

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

Jeffrey T. Fong, Ph.D., P.E.

Physicist and Project Manager

*Applied & Computational Mathematics Division
National Institute of Standards & Technology (NIST)
Gaithersburg, MD 20899-8910, U.S.A.*

<http://www.nist.gov/itl/math/jeffrey-t-fong.cfm>

(301) 975-8217 fong@nist.gov

COMSOL
CONFERENCE
2015 BOSTON

***Co-authored by Fong, Heckert, Filliben, Marcal, and Rainsberger.
This is a contribution of NIST. Not subject to copyright.*

Outline of Talk

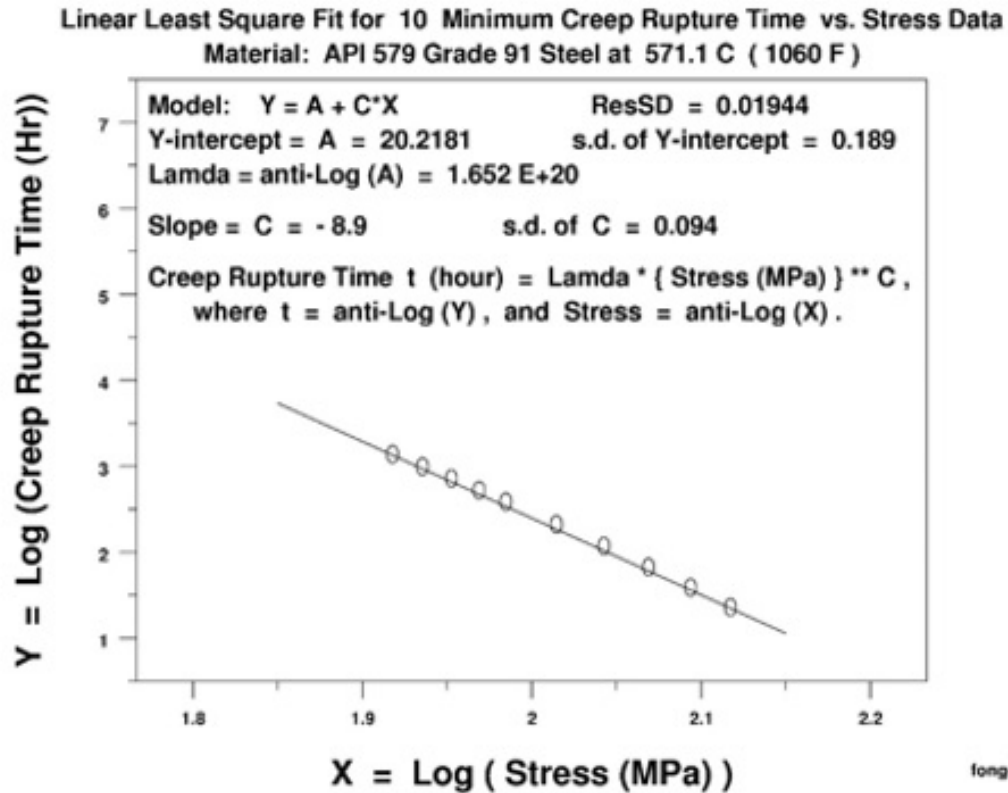
(23 slides)

- (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 = coefficient of variation = s.d. / 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, σ :

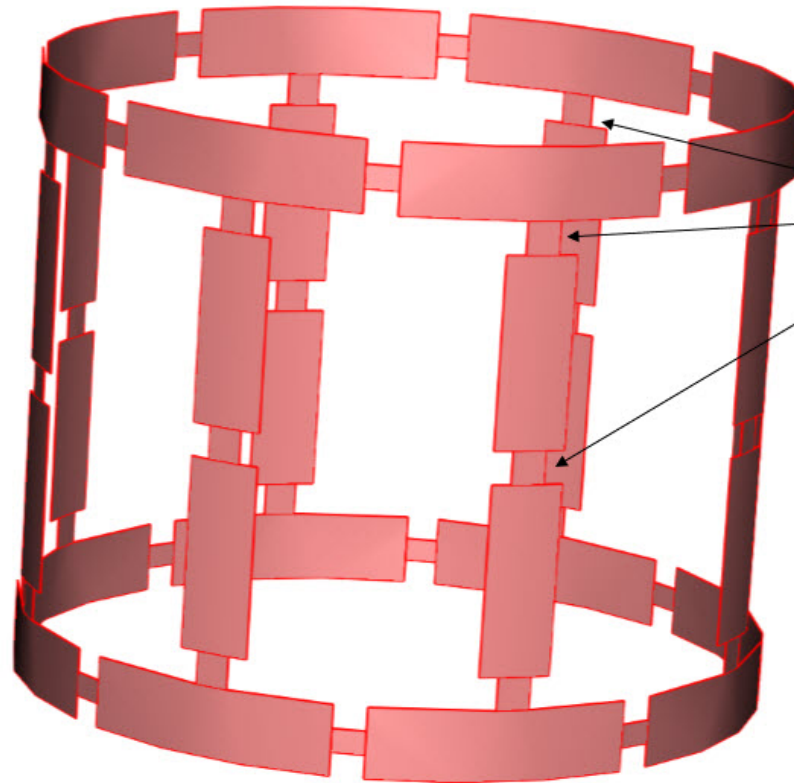
$$cv(t) = |C| * cv(\sigma). \quad (2)$$

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).
- (2) Uncertainty due to Mesh Density (2015).
- (3) Uncertainty due to **Model Parameters (2014)**.
- (4) Uncertainty due to **Solution Platform (2016)**.

- MRI

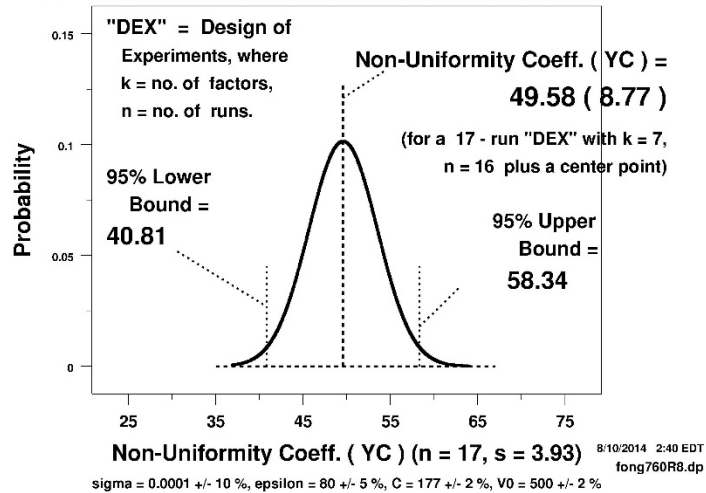


Each flap represents a simple circuit or port element such as a 50 Ohm feed or a tuning capacitor.

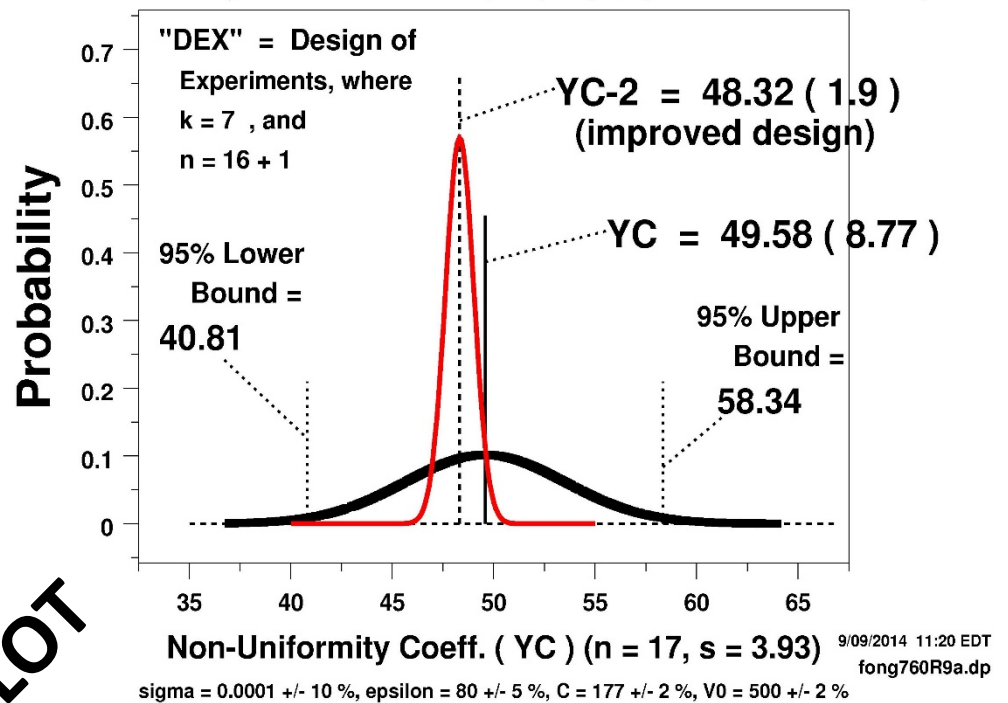
(Standard finite element modeling approach for RF and Microwave components)

$$\nabla \times \mu_r^{-1}(\nabla \times \mathbf{E}) - k_0^2(\epsilon_r - \frac{j\sigma}{\omega\epsilon_0})\mathbf{E} = 0$$

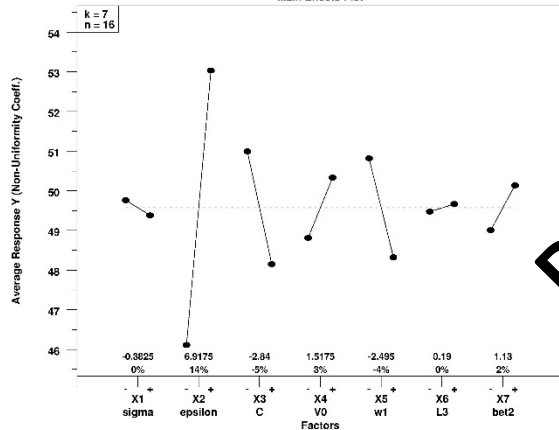
Non-Uniformity of NIRS Coil Magnetic Flux Density in Inner Water Tube
95% Uncertainty Bounds Plot with Dataplot (Fong-Stupic-Keenan-Russek, 2014)



Non-Uniformity of NIRS Coil Magnetic Flux Density in Inner Water Tube
95% Uncertainty Bounds Plot with Dataplot (Fong-Stupic-Keenan-Russek, 2014)



Step 3 COMSOL-RF Analysis of NIRS Birdcage Coil with High C and Inner Water Tube
Main Effects Plot



DATAPLOT

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

Solved with COMSOL Multiphysics 5.0

Stresses and Strains in a Wrench

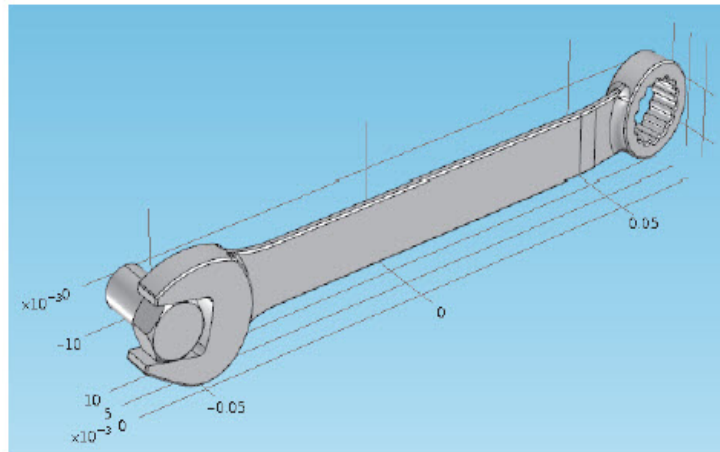
Introduction

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.

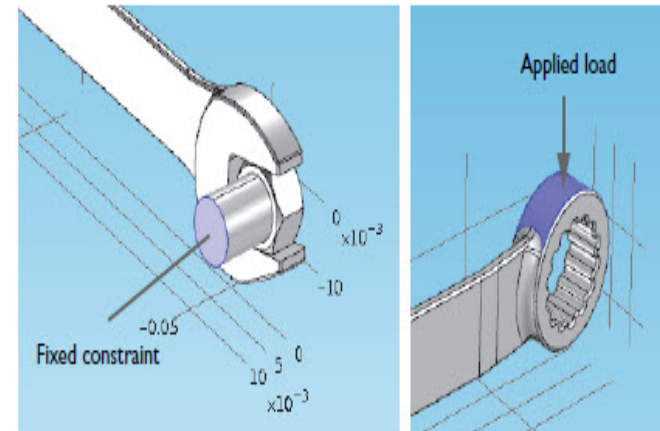
Despite its simplicity, and the fact that very few engineers would run a structural analysis before trying to turn a bolt, the example provides an excellent overview of structural analysis in COMSOL Multiphysics.

Model Definition

The model geometry is shown below.

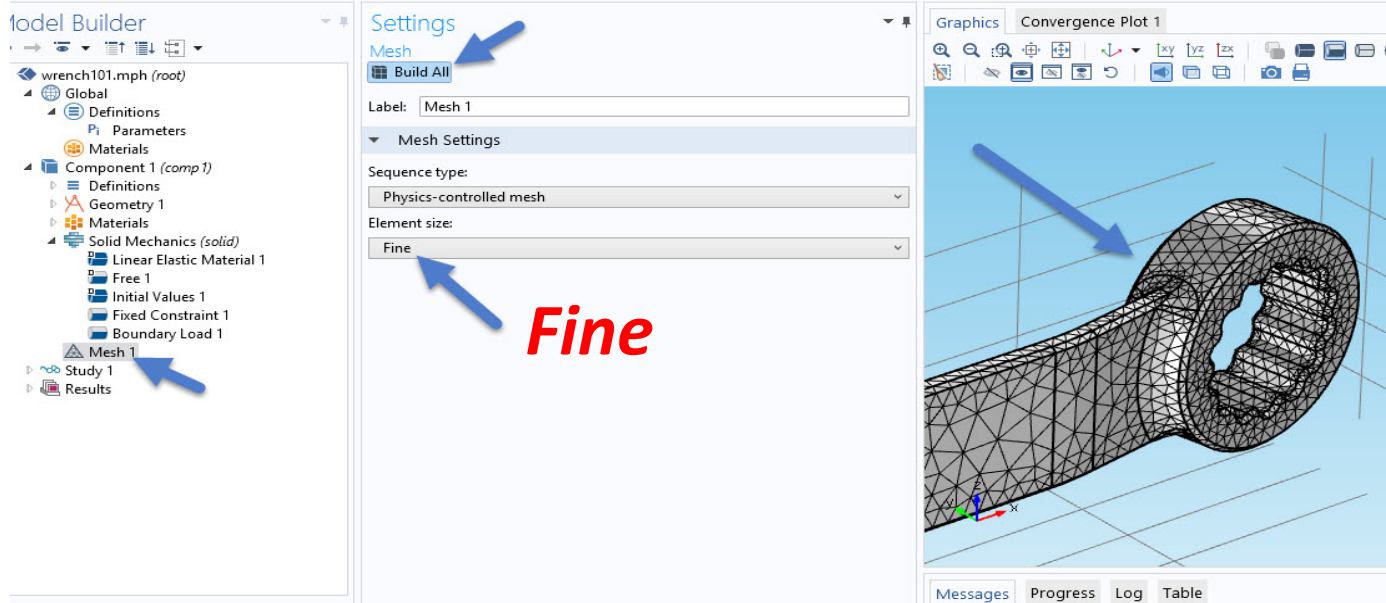
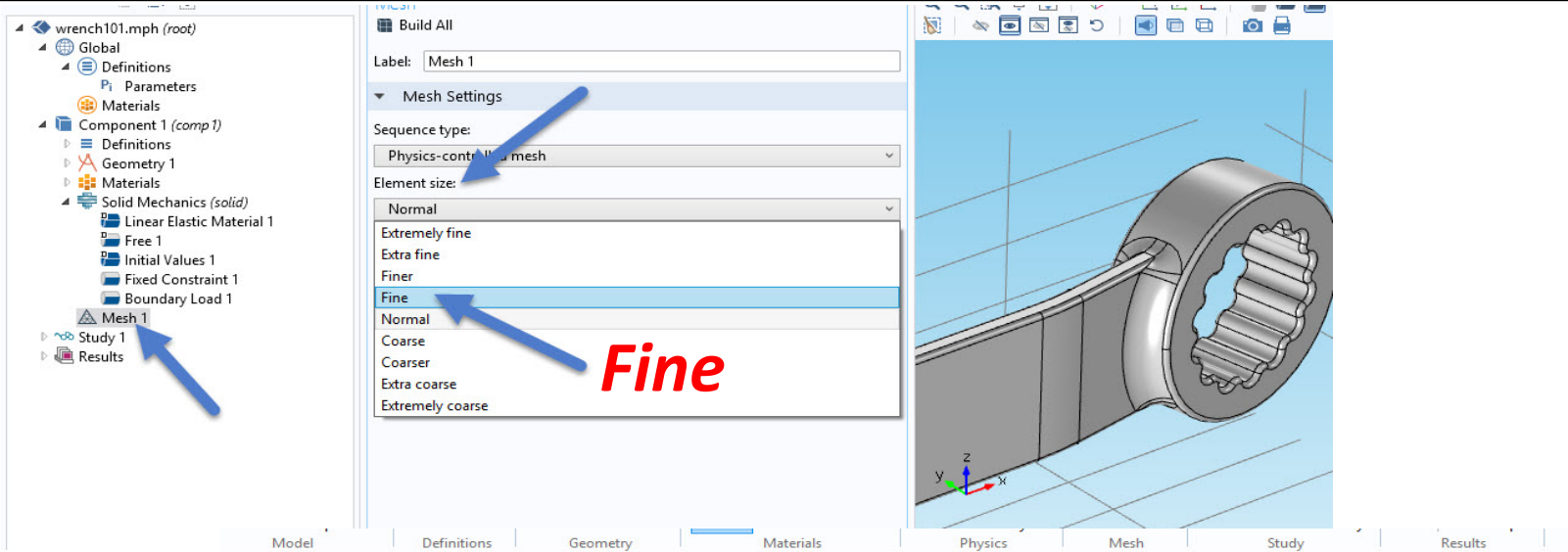


The bolt's fixed constraint is at the cross section shown below. A load is applied at the box end of the combination wrench.



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



Element Size: Fine

24,606 elements

123,657 d.o.f.

Element Size: Fine

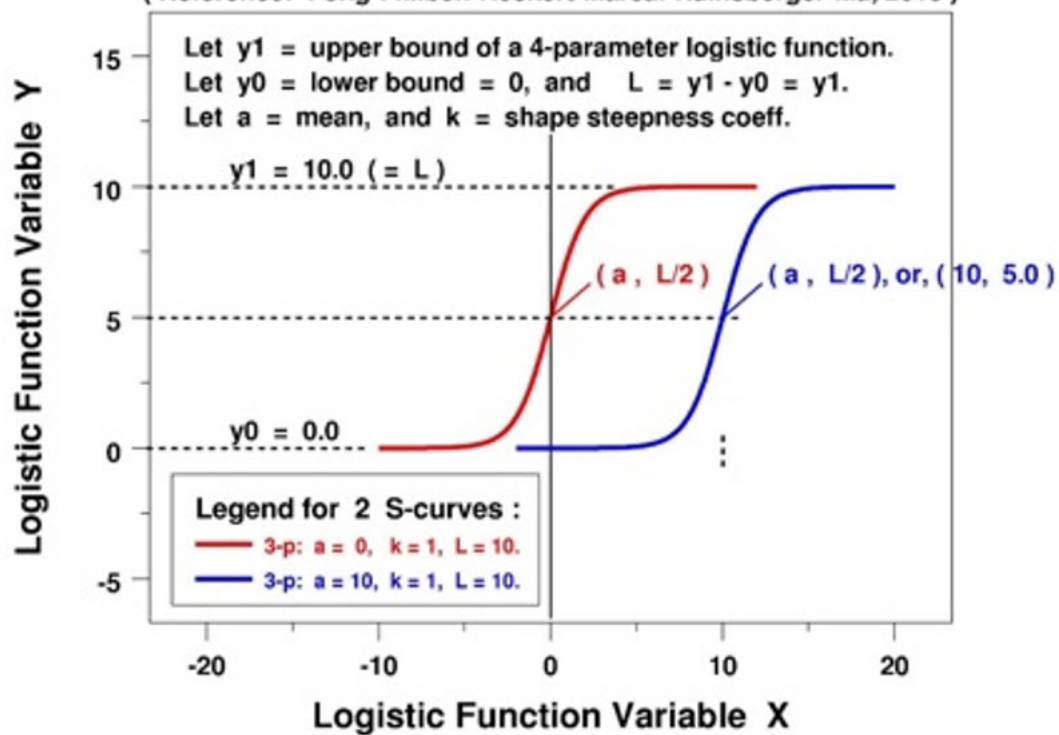
The screenshot displays the ANSYS Workbench interface for a finite element analysis. The 'Model Builder' on the left shows a tree view with 'Component 1' containing 'Solid Mechanics (solid)' and 'Mesh 1'. The 'Settings' panel for 'Volume Maximum' is open, showing the expression 'ppr(solid.mises)' and unit 'MPa'. The 'Graphics' panel shows a 3D model of a wrench handle with a stress distribution. A blue arrow points to the 'Evaluate' button in the Settings panel, and another blue arrow points to the value '364.35' in the Messages panel, which is highlighted in red. The text '364.35 MPa' is written in large red font next to the value.

| Element Size | Degrees of Freedom (d.o.f.) (Log ₁₀ (dof)) | Max. Mises Stress (MPa) | % of Stress (100 for fine) |
|------------------|--|-------------------------|-------------------------------|
| Fine | 123,657 (5.0922) | 364.35 | (100 %) |
| Normal | 74,226 (4.8706) | 355.02 | (97.4 %) |
| Coarse | 47,022 (4.6723) | 339.37 | (93.1 %) |
| Coarser | 31,476 (4.4980) | 326.76 | (89.7 %) |
| Extremely Coarse | 10743 (4.0311) | 322.45 | (88.5 %) |

Pierre Francois Verhulst (1845)

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

3-parameter Logistic : $Y = L - L * \{ \exp[-k*(X-a)] / [1 + \exp[-k*(X-a)]] \}$
 (Reference: Fong-Filliben-Heckert-Marcial-Rainsberger-Ma, 2015)



(4) Uncertainty
of
COMSOL Wrench Solutions
Using
Nonlinear Least Squares
(NL-LSQ) Fit.

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 |

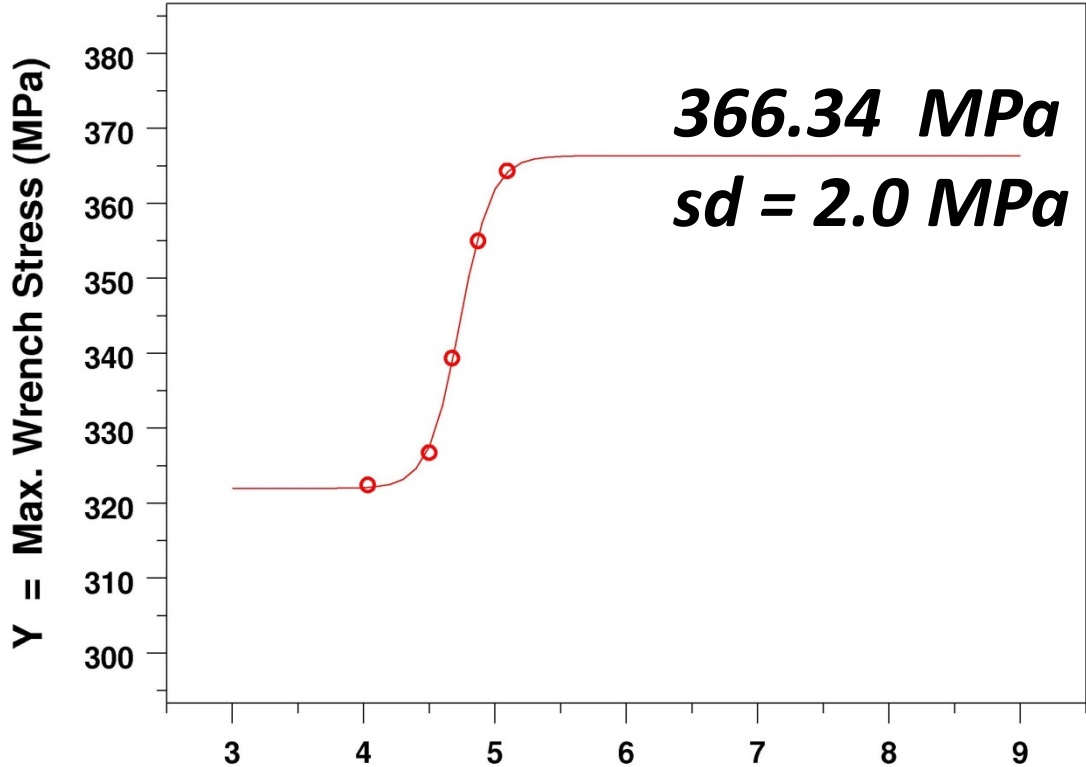
| Final Parameter Estimates | | Approximate Standard Deviation | t-value |
|---------------------------|----|--------------------------------|-----------------|
| 1 | Y1 | 366.3426 | 2.0070 182.5263 |
| 2 | L | 44.3641 | 2.5945 17.0992 |
| 3 | K | 8.2487 | 1.0702 7.7076 |
| 4 | X0 | 4.7336 | 0.0194 243.7687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

366.34 MPa
s.d. = 2.0 MPa

Residual Standard Deviation: 1.2179
Residual Degrees of Freedom: 1

5/02/2015 at 14:30 EDT

Nonlinear Least Squares Logistic Fit for Y versus LOG₁₀ (X)
 (FEM Uncertainty, Fong-Filliben-Heckert-Marcial-Rainsberger, 2015)



| Degrees of Freedom (d.o.f.) (Log ₁₀ (dof)) | Max. Mises Stress (Mpa) |
|---|-------------------------|
| 123,657 (5.0922) | 364.35 |
| 74,226 (4.8706) | 355.02 |
| 47,022 (4.6723) | 339.37 |
| 31,476 (4.4980) | 326.76 |
| 10743 (4.0311) | 322.45 |

LOG₁₀ (X) where X = degrees of freedom (d.o.f.) of
 COMSOL Wrench FEM Solution with Tetra-04 Element from Coarse to Fine Meshes

fem6b.dp

| Element Size | Degrees of Freedom (d.o.f.) (Log ₁₀ (dof)) | Max. Mises Stress (Mpa) |
|------------------|--|-------------------------|
| Fine | 123,657 (5.0922) | 364.35 |
| Normal | 74,226 (4.8706) | 355.02 |
| Coarse | 47,022 (4.6723) | 339.37 |
| Coarser | 31,476 (4.4980) | 326.76 |
| Extremely Coarse | 10743 (4.0311) | 322.45 |

Predicted Max. Mises Stress = **366.34 MPa**, s.d. = **2.0 MPa**.

Question: Is that good enough ?

Settings

Table Graph

Plot

Label: Table Graph 1

Data

Table: Table 2

x-axis data: Number of degrees of freedom (1)

Plot columns: Manual

Columns:

| |
|----------------------------------|
| hd |
| ppr(solid.mises) (MPa) |
| Number of degrees of freedom (1) |

Transformation: None

Plot imaginary part

Preprocessing

Coloring and Style

Line style

Graphics

Convergence Plot 1

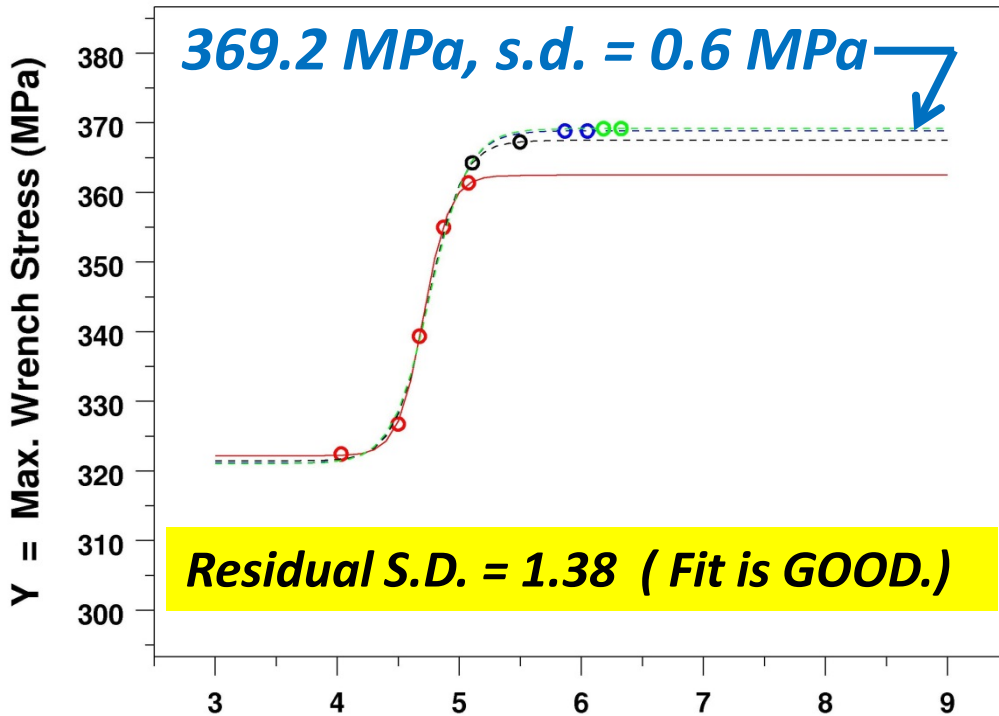
Messages Progress Log Table 2

| hd | ppr(solid.mises) (MPa) | Number of degrees of freedom (1) |
|---------|------------------------|----------------------------------|
| 1.0000 | 361.40 | 1.1875E5 |
| 2.0000 | 368.55 | 3.1397E5 |
| 3.0000 | 369.24 | 7.3222E5 |
| 4.0000 | 369.72 | 1.1196E6 |
| 5.0000 | 369.73 | 1.5178E6 |
| 6.0000 | 369.61 | 2.1136E6 |
| 7.0000 | 369.54 | 2.6701E6 |
| 8.0000 | 369.80 | 3.4118E6 |
| 9.0000 | 369.72 | 4.1930E6 |
| 10.0000 | 369.72 | 5.0332E6 |
| Li | 369.61 | 5.9196E6 |
| C | <u>369.71</u> | <u>6.9329E6</u> |

Max. Mises Stress = 369.71 MPa = 6,932,883 (d.o.f.)

4/30/2015 at 21:30 EDT

Nonlinear Least Squares Logistic Fit for Y versus LOG₁₀ (X)
 (FEM Uncertainty, Fong-Filliben-Heckert-Marcial-Rainsberger, 2015)



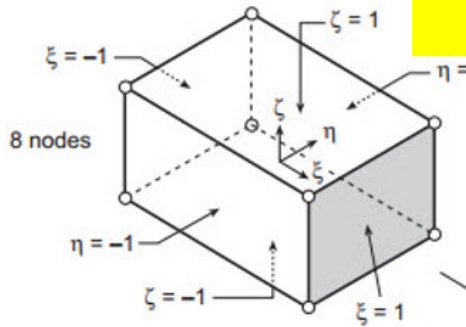
| FEM Result Y (MPa) | Degrees of Freedom (dof) X |
|--------------------|----------------------------|
| 322.45 | 10743 |
| 326.76 | 31476 |
| 339.37 | 47022 |
| 355.02 | 74226 |
| 361.40 | 118750 |
| 364.35 | 127663 |
| 368.55 | 313970 |
| 369.24 | 732220 |
| 369.72 | 1119600 |
| 369.73 | 1517800 |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

LOG₁₀ (X) where X = degrees of freedom (d.o.f.) of
 COMSOL Wrench FEM Solution with Tetra-04 Element from Coarse to Fine Meshes

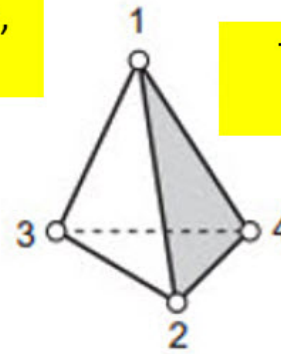
fem7_cms_0506070809_10_12.dp

Ans. Max. Mises Stress at 95 % confidence level = (368.0, , 370.4 MPa)

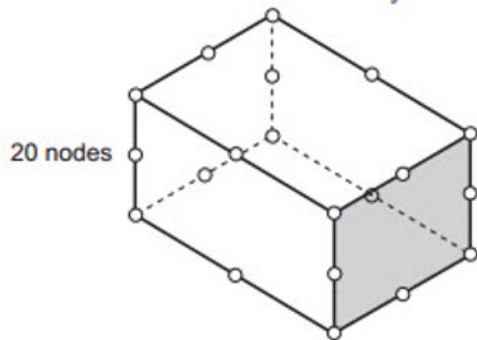
(5) Stresses
in a
Cantilever Beam for
Different
element types.



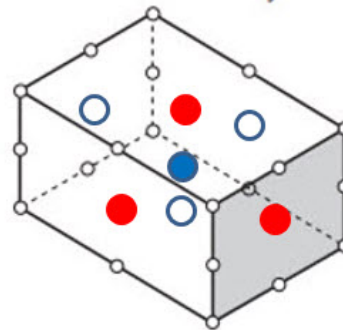
Hexahedron – 8-node,
or, **Hexa-8.**



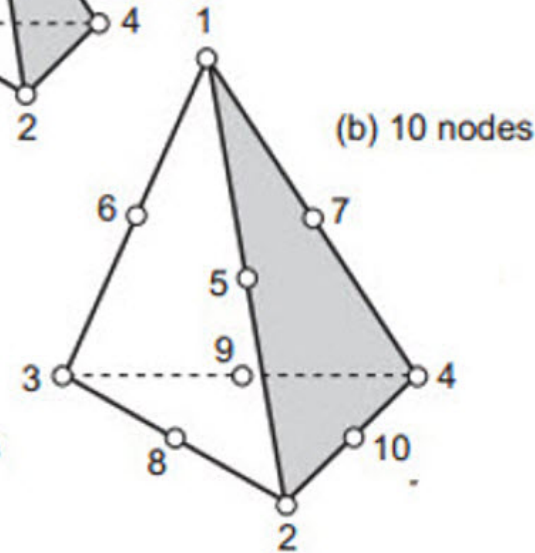
Tetrahedron – 4-node,
or, **Tetra-4.**



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

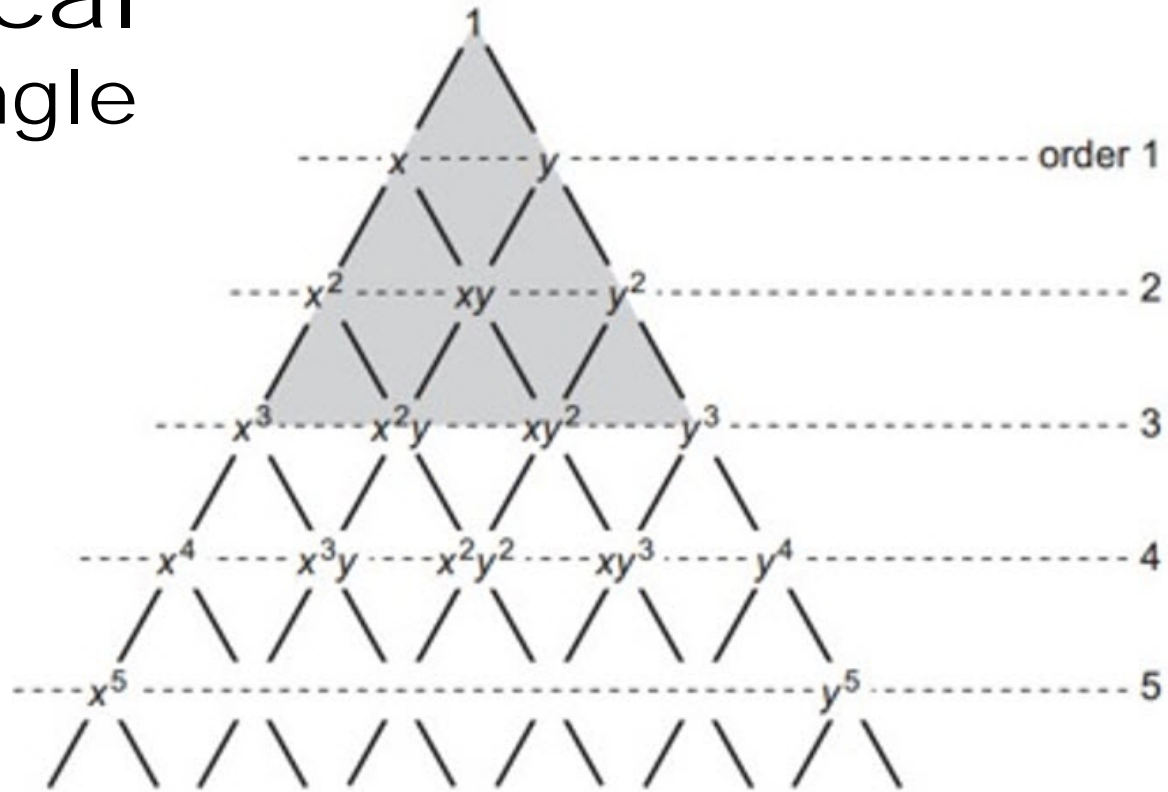


Hexahedron- 27 nodes
or, **Hexa-27**



Tetrahedron – 10-node,
or, **Tetra-10.**

Pascal Triangle



FEM Uncertainty due to Element Type

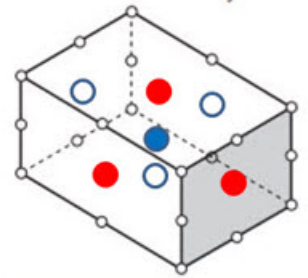
Truncation error in displacement method in FEA, u is a single d.o.f. and $\{a\}$ the undetermined coefficients, and $h(0)^n$ the truncation error.

- For quadrilaterals in 2-D with 9 nodes

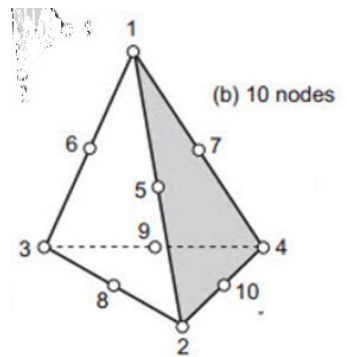
$$u = [1, x, xy, y, x^2, x^2y, x^2y^2, xy^2, y^2] \{a\} + h(0)^3$$

- For simplex elements in 2-D with 6 nodes

$$u = [1, x, xy, y, x^2, y^2] \{a\} + h(0)^2$$

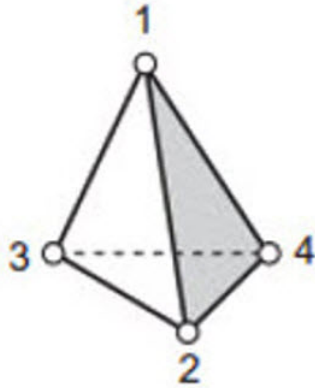


Hexahedron- 27 nodes or, **Hexa-27**

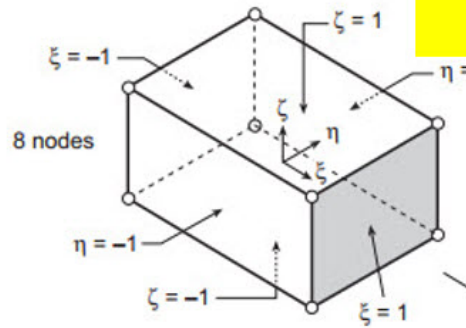


Tetrahedron – 10-node, or, **Tetra-10.**

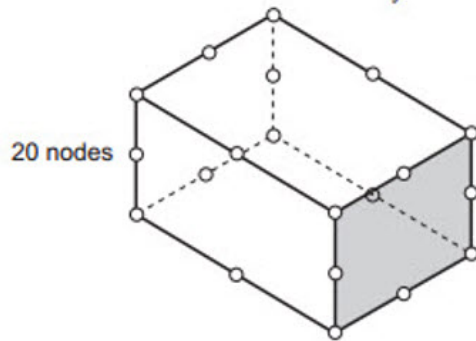
Tetrahedron – 4-node,
or, Tetra-4.



Hexahedron – 8-node,
or, **Hexa-8.**

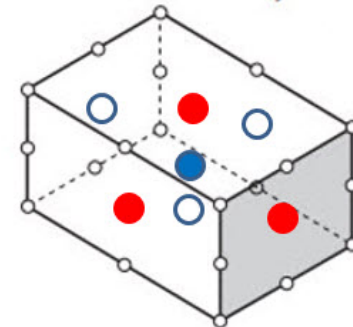


$$h(0)^2$$

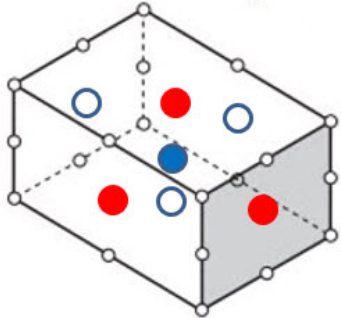


Hexahedron- 20 nodes
or, **Hexa-20**

$$h(0)^3$$

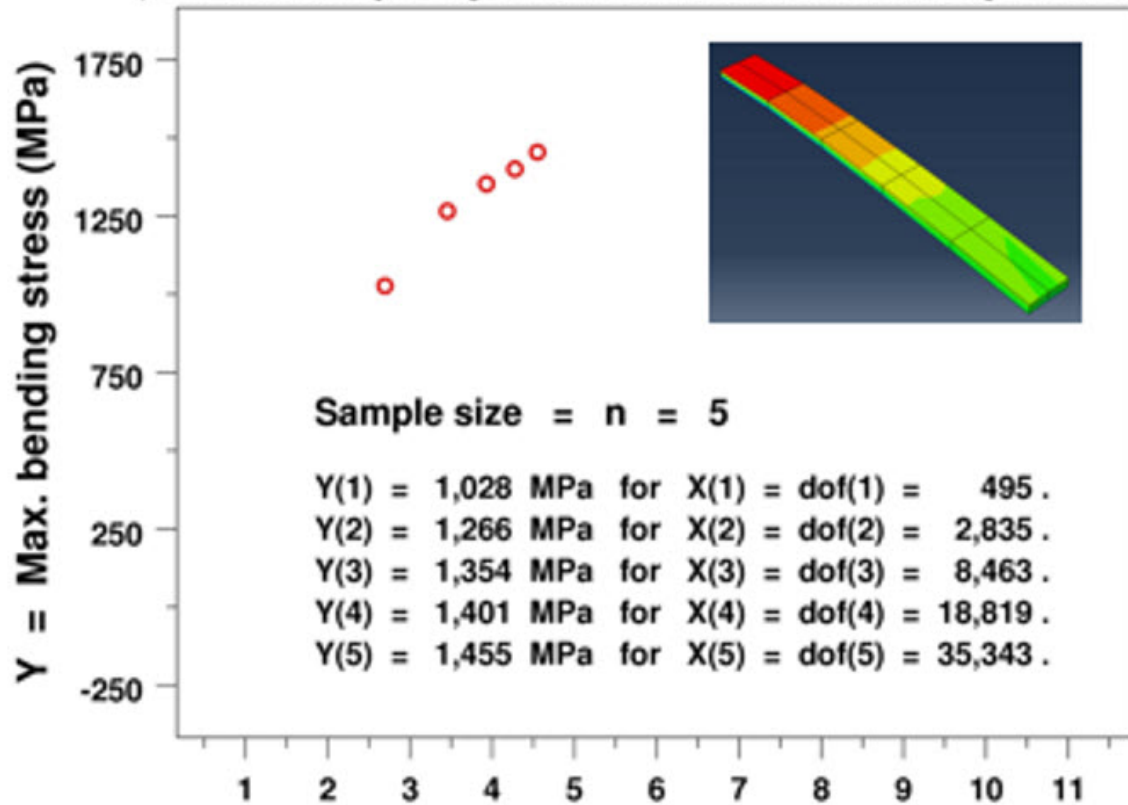


Hexahedron- 27 nodes
or, **Hexa-27**



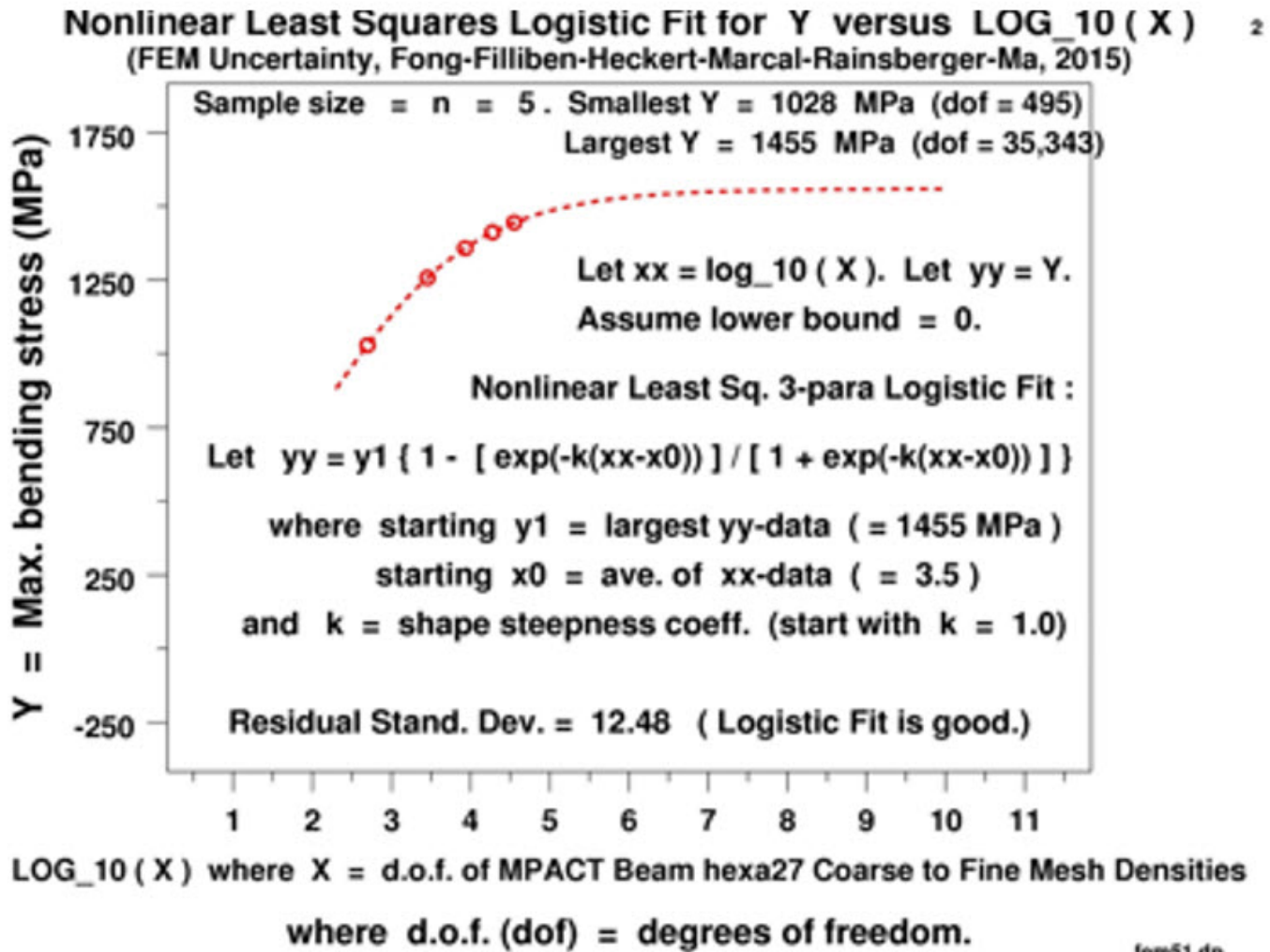
Hexahedron- 27 nodes
or, **Hexa-27**

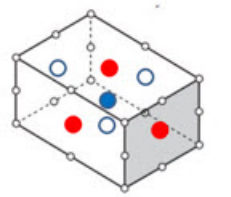
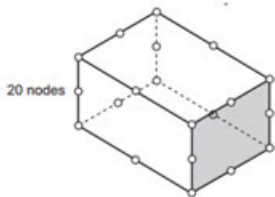
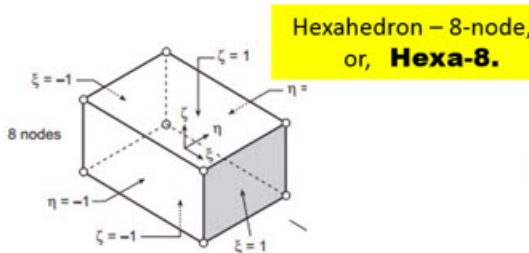
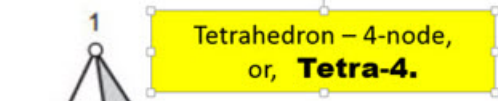
Nonlinear Least Squares Logistic Fit for Y versus LOG₁₀ (X)
(FEM Uncertainty, Fong-Filliben-Heckert-Marcacal-Rainsberger-Ma, 2015)



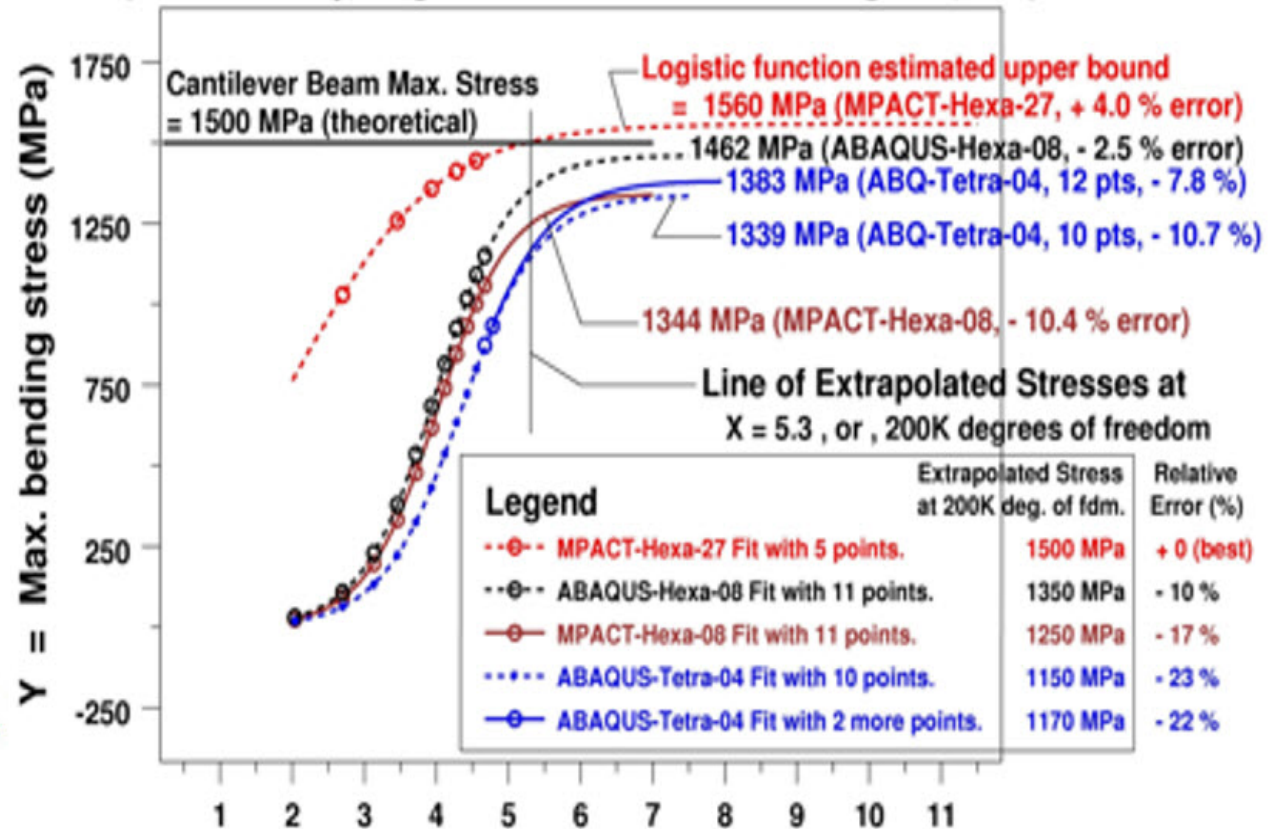
where d.o.f. (dof) = degrees of freedom.

fem51.dp





Nonlinear Least Squares Logistic Fit for Y versus LOG₁₀ (X)
(FEM Uncertainty, Fong-Filliben-Heckert-Marcial-Rainsberger-Ma, 2015)



LOG₁₀ (X) where X = degrees of freedom (d.o.f.) of

ABAQUS Hexa08 (black), Tetra04 (blue), MPACT Beam hexa27 (red) and hexa08 (green)

fem51.dp

(6) Concluding Remarks.

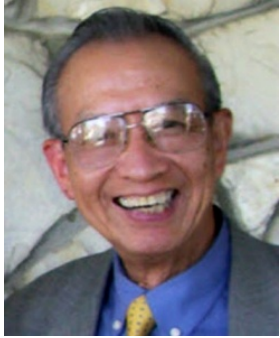
- In this talk, we show how one can quantify FEM uncertainties due to the following three sources:
- (1) Uncertainty due to Element Type (2015).
- (2) Uncertainty due to Mesh Density (2015).
- (3) Uncertainty due to **Model Parameters (2014)**.

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)**.

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.”