-up list to simplify the definition of algebraic constraints expressions. Figure 19 illustrates the Linear Constraints tab panel of the LSSOL Optimization Constraint Window.

Specify constraint expressions for LSSOL in terms of the selected Optimization Variables in a beamline model.

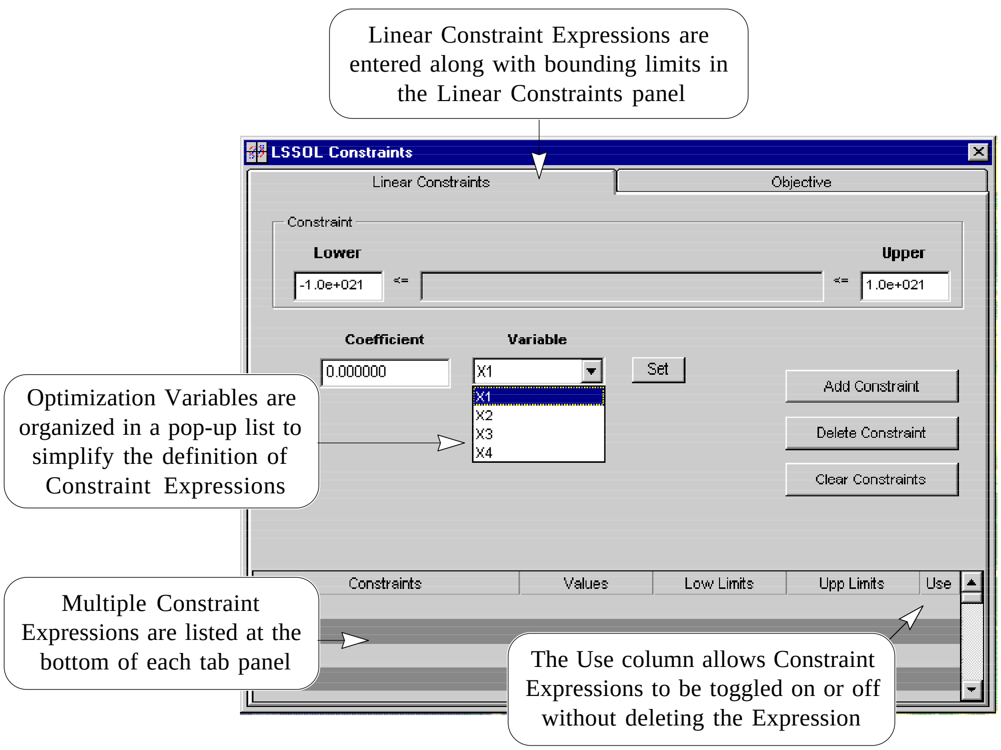

Figure 19. LSSOL Linear Constraints.

A Constraint Expression can be typed directly into the Constraint field at the top of the window, or the pop up for Optimization Variables can be used to construct the expression. The *Set* button is used to make a selection from the Variable pop-up. Defaults are provided for the lower and upper bound values based on an option in the Optimizer Options Window. The *Add Constraint* button is used to accept a Constraint Expression and add it to the list at the bottom of the window. A constraint expression can be removed from the list by selecting it with the mouse and pressing the *Delete Constraint* button. All constraints can be deleted at once using the *Clear Constraints* button.

The Optimization Objective Function for LSSOL is defined in the Objective Function tab panel of the Optimization Constraints Window, illustrated in Figure 20

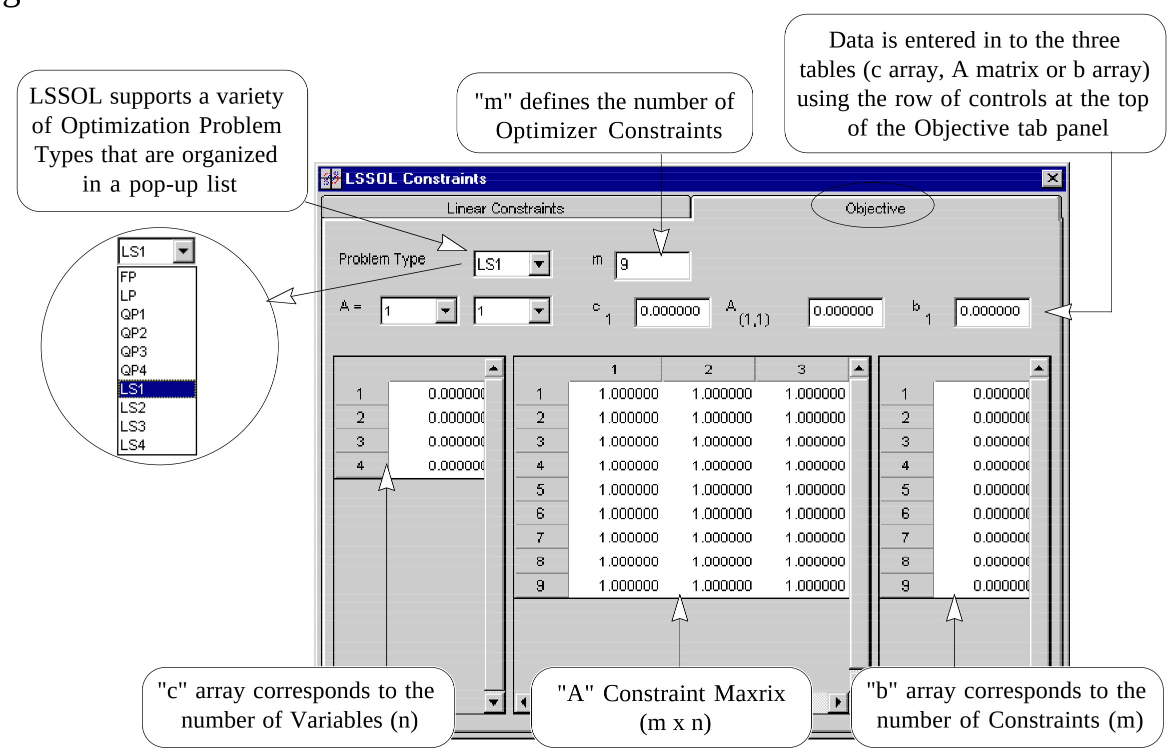

Figure 20. Optimization Objective Function for LSSOL.

LSSOL supports a variety of Optimization Problem Types which are described in the *User's Guide for LSSOL*. The Optimization Type is selected with the Problem Type pop-up in the Objective tab panel of the LSSOL Constraints Window, as illustrated in Figure 20.

The Objective function for LSSOL is specified using the "c" array, corresponding to the number of Optimization Variables, the "b" array, corresponding to the number of constraints and the "A" Constraint Matrix. Data is entered into these three tables using pop-up controls to specify the row and column in the "A" Matrix and then entering the desired value in any of the input fields for "b", "A" or "c". After making a selection using the row and column pop-ups, subscripts will appear next to each of the text fields. Use the Enter key to accept a value from a text input field and it will be updated in the corresponding table.

Refer to the *User's Guide for LSSOL* for a description of the different types of problems that can be examined with LSSOL and the specification of constraints and the objective matrix.

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5. Options & Watch Values

The Tools Menu in the Optimizer Problem Window provides commands for opening the Watch Values Setup Windows for the NPSOL and MINOS optimization engines. Figure 21 illustrates opening the Watch Values Setup Window for NPSOL from the NPSOL Submenu in the Tools Menu. This Watch Values Setup Windows is used to select the Optimization Variables and Constraints that will be displayed during an NPSOL Optimization process. The MINOS Watch Values Setup Window is opened from the MINOS Submenu in the Tools Menu. LSSOL does not support watch values.

The Tools Menu in the Problem Window provides commands for opening the Watch Values Setup Windows for the NPSOL and MINOS.

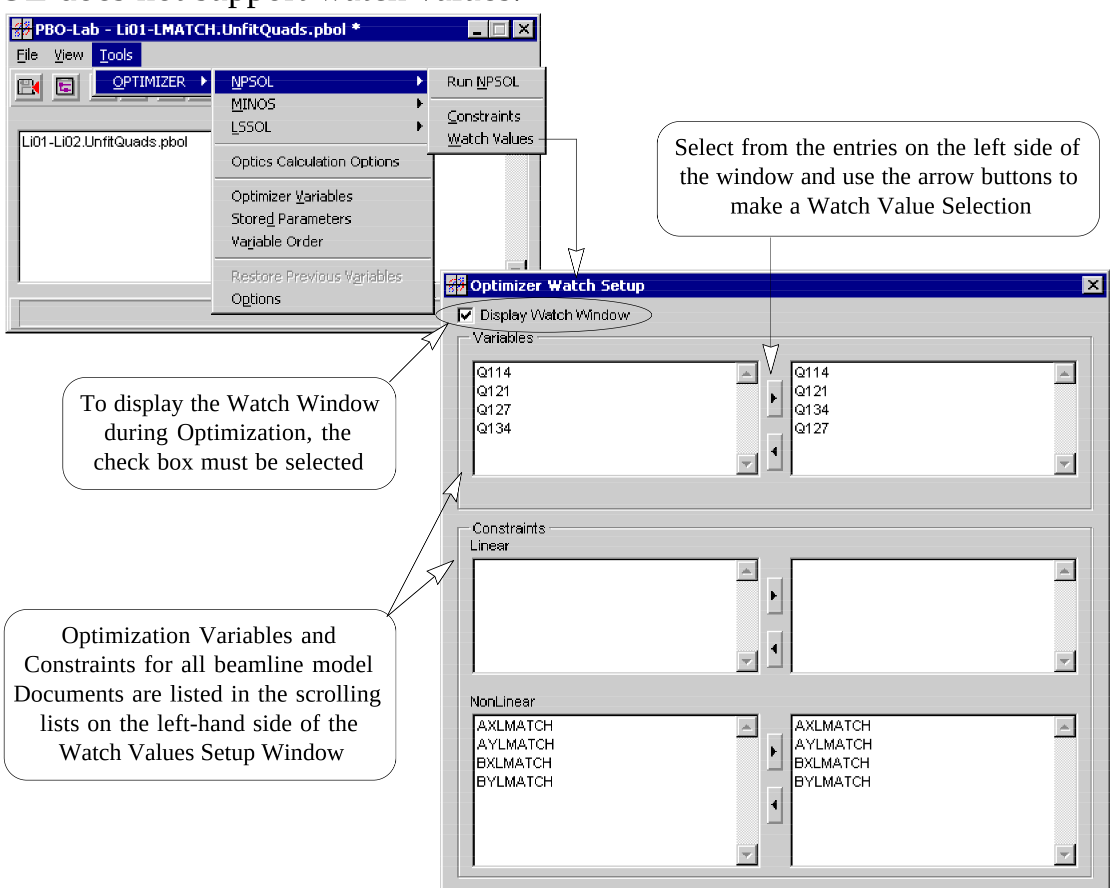

Figure 21. Selecting Watch Values for NPSOL Optimization.

Watch Values Setup Windows

The Watch Values Setup Windows (for NPSOL and MINOS) are divided into Variables and Constraints panels and the Constraints panel is further divided into Linear and Nonlinear Constraints. Setup Watch Values by selecting an entry from the lists of Variables and Constraints on the left side of the window and pressing the right arrow button (in the middle of the window) to copy the selection to the lists on the right side. Entries can also be removed from the watch lists on the right side of the window by selecting them and pressing the left arrow button. The example shown in Figure 21 only contains Variables and Nonlinear Constraints, so the Linear Constraints list is empty.

Watch Values are selected from the lists of Variables and Constraints on the left side of the window and added to the Watch lists on the right side of the window.

In order to display the selected Watch Values during the Optimization process, the check box at the top of the window must also be selected. To disable the display of the Watch Window without deleting any of the selected Watch Values, un-check the box. If there are no Watch Values selected and/or the check box to display the Watch Window has not been checked, then there will be no output until the Optimization process has completed and the native output from the Optimizer is displayed.

Watch Values must be selected and the “Display Watch Window” check box must also be checked in order to get the dynamic Watch Window to display the results during the Optimization Process.

Optics Calculation Options

The Optics Calculation Options Window, shown in Figure 22, is used to select the type of optics calculation that will be used with the different Application Modules (TRANSPORT, TRACE 3D) that may be used in the optimization process. The Optimizer Tool automatically runs an Application Module to get values for application-specific Stored Output Parameters that have been selected in the beamline Model Document Window. These values are then used in the evaluation of Optimization Constraints and the Optimization Objective (merit) function. Each time Optimization Variables are changed, the Application Module is executed in order to update the Stored Output Parameters. Optics Calculation Options are provided so that specific selections can be specified for automatic execution during the optimization process.

The Optics Calculation Options Window is used to select the simulation (Application Module) and the calculation option that will be used during the Optimization process.

After selecting the Simulation Type for a beamline Model Document, the Execution Type must be selected.

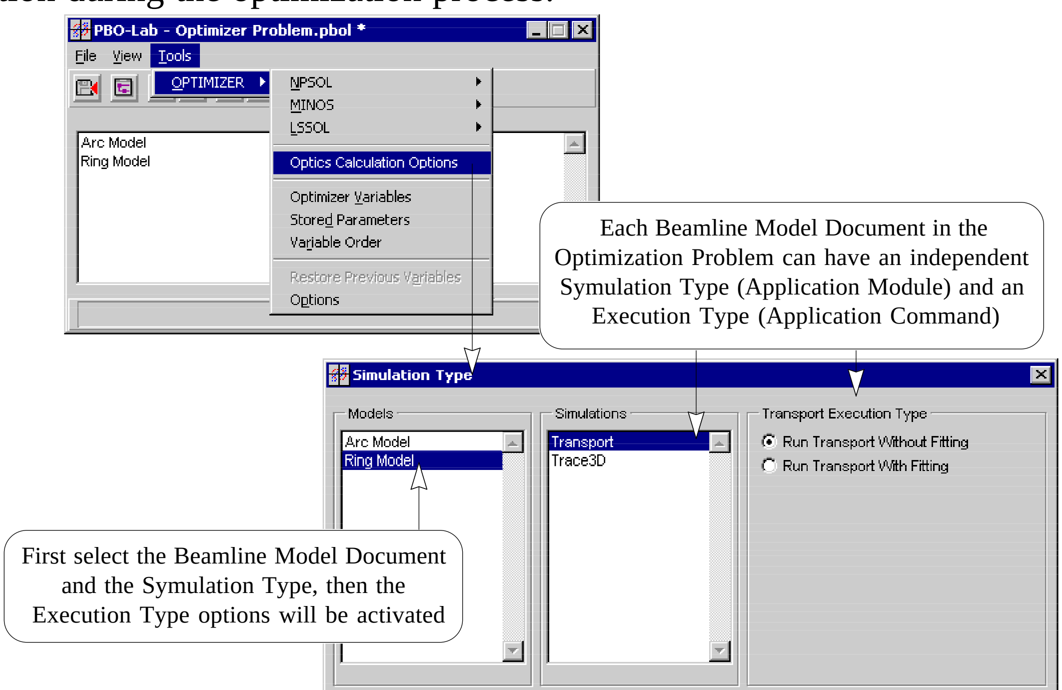

Figure 22. Specifying Optics Calculation Options.

Application Modules have different selections in the Optics Calculation Options Window for specifying the command that will be executed at each iteration in the optimization process. For example, the TRANSPORT Application Module includes selections for running TRANSPORT with or without Fitting, as illustrated in in Figure 22.

There are three panels in the Optics Calculation Options Window. The *Models* panel on the left side of the window contains a list of all the beamline Model Documents in the Optimizer Problem. Clicking on a Model Document in this panel will select that model and activate the middle panel labeled *Simulations*. The *Simulations* panel contains a list of applicable Application Modules. After selecting an Application Module from this list, a third panel will be activated on the right side of the window that contains options for different optics calculations that can be used with the selected Application Module. For example, a hierarchical optimization can be carried out using the TRANSPORT calculation option: *Run Transport With Fitting* to perform a localized fit with TRANSPORT, while a global optimization is performed with the optimization engine.

To specify an Optics Calculation Option, select a beamline Model Document from the Models panel. Then select an Application Module from the Simulations panel. Now select from the available options in the Execution Type panel.

Optimization Problems that contain multiple beamline Model Documents can use different Application Modules and/or different calculation options for each Model Document.

The Optimization Tool determines which Application Modules need to be executed based on the selection of Stored Output Parameters. However, the selections in the Optics Calculation Options Window specify what type of calculation will be performed for each beamline Model when the Application Module is executed.

Optimizer Options Window

The *Options* command in the Tools Menu of the Optimizer Problem Window opens the Optimizer Options Window, as illustrated in Figure 23 This window contains a tab panel for each of the Optimization engines. Each tab panel contains both Options and Preferences. The Options panel is used to set options that are passed directly to the Optimization engine. The Preference panel is used to select different output preferences for the Optimization Tool in PBO Lab.

The Options command in the Tools Menu of the Optimizer Problem Window opens the Optimizer Options Window.

The selections in the Optimizer Options Window are those most commonly used. However, it is also possible to use the native options file of the individual optimization programs to specify any option described in the different user manuals. To use the native options file, check the box for “Use NPSOL.OPT Options File” in the Options panel of the window. Using the native options file will overwrite any options selected in the Optimizer Options Window, but will not effect Preference choices. Refer to the *User’s Guide for NPSOL* for a description of individual options.

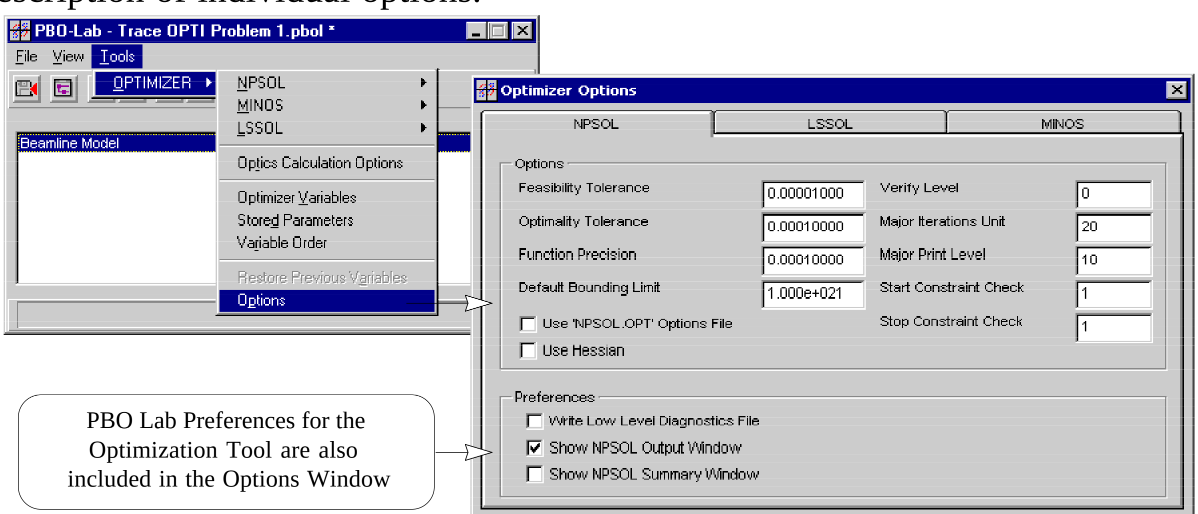

Figure 23. Optimizer Options Window.

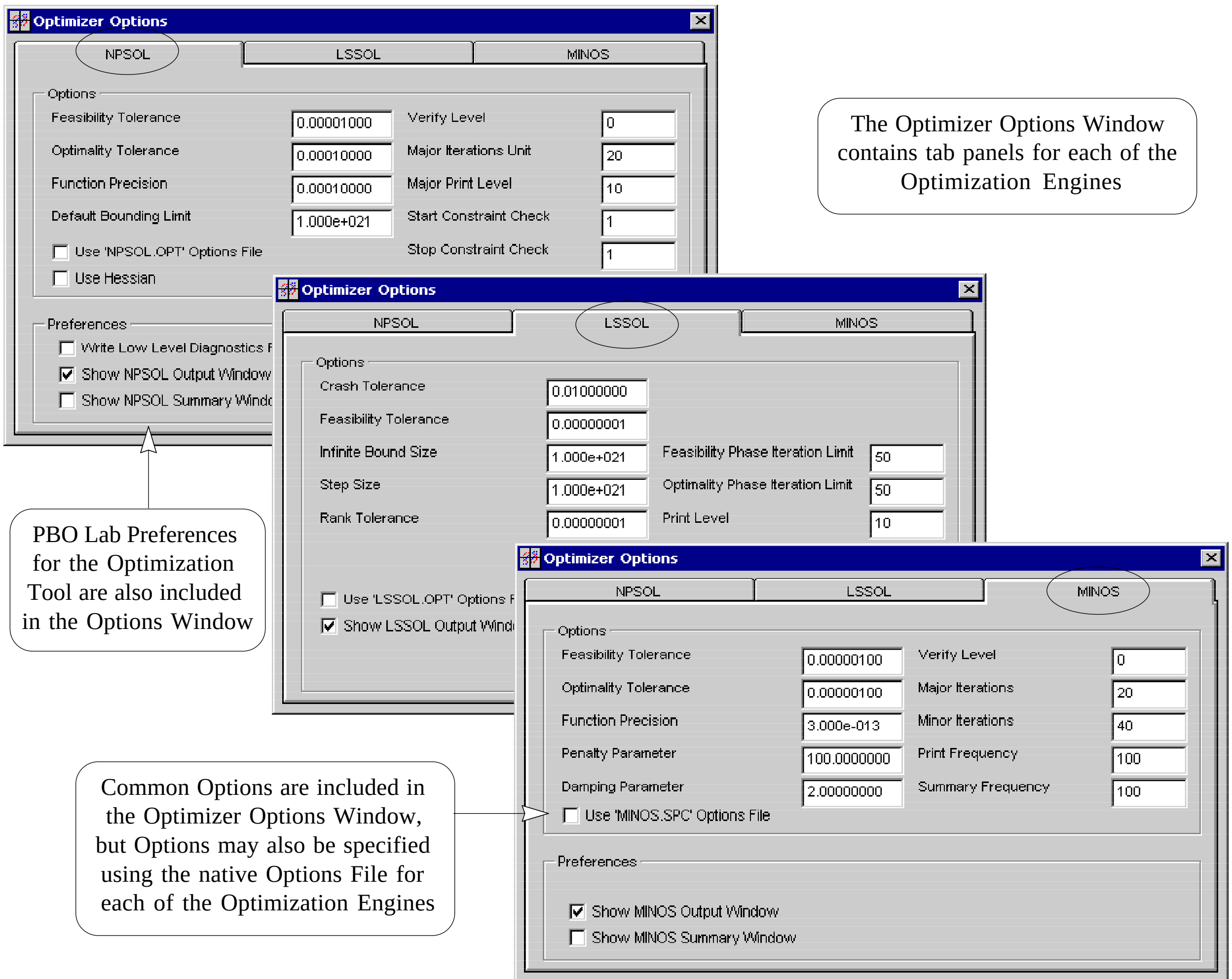

Figure 24. Options tab panels for NPSOL, LSSOL and MINOS.

The PBO Lab preferences for the Optimization Tool differ slightly for the three Optimization Engines. NPSOL includes preferences to automatically open the native NPSOL Output and Summary files, as well as a preference for generating a low level diagnostic output file. LSSOL has one preference for automatically opening its native Output file. LSSOL does not include Summary and Diagnostic output. MINOS preferences include automatically opening native Output and Summary files. There is no low level diagnostic output for MINOS.

7. *Running an Optimization Problem*

An Optimization Problem is defined when Optimization Variables have been selected in the beamline model and Optimization Constraints have been specified for the targeted Optimization Engine. Watch Values must be setup in order to view the optimization process but they are not required to define an Optimization Problem. The optimization process is started using one of the *Run...* commands located in the Optimizer Submenus in the Tools Menu of the Optimizer Problem Window as illustrated in Figure 25.

The optimization process is started using one of the *Run...* commands located in the Optimizer Submenus in the Tools Menu of the Optimizer Problem Window.

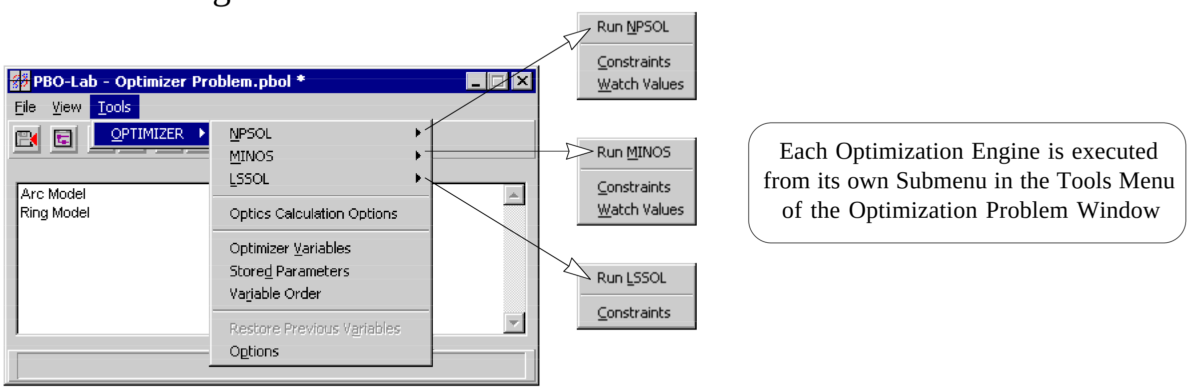

Figure 25. Run an Optimization Problem from the Problem Window Tools Menu.

When the optimization process is complete the native output files are automatically opened in PBO Lab Text Edit Windows. The preferences for automatically opening the native output files are found in the Optimizer Options Window. If these preferences are not checked then the output files will still be generated, but they will not be automatically opened following execution. Previously generated output files may be opened any time using the View Menu commands in the Optimizer Problem Window.

Optimizer Watch Window

The Optimizer Watch Window is opened when the Run Optimizer Command is selected in the Tools Menu, if Watch Values have been selected in the Watch Values Setup Window. If no Watch Values have been selected or the Display Watch Window check box is not selected, then the Watch Window will not be opened during the Optimization process. Figure 26 illustrates running the Optimizer from the Problem Window Tools Menu.

If no Watch Values have been selected or the Display Watch Window check box is not selected, then the Watch Window will not be opened during the Optimization process.

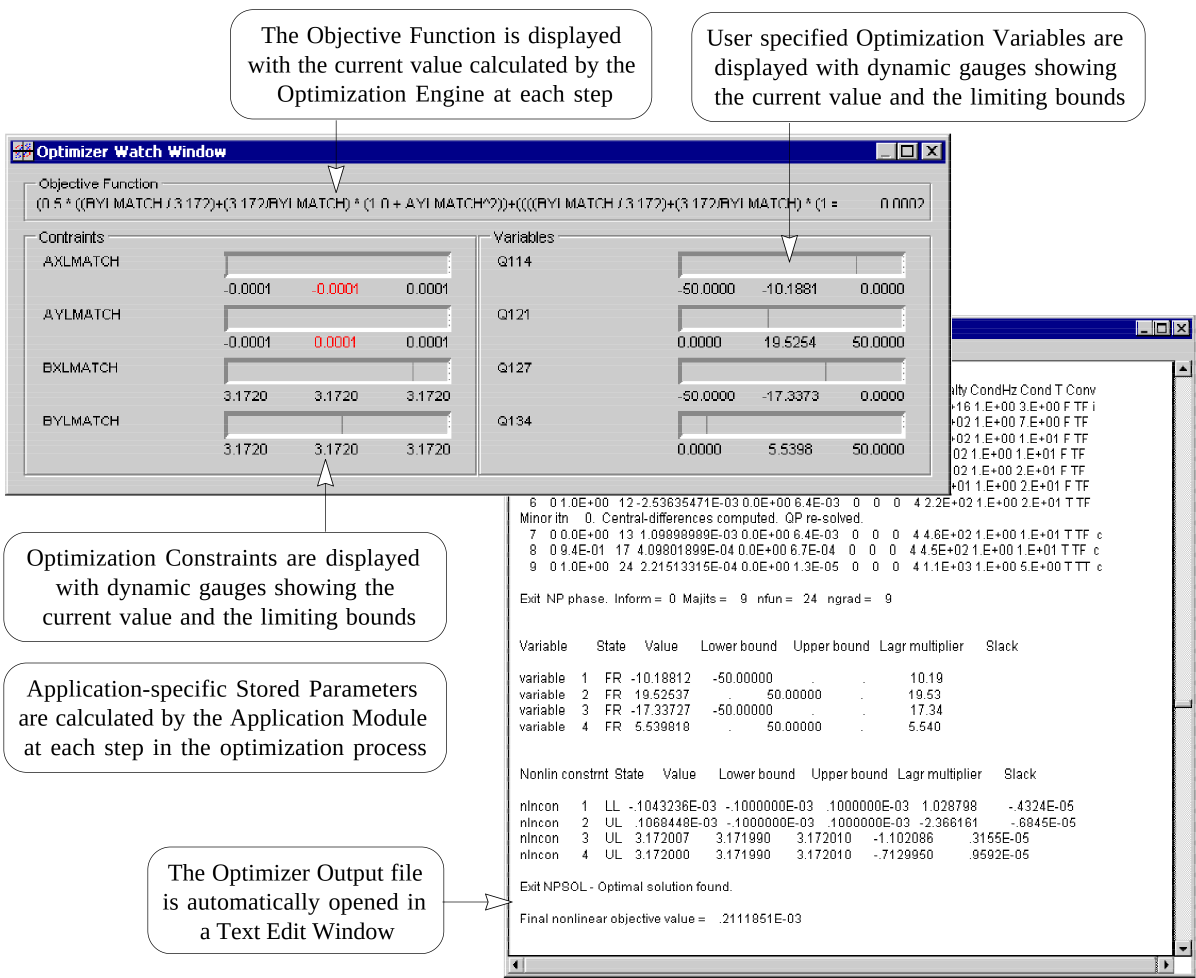

Figure 26. Optimizer Watch Window and NPSOL Output Window.

During optimization the Watch Window is used to monitor the Objective Function as well as Optimization Constraints and Variables. This window dynamically displays the optimization progress during execution. Display gauges that are bound by the user specified limits are updated at each step in the optimization cycle to illustrate the current values for Optimization Constraints and Variables. A display at the top of the window also shows the current value for the Objective Function at each step in the optimization process. An example of the Watch Value Window is shown in Figure 26. The Optimization Variables are used to update the beamline model(s) during the optimization process. Any application-specific Stored Parameters are calculated by the respective Application Module. The Objective Function is evaluated by the Optimizer Tool and its current value is displayed at the top of the Watch Values Window. When the process is complete, the native Output and Summary files are automatically opened in a Text Edit Window as illustrated in Figure 26.

The Watch Window is used to dynamically display the optimization progress during execution.

When the Optimization process is complete, the NPSOL Output file is automatically opened in a Text Edit Window.

In some cases the Optimizer will not find an optimal solution on the first execution. The "Li01-LMATCH.UnfitQuads.pbol" Optimization Problem used in this Supplement is an example. The optimal solution for this problem took two executions of the Optimizer to get the results shown in Figure 25.

Some problems may require multiple executions of the Optimizer to find an optimal solution.

Following the execution of the Optimizer, Optimization Variables selected in the beamline model(s) of the Optimization Problem will be altered. This is true even if the optimal solution is not found. The Optimizer uses the Application Module that has been selected in the Simulation Type Window to evaluate the application-specific Stored Output Parameters each time the Optimization Variables are modified.

Each iteration in the Optimization process updates the beamline model(s) with new Variables chosen by the Optimizer so that the Stored Output Parameters can be recalculated by the Application Module.

At each step in the Optimization process the beamline model(s) are updated with the Variables chosen by the Optimizer, so that the Stored Output Parameters can be recalculated by the Application Module. Consequently, the beamline model(s) will be modified with respect to the Piece Parameters that have been chosen as Optimization Variables.

PBO Lab™ 2.2

(Particle Beam Optics Laboratory)

User Manual Supplement:

Optimization Module

Appendix A

"NPSOL User's Guide"

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User Manual Supplement:

Optimization Module

Appendix B

"MINOS User's Guide"

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Optimization Module

Appendix C

"LSSOL User's Guide"

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