Uncertainty of FEM Solutions Using a Nonlinear Least Squares Fit Method and a Design of Experiments Approach[1]

Jeffrey T. Fong*[2], N. Alan Heckert[2], James J. Filliben[2], Pedro V. Marcal[3], and Robert Rainsberger[4]

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[2]U. S. National Institute of Standards & Technology (NIST), [3]Mpact Corp., [4]XYZ Scientific Applications, Inc.
*Corresponding author: NIST, 100 Bureau Drive, Gaithersburg, MD 20899-8910 U.S.A. fong@nist.gov

Abstract: Uncertainty in COMSOL finite element simulations due to (a) mesh-induced truncation errors, and (b) model parameter uncertainties, is estimated using a nonlinear least squares logistic distribution fit method, and a design-of-experiments approach, respectively. Examples to illustrate both approaches are given using the COMSOL Structural Mechanics module (stress analysis of a wrench), the COMSOL RF module (application of an MRI RF coil design), and other general-purpose FEM software packages. Significance and limitations of both methods are presented and discussed.

Keywords: Design of Experiments, Finite Element Method, Logistic function, Nonlinear Least Squares Fit Method, Uncertainty Quantification.

1. Introduction

Since the 1970s, the availability of powerful computers and general purpose finite element method (FEM) software packages such as NASTRAN, MARK, ANSYS, ABAQUS, LS-DYNA, COMSOL, etc., has drastically changed the engineering design and maintenance practice. More and more design and repair decisions are made today by engineers using the output of an FEM-based simulation.

The problem with any given FEM software package is that it seldom delivers simulations with an estimate of uncertainty due to variability from at least four sources, namely, (S-1) finite element type such as tetrahedron, hexahedron, etc., (S-2) finite element mesh density or degrees of freedom that impacts on the truncation errors, (S-3) model parameters such as material properties, loadings, and boundary constraints, and (S-4) solution method and software platform. For engineering applications, the lack of uncertainty estimates is generally accepted since decisions are made with judgment and code-prescribed safety factors. For advanced engineering and scientific research, where input parameters are not well characterized and the fundamental governing equations are sometimes not even known, the lack of uncertainty quantification (UQ) in FEM simulations falls short for making them credible prior to a process of verification for mathematical and computational correctness and validation against physical reality or experiments.

During the last two decades, advances in model and simulation verification and validation (abbrev. V&V) dealing with (a) uncertain input and uncertainty in modeling (see, e.g., Ayyub[1], 1998; Lord and Wright[2], 2003; and Hlavacek[3], 2004), (b) V&V (see, e.g., Oberkampf [4], 1994; Roache[5], 1998; Oberkampf, Trucano, and Hirsch[6], 2002; Babuska and Oden[7], 2004; and Fong, et al.[8], 2008), and (c) validation in the context of metrology (see, e.g., Butler, et al.[9], 1999; and Fong, et al.[10], 2006), have appeared in the literature. Government agencies and professional societies have also added their concern and made major contributions in the form of directives[11], guides[12, 13, 14], and reviews[15]. Significant advances in V&V of FEM simulations have also been reported (see, e.g., Haldar, Guran, and Ayyub[16], 1997; Haldar and Mahadevan[17], 2000; Yang, et al.[18], 2002; and Fong, et al.[19], 2006. Fong, et al.[20], 2014).

In a recent series of 3 papers[21, 22, 23], Marcal, Fong, et al. addressed all four sources of uncertainties listed earlier, namely, (S-1) element type, (S-2) mesh density, (S-3) model parameters, and (S-4) solution platform, using two computational methods, namely, (1) the application of a nonlinear least squares (NL-LSQ) fit method using a 4-parameter logistic distribution, and (2) the application of a "super-parametric" method.

The purpose of this paper is to apply those two methods to several FEM-based problems using COMSOL[24], and two other platforms named ABAQUS[25] and MPACT[26], such that a stage is set for us to quantify uncertainty due to not only the first three traditionally well-known sources, (S-1), (S-2), and (S-3), but also the less-known source (S-4) involving solution platforms such as COMSOL, ABAQUS, and MPACT. The following table summarizes our attempt to quantify FEM uncertainty in a systematic way using rigorous tools and an ad-hoc set of five test problems (TP-1 through TP-5):

Table 1: FEM Test Problems vs. Uncertainty Sources
Legion: ABQ = ABAQUS[25]; ANS = ANSYS; **CMS** = COMSOL[24]; LSD = LS-DYNA; MPC = MPACT[26] ; ☐ = In this paper.

Source / Test Problem	**S-1** Element Type [Ref. 21]	**S-2** Mesh Density [Ref. 22]	**S-3** Model Parameter [Ref. 23]	S-4 Solution Platform [Ref. 23]
TP-1 Wrench Stress Analysis	*Future Work [Sect. 6]*	**CMS** [This paper, Sect. 3]	*Future Work [Sect. 6]*	*Future Work [Sect. 6]*
TP-2 Simple Cantilever Resonance Frequency	**ABQ MPC** [8,21-23, and this paper, Sect. 4]	**ABQ ANS** [Ref. 8, 21-23]	**ABQ ANS LSD** [Ref. 8]	**ABQ ANS LSD** [Ref. 8]
TP-3 Cantilever with end Load	**ABQ MPC** [Ref. 22]	**ABQ MPC** [Ref. 22]	*Future Work [Sect. 6]*	**ABQ MPC** [Ref. 22]
TP-4 Pipe and welded Elbow with crack	**ABQ MPC** [21-23 & Sect.4 here]	**ABQ MPC** [21-23]	*Future Work [Sect. 6]*	**ABQ MPC** [21-23]
TP-5 MRI Coil Design	*Future Work [Sect. 6]*	*Future Work [Sect. 6]*	**CMS** [Ref. 20, and this paper, Sect. 5]	*Future Work [Sect. 6]*

Throughout this work, we rely heavily on two additional analysis software packages, namely, Dataplot[27], and TrueGrid[28], even though the same results could have been obtained using other similar packages.

In Section 2, we introduce the 4-parameter logistic distribution[29,30], that is the key to an application of the nonlinear least squares (NL-LSQ) fit method[31] in Sections 3 and 4.

In Section 3, we describe an application of the NL-LSQ logistic distribution fit method, using a statistical analysis software package named Dataplot[27], to quantify FEM uncertainty in the stress analysis of a wrench using a parametric feature in the COMSOL Structural Mechanics module.

In Section 4, we introduce a "super-parametric" method, using a FEM pre-processor named TrueGrid[28], by applying it to quantify the FEM uncertainty of the first bending resonance frequency of a simple cantilever beam[32], and the crack tip stress of a steel pipe elbow weldment[21].

In Section 5, we apply a design of experiments approach[33, 34] to the quantification of FEM uncertainty when we design a magnetic resonance imaging (MRI) coil[20] using the COMSOL RF module. This sets the stage for us to expand the investigation of the FEM uncertainty to all four sources, as described in Section 6 under "Future Work."

In Section 7, we discuss the significance and limitations of the two methods (NL-LSQ and super-parametric) for FEM uncertainty quantification, and in Section 8 we end with some concluding remarks. A list of references is given in Section 9.

2. Logistic Distribution

A logistic distribution[29,30], named after Pierre Francois Verhulst[35] for his use in a study of population growth in 1845, is an S-curve with two asymptotes and is commonly represented by the following 4-parameter equation:

$$f(x) = y1 - L \,/\, (1 + \exp(-k * (x - a))), \quad (1)$$

where $y1$ is the upper asymptote, $L = y1 - y0$ with $y0$ equal to the lower asymptote, k is the S-curve shape steepness coefficient, and a, the x-value of the S-curve midpoint (sometimes denoted by $x0$).

To visualize this 4-parameter function, let us simplify it by assigning $y0 = 0$, and $y1 = 1$. Eq. (1) thus becomes a 2-parameter logistic distribution with two example plots given in Fig. 1. The parameter L is, therefore, a scale factor for the difference between the upper and the lower asymptotes.

An interesting property[29,30] of *f(x)* is given by the identity, *f(- x)* = 1 – *f(x).* In this paper, we also use an alternative form of Eq. (1) based on that identity as shown below:

$$f(x) = y1 - L * \{ \exp(-k * (x - a)) / [1 + \exp(-k * (x - a))] \}. \quad (2)$$

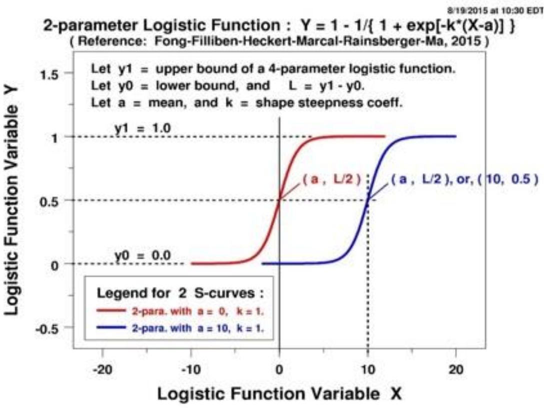


Figure 1. Plots of Two 2-parameter (*a, k*) Logistic distributions where the two asymptotes are assumed to be 0 (lower) and 1.0 (upper).

3. Uncertainty Source S-2 (Mesh Density)

In theory, as the finite element mesh density increases, the sequence of solutions of any variable of interest, say, the max. Mises stress at a specific point, converges to a stable value. This makes the logistic distribution an ideal candidate to model such a sequence. In Figs. 2-5, we show an example of this in the stress analysis of a wrench using a parametric feature of the COMSOL[24] and the nonlinear least squares fit macro of Dataplot[27]. As we increase the number of points from 5 (Fig. 6) to 10 (Fig. 8), we see that the predicted asymptotic stress converges.

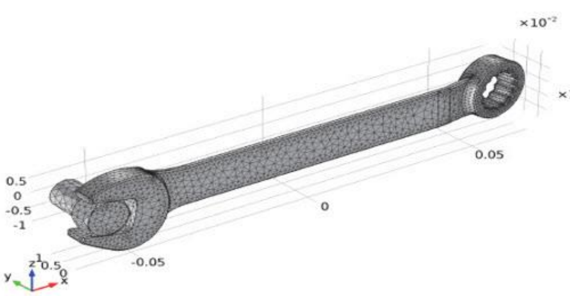


Figure 2. A wrench with a finite element mesh[24].

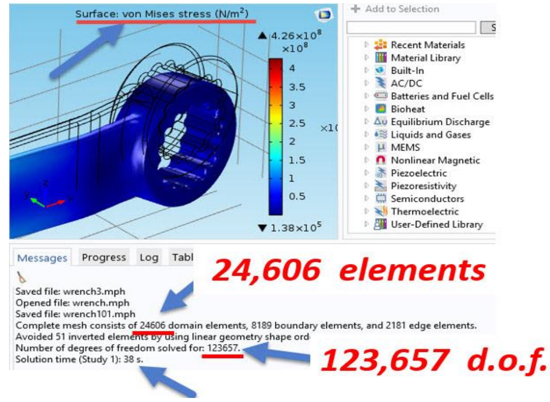


Figure 3. Result of a COMSOL meshing for a fine mesh with 24,606 tetra-04 elements & 123,657 d.o.f.

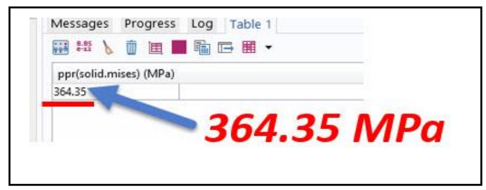
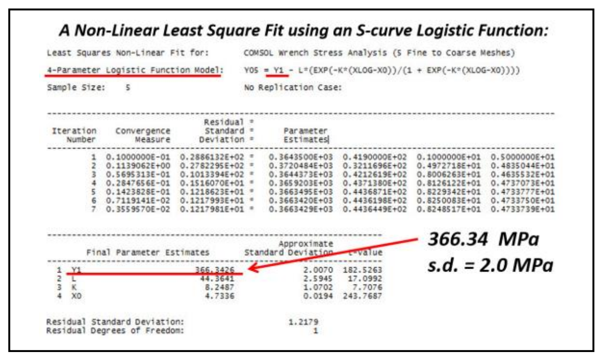


Figure 4. Max. Mises stress from COMSOL analysis.



A Non-Linear Least Square Fit using an S-curve Logistic Function:

Least Squares Non-Linear Fit for: COMSOL Wrench Stress Analysis (5 Fine to Coarse Meshes)
4-Parameter Logistic Function Model: Y05 = Y1 - L*(EXP(-K*(XLOG-X0))/(1 + EXP(-K*(XLOG-X0))))
Sample Size: 5 No Replication Case:

Iteration Number	Convergence Measure	Residual Standard Deviation	Parameter Estimates			
1	0.1000000E-01	0.2886132E+02	0.3643500E+03	0.4190000E+02	0.1000000E+01	0.5000000E+01
2	0.1139062E+00	0.2782295E+02	0.3720484E+03	0.3211696E+02	0.4972718E+01	0.4835044E+01
3	0.5695313E-01	0.1013394E+02	0.3644373E+03	0.4212619E+02	0.8006263E+01	0.4635532E+01
4	0.2847656E-01	0.1516070E+01	0.3659203E+03	0.4371380E+02	0.8126122E+01	0.4737073E+01
5	0.1423828E-01	0.1218623E+01	0.3663495E+03	0.4436871E+02	0.8229342E+01	0.4733777E+01
6	0.7119141E-02	0.1217993E+01	0.3663420E+03	0.4436198E+02	0.8250083E+01	0.4733750E+01
7	0.3559570E-02	0.1217981E+01	0.3663429E+03	0.4436449E+02	0.8248517E+01	0.4733739E+01

	Final Parameter Estimates		Approximate Standard Deviation	t-Value
1	Y1	366.3426	2.0070	182.5263
2	L	44.3641	2.5945	17.0992
3	K	8.2487	1.0702	7.7076
4	X0	4.7336	0.0194	243.7687

Residual Standard Deviation: 1.2179
Residual Degrees of Freedom: 1

Figure 5. Max. stress from a Dataplot[27] NL-LSQ fit.

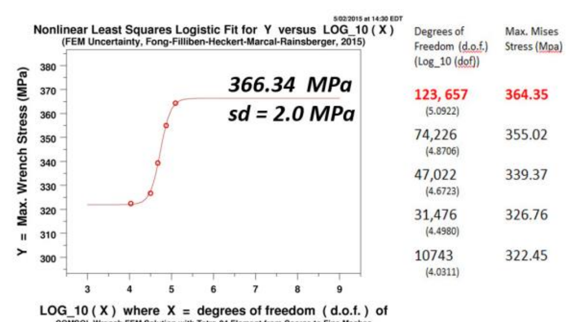


Figure 6. Plot of a 5-point Dataplot[27] NL-LSQ fit.

Table 2. Results of a Parametric Run in COMSOL

FEM Result Y (MPa)	Degrees of Freedom (dof) X
322.45	10743
326.76	31476
339.37	47022
355.02	74226
361.40	118750
364.35	127663
368.55	313970
369.24	732220
369.72	1119600
369.73	1517800
369.61	2113600
369.54	2670100
369.80	3411800
369.72	4193000
369.72	5033200
369.61	5919600
369.71	6,932,883

← 5th point In Fig. 6. (127663)

← 10th point In Fig. 7. (2113600)

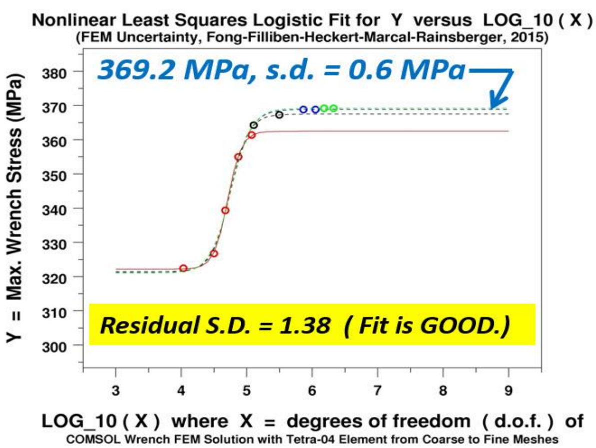


Figure 7. Plot of a 10-point Dataplot[27] NL-LSQ fit of COMSOL solution of stress analysis of a wrench.

4. Uncertainty Source S-1 (Element Type)

The existence of an automatic meshing algorithm for the 4-node tetrahedron element led FEM users to believe that one can obtain accurate result with a tetra-04 mesh by pushing the mesh density to its limit. In a recent paper by Marcal, Fong, et al.[21], that belief has been shown to be false. In other words, element type matters. This has led to the development of a "super-parametric" method, as implemented in TrueGrid[28], where the element type, mesh density, and solution platform are parametric in addition to model parameters. A typical TrueGrid output is given in Fig. 8, and two examples of UQ for S-1 (element type) are shown in Figs. 9 (cantilever) and 10 (elbow).

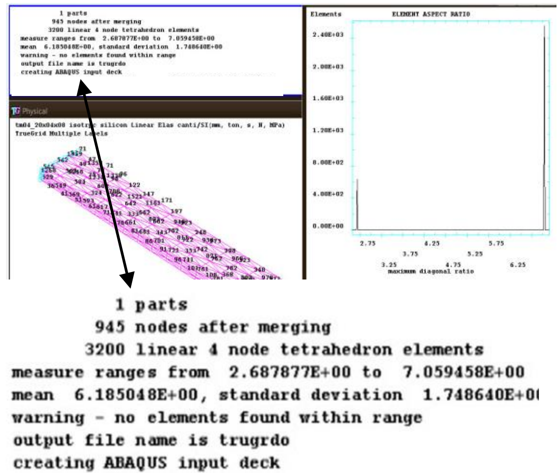


Figure 8. A typical screen output of a TrueGrid[28] code creating an ABAQUS code for a cantilever mesh.

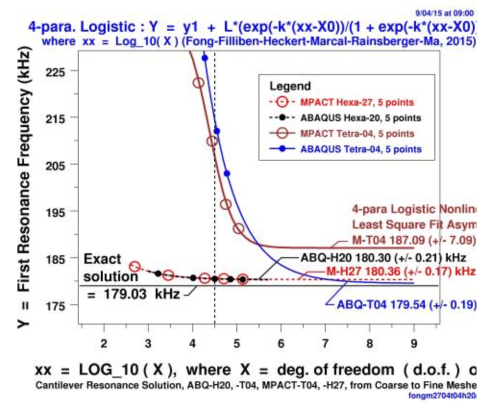


Figure 9. Plot of FEM for 3 element types, two solution platforms, and 5 mesh densities for a cantilever bending resonance frequency problem[23].

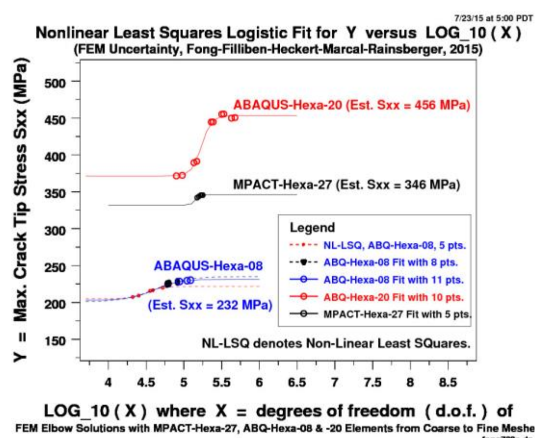
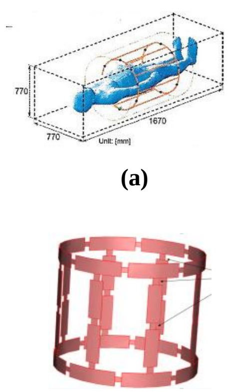


Figure 10. Plot of FEM results for 3 element types for UQ of max. crack-tip stress of an elbow weldment[21].

Excerpt from the Proceedings of the 2015 COMSOL Conference in Boston

5. Uncertainty S-3 (Model Parameters)

In COMSOL, one addresses the S-3 (model parameters) uncertainty problem by parametrizing geometrical parameters, material property coefficients, loadings, and boundary constraints, as shown in a recent UQ paper by Fong, Heckert, et al[20]. In Figs. 10 and 11, we show how one solves an optimization problem for the design of a magnetic resonance imaging (MRI) RF coil by applying a fractional factorial orthogonal design of experiments method[33,34]. In Fig. 12, we show that the UQ of an earlier design with 7 factors led us to an improved design with a much smaller standard deviation.



(a)

(b)

X1	X2	X3	X4	X5	X6	X7
-1	-1	-1	+1	+1	+1	-1
+1	-1	-1	-1	-1	+1	+1
-1	+1	-1	-1	+1	-1	+1
+1	+1	-1	+1	-1	-1	-1
-1	-1	+1	+1	-1	-1	+1
+1	-1	+1	-1	+1	-1	-1
-1	+1	+1	-1	-1	+1	-1
+1	+1	+1	+1	+1	+1	+1
+1	+1	+1	-1	-1	-1	+1
-1	+1	+1	+1	+1	-1	-1
+1	-1	+1	+1	-1	+1	-1
-1	-1	+1	-1	+1	+1	+1
+1	+1	-1	-1	+1	+1	-1
-1	+1	-1	+1	-1	+1	+1
+1	-1	-1	+1	+1	-1	+1
-1	-1	-1	-1	-1	-1	-1

(c)

Figure 11. (a) An MRI facility. (b) A prototype MRI RF coil. (c) A 7-factor 16-run fractional factorial orthogonal experimental design for UQ of the coil.

Table 3. Data for the 7-factor, 16-run UQ experiment

	X1	X2	X3	X4	X5	X6	X7
	Sigma	Epsilonr	C	V0	w1	L3	bet2
Base Run (00)	0.0001	80	177	500	80	35	5
Unit	*S/m*	*1*	*pF*	*volt*	*mm*	*mm*	*degree*
+ / - variation	10 %	5 %	2 %	2 %	5 %	10 %	10 %
Run No. (01)	0.00009	76	173.46	510	84	38.5	4.5
Run No. (02)	0.00011	76	173.46	490	76	38.5	5.5
Run No. (03)	0.00009	84	173.46	490	84	31.5	5.5
Run No. (04)	0.00011	84	173.46	510	76	31.5	4.5
Run No. (05)	0.00009	76	180.54	510	76	31.5	5.5
Run No. (06)	0.00011	76	180.54	490	84	31.5	4.5
Run No. (07)	0.00009	84	180.54	490	76	38.5	4.5
Run No. (08)	0.00011	84	180.54	510	84	38.5	5.5
Run No. (09)	0.00011	84	180.54	490	76	31.5	5.5
Run No. (10)	0.00009	84	180.54	510	84	31.5	4.5
Run No. (11)	0.00011	76	180.54	510	76	38.5	4.5
Run No. (12)	0.00009	76	180.54	490	84	38.5	5.5
Run No. (13)	0.00011	84	173.46	490	84	38.5	4.5
Run No. (14)	0.00009	84	173.46	510	76	38.5	5.5
Run No. (15)	0.00011	76	173.46	510	84	31.5	5.5
Run No. (16)	0.00009	76	173.46	490	76	31.5	4.5

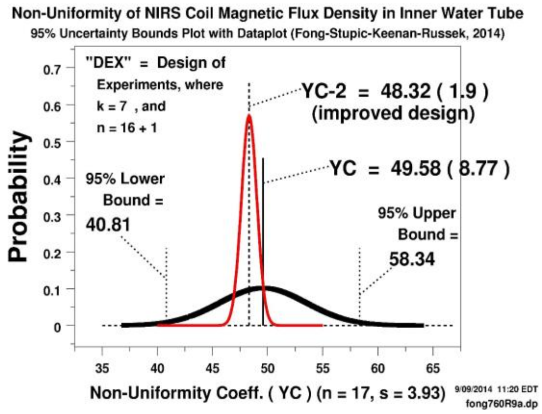


Figure 12. Plots for two UQ experiments with the first design (in black) and the improved design (in red).

6. Future Work

In this paper, we have shown through four test problems that the application of a nonlinear least squares fit method and a super-parametric method allows us to address 3 sources of FEM uncertainty, namely, the element type, the mesh density, and the modeling parameters. As listed in Table 1, we have shown elsewhere[8, 21-23] that the solution platform source can also be addressed using the super-parametric method in 3 test problems, TP-2, TP-3, and TP-4. To complete this investigation with 5 test problems and 4 UQ sources, we need to undertake what are missing in Table 1 as future work.

7. Significance & Limitations

The FEM UQ approach outlined in this paper is significant because both the NL-LSQ method and the super-parametric method are easy to implement to cover all 4 sources of uncertainty. The approach is limited in the sense that it is not applicable to addressing the question whether a model is physically correct.

8. Concluding Remark

We conclude that a rigorous tool using a 4-parameter logistic distribution and a nonlinear least squares fit method has been found to address all four sources of FEM uncertainty, when we combine the tool with a super-parametric and a design of experiments method.

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