A Design-of-Experiments Plug-In for Estimating Uncertainties in Finite Element Simulations (*)

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Abstract: The objective of this paper is to introduce an economical and user-friendly technique for estimating a specific type of finite element simulation uncertainties, or, "error bars," for a class of mathematical models, of which no closed-form or approximate solution is known to exist. Using Python, Abaqus-Python, and a public-domain statistical data analysis software package named Dataplot, we present a design-of-experiments-based Python-Dataplot-Uncertainty Plug-In (PD-UP) to estimate the finite element simulation uncertainties in a mathematical model due to variability in modeling parameters such as material property constants, geometric parameters, loading rates, etc. Examples of finite element simulations of the free vibrations of a single-crystal silicon cantilever beam in an atomic force microscope with an estimation of the uncertainties of the first bending mode resonance frequency of the beam, are included.

Keywords: Abaqus; ANSYS; atomic force microscope, cantilever beam; computational sciences; Dataplot; design of experiments; finite element method; mathematical modeling; mechanics; nanotechnology; plug-in; Python; sensitivity analysis; simulation; single crystal silicon; statistical data analysis; uncertainty analysis; uncertainty quantification; verification; vibration.

1. Introduction

It is well-known that simulation results of the finite element method (FEM) contain errors due to a variety of sources (see, e.g., Hughes 1987, Haldar 1997, Zienkiewicz 2000, Chu 2002, Yang 2002, Lord 2003, Fong 2005, Fong 2006a, Fong 2006b, Fong 2008a). By and large, such errors are of major concern to experimentalists or modelers, when the governing equations and their associated material property constants, boundary conditions, geometric parameters, and loading rates, etc., are known to contain significant uncertainties as defined for physical measurements in ISO 1993 and Taylor 1994, and for black-box computer models by a recent paper of Kennedy 2001. In this paper, we address FEM simulation errors by going beyond Kennedy 2001 in the sense that we no longer treat an FEM model as a black-box. Using a design-of-experiments approach and a 10-step statistical analysis algorithm (Filliben 2002), we develop a plug-in for an FEM model with an uncertainty estimation and a robustness ranking of not only the parametric variables but also the FEM code platforms (e.g., Abaqus vs. ANSYS) and FEM mesh sizes (coarse vs. fine).

2. A Calibrated FEM Model

In the opening section of a 2001 paper by Kennedy and O'Hagan (Kennedy 2001), the authors made the following observation on "computer models and calibration":

> " . . . to use a model to make predictions in a specific context it may be necessary first to *calibrate* the model by using some observed data." [*Italics* by authors of this paper.]

Kennedy and O'Hagan went on to present a "Bayesian approach to calibrating a computer code by using observations from the real process, and subsequent prediction and uncertainty analysis of the process whcih corrects for model inadequacy." They treated the computer code as a "black box," and made no use of information about the mathematical model implemented by the code.

Our interest in developing a *calibrated* FEM model requires us to open up that "black box" and have a closer look at the output of that model as it varies according to three metrics, namely, the finite element mesh size, m, the mesh type, m_t, (e.g., hexahedron vs. tetrahedron), and the FEM code implementation type, c_t, (e.g., Abaqus vs. ANSYS). To facilitate our presentation, we adopt the notation of Kennedy and O'Hagan (see Sections 4.1 and 4.2 of Kennedy 2001) with a minor change in indexing the components of various vectors to avoid confusion with our notation in prior publications using the method of design of experiments (Fong 2006b, Fong 2008a).

Let $\mathbf{x} = (x_1, \ldots, x_k)^T$ be a k-dimensional process input vector, and $\mathbf{t} = (t_1, \ldots, t_{q2})^T$, a q_2-dimensional calibration input vector, such that n runs of a computer code produces an output vector $\mathbf{y} = (y_1, \ldots, y_n)^T$ given by the following relation:

$$\mathbf{y} = \eta\,(\mathbf{x}, \mathbf{t}). \tag{1}$$

Let $\zeta(\mathbf{x})$ denote the true value of a real process when the variable process inputs take values $\mathbf{x}$, and let there be n_o observations denoted by the n_o-dimensional vector, $\mathbf{z} = (z_1, \ldots, z_{no})^T$, where each z_p, $p = 1, \ldots, n_o$, is an observation of $\zeta(\mathbf{x})$ for known variable inputs $\mathbf{x}$, but subject to error. The full set of data that is available for the analysis is $\mathbf{d}^T = (\mathbf{y}^T, \mathbf{z}^T)$, and according to Kennedy 2001, the relationship between the observations z_p, the true process $\zeta(\mathbf{x})$, and the computer model output $\eta\,(\mathbf{x}, \mathbf{t})$, is given by the following equation:

$$z_p \;=\; \zeta(\mathbf{x}) \;+\; e_p \;=\; \rho\,\eta\,(\mathbf{x}, \boldsymbol{\theta}) \;+\; \delta(\mathbf{x}) \;+\; e_p\,, \tag{2}$$

where e_p is the observation error for the pth observation, ρ is an unknown regression parameter, and $\delta(\mathbf{x})$ is a model inadequacy function that is independent of the code output $\eta\,(\mathbf{x}, \boldsymbol{\theta})$, and $\boldsymbol{\theta}$ is the unknown calibration inputs corresponding to the particular real process for which we wish to calibrate the model. Note that when we make the n runs of the computer model, we replace $\boldsymbol{\theta}$ by $\mathbf{t}$, the known values of the calibration inputs, and as pointed out in Kennedy 2001, the important conceptual difference between $\boldsymbol{\theta}$ and $\mathbf{t}$ requires us to emphasize it in equation (2), which can be viewed as defining a non-linear regression model. The computer code itself defines the regression function through the term $\rho\,\eta\,(\mathbf{x}, \boldsymbol{\theta})$, with parameters ρ and $\boldsymbol{\theta}$. The other two terms can be viewed as together representing (non-independent) residuals.

3. A Calibrated FEM Model for a "Simple" Real Process

To illustrate the various quantities in equation (2) in a simple example, let us assume a "simple" real process where a mathematical model exists with a known solution such that both $\delta(\mathbf{x})$ and e_p in equation (2) vanish. In addition, we consider a sufficiently small local region where a linear regression model is valid (ρ = 1), then equation (2) for an FEM model with a two-dimensional input vector, $(X_1, X_2)^T$, may be written in the following form:

$$z = \eta(\mathbf{x}, \mathbf{t}) + \delta(\mathbf{x}) + e = A_0 + A_1 * X_1 , + A_2 * X_2 + t\,(m,\ m_t\ , c_t\ ; \delta , e\,), \qquad (3)$$

where A_0 , A_1, and A_2 are the regression coefficients of a linear model, and t , a calibration input function that could depend on the FEM mesh size, m , mesh type, m_t , the code implementation type, c_t , as well as δ and e . In general, the dimension of the input vector in Equation (3) may be more than two, but for the purpose of illustrating equation (2), we shall present examples only for a two-dimensional input vector.

4. Statistical Theory of Design of Experiments (abbrev. DOE)

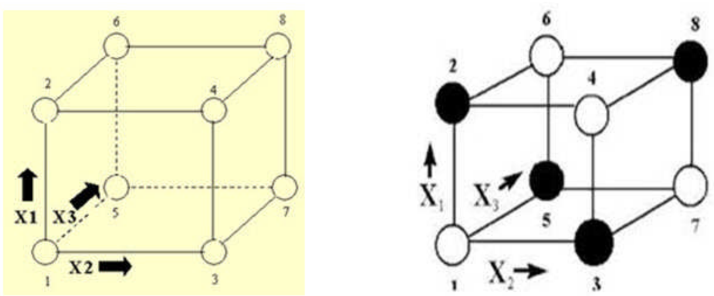

Figure 1. (left) **A full-factorial 8-run orthogonal design for 3 factors.**
(right) **A fractional factorial 4-run orthogonal design for 3 factors.**

To estimate finite element simulation uncertainties due to physical modeling, we propose to do a virtual experiment by changing one or more physical process variables (factors) in order to observe the effect the changes have on one or more response variables. In an earlier paper (Fong 2008a), we propose a DOE-based methodology (Box 1978, Montgomery 2000), because DOE is an efficient procedure for planning experiments so that the data obtained can be analyzed to yield valid and objective conclusions with respect to the relative importance of the factors.

DOE begins with determining the *objectives* of an experiment and selecting the *process factors* for the study. An Experimental Design is the laying out of a detailed experimental plan in advance of doing the experiment. Well chosen experimental designs maximize the amount of "information" that can be obtained for a given amount of experimental effort. The statistical theory underlying DOE begins with the concept of *process models*. A process *model* of the 'black box' type is formulated with several discrete or continuous input *factors* that can be controlled, and one or more measured output *responses.* The output responses are assumed continuous. Real or virtual experimental data are used to derive an empirical (approximate) model linking the outputs and inputs. These empirical models generally contain *first-order (linear) and second-order (quadratic and interactions) terms.* For a complete exposition of this topic, readers are referred to the articles (Box 1978, Montgomery 2000, Croarkin 2003, Fong 2008a) cited in Section 12 (References)

The most popular and cost-effective experimental designs for sensitivity analysis are two-level designs. To illustrate the concept, we show in Fig. 1 (left) a graphical representation of a two-level, full factorial design for three factors, namely, the 2^3 design, and Fig. 4 (right) the same of a two-level, fractional factorial design, or, the 2^{3-1} design. The arrows show the direction of increase of the factors in order to represent the user-defined variability of each factor. The numbers "1" through "8" at the corners of the design box refer to the "Standing Order" of runs (also known in the literature as the "Yates Order").

5. A Calibrated FEM Model of Free Vibrations of a Cantilever Beam

In Table 1, we present the results of an FEM computational experiment (Fong 2008a) for a classical problem in mechanics where the first bending resonance frequency, q_1, of an isotropic elastic cantilever beam of rectangular cross-section is known (Timoshenko 1955, Clough 2003).

Table 1. FEM Computer Modeling of First Bending Resonance Frequency *q1* (kHz) of an Isotropic Elas. Cantilever Beam in an Atomic Force Microscope (Fong 2008a)

3-factor full-factorial DOE	**Figs. 2, 3**	**Fig. 3**	**Fig. 3**		**Figs. 4, 5**	**Figs. 4, 5**
X1 = *L* = Length, X2 = *h* = Thickness, X3 = *E* =Young's Modulus	**Abaqus** v. 6.7	**Abaqus** v. 6.7	**Exact**		**ANSYS** v. 11.0	**ANSYS** v. 11.0
Base value (variation): *L* = 0.232 mm (±1.6 %) *h* = 0.007 mm (±2.5 %) *E* =169,158 MPa (±0.1 %)	Mesh No. ***m* = 4** (20x 4x 8 = 640 elem.)	Mesh No. ***m* = 12** (60x12x24= 17,280 el.)	Theoretical Solution (See Refs. 7 and 37)		Mesh No. ***m* = 4** (20x 4x 8 = 640 elem.)	Mesh No. ***m* = 12** (60x12x24= 17,280 el.)
Run 0 = (0, 0, 0)	181.052	180.503	179.026		181.238	180.523
Run 1 = (-1, -1 , -1)	182.119	181.566	180.049		182.306	181.587
Run 2 = (+1 , -1, -1)	170.807	170.286	168.891		170.981	170.305
Run 3 = (-1 , +1, -1)	191.692	191.113	189.553		191.888	191.135
Run 4 = (+1, +1, -1)	179.786	179.241	177.806		179.970	179.261
Run 5 = (-1, -1, +1)	182.301	181.748	180.229		182.488	181.768
Run 6 = (+1 ,-1, +1)	170.977	170.456	169.060		171.152	170.475
Run 7 = (-1, +1, +1)	191.883	191.304	189.742		192.080	191.326
Run 8 = (+1, +1, +1)	179.966	179.421	177.984		180.150	179.441

The experimental design, as shown in the first column of Table 1, is a 2-level, 3-factor, full-factorial orthogonal design for all five scenarios, i.e., Abaqus (mesh size m = 4), Abaqus (m = 12), Exact, ANSYS (m = 4), and ANSYS (m = 12). Also in the first column of Table 1, we show the base values of the three factors plus their 2-level percent variations. The density of the cantilever beam is assumed to be constant (= 2.329E-06 kg/cu mm). Run 0 is the center point of the design. In Fig. 2, we show the results of a 10-step analysis of the Abaqus (m = 4) run, where a ranking of the absolute values of the effects of the model shows that factors X1 (L) and X2 (h) are dominant and the interactions are negligible. A 2-parameter least square fit of the data yields the estimated mean and 95 % confidence bounds as shown in the upper right corner of Fig. 2. In Fig. 3, we show a comparison of the Abaqus runs for two mesh sizes and found, as expected, the finer mesh (m = 12) to be closer to the exact solution. Using equation (3), we find the calibration constant for Abaqus (m=4) and Abaqus (m=12) to be -2.15 and -1.60, respectively.

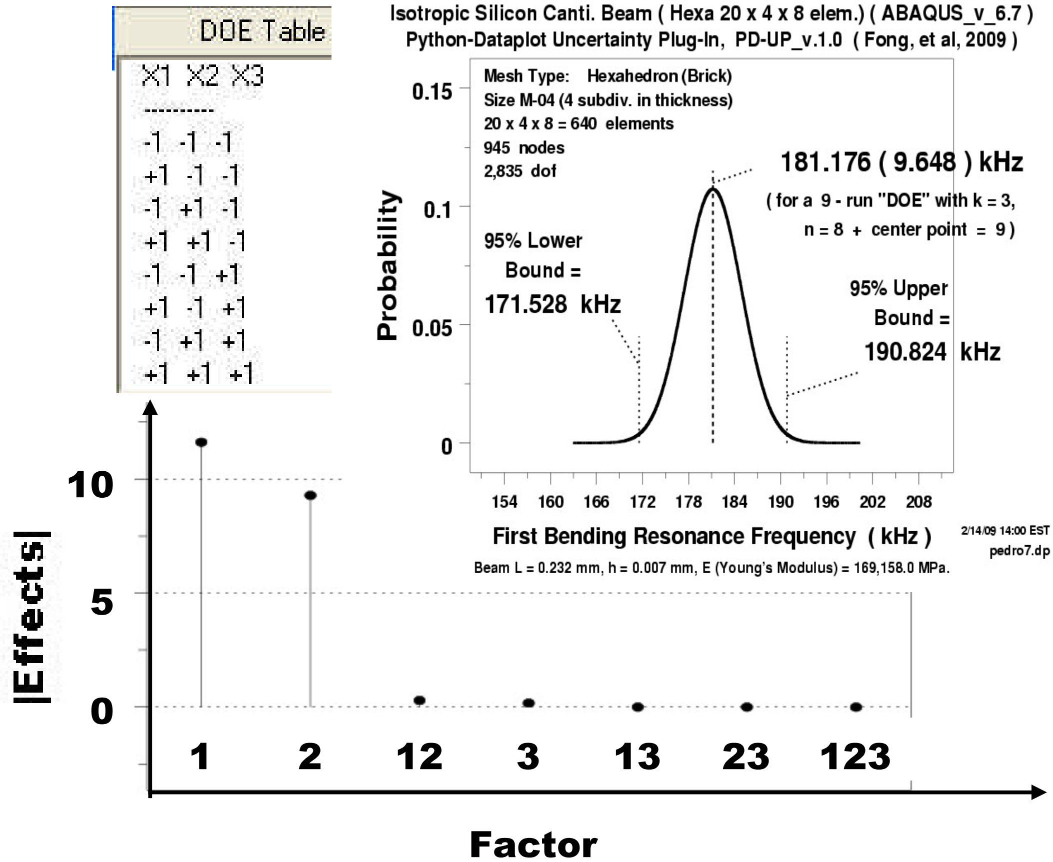

Figure 2. A ranking of main effects plot for Abaqus (mesh size *m* = 4) run with an uncertainty estimation plot in the upper right corner.

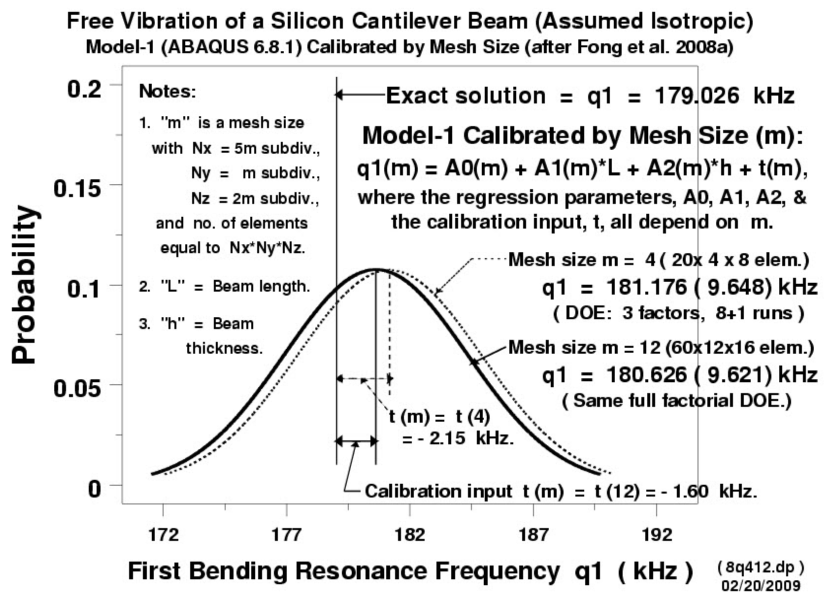

Figure 3. An FEM model showing effect of mesh size from coarse to fine

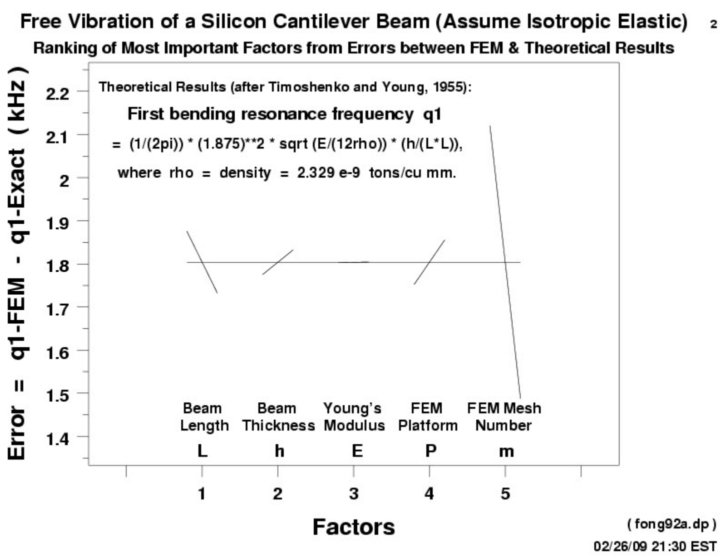

Figure 4. A ranking of five factors based on a DOE analysis of errors.

5. A Calibrated FEM Model (Continued)

Using all the data listed in Table 1, we can answer two questions by adding two more factors (X4 =software platform, X5 = mesh size) to the computer experiment. In Fig. 4, we use a DOE analysis of errors to answer the question which of the five factors is most important (the answer is the factor X5, or, the mesh size). In Fig. 5, we use a block plot to answer the question whether the mesh size effect is "real" (the answer is yes, it is real).

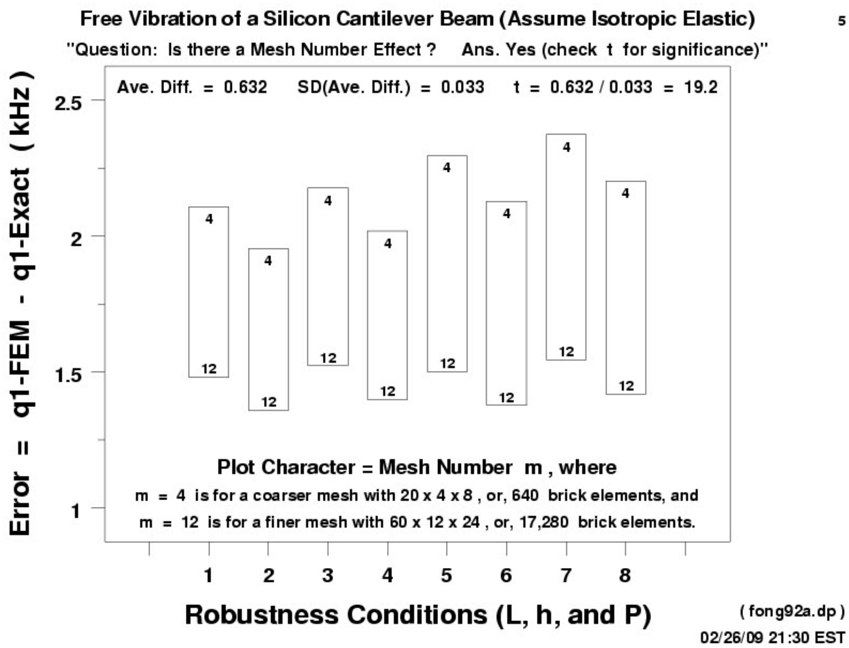

Figure 5. A robustness analysis of FEM data for mesh size effect.

If a real process is not "simple" in the sense that no known solution exists for a plausible mathematical model, we can still use the DOE approach to find a calibrated FEM model provided we have experimental data to guide us (see Fong 2008a). To facilitate this DOE approach, we present in this paper a computational plug-in by using the scripting languages of Python (van Rossum 1999), Abaqus-Python (2008), and a public-domain statistical data analysis software package named Dataplot (Filliben 2002). In Section 6, we present a conceptual design of that plug-in. In Sections 7 and 8, we present a 3-dialog-box design of a Python-Dataplot module. In Sections 9 and 10, we present a real process problem as an example application of the plug-in. A brief discussion and some concluding remarks appear in Section 11, and a list of references in Section 12.

6. A Conceptual Design of a Python-Dataplot Uncertainty Plug-In

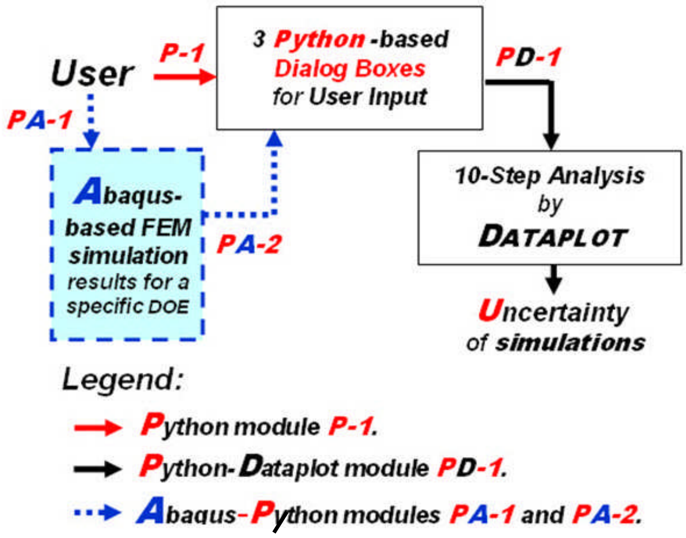

Figure 6. A Conceptual Design of the Python-Dataplot-Uncertainty Plug-In.

Throughout the FEM experiment described in the last section, we were burdened with the task of repeatedly solving the same FEM problem with a different set of parameters prescribed by a DOE. This motivated us to design a computational plug-in to facilitate an FEM uncertainty estimation methodology. As shown in Fig. 6, the so-called Python-Dataplot-Uncertainty Plug-In (abbrev. PD-UP) consists of two separate parts, namely, an FEM part and an Uncertainty Estimation part:

(1) The FEM part, which can be implemented in any packages such as Abaqus, ANSYS, Ls-Dyna, etc., involves the design of two modules, one of which, **PA-1**, is simply to make a single base run of the FEM model, and the other, **PA-2**, to modify the input file of **PA-1** for several more runs according to a design of experiments (DOE) as specified by the user (see, e.g., Box 1978 and Montgomery 2000).

(2) The Uncertainty Estimation part, which is implemented in this paper in Python (van Rossum 1999, Harms 2000, Hammond 2000, Deitel 2005) and a public domain package named Dataplot (Filliben, 2002, Croarkin 2003), also involves the design of two modules, one of which, **P-1**, is to receive input from the user with two dialog boxes, **Dialog_k** and **Dialog_n**, and the other, **PD-1**, to review the input data with the user in Dialog_10-Step before the user clicks a box to execute a 10-step analysis according to a user-defined design of experiments.

Since the second part involves Python, it is advantageous for us to implement the first part with Abaqus for which the Abaqus-Python interface is readily available and facilitates the complete automation of a finite element uncertainty estimation tool as described in Fong 2008a.

7. A Two-Dialog-Box Design for User's Input Module, **P-1**

The user's input module, **P-1**, consists of two dialog boxes, **Dialog_k** (*PyDpGui_1.py*) and **Dialog_n** (*PyDpGui_2.py*). A complete listing of *PyDpGui_1.py* is given in a website and is downloadable.

The user is asked 5 questions in **Dialog_k** (Fig. 7, left) and 3 in **Dialog_n** (Fig. 7, right). The key question, (Q-1.1), in **Dialog_k** is the number of factors, k, in a two-level factorial design of experiments the user wishes to pursue. The other four questions are:

(Q-1.2) the name of an output file,

(Q-1.3) the labels and symbols of the k factors,

(Q-1.4) the values of the k factors for a base run of the finite element simulations (to be known later as the center point of the two-level hypercube design), and

(Q-1.5) the percent variability of each factor in a two-level DOE.

After the value of k is specified in **Dialog_k**, the user is asked in **Dialog_n** another key question, (Q-2.1), namely, n, the number of simulations the user wishes to run with a two-level factorial experimental design. If the user chooses a full factorial design, then $n = 2^k$. If one wishes to conduct an experiment with less than n runs, one may choose a fractional factorial design by selecting a finite number from the set, n_i, $i = 1, 2, . . . p$, where $n_1 = 2^{k-1}$, $n_2 = 2^{k-2}$, . . . , $n_p = 2^{k-p}$, until the smallest n_p that is still greater than k. For example, if $k = 5$, one may choose 2^5 (= 32) runs for a full factorial design, or, either 2^4 (= 16), or, 2^3 (= 8) runs for a fractional factorial design, but not 2^2 (= 4) runs, because 4, being less than 5 (= k), violates the condition that the number of runs must be greater than the number of factors being considered (Box 1978). The other two questions in **Dialog_n** are:

(Q-2.2) the same name of the output file used in the answer for question Q-1.2 to insure continuity, and

(Q-2.3) the label and symbol of the response variable that is being computed from a finite element model involving those k factors and their variability.

At this point, the FEM part of the plug-in is activated (see **PA-1** and **PA-2** in Fig. 6) and the results of ($n+1$) simulations for a user-defined (k, n) design of experiments can be extracted from the FEM runs and stored as input to **Dialog_n** for uncertainty analysis.

7. A Two-Dialog-Box Design for User's Input Module, **P-1** (Cont'd)

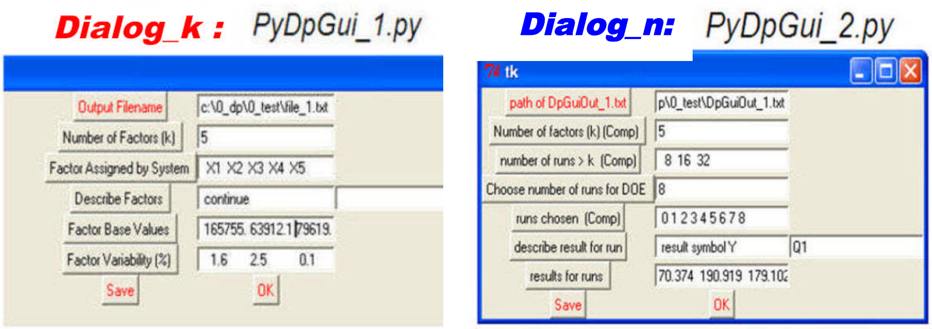

Figure 7. (Left) **Dialog_k** to define ***k*** factors and enter their variability (Right) **Dialog_n** to choose ***n*** runs for a (***k, n***) design and enter results.

8. Design of **Dialog_10-Step**, the Python-Dataplot Module, **PD-1**

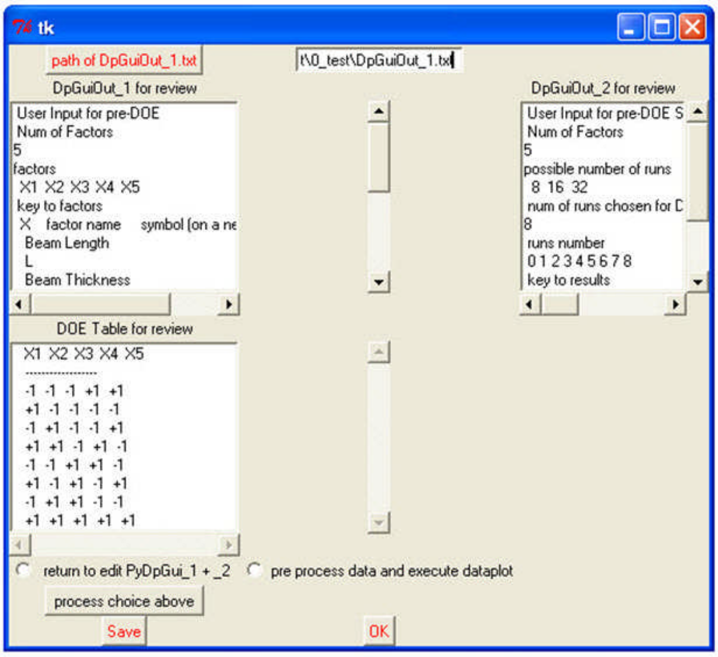

Figure 8. Dialog_10-Step with three output screens.

We are now ready to activate the uncertainty estimation of the PD-UP design by invoking **Dialog_10-Step** (PyDpGui_3.py. See Fig. 8.). The user is first asked to fill in the name of the output file specified earlier in **Dialog_k**. When that name is correct, three screens of input data will be displayed for review. The first screen (upper left of Fig. 8) is a review of the user's input to **Dialog_k**. The second screen (upper right of Fig 8) is a review of the user's input to **Dialog_n**. The third screen (lower left of Fig. 8) is new to the user, and contains the DOE table for the values of k and n furnished by the user in **Dialog_k** and **Dialog_n**.

If the user is not satisfied, the dialog box will return to **Dialog_k** and **Dialog_n**. Otherwise, a dataplot code named "*pedro7.dp*" is activated to run the 10-step statistical analysis and return an 11-plot file for viewing and downloading. The plot 11 is the uncertainty estimation result such as those given in Figs. 2 and 3.

9. An Example of an FEM Model without a Known Solution

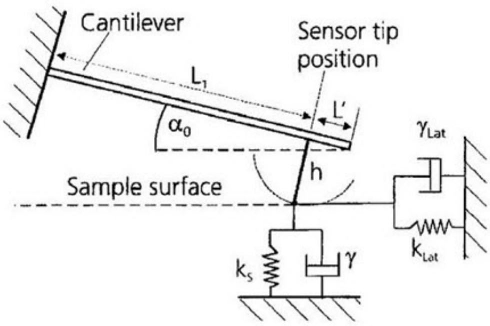

Figure 9. A cantilever beam inside an atomic force microscope (Kester 2000).

In experiments (Rabe 1996, Hurley 2003, and Fig. 9 after Kester 2000) and computational models (Timoshenko 1955, Lekhnitskii 1981, and Fong 2006b) on the resonance frequencies of a single-crystal silicon cantilever beam in an atomic force microscope, Hurley 2003 and Fong 2008a reported a major discrepancy on the two lowest natural bending resonance frequencies of such beam in two different shapes, rectangular and dagger. For our purposes here, it suffices to introduce that well-documented problem as an example of a direct application of the newly developed Python-Dataplot-Uncertainty Plug-in. Using measurement variability data of single-crystal silicon elastic constants first published by McSkimin 1966, and geometric parameter variability data such as beam length and thickness commonly known to laboratory researchers, we propose a two-level, (k = 5, n = 8), fractional factorial orthogonal DOE with the five factors being the beam length (X1), the beam thickness (X2), the cubic-crystal silicon elastic constant C_{11} (X3), the second constant C_{12} (X4), and the third constant C_{44} (X5). The response variable is the first bending resonance frequency of a silicon cantilever beam in an atomic force microscope.

10. Virtual Experimental Data According to an Orthogonal Design

As cited in Fong 2008a, the availability of a public-domain statistical data analysis package named Dataplot and the documentation (Croarkin 2003) of a 10-step exploratory data analysis (EDA) approach to the analysis of 2^k full factorial and 2^{k-p} fractional factorial designs, provided us an opportunity to fully develop an FEM uncertainty estimation tool as the analysis of a screening problem. In general, there are two characteristics to consider in a screening problem: (a) There are many factors to consider. (b) Each of these factors may be either continuous or discrete. The desired output from the analysis of a screening problem consists of: (i) A ranked list (by order of importance) of factors. (ii) The best settings for each of the factors. (iii) A good model. (iv) Some insight. When we use **Dialog_10-Step** (*PyDpGui_3.py*) to estimate finite element uncertainties, we first obtain 10 informative plots (see Fong 2008a for a listing of those 10 plots), one of which is a plot on the ranking of the main effects as well as interactions among k factors (k = 5 in this example). We then used a linear regression fit of the two dominant factors (X1 and X2 in this case) to obtain an uncertainty estimate of the response. Such a computational plug-in is quite useful when we deal with a non-simple real-life process such as the modeling of the resonance frequency of a single-crystal silicon beam in an atomic force microscope. An example of this application is given in Fig. 10.

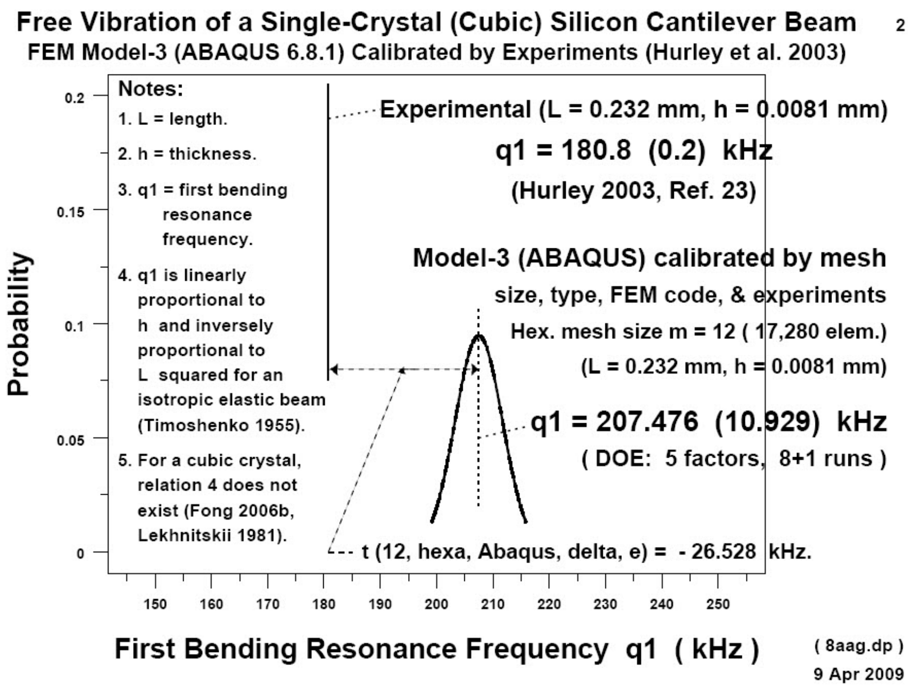

Figure 10. An FEM model calibrated by mesh size, type, code, & experiments.

11. Discussion and Concluding Remarks

In this expository paper on a two-part code implementation of a DOE-based FEM uncertainty estimation methodology, we have presented only the uncertainty estimation part of the plug-in, namely, three Python codes, *PyDpGui_1.py*, *PyDpGui_2.py*, and *PyDpGui_3.py*, and one Dataplot code, *pedro7.dp*. All four codes are available at http://math.nist.gov/mcsd/software.html. We have left the FEM part open, because our purpose is to make the plug-in, PD-UP (v. 1.0), available for any finite element uncertainty estimation effort using either commercially-available, proprietary, or public-domain FEM packages. For instance, when the FEM package is Abaqus, we plan to specialize our PD-UP with a link to Abaqus-Python and name the resulting plug-in the Abaqus-PD-UP. A similar link can be made to another Python-based FEM package named MPACT, and the resulting plug-in will be named MPACT-PD-UP, and so on. All of the new plug-ins, of course, will be coded in Python.

As illustrated in our numerous examples, we conclude that it is feasible to apply a DOE-based methodology to the estimation of FEM uncertainty due not only to model inadequacy, physical parameters, and observation errors, but also to computer black box parameters such as mesh size, type, and code implementation. Recent FEM simulations with or without using Python as a scripting language (see, e.g., Langer 2001, Easley 2007, Chao 2008, Fong 2008b) and new FEM simulations such as Fong 2009 may benefit from this plug-in when uncertainty of the computer code vs. real process observations is a compelling issue.

Based on the results presented in Figs. 4 and 5 of Section 5, where we showed two ways of answering a question whether a specific factor such as the mesh size has an effect, we observe that the computational plug-in, PD-UP, v. 1.0, reported in this paper, is applicable only to the automation of the 10-step sensitivity and uncertainty analysis of FEM calculations (Fig. 2). A future verstion of PD-UP incorporating the block plot methodology (Fig. 5) as well as the remaining FEM part of the plug-in will complete the larger goal of this paper, namely, a cost-effective and user-friendly FEM uncertainty estimation for modeling real processes of multiple factors.

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