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User's Manual for VALMET: Validation Metric Estimator Program

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User's Manual for VALMET: VALIDATION METRIC ESTIMATOR PROGRAM

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Abstract

This manual describes the use of the computer program VALMET, a MATLAB program to estimate validation metrics for quantitative comparisons of computer simulations and experimental measurements. VALMET compares the mean (expected) value from the computational simulation with the estimated mean from the experimental measurements and quantifies the uncertainty in the experimental data using a statistical confidence interval. If the experimental data points are closely spaced over the range of the control parameter, an interpolation function is computed to represent the data. If the experimental measurements are sparse over the range of the control parameter, a regression is performed to obtain a function that approximates the estimated mean of the experimental data. The computational data is also interpolated so that it can be compared with the experimental data over the desired range of the data. The comparison results can be plotted in different ways, along with the desired confidence interval. The VALMET results can also be printed to a data file for further processing.

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Nomenclature

$1-\alpha$	= chosen quantile for the confidence interval
CI	= confidence interval
$\left.\left\lvert\frac{CI}{\bar{y}_e}\right\rvert\right._{avg}$	= average relative error metric confidence indicator
$\left.\left\lvert\frac{CI}{\bar{y}_e}\right\rvert\right._{\max}$	= maximum relative error metric confidence indicator
$\tilde{E}$	= estimated error of the computational simulation (computational simulation results minus the estimated mean of the experimental results)
$\left.\left\lvert\frac{\tilde{E}}{\bar{y}_e}\right\rvert\right._{avg}$	= average of the absolute relative error of the computational simulation results
$\left.\left\lvert\frac{\tilde{E}}{\bar{y}_e}\right\rvert\right._{\max}$	= maximum absolute relative error of the computational simulation results
$F(\nu_1, \nu_2, 1-\alpha)$	= F-distribution function with ν_1 and ν_2 specifying the first and second number of degrees of freedom, respectively, and 1- α is the quantile for the confidence interval specified
n	= number of sets of experimental data
np	= number of data points in the averaged experimental data set
p	= number of regression coefficients
$s(x)$	= standard deviation of the sets of experimental data as a function of x
$S(\vec{\theta})$	= error sum of squares of the regression
SRQ	= system response quantity
$t_{\alpha/2,\nu}$	= 1- α/2 quantile of the t-distribution for ν degrees of freedom
x_i^c	= i^{th} x value of the computational data
$y_e^i(x)$	= array of the i^{th} set of experimental measurements
$\bar{y}_e$	= estimated mean of the experimental data
$\lvert\,\bar{y}_e\,\rvert_{avg}$	= average of the absolute value of the estimated mean of the experimental data
$y_m(x_i)$	= mean of the computational simulation at x_i
$\mu(x)$	= true mean of the parent population of the experimental data as a function of x
ν	= number of degrees of freedom (n-1) of the experimental data

1. INTRODUCTION

The VALMET computer program estimates the error in a computer simulation given a reliable set of experimental data. Here, "reliable" means statistically independent measurements with normal (Gaussian) distributed measurement errors and no significant systematic error. The estimated error, referred to as a validation metric, is computed as the difference between the computational result and the experimental measurements as a function of the control (independent) parameter. VALMET also computes two global metrics, i.e., measures of disagreement between the computational and experimental results over the range of the control parameter. These two global metrics are the average relative error metric and the maximum relative error metric. The local validation metric and the global metrics include a statistical confidence interval to estimate the uncertainty in the comparison that is due to uncertainty in the experimental data. The code implements a new validation metric, as well as the global metrics, presented in Oberkampf and Barone [1]. If a set of experimental data is sparsely sampled over the range of the control parameter, i.e., an interpolation function cannot be confidently constructed over the range of the data, VALMET computes a regression fit of the data. If sufficient experimental data are available over the range of the data, an interpolation function is computed to represent the data. For both the regression case and the interpolation case, the uncertainty in the experimental data is represented with a statistical confidence interval over the range of the data.

Program VALMET can run on a computer with an installed version of the MATLAB software, or as a stand-alone compiled code on a Windows 2000/XP computer. The current version of VALMET is restricted to one-dimensional computational and experimental data, i.e., there can be only one control parameter for the data. User interaction with VALMET is primarily through a graphical user interface (GUI), allowing quick and easy use of the code. The data can be provided to VALMET in the form of Excel spreadsheets or text files. The metrics are displayed as text and in various plots. Some of the plots display the data with confidence intervals corresponding to a user-specified confidence level.

Section 2 of this report briefly discusses the derivation of the validation metrics. Much of Section 2 is taken from Oberkampf and Barone [1]. Section 3 discusses how VALMET implements the metrics and options specific to the code. Section 4 describes the input files that VALMET requires, Section 5 describes the dialog between the user and VALMET needed to run the program, and Section 6 describes the plots and other output that VALMET generates. Section 7 describes some commonly encountered VALMET errors. The new user is particularly encouraged to read Section 7 before executing the program to better understand common errors that are encountered. Installation instructions are contained in Section 8. The Appendices contain two complete examples of VALMET runs, including input files, VALMET – user dialog, and output plots and files. Appendix A presents an interpolation example involving a turbulent buoyant plume of helium and Appendix B presents a regression example involving a compressible free-shear layer.

2. VALIDATION METRICS

Oberkampf and Barone [1] present the validation metrics that are implemented in VALMET. This section contains a brief summary of derivation of the validation metrics from that reference.

Computable measures are needed that can quantitatively compare computational and experimental results over a range of input, or control, variables to sharpen assessment of computational accuracy. This type of difference measure has been recently referred to as a validation metric by Oberkampf and Trucano [2]. Oberkampf and Barone [1] have developed a new validation metric that is based on the statistical concept of a confidence interval. Using this fundamental concept, two versions of this metric are available; one for interpolation of experimental data and one for regression (curve fitting) of experimental data. The local validation metric result is computed as a function of the input variable over the range of the computational and experimental data. Two global metrics are also computed in VALMET: the average relative error metric and the maximum relative error metric. These global metrics provide a broader measure of the deviation of the computational data from the experimental data.

Both the local validation metric and the global metric compute a set of upper and lower confidence intervals for a user-specified confidence value. These confidence intervals estimate the uncertainty in the experimental data, as well as the related uncertainty in the validation metric. Since the confidence interval approach is based on statistical procedures, it is obvious that there must be a minimum of two sets of experimental data.

Note that the discussion in Oberkampf and Barone [1] and the current version of VALMET both limit the data to one dimension, i.e., one control (or input) parameter. The quantity of interest that is compared between the computational simulation and the experiment is referred to as the system response quantity (SRQ). Interpolation of the SRQ is appropriate when it is measured in fine increments over a range of the input variable. Finely spaced increments allow an interpolation function of the experimental measurements to be confidently constructed over the range of the input variable. Regression of the SRQ is appropriate for the situation where the experimental data are sparse over the range of the input variable. This situation is, in general, the more common situation occurring in experimental data.

The equation numbers in curly braces {} are those in Oberkampf and Barone [1].

2.1 Validation Metrics and Confidence Interval for Interpolation Case

Oberkampf and Barone [1] consider the case in which both the computational result and the experimental mean for the SRQ are functions of the input variable x. For the interpolation case, the average of the experimental data at each x provides the best estimate of the true value of the SRQ at that x. Given n sets of experimental measurements, the average for the set of measurements of the SRQ as a function of x is:

$$\bar{y}_e = \frac{1}{n}\sum_{i=1}^{n} y_e^i \qquad (1) \qquad \{8\}$$

where $\bar{y}_e$ is the estimated, or sample, mean based on n experiments.

Let y_m be the SRQ of the computational model. The estimated error in the computational model is:

$$\tilde{E}(x) = y_m(x) - \bar{y}_e(x) \qquad (2) \qquad \{7\}$$

Using the standardized random variable $Z = \frac{\bar{y}_e - \mu}{s/\sqrt{n}}$ with Student's t distribution, it can be shown that the true error as a function of x is in the interval:

$$\left(\tilde{E}(x) - t_{\alpha/2,\nu} \cdot \frac{s(x)}{\sqrt{n}}, \tilde{E}(x) + t_{\alpha/2,\nu} \cdot \frac{S(x)}{\sqrt{n}}\right) \qquad (3) \qquad \{16\}$$

with a confidence level of 100(1-α)% for $\nu = n$-1 degrees of freedom. The population standard deviation as a function of x is approximated by

$$s(x) \sim \left[\frac{1}{n-1}\sum_{i=1}^{n}\left(y_e^i(x) - \bar{y}_e(x)\right)^2\right]^{1/2} \qquad (4) \qquad \{17\}$$

The use of the standard deviation requires $n > 1$, so single sets of experimental data cannot be processed by interpolation in VALMET. The interval given in Eq. (3) gives the bounds on the model error (Eq. (2)) at the desired confidence level.

2.2 Global Metrics and Confidence Intervals for Interpolation Case

Although the equations above provide the results of the validation metric as a function of x, there are some situations where it is desirable to construct a more compact, or global, statement of the validation metric result. A convenient method to compute a global metric would be to use a vector norm of the estimated error over the range of the input variable. The L_1 norm is useful to interpret the estimated average absolute error of the computational model over the range of the data. Using the L_1 norm, one could form an average absolute error or a relative absolute error over the range of the data. We choose to use the relative absolute error by normalizing the absolute error by the estimated experimental mean and then integrating over the range of the data. We define the *average relative error metric* to be

$$\left|\frac{\tilde{E}}{\bar{y}_e}\right|_{avg} = \frac{1}{(x_u - x_l)}\int_{x_l}^{x_u}\left|\frac{y_m(x) - \bar{y}_e(x)}{\bar{y}_e(x)}\right| dx \qquad (5) \qquad \{18\}$$

where x_u is the largest value and x_l is the smallest value, respectively, of the input variable. As long as $\bar{y}_e(x)$ is not near zero, the average relative error metric is a useful quantity.

VALMET excludes data points with $\bar{y}_e(x) \approx 0$ from the calculation of the average relative error metric, the maximum relative error metric, and their confidence indicators.

The confidence interval that should be associated with this average relative error metric is the average confidence interval normalized by the absolute value of the estimated experimental mean over the range of the data. We define the *average relative confidence indicator* as the half-width of the confidence interval averaged over the range of the data:

$$\left|\frac{CI}{\bar{y}_e}\right|_{avg} = \frac{t_{\alpha/2,\nu}}{(x_u - x_l)\sqrt{n}} \int_{x_l}^{x_u} \left|\frac{s(x)}{\bar{y}_e(x)}\right| dx \qquad (6) \quad \{19\}$$

We refer to $\left|\frac{CI}{\bar{y}_e}\right|_{avg}$ as an indicator, as opposed to an average relative confidence interval, because the uncertainty structure of $s(x)$ is not maintained through the integration operator ($s(x)$ is defined only at the points where the experimental data is averaged). $\left|\frac{CI}{\bar{y}_e}\right|_{avg}$ provides a quantity with which to interpret the significance of $\left|\frac{\tilde{E}}{\bar{y}_e}\right|_{avg}$. Stated differently, the magnitude of $\left|\frac{\tilde{E}}{\bar{y}_e}\right|_{avg}$ should be interpreted relative to the magnitude of the normalized uncertainty in the experimental data, $\left|\frac{CI}{\bar{y}_e}\right|_{avg}$.

There may be situations where the average relative error metric may not adequately represent the model accuracy because of the strong smoothing nature of the integration operator. For example, there may be a large error at some particular point over the range of the data that should be noted. It is useful to define a maximum value of the absolute relative error over the range of the data. Using the L_∞ norm to accomplish this, we define the *maximum relative error metric* as

$$\left|\frac{\tilde{E}}{\bar{y}_e}\right|_{\max} = \max_{x_l \le x \le x_u} \left|\frac{y_m(x) - \bar{y}_e(x)}{\bar{y}_e(x)}\right| \qquad (7) \quad \{20\}$$

A significant difference between $\left|\frac{\tilde{E}}{\bar{y}_e}\right|_{avg}$ and $\left|\frac{\tilde{E}}{\bar{y}_e}\right|_{\max}$ would indicate the need to more carefully examine the trend of the model with respect to the trend of the experimental data.

The confidence interval that should be associated with the maximum relative error metric is the confidence interval normalized by the estimated experimental mean. Both the confidence interval and the estimated experimental mean are evaluated at the point where the maximum relative error metric occurs. Let the x value where $\left|\frac{\tilde{E}}{\bar{y}_e}\right|_{\max}$ occurs be defined as $\hat{x}$. Then the confidence interval associated with the maximum relative error metric is

$$\left|\frac{CI}{\bar{y}_e}\right|_{\max} = \frac{t_{\alpha/2,\nu}}{\sqrt{n}}\left|\frac{s(\hat{x})}{\bar{y}_e(\hat{x})}\right| \qquad (8) \quad \{21\}$$

Note that in the last two sections (2.1 and 2.2), all of the functions of x, e.g., $y_m(x)$ and $s(x)$, are considered as continuous functions constructed by interpolation.

In addition to these global metrics, VALMET provides as additional global information the average of the absolute values of the estimated mean of the experimental data:

$$|\bar{y}_e|_{avg} = \frac{1}{np}\sum_{j=1}^{np}|\bar{y}_e(x_j)| \qquad (9)$$

Here np is the number of points in the averaged experimental data set.

2.3 Validation Metrics and Confidence Interval for Regression Case

We now consider the case where the quantity of experimental data for the SRQ is not sufficient to construct an interpolation function. Consequently, a regression function (curve fit) must be constructed to represent the estimated mean over the range of the data. The regression case could be described as: a) given a set of experimental data (containing random variability) that is specified over some range of the input variable, x, and b) given an assumption concerning the functional form of the regression function, then the calculation is made that a) computes the parameters of the regression function that minimizes the square of the error between the experimental data and the regression function, and b) computes the confidence interval for the experimental data. In the regression case, the average relative error metric and maximum relative error metric are calculated in the same manner as for the interpolation case (Section 2.2). Since there are no standard deviations at the x-values of the set of experimental data, the confidence intervals associated with the average relative error metric and the maximum relative error metric are estimated in a different manner.

We wish to determine the confidence interval that results from uncertainty in the regression coefficients over the complete range of the regression function. The regression coefficients are all correlated with one another because they appear in the same regression function that is fitting the experimental data. This type of confidence interval is typically referred to as a simultaneous confidence interval, a simultaneous inference, or a confidence region, so that it can be distinguished from traditional (or single-comparison) confidence intervals [3-5].

Since the quantity of experimental data is not sufficient to construct an interpolating function, we can represent the estimated mean of the data, $\bar{y}_e(x)$, as a general nonlinear regression function

$$\bar{y}_e(x) = f(x, \vec{\theta}) + \varepsilon \qquad (10) \quad \{22\}$$

$f(x; \cdot)$ is the chosen form of the regression function over the range of the input parameter *x*; $\vec{\theta} = \theta_1, \theta_2, \cdots, \theta_p$ are the unknown coefficients of the regression function; and ε is the random error that can be due to either measurement uncertainty, or it can be due to variability in the physical process itself, e.g., variability in multiple samples being tested. Let the set of *m* experimental measurements of the SRQ of interest be given by

$$\left(y_e^i, x_i \right) \ \text{ for } i = 1, 2, \ldots, m \qquad (11) \quad \{23\}$$

Using a least-squares fit of the experimental data, it can be shown [4,5] that the error sum of squares $S(\vec{\theta})$ in *p*-dimensional space is

$$S\left(\vec{\theta}\right) = \sum_{i=1}^{n} \left[y_e^u(x) - f\left(x_i; \vec{\theta}\right) \right]^2 \qquad (12) \quad \{24\}$$

The vector that minimizes $S(\vec{\theta})$ is the solution vector, and it is written as $\hat{\vec{\theta}}$. This system of simultaneous, nonlinear equations can be solved by various software packages that compute solutions to the nonlinear least-squares problem. VALMET uses the MATLAB software package.

Draper and Smith [4] and Seber and Wild [5] discuss a number of methods for the computation of the confidence regions around the point $\hat{\vec{\theta}}$ in *p*-dimensional space. For any specified confidence level $100(1-\alpha)\%$, a unique region envelops the point $\hat{\vec{\theta}}$. For two regression parameters, (θ_1, θ_2), we have a two-dimensional space, and these regions are contours that are similar to ellipses with a curved major axis. For three parameters, $(\theta_1, \theta_2, \theta_3)$, we have a three-dimensional space, and these regions are contours that are similar to bent ellipsoids, e.g., shaped like a banana. A procedure that appears to be the most robust to nonlinear features in the equations [5] and that is practical when *p* is not too large (roughly *p* < 6), is to solve an inequality for the set of $\vec{\theta}$:

$$\vec{\theta} \text{ such that } S(\vec{\theta}) \leq S(\hat{\vec{\theta}}) \left[a + \frac{p}{m-p} F(p, m-p, 1-\alpha) \right] \qquad (13) \quad \{25\}$$

In Eq. (13), $F\left(\nu_1, \nu_2, 1-\alpha\right)$ is the *F* probability distribution, ν_1 is the first parameter specifying the number of degrees of freedom, ν_2 is the second parameter specifying the number of degrees of freedom, $1-\alpha$ is the quantile for the confidence interval of interest, and *m* is the number of experimental measurements.

2.4 Global Metrics and Confidence Intervals for Regression Case

In the regression case, the average relative error metric (Eq. (5)) and the maximum relative error metric (Eq. (7)) are calculated from the same formulas, except that now $\overline{y}_e(x)$ is the value of the regression fit instead of the value of the average experimental data at *x*.

If we would like to make a quantitative assessment of the global modeling error, then we can extend the global measures expressed in Eqs. (8, 10-12). The average relative confidence indicator, Eq. (6), and the confidence interval associated with the maximum relative error, Eq. (8), are based on symmetric confidence intervals given in Section 2.2. For the nonlinear regression case, i.e., nonlinear in the regression coefficients, we no longer have symmetric confidence intervals. As a result, we approximate the confidence intervals by taking the average half-width of the confidence interval over the range of the data and the half-width of the confidence interval at the maximum relative error, respectively. For the average relative error confidence indicator, we now have

$$\left|\frac{CI}{\overline{y}_e}\right|_{avg} = \frac{1}{\left(x_u - x_l\right)} \int_{x_l}^{x_u} \left|\frac{y^+_{CI}(x) - y^-_{CI}(x)}{2\overline{y}_e(x)}\right| dx \,. \qquad (14) \quad \{26\}$$

$y^+_{CI}(x)$ and $y^-_{CI}(x)$ are the upper and lower confidence intervals, respectively, as a function of *x*. As discussed below, $y^+_{CI}(x)$ and $y^-_{CI}(x)$ are found by substituting into the regression function $f(x;\vec{\theta})$, all $\vec{\theta}$ that satisfy Eq. (13). As stated earlier, $\left|\frac{CI}{\overline{y}_e}\right|_{avg}$ provides a quantity with which to interpret the significance of $\left|\frac{\tilde{E}}{\overline{y}_e}\right|_{avg}$.

Also, we have

$$\left|\frac{CI}{\overline{y}_e}\right|_{\max} = \left|\frac{y^+_{CI}(\hat{x}) - y^-_{CI}(\hat{x})}{2\overline{y}_e(\hat{x})}\right| \qquad (15) \quad \{27a\}$$

for the half-width of the confidence interval at the maximum relative error point, $\hat{x}$. $\left|\frac{CI}{\overline{y}_e}\right|_{\max}$ provides a quantity with which to interpret the significance of $\left|\frac{\tilde{E}}{\overline{y}_e}\right|_{\max}$. The maximum relative error point is defined as the *x* value where $\left|\frac{\tilde{E}}{\overline{y}_e}\right|$ achieves its maximum, that is,

$$\hat{x} = x \text{ such that } \left| \frac{y_{CI}^{+}(x) - y_{CI}^{-}(x)}{\bar{y}_e(x)} \right| \text{ is a maximum for } x_l \le x \le x_u \qquad (16) \quad \{27b\}$$

The confidence interval bounds above and below the regression curve are computed point-by-point by a constrained optimization procedure. The lower bound is found by minimizing the regression function, $f(x,\vec{\theta})$, subject to the constraint in Eq. (13). The upper bound is found by maximizing the regression function subject to the constraint in Eq. (13).

3. CAPABILITIES OF THE VALMET CODE

This section discusses some capabilities available in VALMET with regard to the interpolation and regression options. In addition, some comments are made concerning the computation of the confidence intervals for the regression option.

3.1 VALMET Interpolation Processing

Interpolation requires that the experimental and computational data use the same independent variable grid. The user selects one of the following grids to be used:

- the experimental grid (i.e., the computational data is interpolated onto the experimental data grid),
- the computational grid (i.e., the experimental data is interpolated onto the computational data grid), or
- a "round number" grid (i.e., both experimental and computational data are interpolated onto an evenly spaced grid). VALMET computes a default range and step size for the round number grid, which the user may adjust.

The interpolation algorithm omits any points that are outside of the region common to both experimental and computational data.

The experimental and computational data are interpolated onto the selected grid using one of two user-selected methods:

- linear: the data value at each grid point is found using a straight line through the two data points surrounding the grid point, or
- spline: the data value at each grid point is found from VALMET computing a set of piecewise continuous cubic polynomials passing through the data points.

The confidence interval for the interpolation option is symmetric about the average of the experimental data. Since the confidence interval calculation uses the standard deviation of the experimental data as a function of *x*, the distance between the confidence interval curve and the experimental average can vary from point to point.

3.2 VALMET Regression Processing

The following function forms are available for the regression equation:

Forms 1 through 8: polynomials of degree 1 through 8

Form 9: hyperbola: $y = a + \dfrac{b}{1 + cx}$

Form 10: exponential: $y = c + b \cdot e^{ax}$

Form 11: exponential: $y = bx^a$

Form 12: Fermi-Dirac function: $y = \dfrac{a + x^c}{b + x^c}$ (for $x \geq 0 \quad and \quad c \neq 0$)

For c > 0, this function approaches y=1 for $x \to \infty$.
For c < 0, this function approaches y=1 at x = 0.

Form 13: pulse function: $y = a + b\left(\dfrac{1}{1 + \exp(c(x - d))} - \dfrac{1}{1 + \exp(e(x - f))}\right)$

The pulse starts and ends with y=0.

Form 14: Lorentz function: $y = a + \dfrac{b}{1 + \left(\dfrac{x - c}{d}\right)^2}$

Form 15: Fermi-Dirac variant: $y = 1 + a\left(\dfrac{1}{1 + bx^c} - 1\right)$

Additional function forms can be added to the regression equations offered by VALMET. However, this should only be attempted by advanced users who are familiar with VALMET and are comfortable writing MATLAB scripts.

For most of the regression function forms above, the computation of the regression coefficients and the confidence intervals is very robust. However, in testing various applications we have found that the computation of the confidence interval for Forms 12 and 15 will occasionally fail to converge. For Form 13, failures to converge are even more common because of the great flexibility of the function, which includes six regression coefficients.

Regression form 9 is useful when the data appears to have a vertical or horizontal asymptote. It also is useful for data with a smooth change in slope, either concave upwards or downwards. The two branches of the hyperbola are shown in Figure 3-1. VALMET's non-linear fit of the data will select the appropriate branch of the hyperbola for the fit of the data.

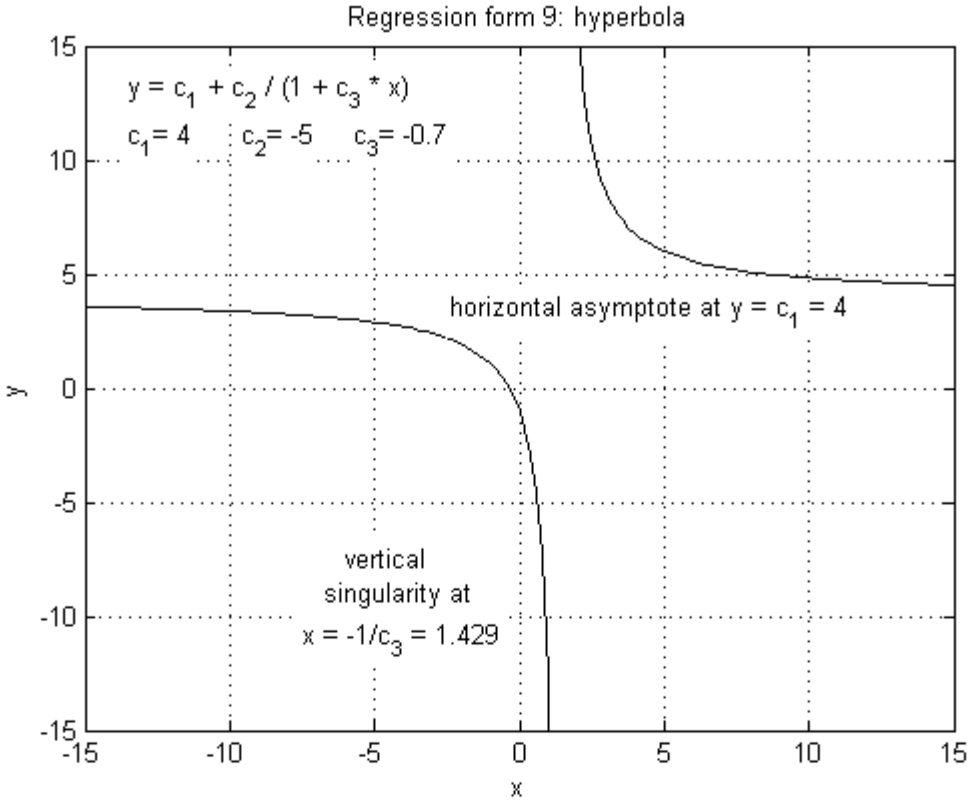

Figure 3-1. Regression Form 9: hyperbola.

Regression form 10 is useful when the data increases or decreases exponentially or according to some power of x. Figure 3-2 shows two versions of the exponential form: a decreasing exponential starting at x,y = (0,100) and dropping off to the right, and an increasing exponential starting at x,y = (0, 20.4) and increasing to the right. The non-linear fit in VALMET will choose the correct version for the data.

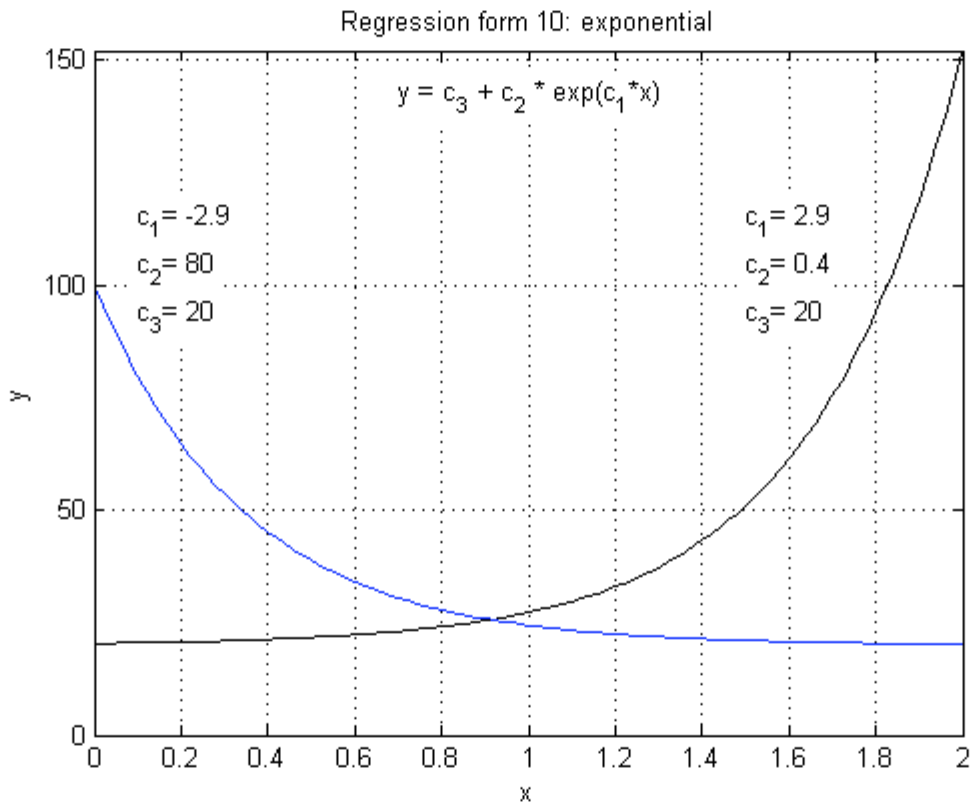

Figure 3-2. Regression Form 10: exponential.

Regression form 11 is a version of the exponential curve that either starts or ends with $y = 0$. Figure 3-3 shows an increasing and a decreasing version of this form.

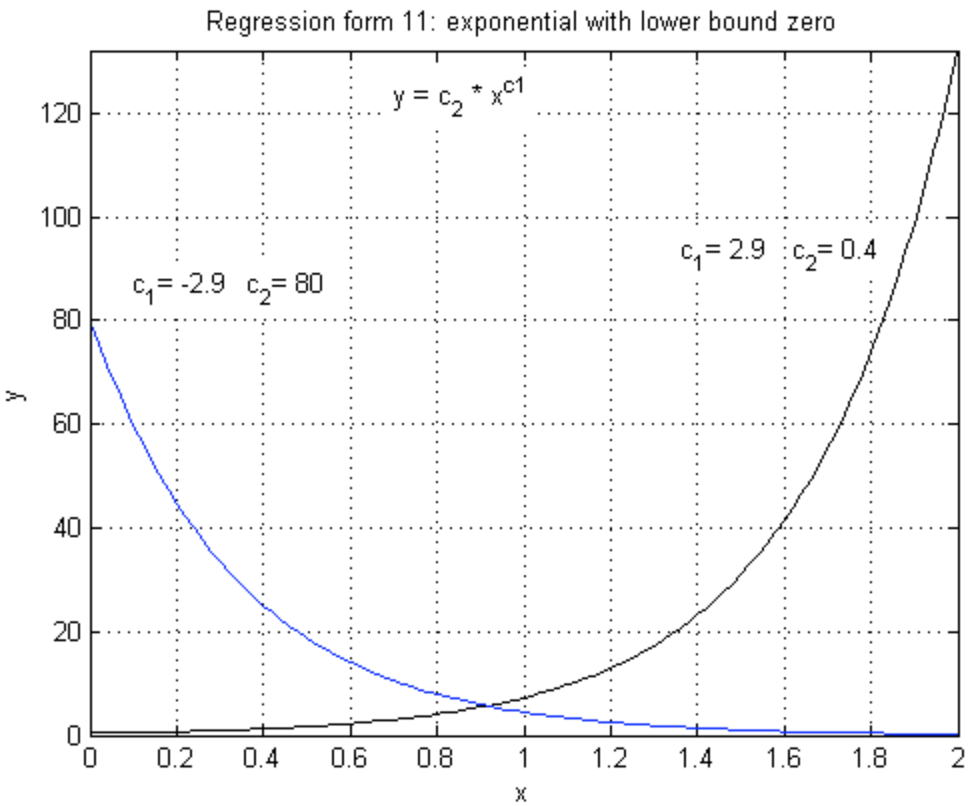

Figure 3-3. Regression Form 11: exponential starting or ending at y=0.

4. DESCRIPTION OF THE INPUT FILES

There are two types of input data expected by VALMET: experimental data and computational data. VALMET expects to read each type of data from a separate file. If there is only one type of data, then that file should be read twice, once as experimental data and again as the computational data.

Both types of data may be input in either an Excel file or a text file. If the computer does not have Excel on it, VALMET may still be able to read the Excel file (with a warning message), but the data should be contained in the first worksheet of the Excel file. The data must be organized in columns, with each column representing a variable. There must be the same number of values (i.e., rows) for each column. Text header lines are permitted before the data, but no text or blank lines are allowed within the data file. For text files, VALMET requests the number of header lines, the column delimiter (usually comma or blank), and the number of columns from the user.

It is important to note that no text or blank lines are allowed after the header lines. (In the remainder of this report, important cautions or warnings for the user are written in a bold-faced type.) In an Excel file, all rows are read up to the final numeric line. If there are blank or text rows (for example, if another table appears after the desired data), these will be read in as NaN's (Not a Number) and will cause a fatal error during processing. In a text file, the first blank or text line signals the end of data, so all data that follow will be ignored.

Each file must have exactly one column of independent variable values (since the code is limited to one dimension). The computational data file should have one column of independent variable data and one column of dependent variable data; other columns are ignored. The experimental data file should have one column of independent variable data and one or more columns of dependent variable data; other columns are ignored. Different experimental measurements may be in separate data files, but the independent variable must be included in each data file, with identical values in each file. The independent variable and the dependent variable may be in any column; VALMET requests the column numbers from the user.

Experimental data files and computational data files for two examples are shown in the appendices. Example text files are shown in Table A-1 and Table A-2; example Excel files are shown in Table B-1 and Table B-2.

5. USER INTERACTIONS WITH THE SOFTWARE

5.1 Starting the Program

To run the MATLAB version of the VALMET program, first start MATLAB by clicking on the MATLAB icon on the desktop, bringing up the MATLAB desktop window. Select the directory where the VALMET.m file resides by browsing in the "Current window" box in the toolbar near the top of the screen. Run the program by typing "VALMET" at the ">>" prompt in the MATLAB command window.

To run the compiled version of the VALMET program, browse for the valmet.exe file and double-click on the file from Windows or type VALMET at a DOS prompt. If an error is displayed, check that VALMET has been properly installed as explained in Section 8.3.

5.2 Graphical User Interface

VALMET uses a graphical user interface to request information from the user. The program requests input using the following constructs:

- "Radio buttons" allow the user to select one or more options. A question is displayed with a set of buttons (circles) underneath; each button is associated with a text option. The user selects an option(s) by clicking on one or more of the buttons. If a "NEXT" box is present, the user should click on the appropriate buttons, then click NEXT to proceed. If the options are mutually exclusive (e.g., yes or no), there may not be a "NEXT" box. In this case, processing proceeds when a button is selected.

- A "dialog box" allows the user to enter text or numeric values. A box appears on top of the current input window. It has a question, a white area for the user's response, and "OK" and "Cancel" boxes. The user should type the appropriate response in the white area, then click on the "OK" box to proceed. The dialog box disappears when OK is clicked. Clicking the "Cancel" box may cause an input error in VALMET.

- A "file selection browser" allows the user to browse for and select a specific file. This VALMET browser is very similar to the Windows browser. Files and folders in the current directory are shown. The user can go up a directory by clicking the up-arrow on the yellow file folder icon, or the user can go down into a folder by double clicking on the folder name. The user can select a file by double clicking on the file name, or by single clicking on the file name and clicking on the "OPEN" box in the lower right corner of the window. There may be a short delay after clicking on a file name before any response is seen. The browser disappears when OPEN is clicked.

To exit the program early, click the "X" in the upper-right corner of the input window or type ctrl-C in the MATLAB command window.

5.3 VALMET – User Dialog

This section details the prompts that VALMET displays (shown in Arial font) and discusses expected replies from the user (indented under the prompt). The expected replies are not described in detail; most should be obvious to the user. Dialog sessions that run two example problems are shown in Appendix Sections A.2 and B.2, with screen shots to illustrate certain information.

VALMET writes output files to the current directory. **Some of the output files have fixed names; thus, output files from previous runs may be overwritten. Copy or rename any output files of interest before VALMET starts. Trying to overwrite files may cause the compiled version of VALMET to abort.** See Section 5.4 for more information.

Output File Options

Do you want a text output file with experimental, computational, and CI data?

> Click on the "yes" or "no" button, then click on the NEXT box.

Enter a name for the output text data file:

> This dialog box appears only if the user clicks "yes" above. Enter the file name and click OK.

Do you want the date and time appended to the plots and text output file?

> Click "yes" or "no".

Experimental Data File Options

Are the experimental data in one file or multiple files?

> Options are "All data in one file" or "Data in multiple files". If the user clicks "Data in multiple files", a message listing the constraints on multiple files (see Section 4) appears for a short time, then the next query appears.

Are your EXPERIMENTAL data in an Excel file or a text file?

> Options are "Excel: .xls", "text: .txt or .dat" or "show all files" (for a text file that does not have a .txt or .dat extension).

The program displays a file browser window so the user can browse for and select the experimental data file.

> Use the file browser to select the experimental data file. There may be a short pause after you click on one of the buttons until the file browser window comes up. There may be another pause before the next query appears.

Choose the worksheet that contains the data:

> This query only appears if an Excel file is being read and if the file contains more than one workbook. The program shows the names of the workbooks as options. The user must know which workbook contains the correct data.

The first eight lines of the Excel file or the text file are shown at the bottom of the input window. For an Excel file, the correct number of header (text) lines may not be shown. This is not important since VALMET does not ask for the number of header lines for an Excel file.

How many header lines precede the data?

This query and the next two queries do not appear for an Excel file. VALMET can determine on its own the number of header lines and columns for an Excel file.

What delimiter character separates the numeric data?

Enter the appropriate delimiter character. If the delimiter is a blank, press the space bar in the dialog box before clicking OK.

How many columns (total) are there in the file?

Enter the total number of columns in the file, not necessarily the number that will be processed.

Which column is the independent variable?

Enter the column number. The independent variable may be in any column.

Do you want to multiply the independent variable by a scale factor?

This allows the user to convert the independent variable from one set of units to another or to normalize it in some fashion. For example, meters can be converted to centimeters by using a scale factor of 100. The scaled data appears in the output text file and on all plots.

Enter the scale factor:

This query only appears if the user selects "yes" above.

Enter a caption with (units) for the independent variable:

This caption will be used for labeling the plot x-axis. The units, if provided, should be enclosed in parentheses.

Do you want to multiply the measured variable by a scale factor?

Enter the scale factor:

This query only appears if the user selects "yes" above.

Enter a caption with (units) for the measured variable:

This caption will be used for labeling the plot y-axis. The units, if provided, should be enclosed in parentheses.

Select the column number(s) of the EXPERIMENTAL data (averaged if two or more):

This query only appears if there are more than two columns of data; otherwise VALMET assumes one column is the independent variable (indicated above) and the other is the dependent variable. Buttons are displayed for every column other than the independent variable, and the user can select one or more columns of data. Click NEXT when all the desired columns have been selected. If more than one column is selected, VALMET uses the average of all the selected columns.

Do you want to read another data file?

This query only appears if the user selected "data in multiple files" at the start of this section. If the user clicks "yes", the program repeats the queries in this section for the next file.

Computational Data File Options

All of the queries for the experimental data file are repeated for the computational data file, except that the names of the independent and dependent variables are not requested since they are assumed to have the same names.

Processing Options

What % confidence interval do you want (50 to 99.99)?

> **Enter the confidence interval as a percent value** rather than as a fraction (i.e., enter 90 instead of 0.9)! The program accepts any confidence interval between 0 and 100 (exclusive), but values outside the range 50 to 99.99 percent have not been tested.

Do you want to use interpolation or regression on the data?

> Options are “interpolation” or “regression”.

The start, end, and average spacing or step size for each grid type are listed. An example of this screen is shown in Figure A-2. Note that any points that are outside of the region common to both experimental and computational data are omitted. Thus, the end points presented are not necessarily the end points of the data but are points that lie at or within the ranges of both the experimental and computational data.

Which interpolate grid do you want to use?

> This query only occurs for interpolation. Options are “Experimental”, “Computational”, or “Round number”. See Section 3.1 for information on the grid choice.

Set roundnumber spacing parameters.

> This query only appears for interpolation with the round number grid and for regression. The step size, interval start, interval end, and number of points are displayed. Examples of this screen are shown in Figure A-2 (interpolation) and Figure B-2 (regression). The user can enter new values for any of the parameters. The other values will be adjusted as needed. For example, if the step size is changed, the number of points will be recalculated. Click DONE when the grid is satisfactory.

What interpolation method do you want to use?

> This query only occurs for interpolation. Options are “linear” or “spline”. See Section 3.1 for information about the interpolation method.

Select a regression form y=f(x) for your data:

> This query only occurs for regression. An example of this screen is shown in Figure B-3. The function forms that are available for the regression equation are listed and explained in Section 3.2. They include polynomial fits of degrees 1 through 8, a hyperbola, two exponential forms, a Fermi-Dirac function, a pulse function, a Lorentz function, and a Fermi-Dirac variant.

Do you want to change the starting point(s)?

> This query only occurs for regression. An example of this screen is shown in Figure B-4. This query allows the user to change the starting points of the optimization problem that is solved for the lower and upper confidence bounds (Section 2.4). This option is useful if the default values did not

converge well. The options are "change lower bound initial coordinates", "change upper bound initial coordinates" or "no". The coordinates refer to the coefficients in the regression equation. Click "no" to leave the starting points unchanged. Note that to change both the lower bound and the upper bound, both the lower bound button and the upper bound button must be clicked! Click NEXT to proceed.

Change initial-point coordinates.

This query only appear if the user chooses to change the lower and/or upper bound initial conditions. An example of this screen is shown in Figure B-5. The screen shows the regression equation, the initial values of the coordinates, the current values, and a button for each coordinate. If a button is clicked, a dialog box appears asking for the new value of that coordinate. Click DONE when the all the desired changes have been made. If the user chooses to change both the lower bound and upper bound initial conditions, a query appears for the lower bound, then for the upper bound.

5.4 Processing

Once the processing options have been requested from the user, VALMET performs the requested calculations. Any processing messages are displayed in the MATLAB command window. Messages are color-coded: *black* for informational messages, *blue* for warnings of non-fatal problems, and *red* for fatal errors.

For a regression calculation, the screen gives a rough estimate of the running time for the optimization for two computers with different CPU speeds. The running times are for the default initial optimization coordinates and may differ significantly if other starting coordinates are specified. The regression calculation screen also tells the user to ignore the many warning and informational messages from VALMET; there may be hundreds. The informational messages usually indicate that the iteration has converged within prescribed tolerances.

When the calculation is complete, the validation metrics screen and the plots described under Section 6.1 and Section 6.2 appear on the screen. The plots are stacked on top of each other. The plots can be moved on the screen, closed by clicking the "X" in the upper-right corner of the figure, or minimized to the task bar by clicking the "-" icon.

The validation metrics screen and plots are also stored as .fig files in the current directory. The output files and plots are written to files with fixed names. Some of the file names include the interpolation/regression option and the confidence interval, but some do not. **Thus, running the program or re-processing the data may overwrite some of the existing output files.** The MATLAB version of VALMET overwrites old files without comment. **The compiled version of VALMET may abort when it tries to overwrite old .fig files, after issuing the following message: "Warning: Objects of uitools.uimodemanager class exist - not clearing this class or any of its super-classes".**

This problem can be prevented by renaming the files or by removing the old .fig files from the current directory before VALMET is run and before re-processing the data.

The following query appears in the input window.

Do you want to process the same data again?

> If the user clicks “yes”, VALMET repeats the queries in the “Processing Options” section and re-processes the data. Be aware that some of the existing output files and plots may be overwritten, as discussed above. If the user clicks “no”, the VALMET program terminates and processing returns to the MATLAB desktop.

5.5 Exiting the Program

When the user indicates that processing is complete, the VALMET program terminates and processing returns to the MATLAB desktop. The plots are still available for examination. The user may also save the plots in another format, as discussed in Section 6. To exit the MATLAB version of the program, type “EXIT” in the MATLAB command window. The compiled version of VALMET terminates when all the figures have been closed by clicking the “X” in the upper-right corner of the figure.

6. DESCRIPTION OF THE OUTPUT

VALMET generates a validation metrics screen, and four or five plots (depending on whether interpolation or regression is requested), and an optional output text file. The validation metrics screen and plot files are displayed as figures in the MATLAB desktop, and also stored as .fig files in the current directory. The output text file, if any, is stored in the current directory, but is not displayed to the user.

Each type of output is explained below, and the Appendices contain examples of each type of output. The user can display a .fig file created during a previous run by clicking “File” on the MATLAB menu bar, then “Open”, and browse for the file. A figure can be saved in other formats by clicking “File” on the figure menu bar, then “Save as”. Several formats are available, including Adobe Illustrator (.ai), bitmap (.bmp), EPS, and JPEG.

6.1 Validation Metrics Screen

The validation metrics are displayed on a screen on the MATLAB desktop, and stored in a “.fig” file. Other data of interest are also shown on this screen. An indication of the order of magnitude of the experimental data is given by $\left|\bar{y}_e\right|_{avg}$, the average of the absolute values of the experimental data (Eq. (9)). This quantity is identified as Avg(abs(y-bar_e)) in the interpolation processing mode and as Avg(abs(yregression)) in the regression processing mode.

6.1.1 Validation Metrics Screen for Interpolation

The validation screen for the interpolation case first lists the interpolation options (percent confidence interval, grid type, and interpolation type). Then it lists $\left|\bar{y}_e\right|_{avg}$ and the two global validation metrics and their associated confidence indicators. These values are explained in Section 2.2, and the appropriate equations are referenced here. The values on the screen are identified as:

- Avg(abs(y-bar_e)) *see Eq. (9)*
- Average relative error metric *see Eq. (5)*
- Average relative confidence indicator *see Eq. (6)*
- Maximum relative error metric *see Eq. (7)*
- Confidence interval for maximum relative error metric *see Eq. (8)*

The file name (listed near the bottom of the screen) is globalmetrics_for_interp_*nn*pct.fig, where *nn* is the percent confidence interval.

An example of this screen is shown in Figure A-3.

6.1.2 Validation Metrics Screen for Regression

The validation screen for the regression case lists $|\bar{y}_e|_{avg}$ and the two global validation metrics and their associated confidence intervals. These values are explained in Sections 2.2, 2.3, and 2.4, and the appropriate equations are referenced here. The values on the screen are identified as:

- Avg(abs(yregression)) *see Eq. (9)*
- Average relative error metric *see Eq. (5)*
- Average relative confidence indicator *see Eq. (14)*
- Maximum relative error metric *see Eq. (7)*
- Confidence interval for maximum relative error metric *see Eq. (15)*

The file name (listed near the bottom of the screen) is globalmetrics_for_rform*xx*_*nn*pct.fig, where *xx* is the regression equation function form number (see Section 3.2) and *nn* is the percent confidence interval.

An example of this screen is shown in Figure B-6.

6.2 Plots

Each plot is displayed on a separate figure on the MATLAB desktop, and stored in a separate ".fig" file.

Note that the axis labels for the independent variable and the dependent variable, if applicable for the plot, are provided by the user in the VALMET – user dialog. If the user provided a scale factor, the data plotted is likewise scaled.

In the descriptions below, *nn* is the percent confidence interval and *xx* is the regression equation function form number (see Section 3.2).

6.2.1 Plots for Interpolation

VALMET displays four plots for the interpolation case. Each plot is described briefly in this section. The plots for an example interpolation problem are shown in Appendix A (Figure A-4 through Figure A-7).

The first plot (experimental_data.fig) is titled "Experimental measurements". The plot shows the data from the experimental data file. The dependent variable is plotted versus the independent variable for each of the selected columns of data.

The second plot (comp_and_exp_mean_with_*nn*pct_ci.fig) is titled "Experimental mean with *nn*% confidence interval and computational result". The plot shows the sample mean of the measurements, calculated from the experimental data. It also shows the interval around the estimated mean in which the true mean will occur with *nn*% confidence, calculated from the interpolated function for the experimental sample mean and the confidence interval for the true mean. The plot also shows the computational solution (from the computational data file).

The third plot (est_error_with_*nn*plus_minus_ci_del.fig) is titled "Validation metric result and *nn* confidence interval". The plot shows the estimated error between computational results and mean experimental results, along with the *nn*% confidence interval from the experiment.

The fourth plot (est_error_with_*nn*pct_bounds.fig) is titled "Estimated error and true error in the model with *nn*% confidence interval". The plot shows the estimated error and the confidence interval of the true error in the dependent variable predicted by the computational model as a function of the independent variable.

6.2.2 Plots for Regression

VALMET displays five plots for the regression case. Each plot is described briefly in this section. The plots for an example regression problem are shown in Appendix B (Figure B-7 through Figure B-11).

The first plot (experimental_data.fig) is titled "Experimental measurements". The plot shows the data from the experimental data file.

The second plot (comp_and_exp_mean_with_*nn*pct_ci_rform*xx*.fig) is titled "Experimental data, computational data, and *nn*% confidence interval around fit". The plot shows the experimental data, the *nn*% confidence interval of the regression fit, and the computational simulation result.

The third plot (est_error_with_*nn*plus_minus_ci_rform*xx*.fig) is titled "Validation metric result and *nn* confidence interval". The plot shows the estimated error between computational results and the regression fit of the experimental data, along with the *nn*% confidence interval from the experiment, representing the uncertainty in the experimental data. The estimated error is $v_c - v_{fit}$, where v_c is the array of computational data and v_{fit} is the array of regression fit values on the computational grid. The upper and lower confidence interval curves are the deviations above and below the regression fit on the round number grid from the optimizations that maximize and minimize the regression function subject to the constraint of Eq. (13).

The fourth plot (est_error_with_*nn*pct_bounds_rform*xx*.fig) is titled "Estimated error and true error in the model with nn% confidence interval". The plot displays the results of the validation metric by plotting the *nn*% confidence interval of the true error in dependent variable predicted by the computational model as a function of the independent variable. Again, the estimated error is $v_c - v_{fit}$, where v_c is the array of computational data and v_{fit} is the array of regression fit values on the computational grid. The upper and lower true error curves are the results on the round number grid from the optimizations that maximize and minimize the regression function subject to the constraint of Eq. (13).

The fifth plot (regression_fit_with_*nn*pct_bounds_rform*xx*.fig) is titled "Regression fit and bounds at *nn*% confidence interval". The plot shows the experimental data and the regression fit with *nn*% confidence interval. The functional form of the regression equation and the regression coefficients are displayed on the plot.

6.3 Output Text File (Optional)

The user can request that VALMET generate a text file that contains the input and output data. The name of the output text file is provided by the user during the VALMET – user dialog (see Section 5.3). If the user provided a scale factor for any data, the output shown in the output text file has been scaled accordingly.

Some of the tables in the output text file are wide (i.e., they have several columns and contain more than 80 characters). The lines in wide tables may be truncated or "wrapped" when printed.

6.3.1 Output Text File for Interpolation

The contents of the output text file for the interpolation case are explained below. An example of the file is shown in Table A-3. The output text file contains several sections. Most sections start with an appropriate header line and end with a blank line.

The first two sections of the output text file list the experimental data and the computational data.

The validation metrics section lists the following validation metrics and confidence indicators for interpolation, which are also output on the validation metrics screen and explained under Section 6.1.1:

- Avg(abs(y-bar_e))
- Average relative error metric
- Average relative confidence indicator
- Maximum relative error metric
- Confidence interval for maximum relative error metric

The validation metrics section also lists the interpolation options (percent confidence interval, grid type, interpolation type).

The next section gives the results of the VALMET run. The following values are listed in tabular form:

- *x*: the independent variable, from the selected grid (computational, experimental, or round number),
- exp avg: the experimental data, averaged over the selected columns in the original data source,
- exp avg + CI: upper confidence interval for the experimental data,
- exp avg – CI : lower confidence interval for the experimental data,
- comp: the computational data, by interpolation if the grid is not the computational grid,
- est cmp err: estimated computational error (computational – experimental average),
- true ce + CI: true computational error at upper confidence interval bound,
- true ce – CI: true computational error at lower confidence interval bound.

6.3.2 Output Text File for Regression

The contents of the output text file for the regression case are explained below. An example of the file is shown in Table B-3. The output text file contains several sections. Most sections start with an appropriate header line and end with a blank line.

The first two sections list the experimental data and the computational data.

The validation metrics section lists the following validation metrics for regression, which are also output on the validation metrics screen and explained under Section 6.1.2:

- Avg(abs(yregression))
- Average relative error metric
- Average relative confidence indicator
- Maximum relative error metric
- Confidence interval for maximum relative error metric

The validation metrics section also lists the percent confidence interval and sum-squared error. The sum-squared error is explained in Section 3.2. The bottom of this section contains the function form of the regression equation, followed by the regression coefficients.

The next section contains a table for output computed at the experimental grid. The table lists the following values:

- xval: values of the experimental independent variable,
- fit(xval): values of the fit at xval,
- fit+CI: values of the upper confidence interval as a function of xval,
- fit–CI: values of the lower confidence interval as a function of xval,

- +CI: upper confidence interval above the fit,
- –CI: lower confidence interval below the fit.

Note that in the regression case it is possible for the confidence bounds to be asymmetric about the fit. This is discussed in Section 2.4.

The next section contains a table for output computed at the computational grid. The table lists the following values:

- xc: values of the computational independent variable,
- vc_fit: the values of the fitted dependent variable (i.e., the regression evaluated at the *x* coordinates of the computational data),
- est error: the estimated computational error (computational value – fitted value).

7. COMMON USER ERRORS AND CODE DEFICIENCIES

Many of the errors and deficiencies discussed here have been mentioned elsewhere in this report. They are summarized here because they might be missed in a cursory reading of the report.

Be aware that VALMET uses fixed names for its output files. Thus, multiple runs of VALMET (and repeated processing within VALMET) may overwrite previous results. The compiled version of VALMET may abort after it issues the message “Warning: Objects of uitools.uimodemanager class exist - not clearing this class or any of its super-classes” if it attempts to overwrite files. This is discussed in Sections 5.3 and 5.4; the output files (and file naming) are discussed in Section 6. To avoid problems, move all existing output files to another area before each VALMET run and before re-processing data within VALMET.

Be aware that the input files cannot contain any text or blank lines after the initial header lines. This is discussed in Section 4. If a blank or text line is found before the end of data in an Excel file, the run will terminate with a “NaN” (Not a Number) diagnostic. Thus, the Excel file cannot contain multiple tables in a single spreadsheet or have additional calculations after the desired table. A blank or text line in a text file will not signal an error, but any following data will be ignored.

To exit the program early, use the “X” in the upper-right corner of the input window or type ctrl-C in the MATLAB command window.

The VALMET – user dialog described in Section 5.3 is not very robust. If an incorrect entry is made, an error may result. The user cannot go back to modify incorrect entries. The “Cancel” box available in a dialog box should not be used; it may cause an error.
When VALMET requests the confidence interval during the VALMET – user dialog, be careful to enter it as a percent value rather than as a fraction (i.e., enter 90 instead of 0.90). The program accepts any confidence interval between 0 and 100 (exclusive), but values outside the range 50 to 99.99 percent have not been tested.

When running the compiled version of VALMET, the error message “The dynamic link library mclmcrrt74.dll could not be found in the specified path” or a similar message about missing dll’s indicates a problem with the PATH environmental variable. See the installation instructions (Section 8.3) for directions on how to correct the problem.

Messages of the form

“Attempted to access xe(0): index must be a positive or logical.”

or

“Attempted to access xe(100); index out of bounds because numel(xe)=99.”

indicate that the ranges of the experimental and computational coordinates do not overlap. This could be caused by selecting the wrong column for the coordinate data or by applying an incorrect scale factor.

Legends are positioned automatically to try to avoid overwriting curves and data. However, any additional text, such as regression coefficients, is placed in fixed positions and may be put on top of curves or data. Note that these plot features may be repositioned using features of the MATLAB program.

Occasionally there are some jagged regions in the output for error bound and/or confidence limit curves. This is caused by improper convergence of the numerical solution of the optimization problem that is solved for these quantities. In our testing of VALMET we have found that the most troublesome case is using Form 13 in the regression option – the pulse function.

8. INSTALLATION INSTRUCTIONS

8.1 System Requirements

There are two versions of VALMET that are available: a) the MATLAB version that requires the user to have a MATLAB software license, and b) the compiled version that does not require any MATLAB software. Both versions of VALMET can be executed on a Windows 2000/XP operating system.

8.2 Installation Instructions for MATLAB Version

The MATLAB version of VALMET requires the following:

- The standard MATLAB package (version 7.2 or later).
- The Statistics Toolbox (version 5.2 or later).
- The Optimization Toolbox (version 3.0.2 or later) if regression is to be used instead of interpolation.

It is likely that the program will work with earlier versions of the MATLAB package and toolboxes, but it has not been tested with them.

The MATLAB version of VALMET is provided in a Winzip file. Simply unzip the files into an appropriate directory.

8.3 Installation Instructions for the Compiled Version

The compiled version of VALMET consists of two files, valmet.exe and valmet.ctf. Place both files in an appropriate directory. However, the user must also load and run the program MCRInstaller.exe. MCRInstaller.exe stores all necessary MATLAB routines and libraries on a computer that does not have MATLAB on it.

You may need administrator privilege to run MCRInstaller.exe on Windows 2000/XP systems. VALMET has not been tested with Windows Vista. This installation process will generate needed libraries and add the location of these libraries to the PATH environment variable. To keep the path string from becoming too long, it is suggested that the libraries be installed in the directory where valmet.exe resides. The installer adds a folder “v76”, which contains thousands of files in hundreds of folders.

If the error message “The dynamic link library mclmcrrt74.dll could not be found in the specified path” or a similar message about missing dll’s appears when valmet.exe is run, the PATH environment variable is either too long or is missing the path to the dll’s. If PATH is too long, shorten the path by removing, at least temporarily, some directories that are not needed. If the path to the dll’s (it usually ends in \win32) is missing, locate the dll’s and add their directory to PATH.

8.4 Support

The VALMET code is available from:

Harold Iuzzolino, hjiuzzo@sandia.gov, 505-998-0048,

Matthew Barone, mbarone@sandia.gov, 505-844-4523, or

William Oberkampf, wloberk@sandia.gov, 505-844-3799.

To report bugs or request assistance on the code, contact the above.

9. REFERENCES

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APPENDIX A: INTERPOLATION EXAMPLE – TURBULENT BUOYANT PLUME

Section 5.3 of Oberkampf and Barone [1] describes an example using their validation metric, for the interpolation case, applied to a vertical turbulent buoyant plume of helium. This appendix contains the VALMET input files, the VALMET – user dialog, and the VALMET output for this interpolation example.

The experimental data for this example consists of four sets of experimental measurements of time-averaged vertical velocity along the centerline of the jet as a function of axial distance from the exit of the helium jet. The VALMET output given here is very close to that described in Oberkampf and Barone [1], but it may not be identical due to slight differences in the input data.

A.1 Input Files for Interpolation Example

The experimental data file, *helium_exp_data.txt*, shown in Table A-1 has five columns of data: the independent variable (distance) and four columns of velocity measurements.

The computational data file, *helium_comp_data.txt*, shown in Table A-2 has two columns, with the independent variable (distance) in the first column.

The input files listed below are in text format, and the VALMET – user dialog refers to these text files. The installation package includes the input files in both formats for the user's convenience; i.e., a text file and an Excel file. See Section 4 for more information on the format of a VALMET input file.

Table A-1. Text experimental data file *helium_exp_data.txt*.

```
distance,test25,test29,test32,test36
0.01910,0.2180,0.2170,0.2730,0.1250
0.02860,0.2280,0.2200,0.3100,0.2060
0.03820,0.2930,0.3000,0.3360,0.2270
0.04770,0.3480,0.3410,0.3650,0.3180
0.05720,0.3770,0.3870,0.3980,0.3390
0.06680,0.4000,0.4390,0.4430,0.3770
0.07630,0.4170,0.5050,0.5380,0.4270
0.08590,0.4450,0.5800,0.6860,0.4750
0.09540,0.5040,0.6470,0.7480,0.5390
0.10500,0.5870,0.7180,0.8120,0.6120
0.11400,0.6720,0.8020,0.8870,0.6880
0.12400,0.7630,0.8810,0.9620,0.7550
0.13400,0.8550,0.9740,1.0300,0.8170
0.14300,0.9330,1.0800,1.1100,0.8830
0.15300,1.0100,1.1900,1.1900,0.9720
0.16200,1.1000,1.3000,1.2700,1.0700
0.17200,1.2000,1.3900,1.3500,1.1700
0.18100,1.3000,1.4700,1.4400,1.2500
0.19100,1.3900,1.5600,1.5100,1.3300
```

```
0.20000,1.4800,1.6600,1.5800,1.4100
0.21000,1.5600,1.7400,1.6800,1.4900
0.21900,1.6500,1.8100,1.7500,1.5500
0.22900,1.7300,1.8900,1.8300,1.6200
0.23900,1.7900,1.9800,1.8900,1.7000
0.24800,1.8500,2.0600,1.9600,1.7600
0.25800,1.9100,2.1300,2.0300,1.8100
0.26700,1.9700,2.1900,2.0900,1.8600
0.27700,2.0200,2.2400,2.1600,1.9100
0.28600,2.0700,2.2900,2.2300,1.9600
0.29600,2.1100,2.3300,2.3000,2.0100
0.30500,2.1600,2.3800,2.3400,2.0600
0.31500,2.2100,2.4400,2.3800,2.1100
0.32400,2.2500,2.4900,2.4300,2.1500
0.33400,2.3000,2.5400,2.4900,2.2000
0.34300,2.3200,2.5800,2.5400,2.2400
0.35300,2.3500,2.6200,2.5900,2.2700
0.36300,2.3800,2.6500,2.6300,2.3200
0.37200,2.4000,2.6800,2.6700,2.3600
0.38200,2.4300,2.7100,2.7100,2.3800
0.39100,2.4600,2.7400,2.7500,2.4100
0.40100,2.5000,2.7600,2.7900,2.4400
0.41000,2.5200,2.7800,2.8300,2.4700
0.42000,2.5500,2.8000,2.8800,2.5100
0.42900,2.5800,2.8200,2.9200,2.5400
0.43900,2.6000,2.8300,2.9500,2.5600
0.44800,2.6300,2.8400,2.9500,2.5900
0.45800,2.6500,2.8500,2.9600,2.6100
0.46800,2.6600,2.8700,2.9900,2.6400
0.47700,2.6800,2.8800,3.0300,2.6700
0.48700,2.7000,2.8700,3.0300,2.7000
0.49600,2.7100,2.8900,3.0400,2.7100
0.50600,2.7200,2.8800,3.0700,2.7300
0.51500,2.7300,2.8700,3.0900,2.7600
0.52500,2.7400,2.8600,3.1000,2.7800
0.53400,2.7600,2.8700,3.1000,2.8000
0.54400,2.7800,2.8800,3.1000,2.8100
0.55300,2.8000,2.9000,3.1300,2.8100
0.56300,2.8000,2.9000,3.1600,2.8200
0.57200,2.8000,2.9000,3.1800,2.8400
0.58200,2.8100,2.9000,3.1700,2.8600
0.59200,2.8300,2.9000,3.1800,2.8800
0.60100,2.8500,2.9000,3.2000,2.8900
0.61100,2.8400,2.9000,3.2100,2.8900
0.62000,2.8500,2.9100,3.2200,2.9000
0.63000,2.8700,2.9200,3.2300,2.9300
0.63900,2.8800,2.9200,3.2500,2.9500
0.64900,2.8900,2.9300,3.2600,2.9600
0.65800,2.8900,2.9200,3.2500,2.9700
0.66800,2.8900,2.9000,3.2700,2.9900
0.67700,2.9000,2.8900,3.2900,3.0000
0.68700,2.8900,2.8700,3.3100,3.0200
0.69600,2.8600,2.8600,3.3300,3.0500
0.70600,2.8500,2.8600,3.3300,3.0600
0.71600,2.8400,2.8700,3.3400,3.0700
0.72500,2.8400,2.8700,3.3500,3.0700
0.73500,2.8200,2.8500,3.3600,3.0800
```

```
0.74400,2.8100,2.8400,3.3500,3.0800
0.75400,2.7900,2.8300,3.3500,3.0900
0.76300,2.8000,2.8300,3.3600,3.0900
```

Table A-2. Text computational data file *helium_comp_data.txt*.

```
axial distance (m)  TFNS solution (m/s)
0.010500  0.32489
0.021021  0.25350
0.031542  0.19927
0.042063  0.17202
0.052583  0.16736
0.063104  0.18068
0.073625  0.20747
0.084146  0.24543
0.094667  0.30602
0.10519  0.38006
0.11571  0.45638
0.12623  0.53797
0.13675  0.63034
0.14727  0.73401
0.15779  0.84443
0.16831  0.95630
0.17883  1.0687
0.18935  1.1811
0.19987  1.2871
0.21040  1.3873
0.22092  1.4805
0.23144  1.5687
0.24196  1.6548
0.25248  1.7395
0.26300  1.8231
0.27352  1.9039
0.28404  1.9816
0.29456  2.0567
0.30508  2.1295
0.31560  2.2000
0.32612  2.2678
0.33665  2.3315
0.34717  2.3905
0.35769  2.4442
0.36821  2.4923
0.37873  2.5349
0.38925  2.5721
0.39977  2.6053
0.41029  2.6358
0.42081  2.6633
0.43133  2.6880
0.44185  2.7101
0.45237  2.7303
0.46290  2.7490
0.47342  2.7670
0.48394  2.7844
0.49446  2.8009
0.50498  2.8166
```

```
0.51550  2.8311
0.52602  2.8447
0.53654  2.8580
0.54706  2.8710
0.55758  2.8845
0.56810  2.8986
0.57862  2.9134
0.58915  2.9282
0.59967  2.9427
0.61019  2.9565
0.62071  2.9698
0.63123  2.9819
0.64175  2.9925
0.65227  3.0016
0.66279  3.0094
0.67331  3.0157
0.68383  3.0203
0.69435  3.0233
0.70488  3.0247
0.71540  3.0250
0.72592  3.0242
0.73644  3.0225
0.74696  3.0202
0.75748  3.0173
0.76800  3.0142
```

A.2 VALMET – User Dialog for Interpolation Example

This section gives the appropriate responses to the VALMET prompts needed to run the interpolation example. Most responses are enclosed in quotes; the quotes should not be typed as part of the response. For more information on the VALMET – user dialog, see Sections 6.2 and 5.3.

Output File Options

Do you want a text output file with experimental, computational, and CI data?

Click "Yes", then NEXT.

Enter a name for the output text data file:

Enter "helium_output.txt", then click OK.

Do you want the date and time appended to the plots and text output file?

Click "Yes".

Experimental Data File Options

Are the EXPERIMENTAL data in one file or multiple files?

Click "All data in one file".

Are your EXPERIMENTAL data in an Excel file or a text file?

Click "Text: .txt or .dat".

Browse for the experimental data file *helium_exp_data.txt*.

Browse to the folder where the data file resides, click on file *helium_exp_data.txt*, and click OPEN. The first eight lines of file *helium_exp_data.txt* are displayed. Figure A-1 shows a screen shot of the file display. The next few questions deal with file *helium_exp_data.txt* shown in Table A-1.

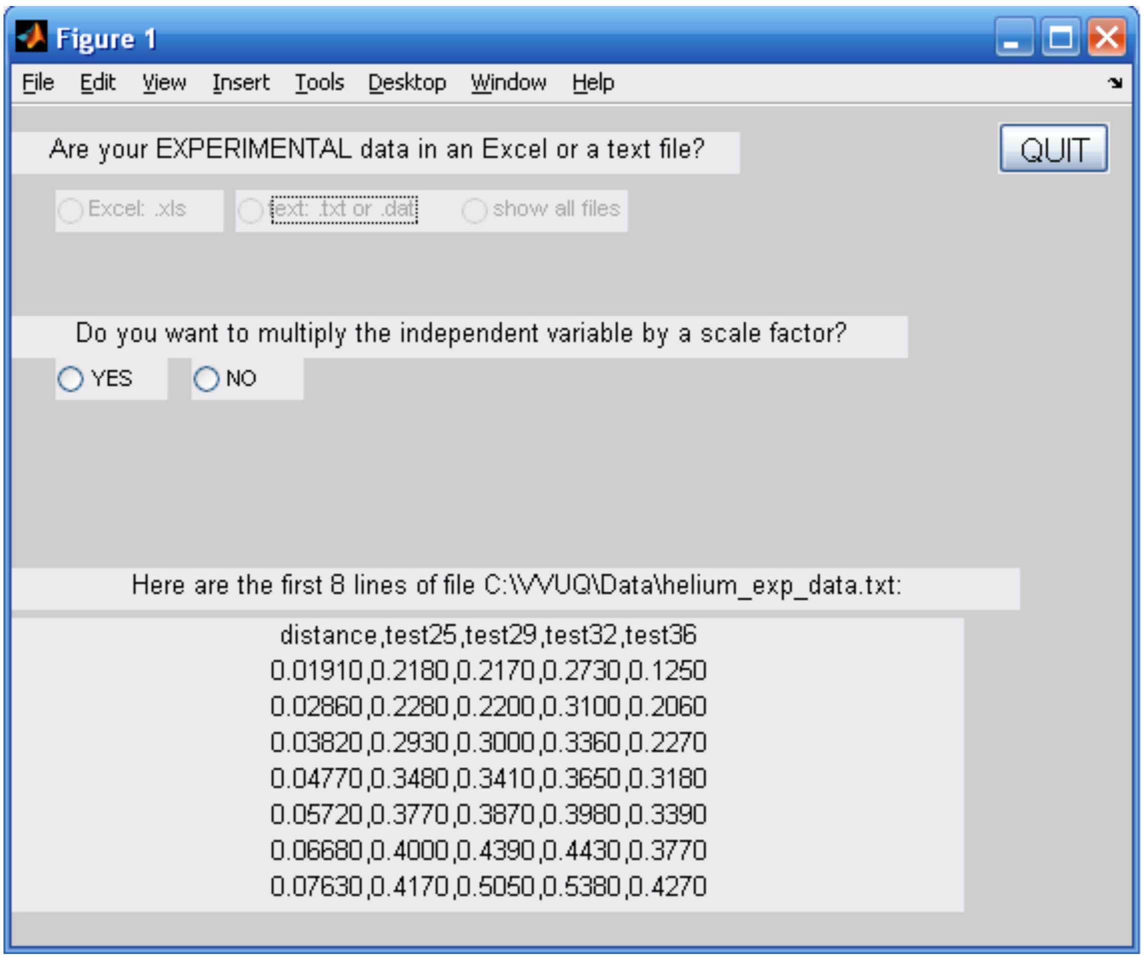

Figure A-1. Screen shot of experimental data query.

How many header lines precede the data?

Enter “1”.

What delimiter character separates the numeric data?

Enter a comma (“,”).

How many columns (total) are there in the file?

Enter “5”.

Which column is the independent variable?

Enter “1”.

Do you want to multiply the independent variable by a scale factor?

Click “No”.

Enter a caption with (units) for the independent variable:

Enter “Distance (m)”; remember to omit the quotes.

Do you want to multiply the measured variable by a scale factor?

Click “No”.

Enter a caption with (units) for the measured variable:

Enter “Vertical velocity (m/s)”.

Select the column number(s) of the EXPERIMENTAL data (averaged if two or more)

Click the buttons for column “2”, “3”, “4”, and “5”.

Computational Data File Options

Are your COMPUTATIONAL data in an Excel file or a text file?

Click “Text: .txt or .dat”.

Browse for the computational data file *helium_comp_data.txt*.

Browse to the folder where the data file resides, click on file *helium_comp_data.txt*, and click OPEN. The first eight lines of file *helium_comp_data.txt* are displayed. The next few questions deal with the file *helium_comp_data.txt* shown in Table A-2.

How many header lines precede the data?

Enter “1”.

What delimiter character separates the numeric data?

Enter a blank (i.e., press the space bar, then click OK).

How many columns (total) are there in the file?

Enter “2”.

Which column is the independent variable?

Enter “1”.

Do you want to multiply the independent variable by a scale factor?

Click “No”.

Do you want to multiply the computed variable by a scale factor?

Click “No”.

The computed data is assumed to be in column 2 since there are only two columns of data and the independent variable is in column 1.

Processing Options

What % confidence interval do you want (50 to 99.99)?

Enter “90”.

Do you want to use interpolation or regression on the data?

Click “Interpolation”.

Which interpolation grid do you want to use?

Click “Round number”.

Set round number spacing parameters.

Figure A-2 shows a screen shot with these parameters and the query. Click DONE.

What interpolation method do you want to use?

Click “Spline”.

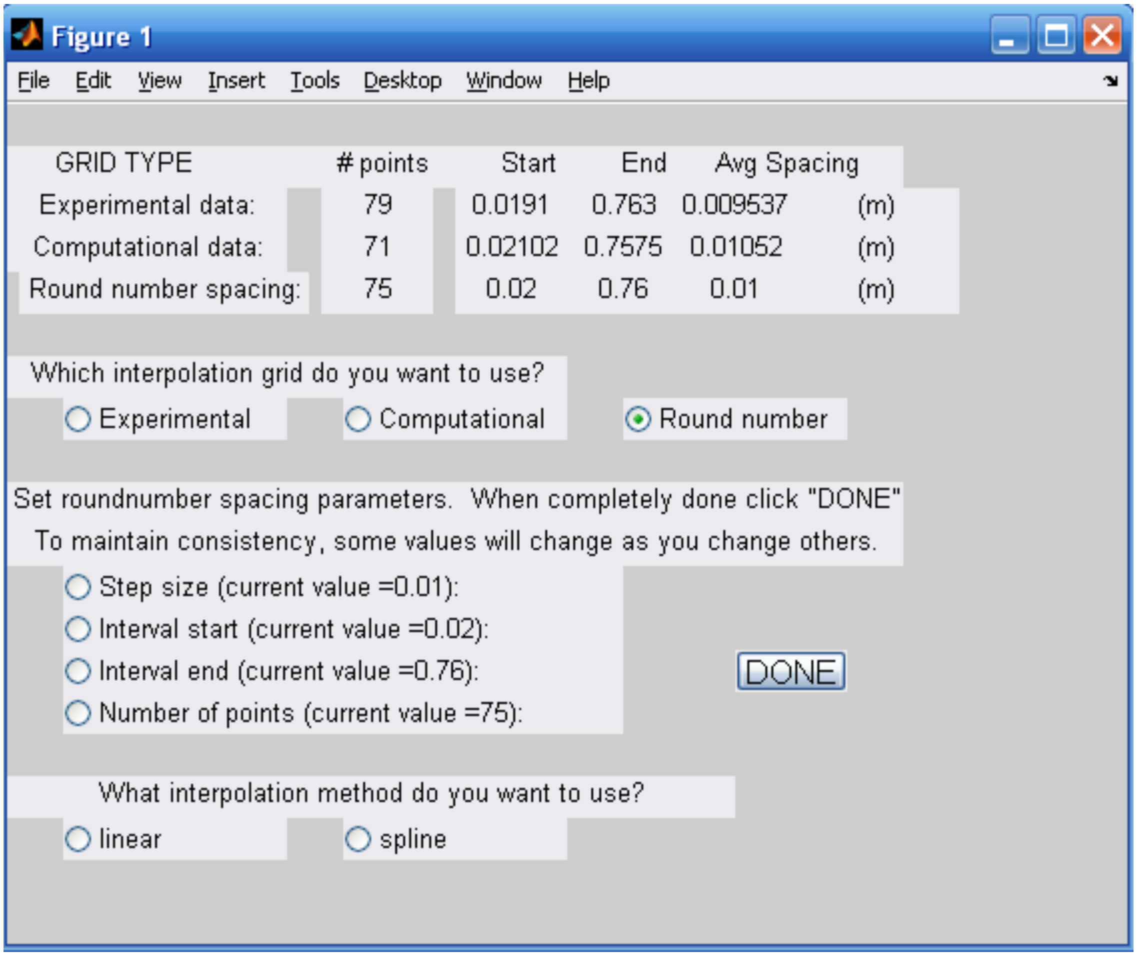

Figure A-2. Screen shot of grid parameters query.

Processing

VALMET performs the requested calculation. No warning (blue) or fatal (red) messages should appear. If such messages appear, either the user has not responded to the queries correctly or the program or data files have been corrupted.

After a few seconds pause, the validation metrics screen and the plots will appear. The plots are stacked on top of each other, but the plots can be moved on the screen or minimized to the task bar using the “-” icon.

The following query appears in the input window.

Do you want to process the same data again?

Click “No”.

A.3 Output for Interpolation Example

The VALMET output for the interpolation example is presented in this section. The validation metrics screen, the four plots, and the output text file are shown along with a brief discussion of each. Oberkampf and Barone [1] contains very similar plots; it includes a more thorough discussion of the information that can be gleaned from them.

Figure A-3 shows the two global validation metrics and their associated confidence indicators. This screen is in more detail in Section 6.1.1. Note that the values on this screen are reflected in the output plots.

The screen shown in Figure A-3 is stored in file globalmetrics_for_interp_90pct.fig.

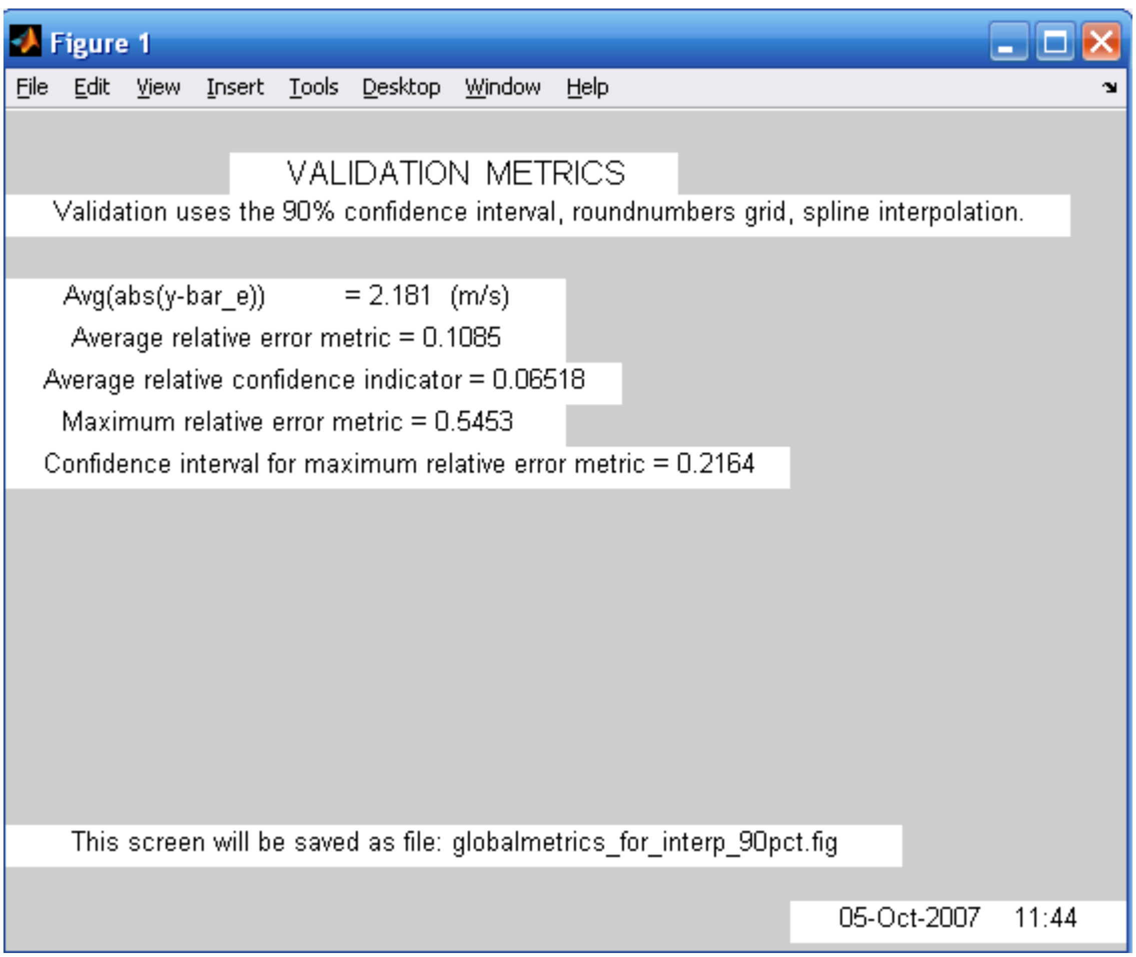

Figure A-3. Validation metrics screen (interpolation).

Figure A-4 is very similar to Figure 5 in Oberkampf and Barone [1]. The plot shows the data from the experimental data file. The dependent variable (velocity) is plotted versus the independent variable (distance) for each of the four selected columns of data.

The Figure A-4 plot is stored in file experimental_data.fig.

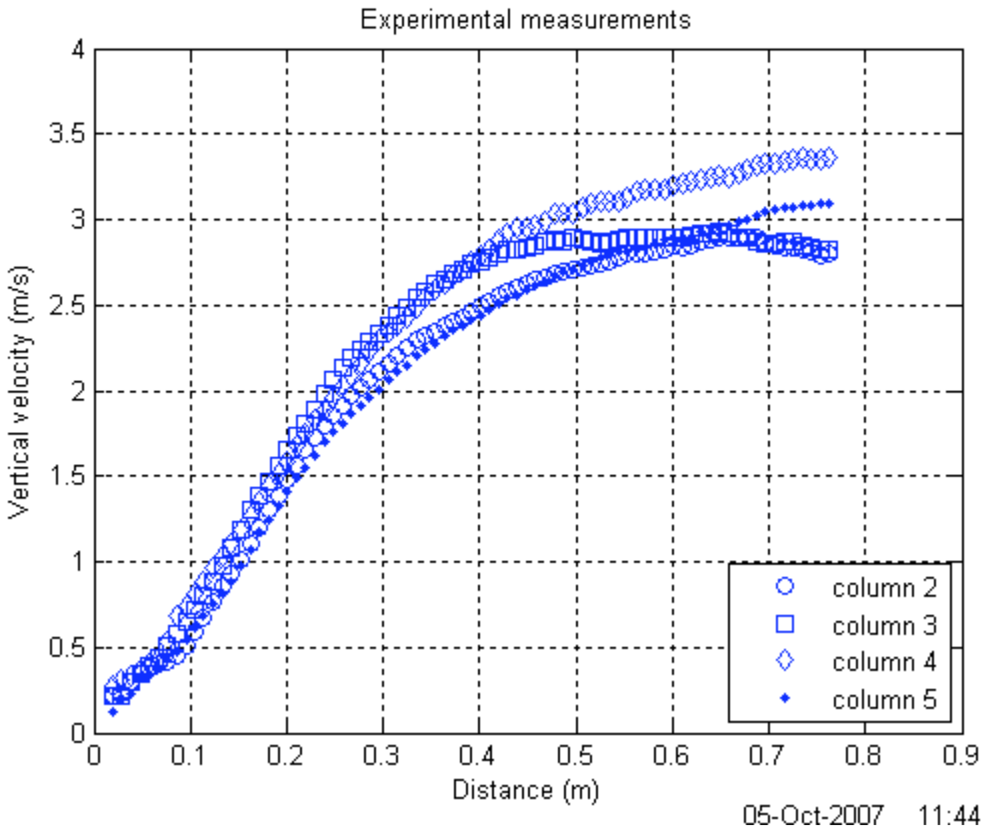

Figure A-4. Plot of experimental data (interpolation).

Figure A-5 is very similar to Figure 6 in Oberkampf and Barone [1]. The plot shows the sample mean of the measurements, $\bar{y}_e(x)$, calculated from the experimental data (Figure A-4). It also shows the interval around the estimated mean in which the true mean will occur with 90% confidence, calculated from the interpolated function for the experimental sample mean and the confidence interval for the true mean. The computational solution (from the computational data file) is also shown.

The Figure A-5 plot is stored in file comp_and_exp_mean_with_90pct_ci.fig.

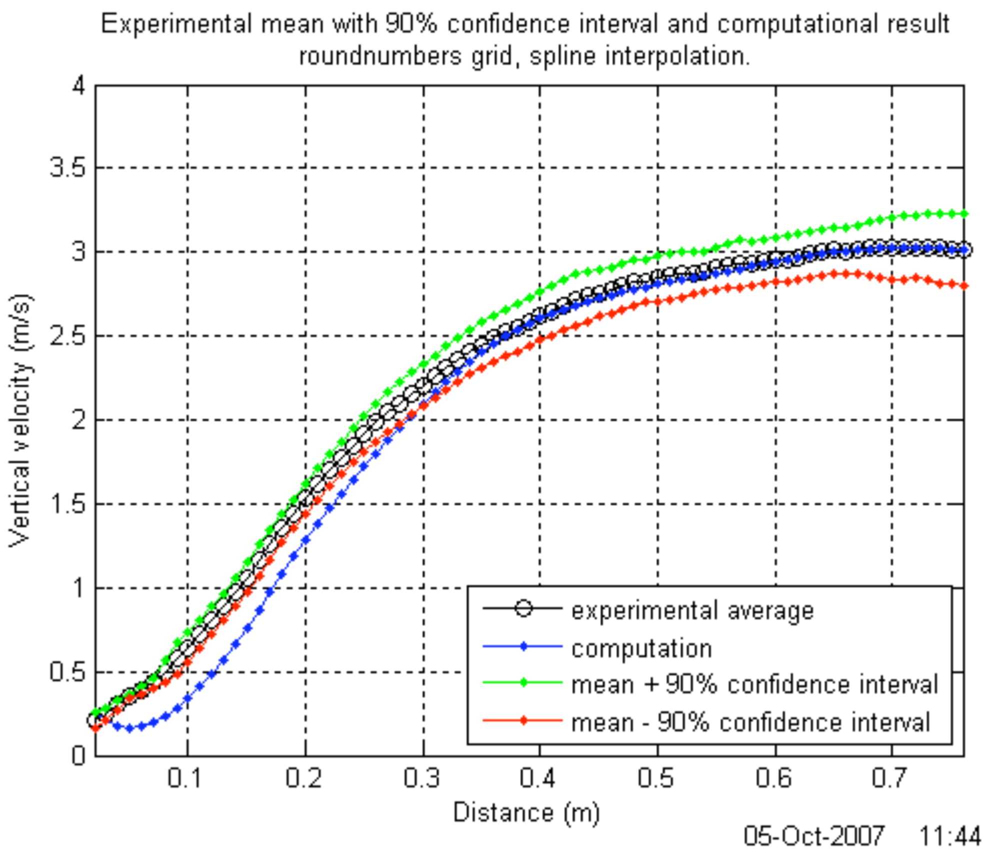

Figure A-5. Plot of experimental mean with 90% CI and computational result (interpolation).

Figure A-6 is very similar to Figure 7 in Oberkampf and Barone [1]. It shows the estimated error between computational results and mean experimental results, $\tilde{E}(x) = y_m(x) - \bar{y}_e(x)$, along with the 90% confidence interval from the experiment. These results are computed using Eqs. (2) – (4).

This plot allows the level of disagreement between computational and experimental results to be more critically examined. Oberkampf and Barone [1] discuss how this type of plot provides a magnifying glass, as it were, to both the error in the computational model and the uncertainty in the experimental data. The validation metric result shown in the plot can be quantitatively summarized or condensed using the validation metrics displayed in Figure A-3.

The Figure A-6 plot is stored in file est_error_with_90plus_minus_ci_del.

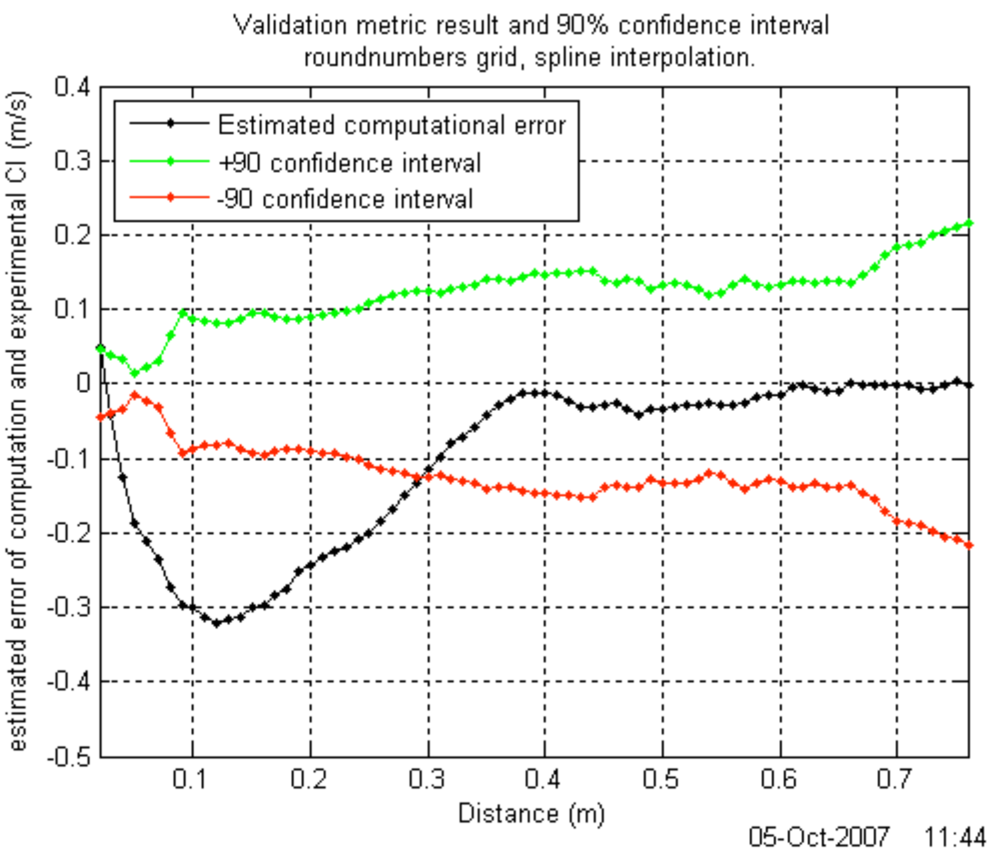

Figure A-6. Plot of validation metric result and 90% CI (interpolation).

Figure A-7 is very similar to Figure 8 in Oberkampf and Barone [1]. The final method of displaying the results of the validation metric is to plot the 90% confidence interval of the true error in velocity predicted by the computational model as a function of the axial distance from the exit of the jet. The true error is approximated by the estimated error, and the confidence interval is calculated using Eq. (16).

Although Figure A-7 displays essentially the same data as shown in Figure A-6, Oberkampf and Barone [1] explains how Figure A-7 allows us to consider slightly different perspectives for assessing the model.

The Figure A-7 plot is stored in file est_error_with_90pct_bounds.fig.

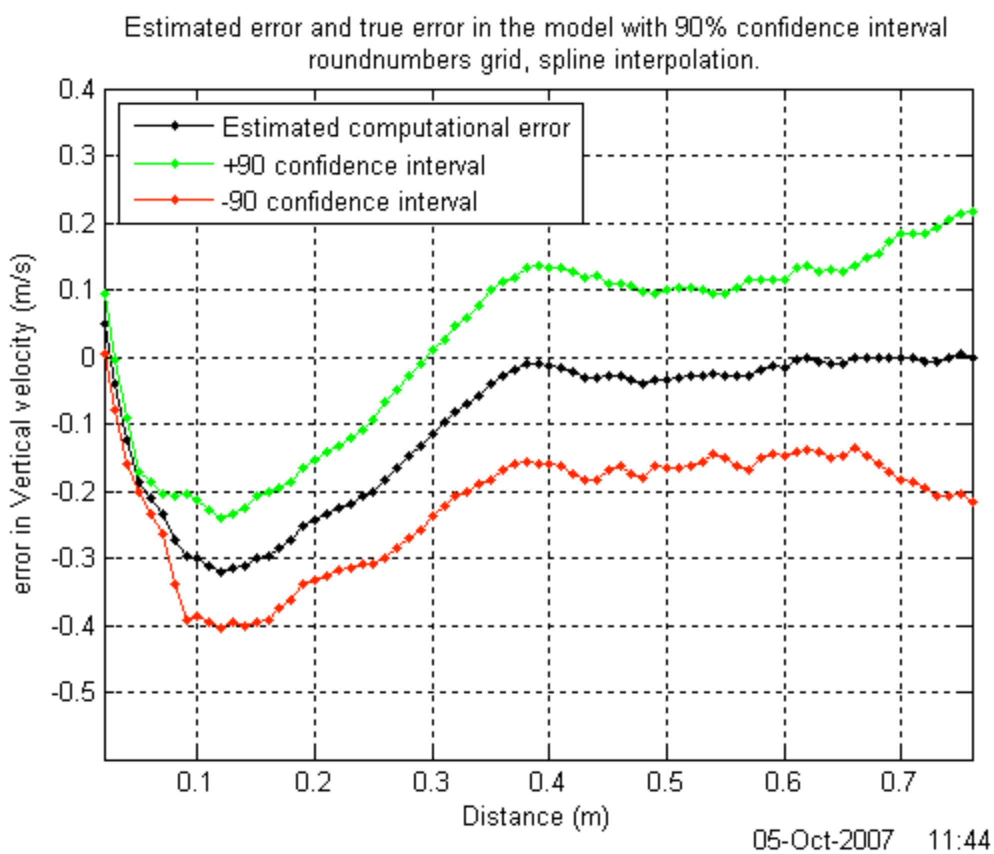

Figure A-7. Plot of estimated error and true error with 90% CI (interpolation).

Table A-3 contains a listing of the optional output text file. It contains the experimental data, the computational data, the verification metrics and confidence indicators (as displayed in the validation metrics screen shown in Figure A-3), and a table of results from the VALMET run. The contents of this file are discussed in more detail in Section 6.3.1.

Note that most of the tables in the output text file are preceded by a line with two numbers: the number of columns in the table minus 1, and the number of rows of data in the table (not including the header line).

Table A-3. Output text file *helium_output.txt* (interpolation).

```
05-Oct-2007    11:44
experimental data
Distance (m)
Vertical velocity (m/s)
   4   79
     xe         col_2         col_3         col_4         col_5
  1.910e-002  2.180e-001  2.170e-001  2.730e-001  1.250e-001
  2.860e-002  2.280e-001  2.200e-001  3.100e-001  2.060e-001
  3.820e-002  2.930e-001  3.000e-001  3.360e-001  2.270e-001
  4.770e-002  3.480e-001  3.410e-001  3.650e-001  3.180e-001
  5.720e-002  3.770e-001  3.870e-001  3.980e-001  3.390e-001
  6.680e-002  4.000e-001  4.390e-001  4.430e-001  3.770e-001
  7.630e-002  4.170e-001  5.050e-001  5.380e-001  4.270e-001
  8.590e-002  4.450e-001  5.800e-001  6.860e-001  4.750e-001
  9.540e-002  5.040e-001  6.470e-001  7.480e-001  5.390e-001
  1.050e-001  5.870e-001  7.180e-001  8.120e-001  6.120e-001
  1.140e-001  6.720e-001  8.020e-001  8.870e-001  6.880e-001
  1.240e-001  7.630e-001  8.810e-001  9.620e-001  7.550e-001
  1.340e-001  8.550e-001  9.740e-001  1.030e+000  8.170e-001
  1.430e-001  9.330e-001  1.080e+000  1.110e+000  8.830e-001
  1.530e-001  1.010e+000  1.190e+000  1.190e+000  9.720e-001
  1.620e-001  1.100e+000  1.300e+000  1.270e+000  1.070e+000
  1.720e-001  1.200e+000  1.390e+000  1.350e+000  1.170e+000
  1.810e-001  1.300e+000  1.470e+000  1.440e+000  1.250e+000
  1.910e-001  1.390e+000  1.560e+000  1.510e+000  1.330e+000
  2.000e-001  1.480e+000  1.660e+000  1.580e+000  1.410e+000
  2.100e-001  1.560e+000  1.740e+000  1.680e+000  1.490e+000
  2.190e-001  1.650e+000  1.810e+000  1.750e+000  1.550e+000
  2.290e-001  1.730e+000  1.890e+000  1.830e+000  1.620e+000
  2.390e-001  1.790e+000  1.980e+000  1.890e+000  1.700e+000
  2.480e-001  1.850e+000  2.060e+000  1.960e+000  1.760e+000
  2.580e-001  1.910e+000  2.130e+000  2.030e+000  1.810e+000
  2.670e-001  1.970e+000  2.190e+000  2.090e+000  1.860e+000
  2.770e-001  2.020e+000  2.240e+000  2.160e+000  1.910e+000
  2.860e-001  2.070e+000  2.290e+000  2.230e+000  1.960e+000
  2.960e-001  2.110e+000  2.330e+000  2.300e+000  2.010e+000
  3.050e-001  2.160e+000  2.380e+000  2.340e+000  2.060e+000
  3.150e-001  2.210e+000  2.440e+000  2.380e+000  2.110e+000
  3.240e-001  2.250e+000  2.490e+000  2.430e+000  2.150e+000
  3.340e-001  2.300e+000  2.540e+000  2.490e+000  2.200e+000
  3.430e-001  2.320e+000  2.580e+000  2.540e+000  2.240e+000
  3.530e-001  2.350e+000  2.620e+000  2.590e+000  2.270e+000
  3.630e-001  2.380e+000  2.650e+000  2.630e+000  2.320e+000
  3.720e-001  2.400e+000  2.680e+000  2.670e+000  2.360e+000
  3.820e-001  2.430e+000  2.710e+000  2.710e+000  2.380e+000
  3.910e-001  2.460e+000  2.740e+000  2.750e+000  2.410e+000
  4.010e-001  2.500e+000  2.760e+000  2.790e+000  2.440e+000
  4.100e-001  2.520e+000  2.780e+000  2.830e+000  2.470e+000
  4.200e-001  2.550e+000  2.800e+000  2.880e+000  2.510e+000
  4.290e-001  2.580e+000  2.820e+000  2.920e+000  2.540e+000
  4.390e-001  2.600e+000  2.830e+000  2.950e+000  2.560e+000
  4.480e-001  2.630e+000  2.840e+000  2.950e+000  2.590e+000
  4.580e-001  2.650e+000  2.850e+000  2.960e+000  2.610e+000
```

4.680e-001	2.660e+000	2.870e+000	2.990e+000	2.640e+000
4.770e-001	2.680e+000	2.880e+000	3.030e+000	2.670e+000
4.870e-001	2.700e+000	2.870e+000	3.030e+000	2.700e+000
4.960e-001	2.710e+000	2.890e+000	3.040e+000	2.710e+000
5.060e-001	2.720e+000	2.880e+000	3.070e+000	2.730e+000
5.150e-001	2.730e+000	2.870e+000	3.090e+000	2.760e+000
5.250e-001	2.740e+000	2.860e+000	3.100e+000	2.780e+000
5.340e-001	2.760e+000	2.870e+000	3.100e+000	2.800e+000
5.440e-001	2.780e+000	2.880e+000	3.100e+000	2.810e+000
5.530e-001	2.800e+000	2.900e+000	3.130e+000	2.810e+000
5.630e-001	2.800e+000	2.900e+000	3.160e+000	2.820e+000
5.720e-001	2.800e+000	2.900e+000	3.180e+000	2.840e+000
5.820e-001	2.810e+000	2.900e+000	3.170e+000	2.860e+000
5.920e-001	2.830e+000	2.900e+000	3.180e+000	2.880e+000
6.010e-001	2.850e+000	2.900e+000	3.200e+000	2.890e+000
6.110e-001	2.840e+000	2.900e+000	3.210e+000	2.890e+000
6.200e-001	2.850e+000	2.910e+000	3.220e+000	2.900e+000
6.300e-001	2.870e+000	2.920e+000	3.230e+000	2.930e+000
6.390e-001	2.880e+000	2.920e+000	3.250e+000	2.950e+000
6.490e-001	2.890e+000	2.930e+000	3.260e+000	2.960e+000
6.580e-001	2.890e+000	2.920e+000	3.250e+000	2.970e+000
6.680e-001	2.890e+000	2.900e+000	3.270e+000	2.990e+000
6.770e-001	2.900e+000	2.890e+000	3.290e+000	3.000e+000
6.870e-001	2.890e+000	2.870e+000	3.310e+000	3.020e+000
6.960e-001	2.860e+000	2.860e+000	3.330e+000	3.050e+000
7.060e-001	2.850e+000	2.860e+000	3.330e+000	3.060e+000
7.160e-001	2.840e+000	2.870e+000	3.340e+000	3.070e+000
7.250e-001	2.840e+000	2.870e+000	3.350e+000	3.070e+000
7.350e-001	2.820e+000	2.850e+000	3.360e+000	3.080e+000
7.440e-001	2.810e+000	2.840e+000	3.350e+000	3.080e+000
7.540e-001	2.790e+000	2.830e+000	3.350e+000	3.090e+000
7.630e-001	2.800e+000	2.830e+000	3.360e+000	3.090e+000

computational data
Distance (m)
Vertical velocity (m/s)
1 73

xc	col_2
1.050e-002	3.249e-001
2.102e-002	2.535e-001
3.154e-002	1.993e-001
4.206e-002	1.720e-001
5.258e-002	1.674e-001
6.310e-002	1.807e-001
7.362e-002	2.075e-001
8.415e-002	2.454e-001
9.467e-002	3.060e-001
1.052e-001	3.801e-001
1.157e-001	4.564e-001
1.262e-001	5.380e-001
1.368e-001	6.303e-001
1.473e-001	7.340e-001
1.578e-001	8.444e-001
1.683e-001	9.563e-001
1.788e-001	1.069e+000
1.893e-001	1.181e+000
1.999e-001	1.287e+000
2.104e-001	1.387e+000
2.209e-001	1.480e+000
2.314e-001	1.569e+000
2.420e-001	1.655e+000
2.525e-001	1.740e+000
2.630e-001	1.823e+000
2.735e-001	1.904e+000
2.840e-001	1.982e+000
2.946e-001	2.057e+000
3.051e-001	2.130e+000
3.156e-001	2.200e+000
3.261e-001	2.268e+000
3.367e-001	2.332e+000
3.472e-001	2.390e+000

3.577e-001	2.444e+000
3.682e-001	2.492e+000
3.787e-001	2.535e+000
3.892e-001	2.572e+000
3.998e-001	2.605e+000
4.103e-001	2.636e+000
4.208e-001	2.663e+000
4.313e-001	2.688e+000
4.419e-001	2.710e+000
4.524e-001	2.730e+000
4.629e-001	2.749e+000
4.734e-001	2.767e+000
4.839e-001	2.784e+000
4.945e-001	2.801e+000
5.050e-001	2.817e+000
5.155e-001	2.831e+000
5.260e-001	2.845e+000
5.365e-001	2.858e+000
5.471e-001	2.871e+000
5.576e-001	2.885e+000
5.681e-001	2.899e+000
5.786e-001	2.913e+000
5.891e-001	2.928e+000
5.997e-001	2.943e+000
6.102e-001	2.957e+000
6.207e-001	2.970e+000
6.312e-001	2.982e+000
6.418e-001	2.993e+000
6.523e-001	3.002e+000
6.628e-001	3.009e+000
6.733e-001	3.016e+000
6.838e-001	3.020e+000
6.944e-001	3.023e+000
7.049e-001	3.025e+000
7.154e-001	3.025e+000
7.259e-001	3.024e+000
7.364e-001	3.023e+000
7.470e-001	3.020e+000
7.575e-001	3.017e+000
7.680e-001	3.014e+000

validation metrics
90 percent confidence interval
2.181e+000 Avg(abs(y-bar_e))
1.085e-001 Average relative error metric
6.518e-002 Average relative confidence indicator
5.453e-001 Maximum relative error metric
2.164e-001 Confidence interval for maximum relative error metric
roundnumbers grid, spline interpolation

7 75

x	exp avg	exp avg +CI	exp avg -CI	comp	est cmp err	true ce+CI	true ce-CI
2.000e-002	2.108e-001	2.564e-001	1.652e-001	2.599e-001	4.913e-002	9.473e-002	3.530e-003
3.000e-002	2.470e-001	2.850e-001	2.091e-001	2.056e-001	-4.141e-002	-3.457e-003	-7.937e-002
4.000e-002	2.997e-001	3.339e-001	2.655e-001	1.754e-001	-1.244e-001	-9.017e-002	-1.585e-001
5.000e-002	3.524e-001	3.671e-001	3.377e-001	1.667e-001	-1.857e-001	-1.710e-001	-2.004e-001
6.000e-002	3.851e-001	4.080e-001	3.621e-001	1.751e-001	-2.100e-001	-1.870e-001	-2.329e-001
7.000e-002	4.316e-001	4.618e-001	4.014e-001	1.972e-001	-2.344e-001	-2.042e-001	-2.646e-001
8.000e-002	5.002e-001	5.659e-001	4.346e-001	2.283e-001	-2.720e-001	-2.063e-001	-3.376e-001
9.000e-002	5.746e-001	6.688e-001	4.803e-001	2.766e-001	-2.980e-001	-2.037e-001	-3.922e-001
1.000e-001	6.421e-001	7.292e-001	5.551e-001	3.428e-001	-2.993e-001	-2.123e-001	-3.864e-001
1.100e-001	7.268e-001	8.103e-001	6.433e-001	4.147e-001	-3.121e-001	-2.286e-001	-3.956e-001
1.200e-001	8.103e-001	8.925e-001	7.280e-001	4.886e-001	-3.216e-001	-2.394e-001	-4.039e-001
1.300e-001	8.859e-001	9.663e-001	8.054e-001	5.697e-001	-3.162e-001	-2.357e-001	-3.966e-001
1.400e-001	9.740e-001	1.062e+000	8.865e-001	6.613e-001	-3.127e-001	-2.252e-001	-4.002e-001
1.500e-001	1.062e+000	1.157e+000	9.682e-001	7.623e-001	-3.001e-001	-2.060e-001	-3.943e-001
1.600e-001	1.164e+000	1.260e+000	1.068e+000	8.679e-001	-2.965e-001	-2.004e-001	-3.925e-001
1.700e-001	1.259e+000	1.349e+000	1.169e+000	9.743e-001	-2.846e-001	-1.943e-001	-3.749e-001
1.800e-001	1.356e+000	1.443e+000	1.269e+000	1.081e+000	-2.746e-001	-1.872e-001	-3.619e-001
1.900e-001	1.439e+000	1.526e+000	1.352e+000	1.188e+000	-2.510e-001	-1.644e-001	-3.377e-001
2.000e-001	1.532e+000	1.623e+000	1.442e+000	1.288e+000	-2.441e-001	-1.541e-001	-3.342e-001

2.100e-001	1.617e+000	1.710e+000	1.525e+000	1.384e+000	-2.339e-001	-1.411e-001	-3.266e-001
2.200e-001	1.698e+000	1.792e+000	1.604e+000	1.473e+000	-2.254e-001	-1.315e-001	-3.193e-001
2.300e-001	1.775e+000	1.872e+000	1.678e+000	1.557e+000	-2.180e-001	-1.209e-001	-3.152e-001
2.400e-001	1.848e+000	1.948e+000	1.748e+000	1.639e+000	-2.087e-001	-1.087e-001	-3.087e-001
2.500e-001	1.921e+000	2.029e+000	1.812e+000	1.720e+000	-2.012e-001	-9.259e-002	-3.098e-001
2.600e-001	1.983e+000	2.098e+000	1.868e+000	1.799e+000	-1.834e-001	-6.816e-002	-2.986e-001
2.700e-001	2.044e+000	2.163e+000	1.926e+000	1.877e+000	-1.672e-001	-4.903e-002	-2.853e-001
2.800e-001	2.101e+000	2.222e+000	1.980e+000	1.952e+000	-1.487e-001	-2.761e-002	-2.698e-001
2.900e-001	2.158e+000	2.283e+000	2.034e+000	2.024e+000	-1.340e-001	-9.540e-003	-2.585e-001
3.000e-001	2.208e+000	2.333e+000	2.083e+000	2.095e+000	-1.137e-001	1.121e-002	-2.385e-001
3.100e-001	2.260e+000	2.384e+000	2.137e+000	2.163e+000	-9.771e-002	2.552e-002	-2.209e-001
3.200e-001	2.310e+000	2.437e+000	2.182e+000	2.229e+000	-8.077e-002	4.628e-002	-2.078e-001
3.300e-001	2.362e+000	2.492e+000	2.232e+000	2.292e+000	-7.041e-002	5.969e-002	-2.005e-001
3.400e-001	2.408e+000	2.542e+000	2.275e+000	2.351e+000	-5.755e-002	7.591e-002	-1.910e-001
3.500e-001	2.446e+000	2.588e+000	2.305e+000	2.405e+000	-4.084e-002	1.005e-001	-1.822e-001
3.600e-001	2.484e+000	2.624e+000	2.344e+000	2.455e+000	-2.844e-002	1.115e-001	-1.684e-001
3.700e-001	2.521e+000	2.660e+000	2.381e+000	2.500e+000	-2.089e-002	1.184e-001	-1.602e-001
3.800e-001	2.551e+000	2.695e+000	2.407e+000	2.540e+000	-1.155e-002	1.326e-001	-1.557e-001
3.900e-001	2.586e+000	2.734e+000	2.439e+000	2.575e+000	-1.180e-002	1.358e-001	-1.594e-001
4.000e-001	2.619e+000	2.765e+000	2.474e+000	2.606e+000	-1.347e-002	1.325e-001	-1.594e-001
4.100e-001	2.650e+000	2.798e+000	2.502e+000	2.635e+000	-1.500e-002	1.335e-001	-1.635e-001
4.200e-001	2.685e+000	2.835e+000	2.535e+000	2.661e+000	-2.371e-002	1.259e-001	-1.733e-001
4.300e-001	2.718e+000	2.869e+000	2.566e+000	2.685e+000	-3.250e-002	1.188e-001	-1.839e-001
4.400e-001	2.737e+000	2.889e+000	2.585e+000	2.706e+000	-3.055e-002	1.211e-001	-1.822e-001
4.500e-001	2.756e+000	2.894e+000	2.617e+000	2.726e+000	-2.982e-002	1.085e-001	-1.681e-001
4.600e-001	2.771e+000	2.907e+000	2.635e+000	2.744e+000	-2.709e-002	1.088e-001	-1.630e-001
4.700e-001	2.796e+000	2.936e+000	2.656e+000	2.761e+000	-3.480e-002	1.050e-001	-1.746e-001
4.800e-001	2.819e+000	2.958e+000	2.681e+000	2.778e+000	-4.136e-002	9.734e-002	-1.801e-001
4.900e-001	2.829e+000	2.957e+000	2.700e+000	2.794e+000	-3.462e-002	9.394e-002	-1.632e-001
5.000e-001	2.843e+000	2.975e+000	2.710e+000	2.809e+000	-3.328e-002	9.915e-002	-1.657e-001
5.100e-001	2.856e+000	2.990e+000	2.722e+000	2.824e+000	-3.227e-002	1.019e-001	-1.665e-001
5.200e-001	2.866e+000	2.999e+000	2.733e+000	2.837e+000	-2.917e-002	1.042e-001	-1.625e-001
5.300e-001	2.877e+000	3.005e+000	2.749e+000	2.850e+000	-2.717e-002	1.012e-001	-1.555e-001
5.400e-001	2.888e+000	3.007e+000	2.769e+000	2.862e+000	-2.558e-002	9.376e-002	-1.449e-001
5.500e-001	2.904e+000	3.027e+000	2.782e+000	2.875e+000	-2.965e-002	9.270e-002	-1.520e-001
5.600e-001	2.917e+000	3.050e+000	2.785e+000	2.888e+000	-2.970e-002	1.031e-001	-1.625e-001
5.700e-001	2.928e+000	3.069e+000	2.788e+000	2.901e+000	-2.687e-002	1.137e-001	-1.675e-001
5.800e-001	2.934e+000	3.068e+000	2.800e+000	2.915e+000	-1.850e-002	1.152e-001	-1.522e-001
5.900e-001	2.944e+000	3.073e+000	2.815e+000	2.929e+000	-1.490e-002	1.141e-001	-1.439e-001
6.000e-001	2.959e+000	3.091e+000	2.828e+000	2.943e+000	-1.613e-002	1.155e-001	-1.478e-001
6.100e-001	2.960e+000	3.098e+000	2.822e+000	2.956e+000	-3.555e-003	1.342e-001	-1.413e-001
6.200e-001	2.970e+000	3.108e+000	2.832e+000	2.969e+000	-1.068e-003	1.371e-001	-1.392e-001
6.300e-001	2.987e+000	3.122e+000	2.853e+000	2.981e+000	-6.939e-003	1.272e-001	-1.411e-001
6.400e-001	3.001e+000	3.140e+000	2.862e+000	2.991e+000	-1.050e-002	1.284e-001	-1.494e-001
6.500e-001	3.010e+000	3.148e+000	2.872e+000	3.000e+000	-1.034e-002	1.276e-001	-1.483e-001
6.600e-001	3.008e+000	3.144e+000	2.871e+000	3.007e+000	-9.666e-005	1.361e-001	-1.363e-001
6.700e-001	3.014e+000	3.162e+000	2.867e+000	3.014e+000	-4.532e-004	1.468e-001	-1.477e-001
6.800e-001	3.021e+000	3.177e+000	2.865e+000	3.019e+000	-2.369e-003	1.536e-001	-1.583e-001
6.900e-001	3.023e+000	3.195e+000	2.851e+000	3.022e+000	-1.138e-003	1.708e-001	-1.730e-001
7.000e-001	3.025e+000	3.209e+000	2.841e+000	3.024e+000	-7.318e-004	1.835e-001	-1.849e-001
7.100e-001	3.027e+000	3.212e+000	2.841e+000	3.025e+000	-1.560e-003	1.842e-001	-1.873e-001
7.200e-001	3.032e+000	3.222e+000	2.842e+000	3.025e+000	-7.034e-003	1.827e-001	-1.968e-001
7.300e-001	3.031e+000	3.230e+000	2.832e+000	3.024e+000	-7.232e-003	1.918e-001	-2.063e-001
7.400e-001	3.023e+000	3.229e+000	2.818e+000	3.022e+000	-1.543e-003	2.042e-001	-2.072e-001
7.500e-001	3.016e+000	3.225e+000	2.807e+000	3.019e+000	3.312e-003	2.126e-001	-2.060e-001
7.600e-001	3.017e+000	3.232e+000	2.801e+000	3.017e+000	-3.761e-004	2.151e-001	-2.159e-001

APPENDIX B: REGRESSION EXAMPLE – COMPRESSIBLE FREE-SHEAR LAYER

Section 6.3 of Oberkampf and Barone [1] describes an example using their validation metric, for the regression case, applied to the growth rate of a turbulent free-shear layer. This appendix contains the VALMET input files, the VALMET – user dialog, and the VALMET output for this regression example.

The experimental data for this example consists of a set of experimental measurements of compressibility factor, Φ, as a function of convective Mach number, M_c. Note that regression must be used because the experimental measurements, from many different experimental facilities, are scattered over a range of M_c. The VALMET output given here is very close to that described in Oberkampf and Barone [1], but it may not be identical due to slight differences in the input data.

B.1 Input Files for Regression Example

The experimental data file, *sl_exp.xls*, shown in Table B-1 has two columns of data: the independent variable (convective Mach number, M_c or Mc) and one column of test results (compressibility factor, Φ or phi).

The computational data file, *sl_exp.xls*, shown in Table B-2 has four columns, with the independent variable in the first column, and the dependent variable in the fourth column. The two other columns of data are ignored.

The input files listed below are in text format, and the VALMET – user dialog refers to these text files. The installation package includes the input files in both text format and Excel format for the user's convenience. See Section 4 for more information on the format of a VALMET input file.

Table B-1. Excel experimental data file *sl_exp.xls*.

Mc_exp	Phi_exp
0.0590	1.0000
0.2060	0.9850
0.3420	0.9780
0.4110	0.9730
0.4550	0.9650
0.4550	0.8170
0.5100	0.9710
0.5190	0.9570
0.5250	1.0580
0.5350	0.8100
0.5800	0.9270
0.5890	0.8120
0.6400	0.7620

0.6400	0.8410
0.6680	0.7330
0.6770	0.6980
0.6910	0.5650
0.7200	0.6330
0.7950	0.5020
0.8250	0.5350
0.8380	0.5700
0.8600	0.5750
0.8620	0.4570
0.9450	0.4890
0.9850	0.4000
0.9920	0.4640
0.9920	0.4640
1.0400	0.5180
1.1220	0.4740
1.3120	0.4360
1.4490	0.4420

Table B-2. Excel computational data file *sl_comp.xls*, worksheet *comp_only*.

Fine Grid Computational Result			
Mc	incomp. Growth rate	Comp. Growth Rate	Phi
0.1000	0.0514	0.0514	1.0000
0.2400	0.0711	0.0712	1.0014
0.3800	0.0792	0.0760	0.9596
0.5200	0.0836	0.0738	0.8828
0.6600	0.0865	0.0690	0.7977
0.8000	0.0884	0.0630	0.7127
0.9400	0.0894	0.0568	0.6353
1.0800	0.0895	0.0508	0.5676
1.2200	0.0873	0.0455	0.5212
1.3600	0.0838	0.0407	0.4857
1.5000	0.0756	0.0367	0.4854

B.2 VALMET – User Dialog for Regression Example

This section gives the appropriate responses to the VALMET prompts needed to run the regression example. Most responses are enclosed in quotes; the quotes should not be typed as part of the response. For more information on the VALMET – user dialog, see Sections 6.2 and 5.3.

Output File Options

Do you want a text output file with experimental, computational, and CI data?

Click “Yes”, then NEXT.

Enter a name for the output text data file:

Enter “sl_output.txt”, then click OK.

Do you want the date and time appended to the plots and text output file?

Click “No”.

Experimental Data File Options

Are the EXPERIMENTAL data in one file or multiple files?

Click “All data in one file”.

Are your EXPERIMENTAL data in an Excel file or a text file?

Click “Excel: .xls”.

Browse for the experimental data file *sl_exp.xls*.

Browse to the folder where the data file resides, click on file *sl_exp.xls*, and click OPEN. The first eight lines of file *sl_exp.xls* are displayed. The next few questions deal with file *sl_exp.xls* shown in Table B-1. Since this is an Excel file, VALMET does not need to ask about header lines, delimiters, or columns.

Which column is the independent variable?

Enter “1”.

Do you want to multiply the independent variable by a scale factor?

Click “No”.

Enter a caption with (units) for the independent variable:

Enter “Mc” ; remember to omit the quotes. Note that units are not entered because Mc is dimensionless.

Do you want to multiply the measured variable by a scale factor?

Click “No”.

Enter a caption with (units) for the measured variable:

Enter “phi”.

The measured variable is assumed to be in column 2 since there are only two columns of data and the independent variable is in column 1.

Computational Data File Options

Are your COMPUTATIONAL data in an Excel file or a text file?

Click “Excel: .xls”.

Browse for the computational data file *sl_comp.xls*.

Browse to the folder where the data file resides, click on file *sl_comp.xls*, and click OPEN. The Excel file contains two worksheets: *comp_only* and *comp*. Since worksheet *comp* contains both the computational and experimental data, it is not in the proper format for VALMET.

Choose the worksheet that contains the data:

Click “comp_only”. The first eight lines of worksheet *comp_only* in file *sl_comp.xls* are displayed. Figure B-1 shows a screen shot of the file display. Note that the screen shot only shows one header line, but there are two header lines in the worksheet (Table B-2). As mentioned in Section 5.3, the header from an Excel file may not be displayed correctly. The next few questions deal with file *sl_comp.xls* worksheet *comp_only* shown in Table B-2.

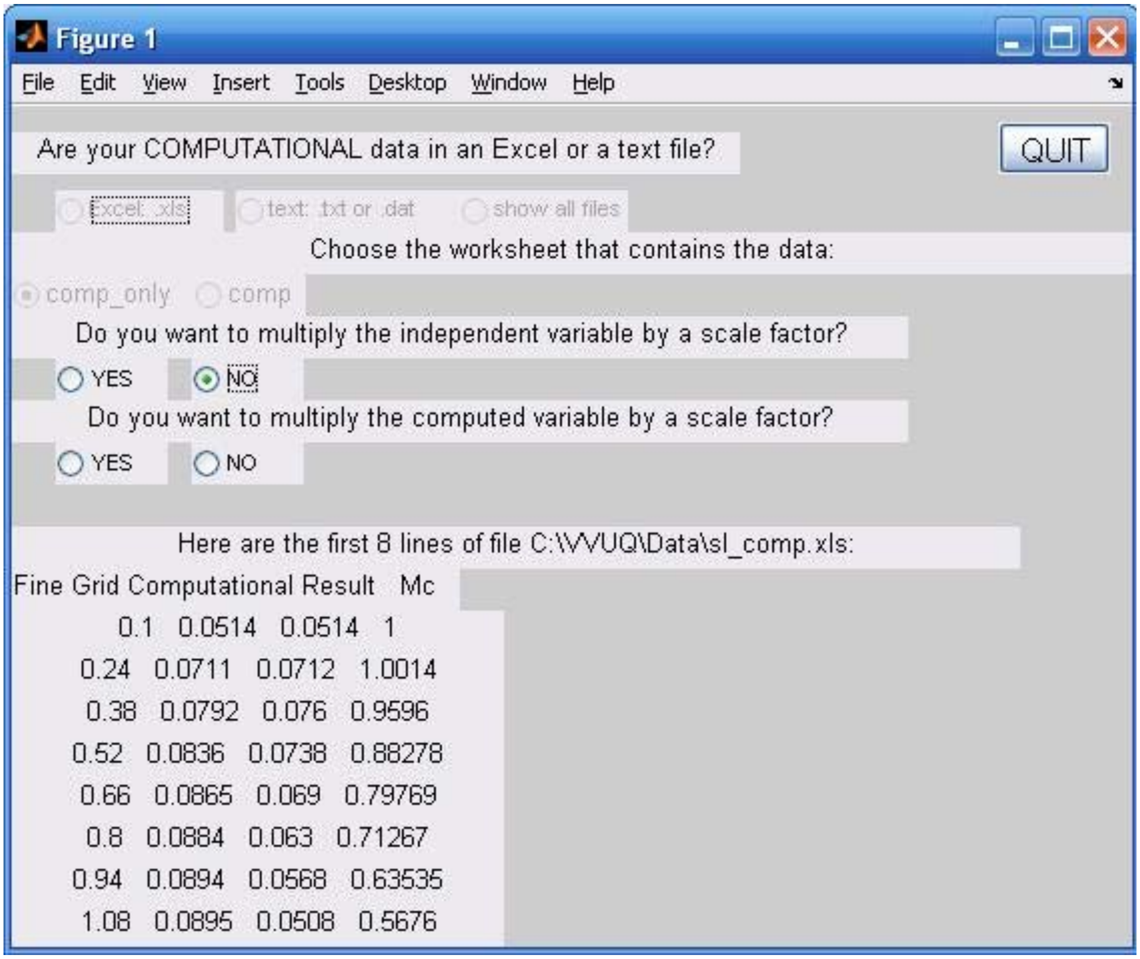

Figure B-1. Screen shot of computational data query.

Which column is the independent variable?

Enter “1”.

Do you want to multiply the independent variable by a scale factor?

Click “No”.

Do you want to multiply the computed variable by a scale factor?

Click “No”.

Select the column number(s) of the EXPERIMENTAL data (averaged if two or more)

Click “4” for the phi column.

Processing Options

What % confidence interval do you want (50 to 99.99)?

Enter “90”.

Do you want to use interpolation or regression on the data?

Click "Regression".

Set round number spacing parameters.

Click "Step size (current value =0.01)".

Enter step size (min=0.0001, max=1.43):

Enter "0.04". Note that when the step size changes, the interval end and number of points also change. Figure B-2 shows a screen shot of the final grid parameters. Click DONE.

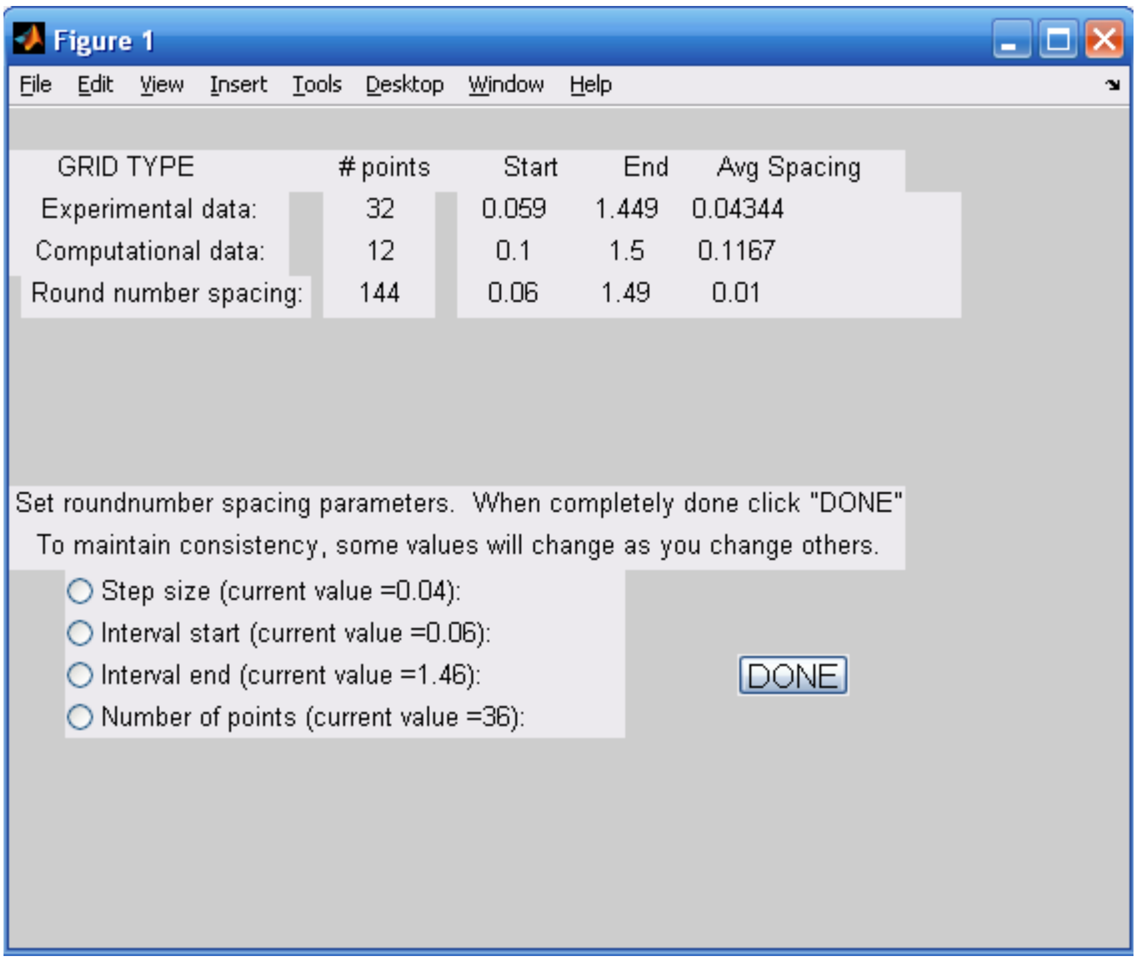

Figure B-2. Screen shot of final grid parameters query.

Select a regression form y=f(x) for your data:

Click "Fermi_Dirac function". Figure B-3 shows a screen shot of this query.

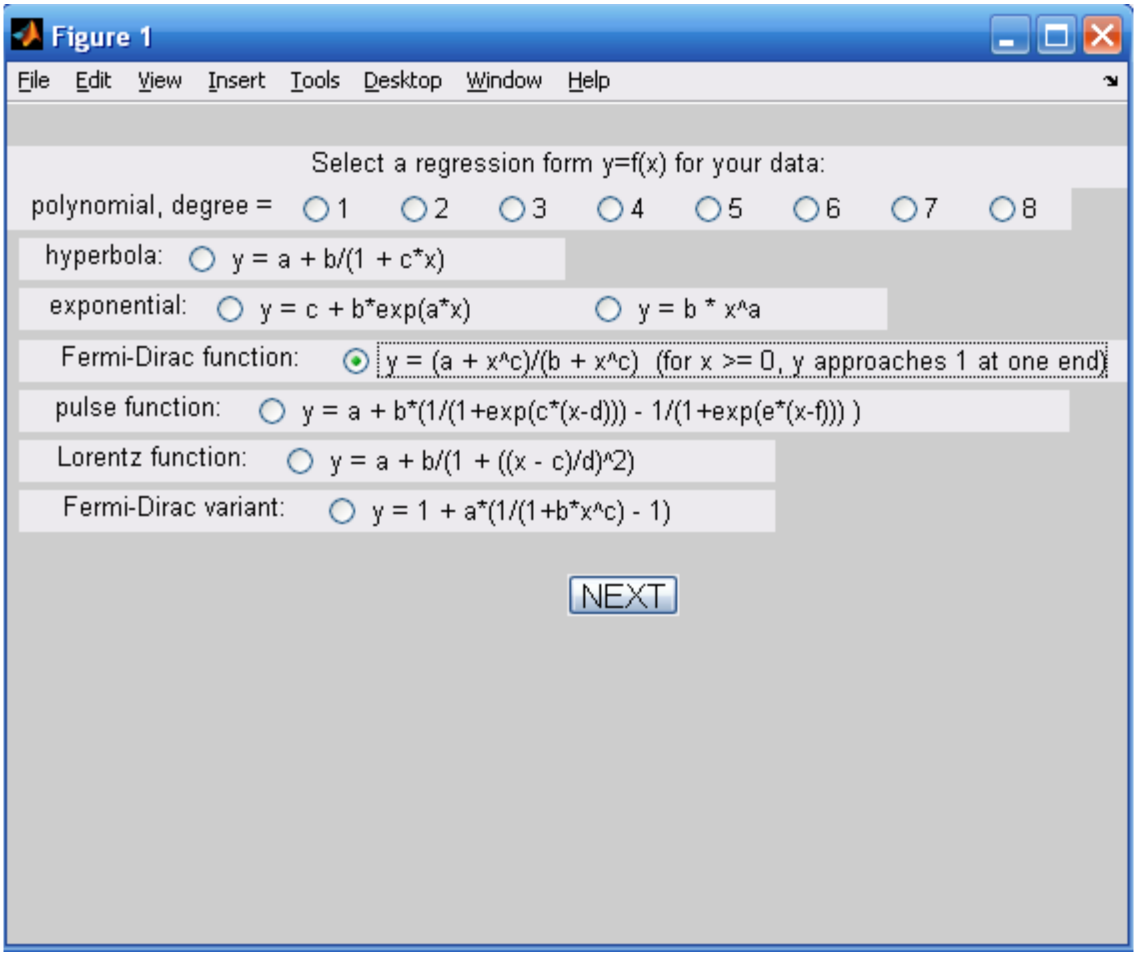

Figure B-3. Screen shot of regression equation function form query.

Do you want to change the starting points(s)?

This query allows the user to change the starting points of the optimization for the lower and upper confidence bounds. Figure B-4 shows a screen shot of this query. Figure B-5 shows a screen shot of the query that would appear if the user clicked “Change lower bound initial coordinates”. Click “No” then click NEXT.

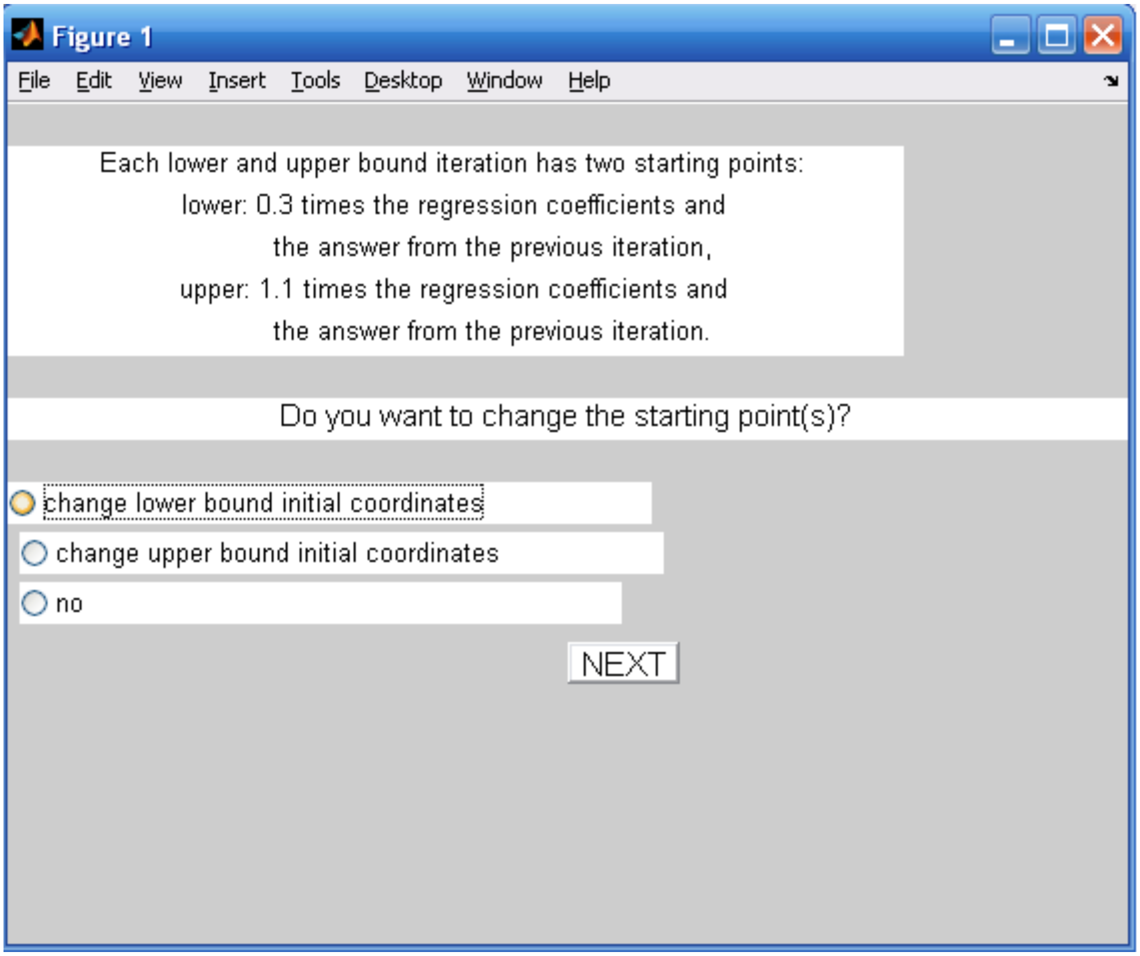

Figure B-4. Screen shot of regression coefficient bound query.

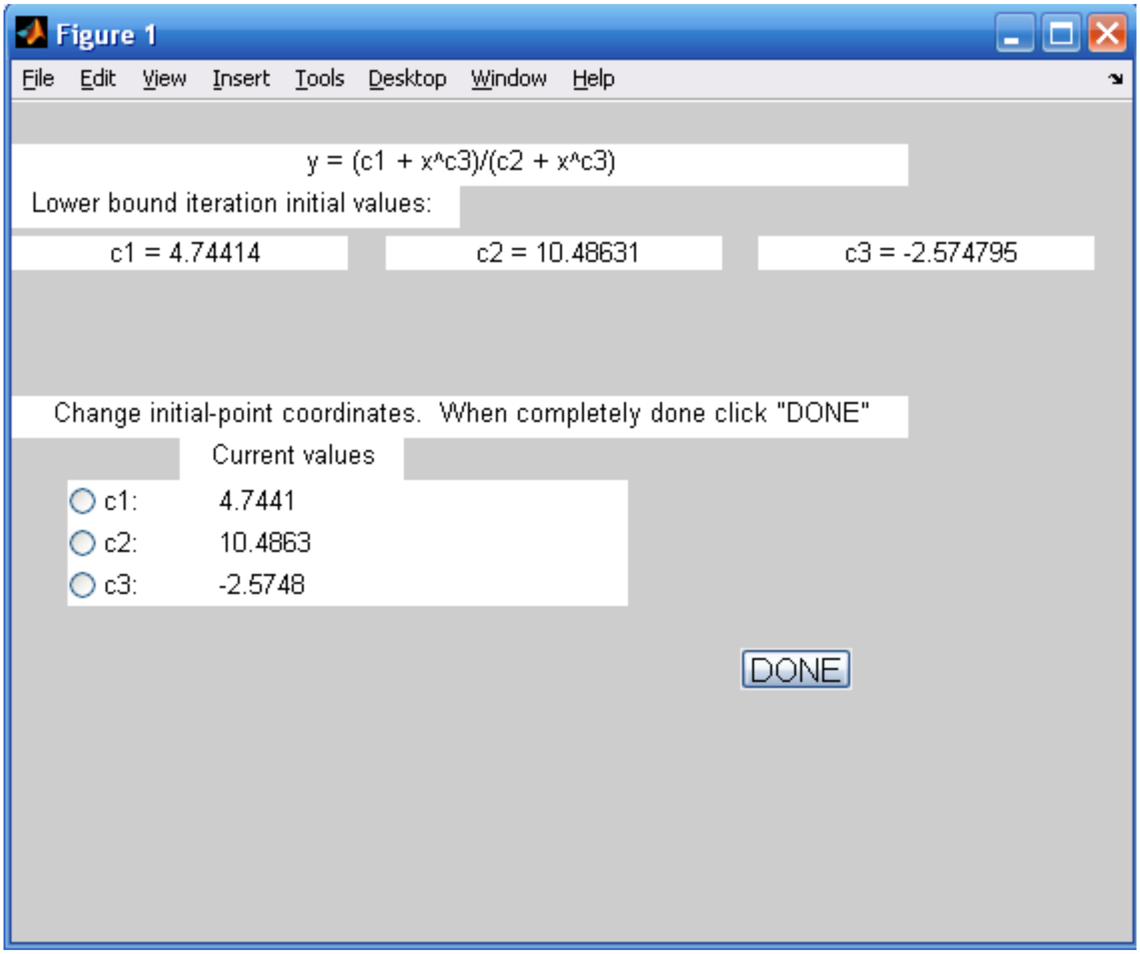

Figure B-5. Screen shot of lower bound initial point coordinates query.

Processing

VALMET performs the requested calculation. Hundreds of informational messages appear (in black). Warning (blue) messages will appear for some small values of x ($x < 0.34$). No fatal (red) messages should appear. If such messages appear, either the user has not responded to the queries correctly or the program or data files have been corrupted.

After a pause (a few seconds to a few minutes, depending on the speed of computer), the validation metrics screen and the plots will appear. The plots are stacked on top of each other, but the plots can be moved on the screen or minimized to the task bar using the "-" icon.

The following query appears in the input.

Do you want to process the same data again?

Click "No".

B.3 Output for Regression Example

The VALMET output for the regression example is presented in this section. The validation metrics screen, the five plots, and the output text file are shown along with a brief discussion of each. Oberkampf and Barone [1] contains very similar plots; it includes a more thorough discussion of the information that can be gleaned from them.

Figure B-6 shows the two global validation metrics and their associated confidence indicators. This screen is discussed in more detail in Section 6.1.2. Note that the values on this screen are reflected in the output plots.

The screen shown in Figure B-6 is stored in file globalmetrics_for_rform12_90pct.fig.

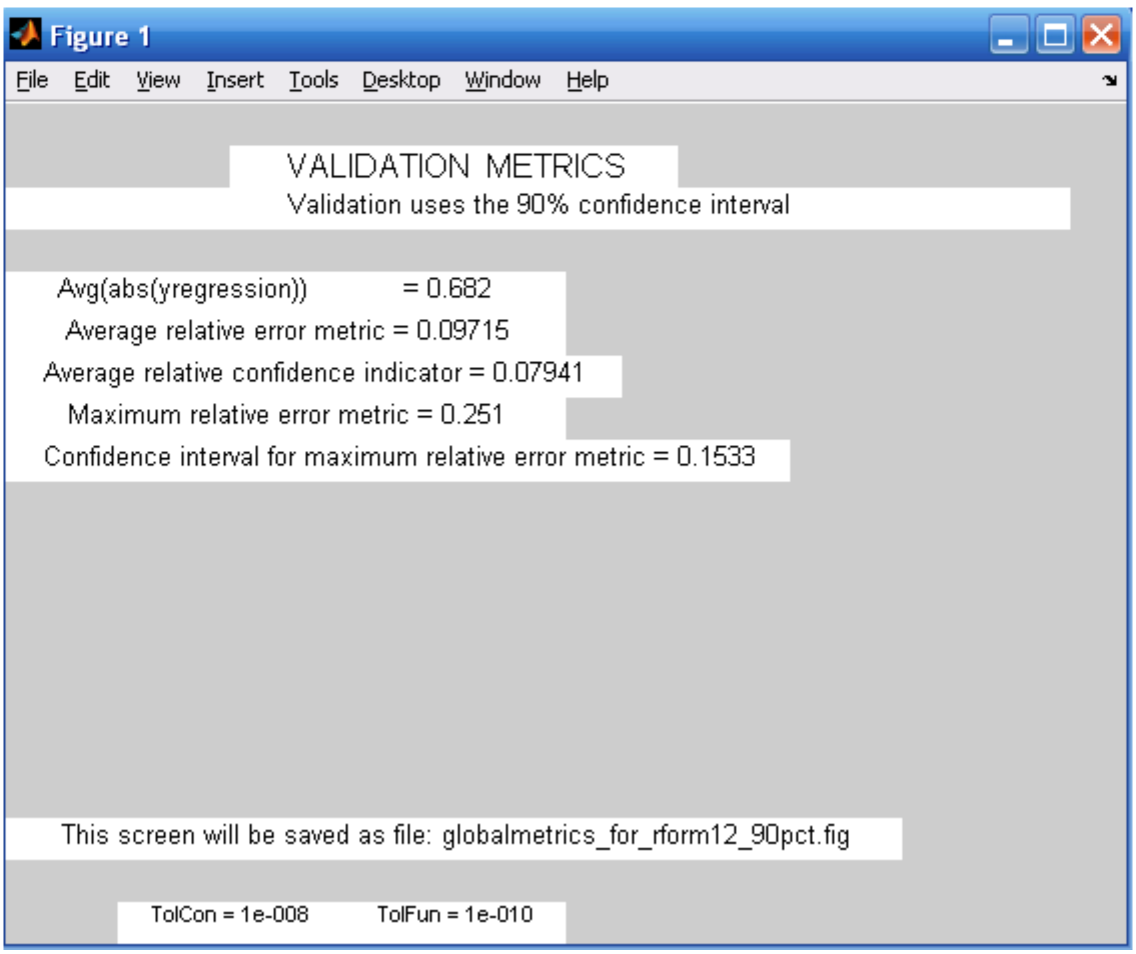

Figure B-6. Validation metrics screen (regression).

Figure B-7 is very similar to Figure 11 in Oberkampf and Barone [1]. It shows the data from the experimental data file. The dependent variable (phi) is plotted versus the independent variable (Mc) for the single column of data.

The Figure B-7 plot is stored in file experimental_data.fig.

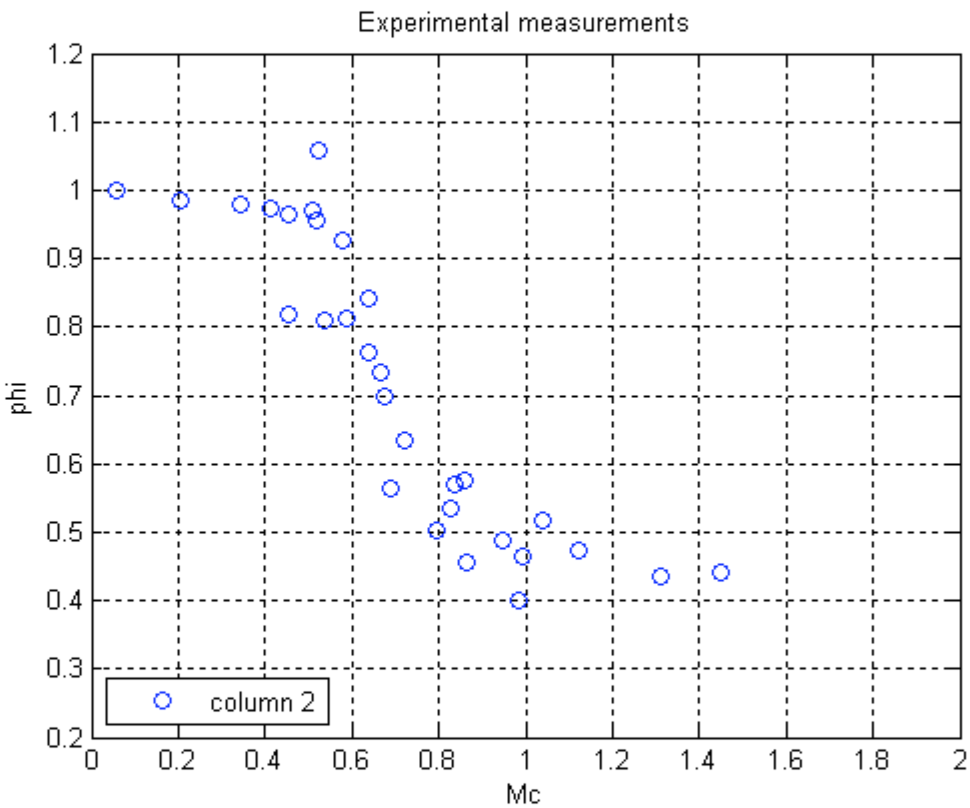

Figure B-7. Plot of experimental data (regression).

Figure B-8 is very similar to Figure 13 in Oberkampf and Barone [1]. The plot shows the experimental data, the 90% confidence interval of the regression fit, and the computational simulation result.

From the confidence interval in Figure B-8, it is seen that the largest uncertainty in the experimental data occurs for large values of Mc. Oberkampf and Barone [1] discuss the analysis of this plot with respect to future validation experiments.

The Figure B-8 plot is stored in file comp_and_exp_mean_with_90pct_ci_rform12.fig. When printed on a printer, the legend box no longer covers part of the lower confidence interval.

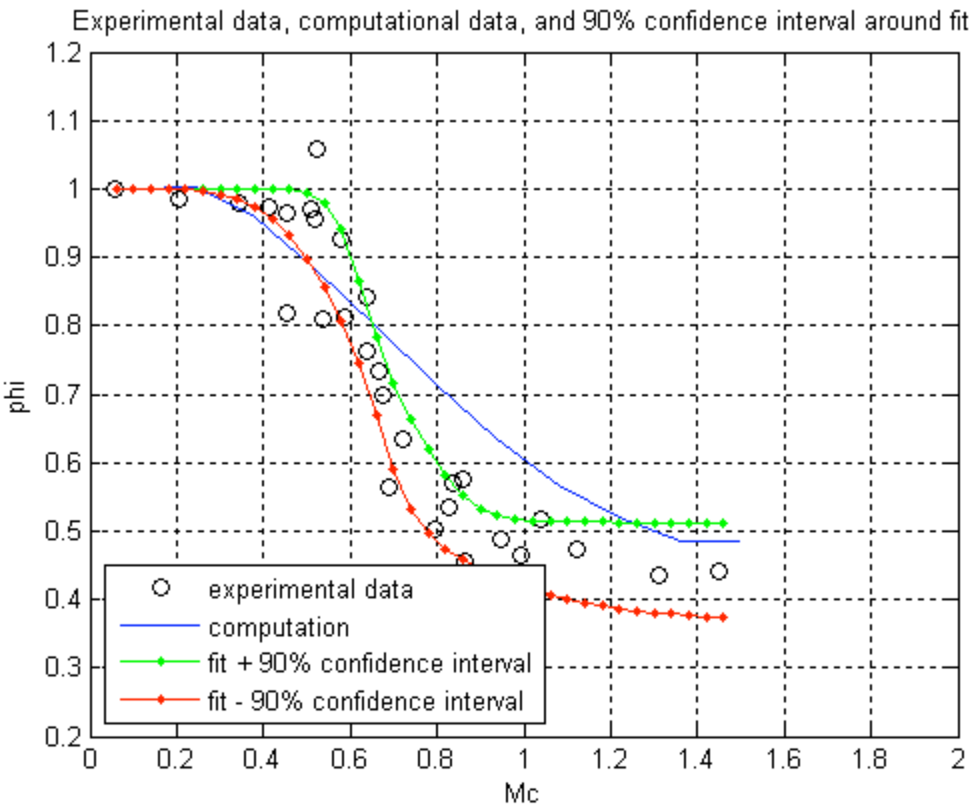

Figure B-8. Plot of experimental data, 90% CI of regression fit, and computational result (regression).

Figure B-9 is very similar to Figure 14 in Oberkampf and Barone [1]. It shows the estimated error, $\tilde{E}(x)$, of the model as a function of Mc along with the 90% confidence interval from the experimental data.

This plot presents the validation metric result, i.e., the difference between computational and the regression fit of the experimental data, along with the 90% confidence interval representing the uncertainty in the experimental data. As pointed out in the discussion of the corresponding plot for the interpolation example (Figure A-6) and in Oberkampf and Barone [1], the validation metric makes a critical examination of both a computational model and the experimental data.

Note that the confidence intervals are not symmetric with respect to zero. This is explained in Section 2.4 and in Oberkampf and Barone [1].

The Figure B-9 plot is stored in file est_error_with_90plus_minus_ci_rform12.fig.

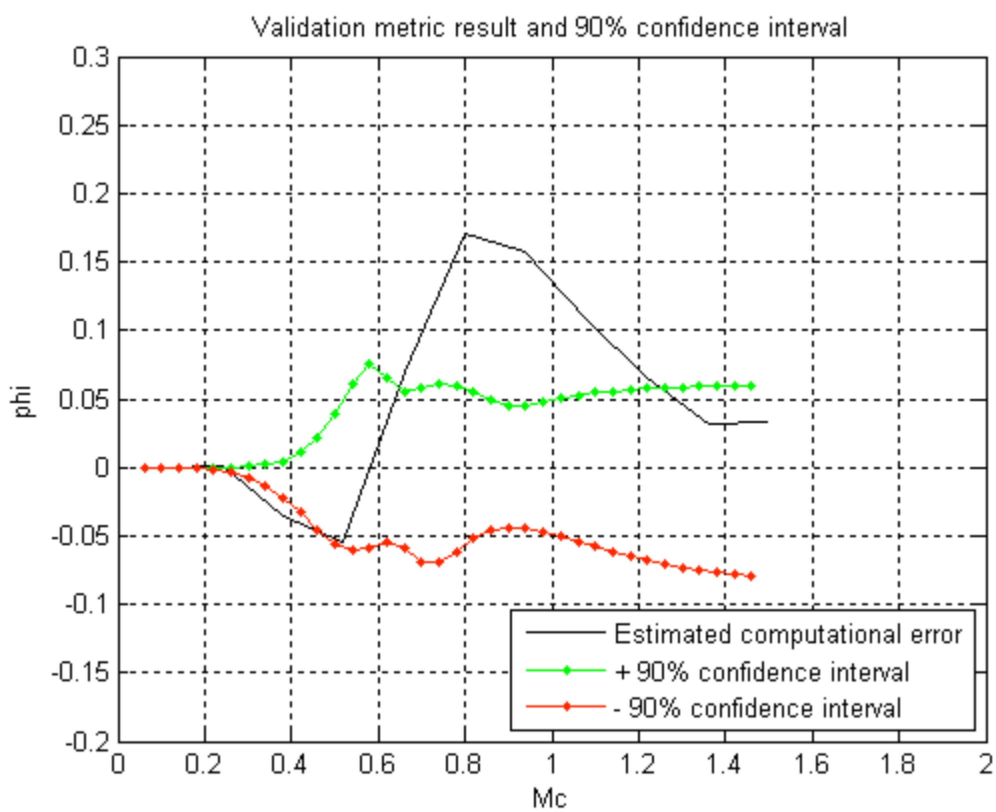

Figure B-9. Plot of validation metric result and 90% CI (regression).

Figure B-10 displays the results of the validation metric by plotting the 90% confidence interval of the true error in phi predicted by the computational model as a function of Mc.

The Figure B-10 plot is stored in file est_error_with_90pct_bounds_rform12.fig.

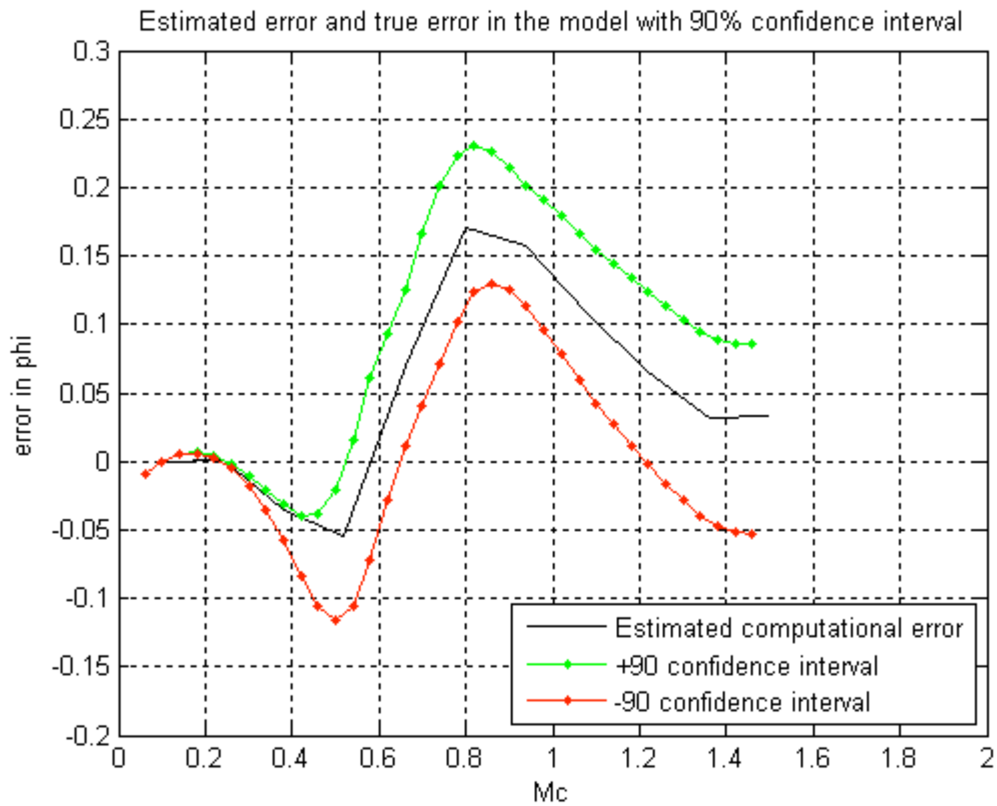

Figure B-10. Plot of estimated error and true error with 90% CI (regression).

Figure B-11 shows the experimental data and the regression fit with 90% confidence interval. The functional form of the regression equation and the regression coefficients are displayed on the plot. Note that the experimental data and confidence interval were also shown in Figure B-8 and Figure 13 in Oberkampf and Barone [1].

The Figure B-11 plot is stored in file regression_fit_with_90pct_bounds_rform12.fig. When printed on a printer, the legend box no longer covers part of the lower confidence interval.

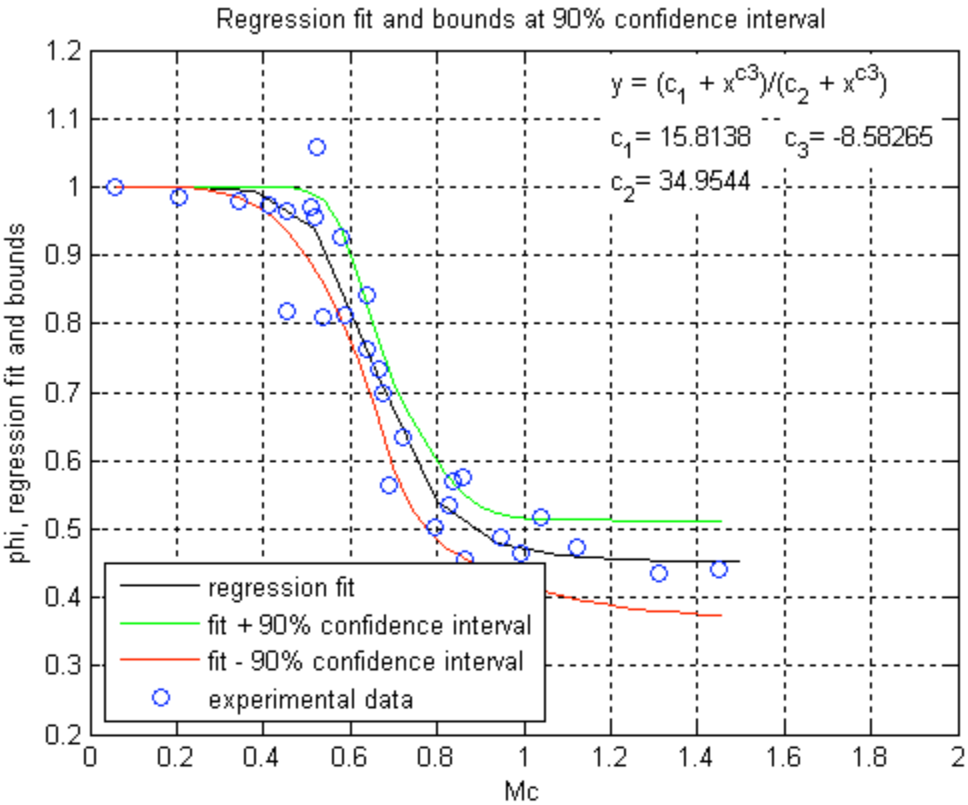

Figure B-11. Plot of experimental data and regression fit with 90% CI (regression).

Table B-3 contains a listing of the optional output text file. It contains the experimental data, the computational data, the verification metrics and confidence indicators (as displayed in the validation metrics screen shown in Figure B-6), a table of output computed at the experimental grid, and a table for output computed at the computational grid. The contents of this file are discussed in more detail in Section 6.3.2.

Note that most of the tables in the file are preceded by a line with two numbers: the number of columns in the table minus 1, and the number of rows of data in the table (not including the header line).

Table B-3. Output text file *sl_output.txt* (regression).

```
experimental data
Mc
phi
   1   31
     xe        col_2
  5.900e-002  1.000e+000
  2.060e-001  9.850e-001
  3.420e-001  9.780e-001
  4.110e-001  9.730e-001
  4.550e-001  9.650e-001
  4.550e-001  8.170e-001
  5.100e-001  9.710e-001
  5.190e-001  9.570e-001
  5.250e-001  1.058e+000
  5.350e-001  8.100e-001
  5.800e-001  9.270e-001
  5.890e-001  8.120e-001
  6.400e-001  7.620e-001
  6.400e-001  8.410e-001
  6.680e-001  7.330e-001
  6.770e-001  6.980e-001
  6.910e-001  5.650e-001
  7.200e-001  6.330e-001
  7.950e-001  5.020e-001
  8.250e-001  5.350e-001
  8.380e-001  5.700e-001
  8.600e-001  5.750e-001
  8.620e-001  4.570e-001
  9.450e-001  4.890e-001
  9.850e-001  4.000e-001
  9.920e-001  4.640e-001
  9.920e-001  4.640e-001
  1.040e+000  5.180e-001
  1.122e+000  4.740e-001
  1.312e+000  4.360e-001
  1.449e+000  4.420e-001

computational data
Mc
phi
   1   11
```

xc	col_4
1.000e-001	1.000e+000
2.400e-001	1.001e+000
3.800e-001	9.596e-001
5.200e-001	8.828e-001
6.600e-001	7.977e-001
8.000e-001	7.127e-001
9.400e-001	6.353e-001
1.080e+000	5.676e-001
1.220e+000	5.212e-001
1.360e+000	4.857e-001
1.500e+000	4.854e-001

```
validation metrics
90      1.2596e-001    % confidence interval, sum squared error
  6.820e-001         Avg(abs(yregression))
  9.715e-002          Average relative error metric
  7.941e-002          Average relative confidence indicator
  2.510e-001          Maximum relative error metric
  1.533e-001          Confidence interval for maximum relative error
metric
regression: y = (c1 + x^c3)/(c2 + x^c3)
    3
  1.5814e+001  3.4954e+001 -8.5826e+000

    5   31
```

xval	fit(xval)	fit+CI	fit-CI	+CI	-CI
6.000e-002	1.000e+000	1.000e+000	1.000e+000	5.627e-010	-3.589e-007
1.000e-001	1.000e+000	1.000e+000	1.000e+000	4.241e-008	-2.556e-005
1.400e-001	1.000e+000	1.000e+000	9.999e-001	7.156e-007	-1.475e-004
1.800e-001	1.000e+000	1.000e+000	9.994e-001	5.805e-006	-5.440e-004
2.200e-001	1.000e+000	1.000e+000	9.984e-001	3.573e-005	-1.531e-003
2.600e-001	9.998e-001	1.000e+000	9.962e-001	1.426e-004	-3.580e-003
3.000e-001	9.994e-001	1.000e+000	9.921e-001	6.203e-004	-7.296e-003
3.400e-001	9.982e-001	1.000e+000	9.849e-001	1.804e-003	-1.330e-002
3.800e-001	9.953e-001	9.999e-001	9.733e-001	4.619e-003	-2.196e-002
4.200e-001	9.890e-001	9.996e-001	9.560e-001	1.057e-002	-3.304e-002
4.600e-001	9.766e-001	9.983e-001	9.315e-001	2.170e-002	-4.512e-002
5.000e-001	9.542e-001	9.937e-001	8.988e-001	3.944e-002	-5.543e-002
5.400e-001	9.179e-001	9.790e-001	8.573e-001	6.114e-002	-6.052e-002
5.800e-001	8.654e-001	9.403e-001	8.066e-001	7.494e-002	-5.884e-002
6.200e-001	7.995e-001	8.655e-001	7.447e-001	6.601e-002	-5.481e-002
6.600e-001	7.279e-001	7.831e-001	6.693e-001	5.523e-002	-5.859e-002
7.000e-001	6.601e-001	7.174e-001	5.915e-001	5.734e-002	-6.855e-002
7.400e-001	6.030e-001	6.636e-001	5.332e-001	6.063e-002	-6.971e-002
7.800e-001	5.589e-001	6.189e-001	4.974e-001	6.006e-002	-6.143e-002
8.200e-001	5.268e-001	5.824e-001	4.746e-001	5.560e-002	-5.219e-002
8.600e-001	5.042e-001	5.536e-001	4.580e-001	4.941e-002	-4.618e-002
9.000e-001	4.886e-001	5.330e-001	4.447e-001	4.444e-002	-4.386e-002
9.400e-001	4.778e-001	5.220e-001	4.334e-001	4.420e-002	-4.443e-002
9.800e-001	4.704e-001	5.176e-001	4.236e-001	4.716e-002	-4.686e-002
1.020e+000	4.653e-001	5.155e-001	4.150e-001	5.015e-002	-5.031e-002
1.060e+000	4.618e-001	5.143e-001	4.076e-001	5.257e-002	-5.419e-002
1.100e+000	4.592e-001	5.137e-001	4.012e-001	5.441e-002	-5.809e-002
1.140e+000	4.575e-001	5.133e-001	3.957e-001	5.580e-002	-6.178e-002
1.180e+000	4.562e-001	5.130e-001	3.910e-001	5.683e-002	-6.514e-002
1.220e+000	4.552e-001	5.128e-001	3.871e-001	5.760e-002	-6.813e-002

```
1.260e+000  4.546e-001  5.127e-001  3.838e-001  5.818e-002 -7.075e-002

  2   11
    xc        vc_fit    est error
1.000e-001  1.000e+000  5.004e-008
2.400e-001  9.999e-001  1.498e-003
3.800e-001  9.953e-001 -3.571e-002
5.200e-001  9.380e-001 -5.523e-002
6.600e-001  7.279e-001  6.981e-002
8.000e-001  5.415e-001  1.712e-001
9.400e-001  4.778e-001  1.575e-001
1.080e+000  4.604e-001  1.072e-001
1.220e+000  4.552e-001  6.595e-002
1.360e+000  4.535e-001  3.215e-002
1.500e+000  4.529e-001  3.255e-002
```

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