Uncertainty of FEM Solutions using a Nonlinear Least Squares Fit Method and a Design of Experiments Approach

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**Co-authored by Fong, Heckert, Filliben, Marcal, and Rainsberger. This is a contribution of NIST. Not subject to copyright.**
Outline of Talk
(23 slides)

- (5) Why Accuracy in FEM Stress Estimates are Important?
- (5) COMSOL Solutions for a Wrench at different mesh densities.
- (1) What is a logistic distribution?
- (5) Uncertainty of COMSOL Wrench Solutions using NL-LSQ.
- (7) Stresses in a Cantilever Beam for different element types.
(1) Why Accuracy In FEM Stress Estimates Are Important?
Fig 1. plot of Log(Creep Rupture Time) vs Log (Stress)

slope \( C = -8.9 \)
Recent experimental results on Creep Rupture in Fig.1

Let $cv = \text{coefficient of variation} = \text{s.d.} / \text{estimated mean}$. 

Following Fong et al [2015] considering classical laws of error propagation, we establish Eq. (2) for the coefficient of variation ($cv$) of the creep rupture time, $t$, as a linear function of the $cv$ of stress, $\sigma$:

$$cv(t) = |C| \times cv(\sigma). \quad (2)$$

Need to assess carefully the uncertainty of the stress estimate,

1% variation in stress = 9% var. in creep rupture time
There are at least four sources of uncertainty in FEM:

1. Uncertainty due to **Element Type** (2015).
4. Uncertainty due to **Solution Platform** (2016).
Each flap represents a simple circuit or port element such as a 50 Ohm feed or a tuning capacitor.

(Standard finite element modeling approach for RF and Microwave components)

\[
\nabla \times \mu^{-1}_r (\nabla \times \mathbf{E}) - k_0^2 (\varepsilon_r - \frac{j \sigma}{\omega \varepsilon_0}) \mathbf{E} = 0
\n\]
Before:
NUC = 49.58 (8.77)

After:
NUC = 48.32 (1.90)
(2) COMSOL Solutions for a Wrench at different mesh densities.
Solved with COMSOL Multiphysics 5.0

Stresses and Strains in a Wrench

Introduction

This tutorial demonstrates how to set up a simple static structural analysis. The analysis is exemplified on a combination wrench during the application of torque on a bolt.

Despite its simplicity, and the fact that very few engineers would run a structural analysis before trying to turn a bolt, the example provides an excellent overview of structural analysis in COMSOL Multiphysics.

Model Definition

The model geometry is shown below.

For the purpose of this model, assume that there is perfect contact between the wrench and the bolt. A possible extension of the model is to apply a contact condition between the wrench and the bolt where the friction and the contact pressure determines the position of the contact surface.

Model Library path: COMSOL_Multiphysics/Structural_Mechanics/wrench
Oct. 8, 2015, 1:00 p.m. Boston Conf. Session on Optimization & Simulation Methods

Fine

Fine
Element Size: Fine

Oct. 8, 2015, 1:00 p.m. Boston Conf. Session on Optimization & Simulation Methods

24,606 elements
123,657 d.o.f.
Element Size: Fine

364.35 MPa
<table>
<thead>
<tr>
<th>Element Size</th>
<th>Degrees of Freedom (d.o.f.) (Log₁₀ (dof))</th>
<th>Max. Mises Stress (MPa)</th>
<th>% of Stress (100 for fine)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fine</td>
<td>123,657 (5.0922)</td>
<td>364.35</td>
<td>(100 %)</td>
</tr>
<tr>
<td>Normal</td>
<td>74,226 (4.8706)</td>
<td>355.02</td>
<td>(97.4 %)</td>
</tr>
<tr>
<td>Coarse</td>
<td>47,022 (4.6723)</td>
<td>339.37</td>
<td>(93.1 %)</td>
</tr>
<tr>
<td>Coarser</td>
<td>31,476 (4.4980)</td>
<td>326.76</td>
<td>(89.7 %)</td>
</tr>
<tr>
<td>Extremely Coarse</td>
<td>10743 (4.0311)</td>
<td>322.45</td>
<td>(88.5 %)</td>
</tr>
</tbody>
</table>
(3) What is a logistic distribution?

Pierre Francois Verhulst (1845)

\[ f(x) = y_1 - L / \left( 1 + \exp \left( -k \ast (x - a) \right) \right), \]

3-parameter Logistic: \( Y = L - L \ast \left\{ \exp[-k\ast(X-a)] / [1 + \exp[-k\ast(X-a)]] \right\} \)

Legend for 2 S-curves:
- 3-p: \( a = 0, k = 1, L = 10 \)
- 3-p: \( a = 10, k = 1, L = 10 \)

Let \( y_1 \) = upper bound of a 4-parameter logistic function.
Let \( y_0 \) = lower bound = 0, and \( L = y_1 - y_0 = y_1 \).
Let \( a \) = mean, and \( k \) = shape steepness coeff.

\( y_1 = 10.0 \) (\( \approx L \))
\( y_0 = 0.0 \)
\( (a, L/2) \) or \( (10, 5.0) \)
A Non-Linear Least Square Fit using an S-curve Logistic Function:

\[
Y_0 = Y_1 - L \times \frac{\exp(-K \times (X_{LOG} - X_0))}{1 + \exp(-K \times (X_{LOG} - X_0))}
\]

Sample Size: 5

<table>
<thead>
<tr>
<th>Iteration Number</th>
<th>Convergence Measure</th>
<th>Residual Standard Deviation</th>
<th>Parameter Estimates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1000000E-01</td>
<td>0.2886132E+02</td>
<td>0.3643500E+03</td>
</tr>
<tr>
<td>2</td>
<td>0.1139062E+00</td>
<td>0.2782295E+02</td>
<td>0.3720484E+03</td>
</tr>
<tr>
<td>3</td>
<td>0.5695131E-01</td>
<td>0.1013394E+02</td>
<td>0.3644373E+03</td>
</tr>
<tr>
<td>4</td>
<td>0.2847656E-01</td>
<td>0.1516070E+01</td>
<td>0.3659203E+03</td>
</tr>
<tr>
<td>5</td>
<td>0.1423828E-01</td>
<td>0.1218623E+01</td>
<td>0.3663493E+03</td>
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<tr>
<td>6</td>
<td>0.7119141E-02</td>
<td>0.1217993E+01</td>
<td>0.3663420E+03</td>
</tr>
<tr>
<td>7</td>
<td>0.3559570E-02</td>
<td>0.1217981E+01</td>
<td>0.3663429E+03</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Final Parameter Estimates</th>
<th>Approximate Standard Deviation</th>
<th>t-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Y_1</td>
<td>366.3426</td>
<td></td>
</tr>
<tr>
<td>L</td>
<td>44.3641</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>8.2487</td>
<td></td>
</tr>
<tr>
<td>X_0</td>
<td>4.7336</td>
<td></td>
</tr>
</tbody>
</table>

Residual Standard Deviation: 1.2179
Residual Degrees of Freedom: 1

366.34 MPa
s.d. = 2.0 MPa
Nonlinear Least Squares Logistic Fit for $Y$ versus $\log_{10}(X)$
(FEM Uncertainty, Fong-Filliben-Heckert-Marcal-Rainsberger, 2015)

$Y = \text{Max. Wrench Stress (MPa)}$

$366.34 \text{ MPa}$

$sd = 2.0 \text{ MPa}$

LOG$_{10}(X)$ where $X =$ degrees of freedom (d.o.f.) of
COMSOL Wrench FEM Solution with Tetra-04 Element from Coarse to Fine Meshes

Degrees of Freedom (d.o.f.)
(Log$_{10}$ (dof))

<table>
<thead>
<tr>
<th>Degrees of Freedom</th>
<th>Max. Mises Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>123, 657</td>
<td>364.35</td>
</tr>
<tr>
<td>(5.0922)</td>
<td></td>
</tr>
<tr>
<td>74,226</td>
<td>355.02</td>
</tr>
<tr>
<td>(4.8706)</td>
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<td></td>
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<td>10743</td>
<td>322.45</td>
</tr>
<tr>
<td>(4.0311)</td>
<td></td>
</tr>
</tbody>
</table>
Predicted Max. Mises Stress = 366.34 MPa, s.d. = 2.0 MPa.

Question: Is that good enough?
Max. Mises Stress = 369.71 MPa = 6,932,883 (d.o.f.)
Nonlinear Least Squares Logistic Fit for $Y$ versus $\log_{10}(X)$
(FEM Uncertainty, Fong-Filliben-Heckert-Marcal-Rainsberger, 2015)

369.2 MPa, s.d. = 0.6 MPa

Residual S.D. = 1.38 (Fit is GOOD.)

$Y = \text{Max. Wrench Stress (MPa)}$

$\log_{10}(X)$ where $X = \text{degrees of freedom (d.o.f.) of COMSOL Wrench FEM Solution with Tetra-04 Element from Coarse to Fine Meshes}$

Ans. Max. Mises Stress at 95% confidence level = (368.0, ..., 370.4 MPa)
(5) Stresses in a Cantilever Beam for Different element types.
Hexahedron – 8-node, or, Hexa-8.

Tetrahedron – 4-node, or, Tetra-4.

Hexahedron – 20 nodes or, Hexa-20

Hexahedron – 27 nodes or, Hexa-27

Tetrahedron – 10-node, or, Tetra-10.
Pascal Triangle
FEM Uncertainty due to Element Type

Truncation error in displacement method in FEA, \( u \) is a single d.o.f. and \( \{a\} \) the undetermined coefficients, and \( h(0)^n \) the truncation error.

- For quadrilaterals in 2-D with 9 nodes
  \[
  u = [1, x, xy, y, x^2, x^2y, x^2y^2, xy^2, y^2] \{a\} + h(0)^3
  \]

- For simplex elements in 2-D with 6 nodes
  \[
  u = [1, x, xy, y, x^2, y^2] \{a\} + h(0)^2
  \]
Tetrahedron – 4-node, 
or, **Tetra-4.**

Hexahedron – 8-node, 
or, **Hexa-8.**

Hexahedron- 20 nodes 
or, **Hexa-20**

Hexahedron- 27 nodes 
or, **Hexa-27**
Nonlinear Least Squares Logistic Fit for $Y$ versus $\text{LOG}_{10}(X)$

(FEM Uncertainty, Fong-Filliben-Heckert-Marcal-Rainsberger-Ma, 2015)

Sample size = $n = 5$

$Y(1) = 1,028$ MPa for $X(1) = \text{dof}(1) = 495$.
$Y(2) = 1,266$ MPa for $X(2) = \text{dof}(2) = 2,835$.
$Y(3) = 1,354$ MPa for $X(3) = \text{dof}(3) = 8,463$.
$Y(4) = 1,401$ MPa for $X(4) = \text{dof}(4) = 18,819$.
$Y(5) = 1,455$ MPa for $X(5) = \text{dof}(5) = 35,343$.

$Y = \text{Max. bending stress (MPa)}$

$\text{LOG}_{10}(X)$ where $X = \text{d.o.f. of MPACT Beam hexa27 Coarse to Fine Mesh Densities}$

where d.o.f. (dof) = degrees of freedom.
Nonlinear Least Squares Logistic Fit for $Y$ versus $\text{LOG}_{10} (X)$

(FEM Uncertainty, Fong-Filliben-Heckert-Marcal-Rainsberger-Ma, 2015)

Sample size $= n = 5$. Smallest $Y = 1028$ MPa (dof = 495)
Largest $Y = 1455$ MPa (dof = 35,343)

Let $xx = \log_{10} (X)$. Let $yy = Y$.
Assume lower bound $= 0$.

Nonlinear Least Sq. 3-para Logistic Fit:

Let $yy = y1 \left\{ \frac{1}{1 + \exp(-k(xx-x0))} \right\}$
where starting $y1 =$ largest $yy$-data ($= 1455$ MPa)
starting $x0 =$ ave. of $xx$-data ($= 3.5$)
and $k =$ shape steepness coeff. (start with $k = 1.0$)

Residual Stand. Dev. $= 12.48$ (Logistic Fit is good.)

$Y =$ Max. bending stress (MPa)

$\text{LOG}_{10} (X)$ where $X =$ d.o.f. of MPACT Beam hexa27 Coarse to Fine Mesh Densities

where d.o.f. (dof) = degrees of freedom.
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Tetrahedron – 4-node, or, Tetra-4.

Hexahedron – 8-node, or, Hexa-8.

Hexahedron – 20 nodes or, Hexa-20

Hexahedron – 27 nodes or, Hexa-27

Nonlinear Least Squares Logistic Fit for $Y$ versus $\log_{10}(X)$
(FEM Uncertainty, Fong-Filliben-Heckert-Marcal-Rainsberger-Ma, 2015)

Cantilever Beam Max. Stress
= 1500 MPa (theoretical)

Logistic function estimated upper bound
= 1560 MPa (MPACT-Hexa-27, + 4.0% error)
= 1462 MPa (ABAQUS-Hexa-08, - 2.5% error)
= 1383 MPa (ABQ-Tetra-04, 12 pts., -7.8%)
= 1339 MPa (ABQ-Tetra-04, 10 pts., -10.7%)
= 1344 MPa (MPACT-Hexa-08, -10.4% error)

Line of Extrapolated Stresses at
$X = 5.3$, or, 200K degrees of freedom

Legend
- -. MPACT-Hexa-27 Fit with 5 points.
- -. ABAQUS-Hexa-08 Fit with 11 points.
- -. MPACT-Hexa-08 Fit with 11 points.
- -. ABAQUS-Tetra-04 Fit with 10 points.
- -. ABAQUS-Tetra-04 Fit with 2 more points.

$Y = \text{Max. bending stress (MPa)}$

$\log_{10}(X)$ where $X = \text{degrees of freedom (d.o.f.)}$ of
ABAQUS Hexa08 (black), Tetra04 (blue), MPACT Beam hexa27 (red) and hexa08 (green)

fem51.dp
In this talk, we show how one can quantify FEM uncertainties due to the following three sources:

1. Uncertainty due to **Element Type (2015)**.
2. Uncertainty due to **Mesh Density (2015)**.
3. Uncertainty due to **Model Parameters (2014)**.

In 2016, we will show that a combination of the NL-LSQ fit method and the design of experiments approach can address uncertainty due to the 4th source, namely,

4. Uncertainty due to **Solution Platform (2016)**.

(6) Concluding Remarks.
Disclaimer

Certain commercial equipment, instruments, materials, or computer software are identified in this talk in order to specify the experimental or computational procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards & Technology, nor is it intended to imply that the materials, equipment, or software identified are necessarily the best available for the purpose.
Dr. Jeffrey T. Fong has been Physicist and Project Manager at the Applied and Computational Mathematics Division, Information Technology Laboratory, National Institute of Standards and Technology (NIST), Gaithersburg, MD, since 1966.

He was educated at the University of Hong Kong (B.Sc., Engineering, first class honors, 1955), Columbia University (M.S., Engineering Mechanics, 1961), and Stanford (Ph.D., Applied Mechanics and Mathematics, 1966). Prior to 1966, he worked as a design engineer (1955-63) on numerous power plants (hydro, fossil-fuel, nuclear) at Ebasco Services, Inc., in New York City, and as teaching & research assistant (1963-66) on engineering mechanics at Stanford University.

During his 40+ years at NIST, he has conducted research, provided consulting services, and taught numerous short courses on mathematical and computational modeling with uncertainty estimation for fatigue, fracture, high-temperature creep, nondestructive evaluation, electromagnetic behavior, and failure analysis of a broad range of materials ranging from paper, ceramics, glass, to polymers, composites, metals, semiconductors, and biological tissues.

A licensed professional engineer (P.E.) in the State of New York since 1962 and a chartered civil engineer in the United Kingdom and British Commonwealth (A.M.I.C.E.) since 1968, he has authored or co-authored more than 100 technical papers, and edited or co-edited 17 national or international conference proceedings. He was elected Fellow of ASTM in 1982 and Fellow of ASME in 1984. In 1993, he was awarded the prestigious ASME Pressure Vessels and Piping Medal. Most recently, he was honored at the 2014 International Conference on Computational & Experimental Engineering & Sciences (ICCES) with a Lifetime Achievement Medal.

Since 2006, he has been Adjunct Professor of Mechanical Engineering and Mechanics at Drexel University and taught a graduate-level 3-credit course on “Finite Element Method Uncertainty Analysis.” Since Jan. 2010, he has given every 6 months an on-line 3-hour short course at Stanford University on “Reliability and Uncertainty Estimation of FEM Models of Composite Structures.” In 2012, he was appointed Adjunct Professor of Nuclear and Risk Engineering at the City University of Hong Kong, and Distinguished Guest Professor at the East China University of Science & Technology, Shanghai, China, to teach annually a 1-credit 16-hour short course on “Engineering Reliability and Risk Analysis.”