New developments in LS-OPT Version 3.2

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ABSTRACT:

An overview of LS-OPT features is given with special emphasis on the major new optimization features available in LS-OPT Version 3.2. These include GUI support for parameter identification, confidence intervals for individual optimal parameters, point plotting as an enhancement to 3-D metamodel plotting, matrix expressions, coordinate-based result extraction and retry features for job distribution

Keywords:

LS-OPT, optimization, robust design, parameter identification

INTRODUCTION

In today's CAE environment it is unusual to make engineering decisions based on a single physics simulation. A typical user conducts multiple analyses by varying the design and uses the combined results for design improvement. LS-OPT [1] provides an environment for design and is tightly interfaced to LS-DYNA and LS-PREPOST with the goal of allowing the user to organize input for multiple simulations and gather and display the results and statistics. More specifically, LS-OPT has capabilities for improving design performance in an uncertain environment and conducting system and material identification. These objectives can be achieved through the use of statistical tools and optimization. The individual tasks that can thus be accomplished are:

- Identify important design variables
- Optimize the design
- Explore the design space using surrogate design models
- Identify sources of uncertainty in FE models
- Visualize statistics of multiple runs
- Optimize the design with consideration of uncertainties
- Conduct robust parameter design

The typical applications are: Multidisciplinary Design Optimization (crashworthiness, modal analysis, durability analysis, etc.), system and material identification (biomaterials, metal alloys, concrete, airbag properties, etc.) and process design (metal forming).

The main technologies available in LS-OPT are:

Experimental Design (DOE). D-Optimal design, Latin Hypercube sampling, Space Filling and others. DOE allows the user to automatically select a set of different designs to be analyzed. The main types mentioned here are each suited to a different type of analysis: *D*-Optimal for polynomials and sequential optimization, Latin Hypercube for stochastic analysis and Space Filling for Neural Networks.

Metamodels (approximations). Response Surface Methodology and Neural Networks are the only options. With these tools, the user can explore the design space and quantify the predictability of a response, i.e. identify sources of noisy response.

Variable screening [4] provides information on the relative importance of design variables.

Optimization. Used for automated design improvement. The Successive Response Surface Method (SRSM) [5] is the principal iterative tool for finding a converged optimum. A similar methodology is used for finding a converged result using neural net updating with adaptive Space Filling.

Probabilistic analysis includes Reliability Analysis, Outlier Analysis, Robust Parameter Design and Reliability-Based Design Optimization (RBDO)[3]. Reliability analysis allows the user to evaluate the probability of failure while Outlier Analysis allows the identification of parts of a model that contribute to noisy response and therefore may affect the overall predictability of the results. Robust Parameter Design and RBDO allow for defining robustness as an objective and the consideration of the probability of failure as a constraint option in optimization. The outlier analysis uses integrated LS-PREPOST features to visualize structural zones with unpredictable behavior.

Features are available to distribute simulation jobs across a network, using a queuing system.

PARAMETER IDENTIFICATION (GUI SUPPORT)

The parameter identification capability has been available since Version 3.0, but without GUI support. For version 3.2, the following features have been added:

Specification of crossplot curves (vectors)

This feature allows the user to combine time-histories such as stress and strain histories into a crossplot, i.e. stress vs. strain. Figure 1 depicts the history panel with an example selection of a crossplot. Note that general expressions are allowed for the component histories.

Specification of the Mean Squared Error (MSE) composite function

The MSE norm defined by

$$\varepsilon = \frac{1}{P}\sum_{p=1}^{P} W_p \left(\frac{f_p(\boldsymbol{x}) - G_p}{s_p} \right)^2 = \frac{1}{P}\sum_{p=1}^{P} W_p \left(\frac{e_p(\boldsymbol{x})}{s_p} \right)^2$$

can be specified using the feature shown in Figure 2. In the example the computational vector f_p is represented by F2_vs_d2 and the measured results G_p by Test2. P is the number of points. Because the number of points is not specified, the value defaults to the number of points in the test file. Otherwise interpolated values are used. The expert mode allows advanced attributes to be entered manually.

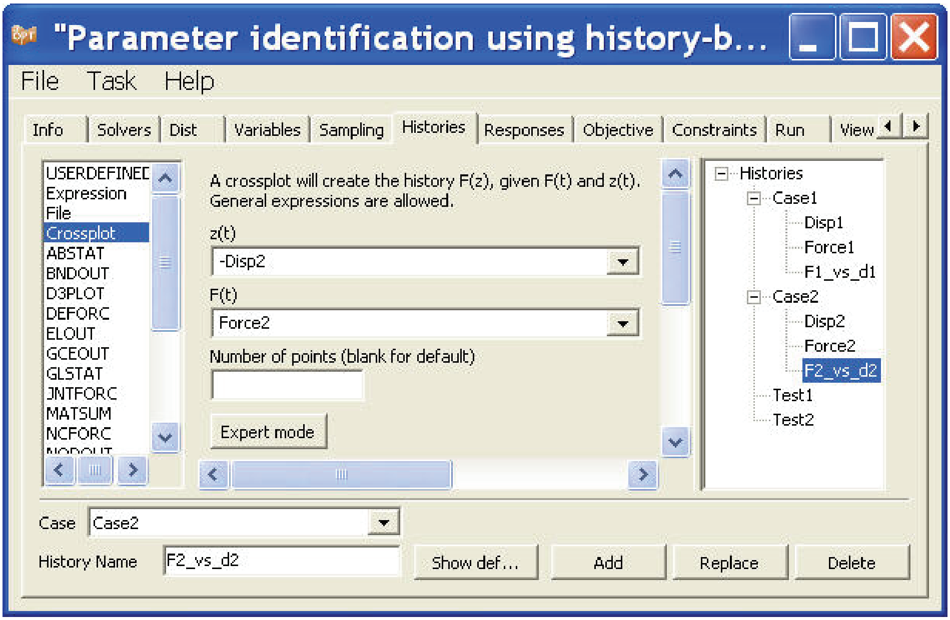


Figure 1: Histories panel showing crossplot selection in a multi-case example

Viewing comparisons of the computed and measured curves

The optimal computational and measured curves can be compared as shown in Figure 3.

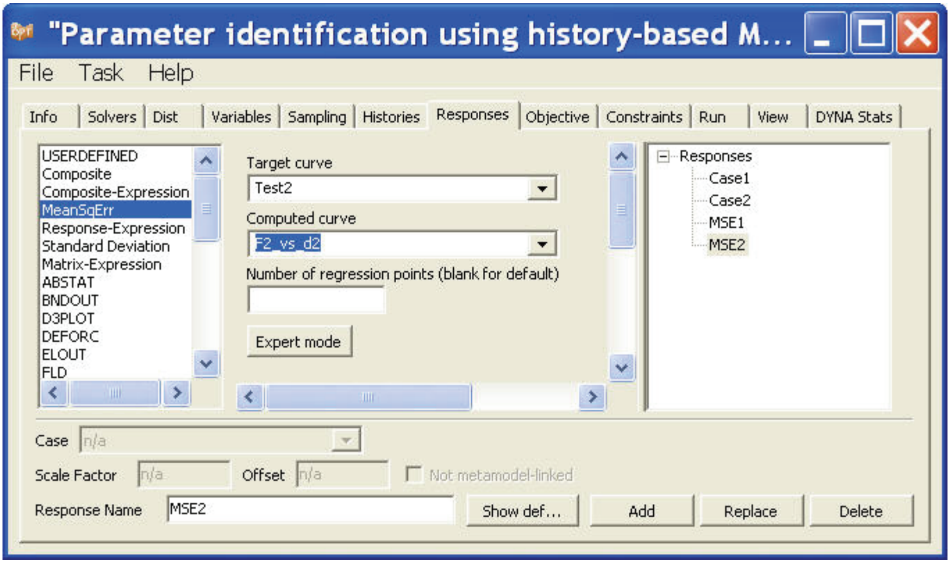


Figure 2: Responses panel showing MeanSqErr selection for MSE2

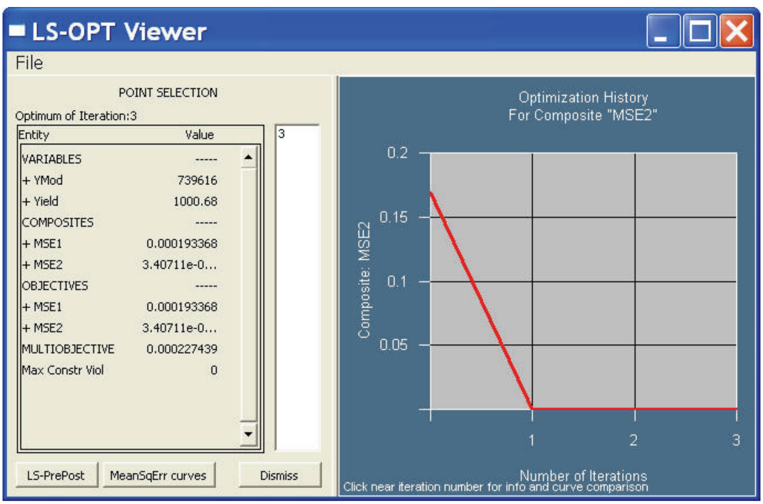
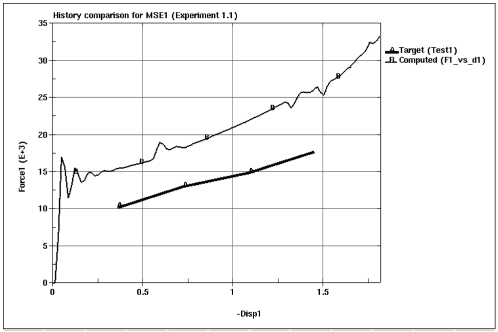


Figure 3a: Optimization history of Mean Squared Error MSE2. Comparison plots can be displayed by clicking near the iteration numbers on the abscissa.



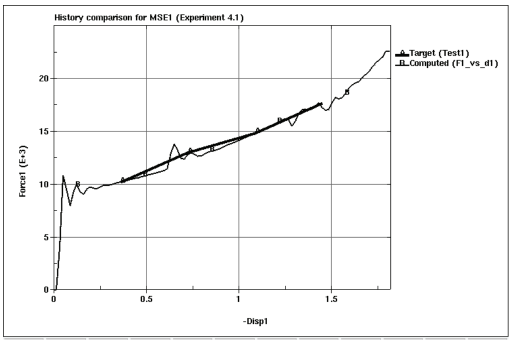


Figure 3b: Initial and optimal curve comparison when selecting the "MeanSqErr curves" option for iteration numbers 0 (baseline) and 3 (optimal) respectively. The heavy line represents the test curve. The comparison plots are generated automatically.

Confidence intervals of individual parameters

Confidence intervals are required to assess the reliability of the material parameters obtained from the optimization run. Assume the nonlinear regression model:

$$G(t) = F(t, \boldsymbol{x}) + \varepsilon$$

where the measured result G is approximated by F and $\boldsymbol{x}$ is a vector of unknown parameters. The nonlinear least squares problem is obtained from the discretization:

$$\min_{\boldsymbol{x}} \frac{1}{P} \sum_{p=1}^{P} (G_p - F_p(\boldsymbol{x}))^2$$

which is minimized to obtain x^*. The variance σ^2 is estimated by

$$\hat{\sigma}^2 = \frac{\left\| \boldsymbol{G} - \boldsymbol{F}(\boldsymbol{x}^*) \right\|^2}{P - n}$$

where $\boldsymbol{F}$ is the P-vector of function values predicted by the model and n is the number of parameters. The 100(1-α)% confidence interval for each x^*_i is:

$$\left(\left[x_i : \left| x_i^* - x_i \right| \leq \sqrt{\hat{C}_{ii}} t_{P-n}^{\alpha/2} \} \right] \right)$$

where

$$\hat{\boldsymbol{C}} := \hat{\sigma}^2 \left[\nabla \boldsymbol{F}\left(x^*\right)^T \nabla \boldsymbol{F}\left(x^*\right) \right]^{-1}$$

and $t_{P-n}^{\alpha/2}$ is the Student *t*-distribution for α.

$\nabla \boldsymbol{F}$ is the $P \times n$ matrix obtained from the n derivatives of the P response functions representing P points at the optimum x. The optimal solution is therefore calculated first, followed by the confidence interval.

A critical issue is to ensure that $\nabla \boldsymbol{F}$ is not based on a gradient obtained from a spurious response surface (e.g. occurring due to noise in the response). Monitoring convergence and selected statistical parameters such as the RMS error and R^2 can help to estimate a converged result. In many cases material identification problems involve smooth functions (e.g. tensile tests) so that spurious gradients would normally not be a problem.

Confidence interval data is presently only available in the `lsopt_report` file:

```
------------------------------------------------------------
90% Confidence intervals for individual optimal parameters
------------------------------------------------------------
Name                  Value        Confidence Interval
                                      Lower      Upper
------------------------------------------------------------
Youngs_Modulus   739559.415      72970.5803 1406148.25
Yield_Stress     1009.14575      978.501323 1039.79017
------------------------------------------------------------
```

SAMPLING AT DISCRETE DESIGN POINTS

The discrete optimization feature in LS-OPT is based on the construction of a response surface which, although only discrete variables are allowed during optimization, is typically built from the continuous variables. That means that discretization is only introduced after response surface construction. This can make sense for variables such as plate thicknesses but will be inappropriate for integer variables (such as the number of ribs in a structure) where no design variable continuity exists. A flag is therefore provided to select the sampling points at the specified discrete values of the variables. Discrete sampling will also handle discrete-continuous problems correctly, using "integer" values only for the discrete variables.

In the GUI, a check box is located as a *D*-Optimal advanced option for basis points for each case (only when discrete variables are available). Discrete sampling is based on selecting a discrete basis set for *D*-Optimality and is therefore not available for other point selection schemes.

MATRIX EXPRESSIONS

Matrix operations can be performed by initializing a matrix, performing multiple matrix operations, and extracting components of the matrix as response functions or results.

There are two functions available to initialize a matrix, namely `Matrix3x3Init` and `Rotate`. Both functions create 3×3 matrices. `Matrix3x3Init` is used to initialize a 3×3 matrix while `Rotate` creates an orthogonal matrix from 3 specified points.

The component of a matrix is extracted using the format `A.aij` (or the 0-based `A[i-1][j-1]`) e.g. `Strain.a23` (or `Strain[1][2]`) where *i* and *j* are limited to 1,2 or 3.

The matrix operation $\boldsymbol{A} - \boldsymbol{I}$ (where $\boldsymbol{I}$ is the unit matrix) is coded as `A-1`.

Example: The deformation gradient matrices corresponding to two time instances are $\boldsymbol{F}_D$ and $\boldsymbol{F}_S$ respectively. A new deformation gradient referred to t_D can be computed as

$$\boldsymbol{F}_{SD} = \boldsymbol{F}_S \boldsymbol{F}_D^{-1}$$

which is then used to compute the Green-Lagrange strain

$$2\boldsymbol{E}_{SD} = \boldsymbol{F}_{SD}^T \boldsymbol{F}_{SD} - \boldsymbol{I} .$$

Because the strains are given in a cylindrical coordinate system, a transformation is required:

$$\boldsymbol{E}'_{SD} = \boldsymbol{A}^T \boldsymbol{E}_{SD} \boldsymbol{A}.$$

In LS-OPT command language, this would be:

```
matrix 'Fd' {Matrix3x3Init(Fd11,Fd12,Fd13,Fd21,Fd22,Fd23,Fd31,Fd32,Fd33)}
matrix 'Fs' {Matrix3x3Init(Fs11,Fs12,Fs13,Fs21,Fs22,Fs23,Fs31,Fs32,Fs33)}
matrix 'A' {Rotate(0, -1.858, 1.858,  X2,Y2,Z2,  X3,Y3,Z3)}

matrix 'FSD' {Fs * inv (Fd)}
matrix 'epsGlobal' {.5 * ( tr ( FSD ) * FSD  -  1  )}
matrix 'epsCyl' {tr(A) * epsGlobal * A}

response 'Ell' expression {epsCyl.a11}
```

POINT PLOTTING IN 3-D

A point plotting option has been provided in conjunction with 3-D metamodel plotting. Several options and status settings (colors-coded) are available.

Point plotting options:

Selection	Description
Analysis Results	Points are plotted for current iteration
All iterations	Points for previous iterations are added
Project points to surface	The points are projected on the surface to improve visibility. Future versions will have a transparency option.
Residuals	Shows a black vertical line connecting the computed and predicted values.
Feasible runs	Show feasible runs only
Infeasible runs	Show infeasible runs only
Failed runs on surface	Failed runs such as error terminations are projected to the surface in grey

Point status:

Selection	Description
Feasibility	Feasible points are shown in green, infeasible points in red (Figure 4).
Previous b/w	The points for the current iteration are shown in green (feasible) or red (infeasible). Previous points as light grey (feasible) or dark grey (infeasible)
Iterations	The iteration sequence is shown using a color progression from blue through red.
Optimum runs	Optimal points are shown in green/red and all other points in white.

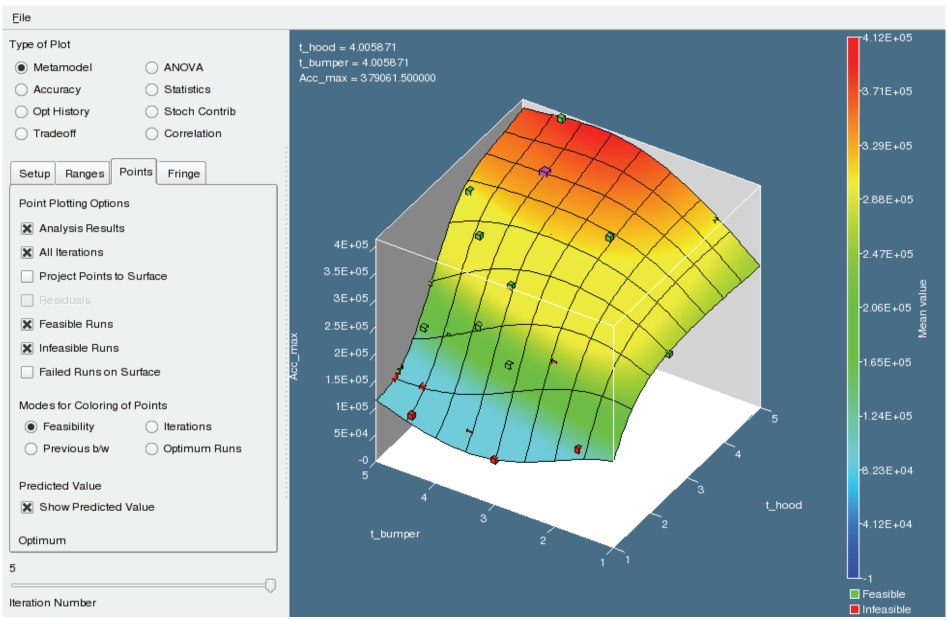


Figure 4: Metamodel plot showing feasible (green) and infeasible (red) points. The prediction point is shown in violet (*t_hood* = 4, *t_bumper* = 4) with the values displayed at the top left. The prediction point can be moved by moving the sliders in the Setup panel.

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