

A *2-Metric* Verification
of a
***COMSOL* Example Problem**
on the
***Fluid-Structure Interaction* in a**
Network of *Blood Vessels* (*)

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[1] **Verification & Validation (**Ve & Va**) of FEM Solutions**

[1] **COMSOL Example-1: Wrench Max. Stress .**

[4] **Metric Ve-1: Uncertainty at one billion DOF (10^{**9})**

[2] **A 2-metric Verification of COMSOL Example-1.**

[2] **COMSL Ex-2: Fluid-Structure Interaction.**

[3] **Metric Ve-2: Rel. Error Rate at one billion DOF.**

[4] **A 2-metric Verification of COMSOL Example-2.**

[1] **Concluding Remarks .**

Verification & Validation (**Ve** & **Va**) of an **F. E. M.** Numerical Experiment

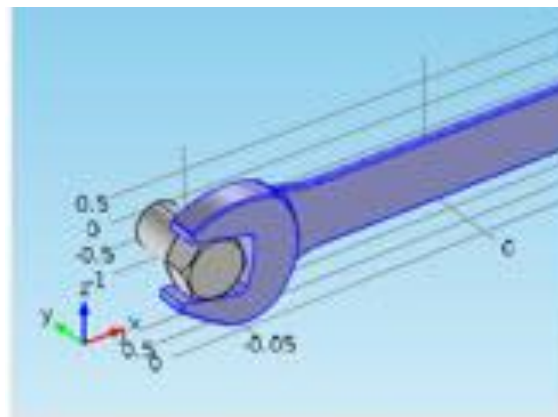
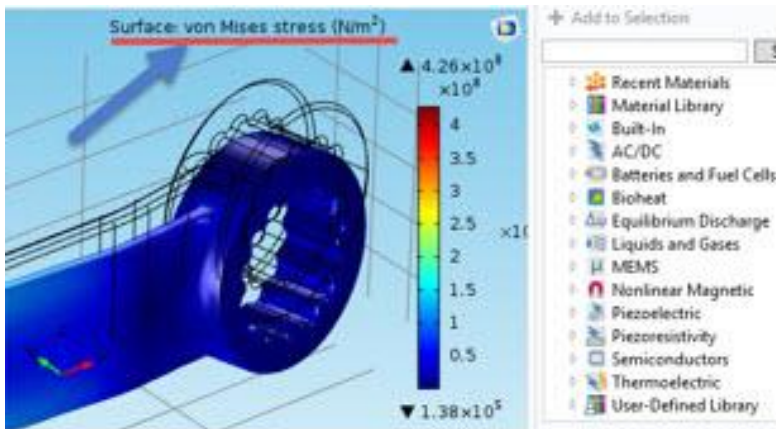
Def. of FEM Solution Verification (**Ve**):

Solution is verified if its **mathematics** is correct.

Def. of FEM solution Validation (**Va**):

Solution is validated if its **physics** is correct (**Va**).

COMSOL Example-1: Wrench Max. Mises Stress



Messages Progress Log Table

24,606 elements

Saved file: wrench3.mph
 Opened file: wrench.mph
 Saved file: wrench101.mph
 Complete mesh consists of 24606 domain elements, 8189 boundary elements, and 2181 edge elements.
 Avoided 51 inverted elements by using linear geometry shape ord
 Number of degrees of freedom solved for: **123,657**
 Solution time (Study 1): 38 s.

Messages Progress Log Table 1

ppr(solid.mises) (MPa)
364.35

364.35 MPa

Metric **Ve-1**: **Uncertainty** at one billion DOF (10^{**9})

What is a **Nonlinear Least Squares Logistic Function fit** ?

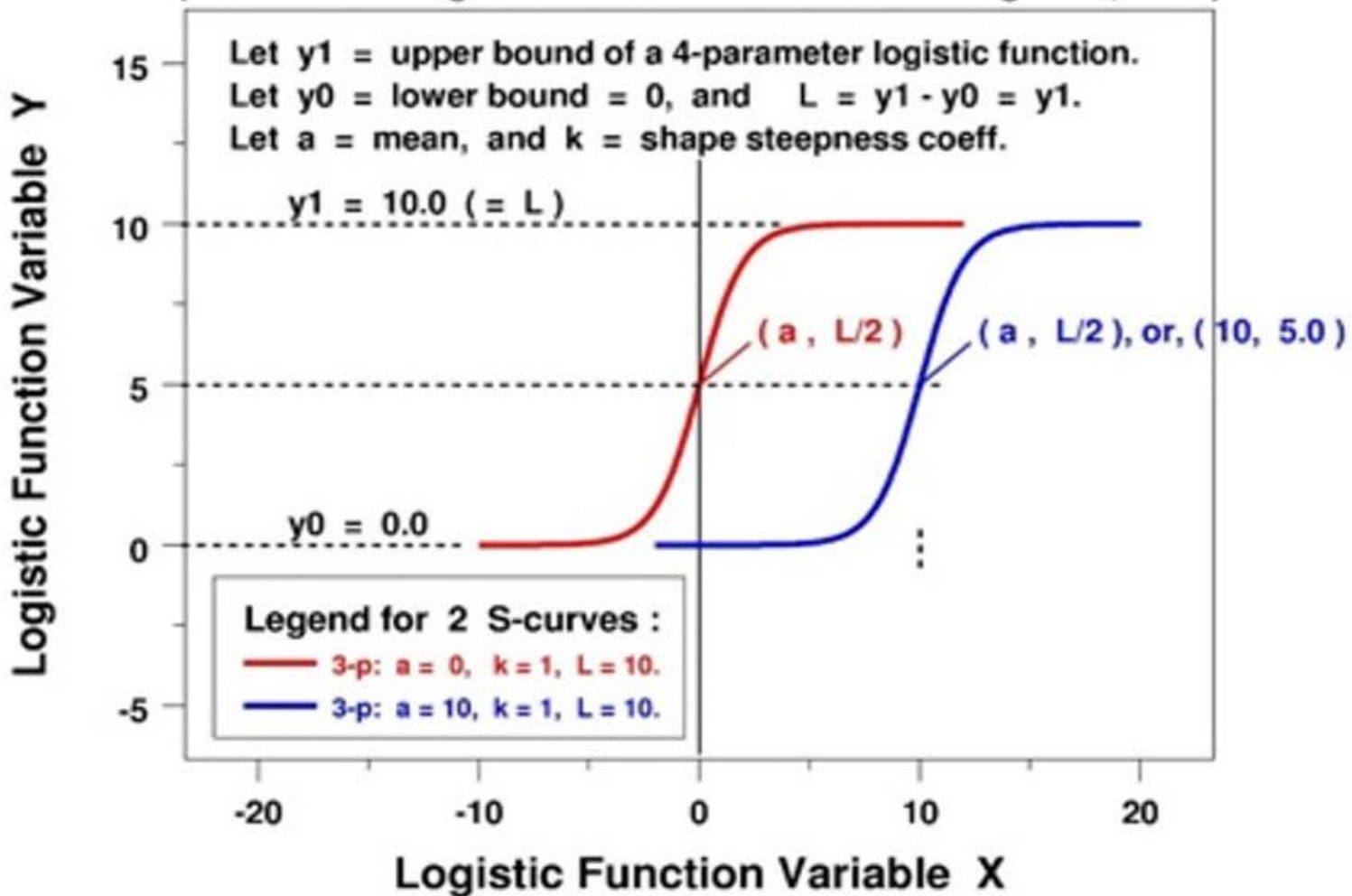
Ans. **Pierre Francois Verhulst (1845)**

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

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



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

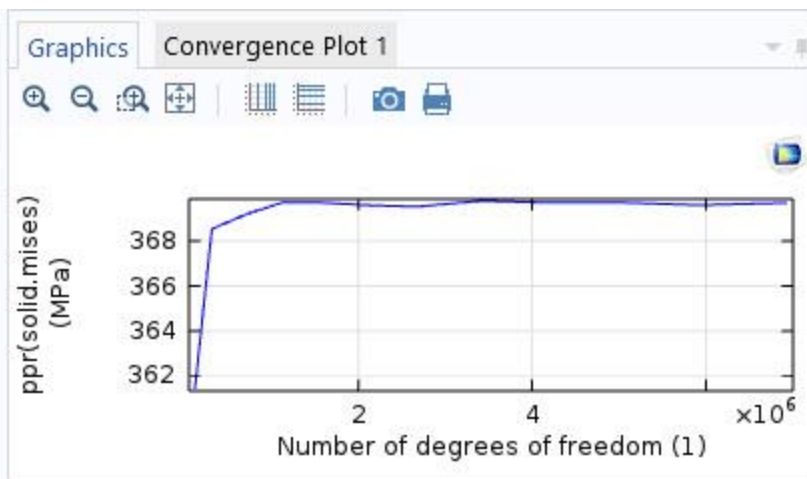
Preprocessing

Coloring and Style

Line style

Li

C



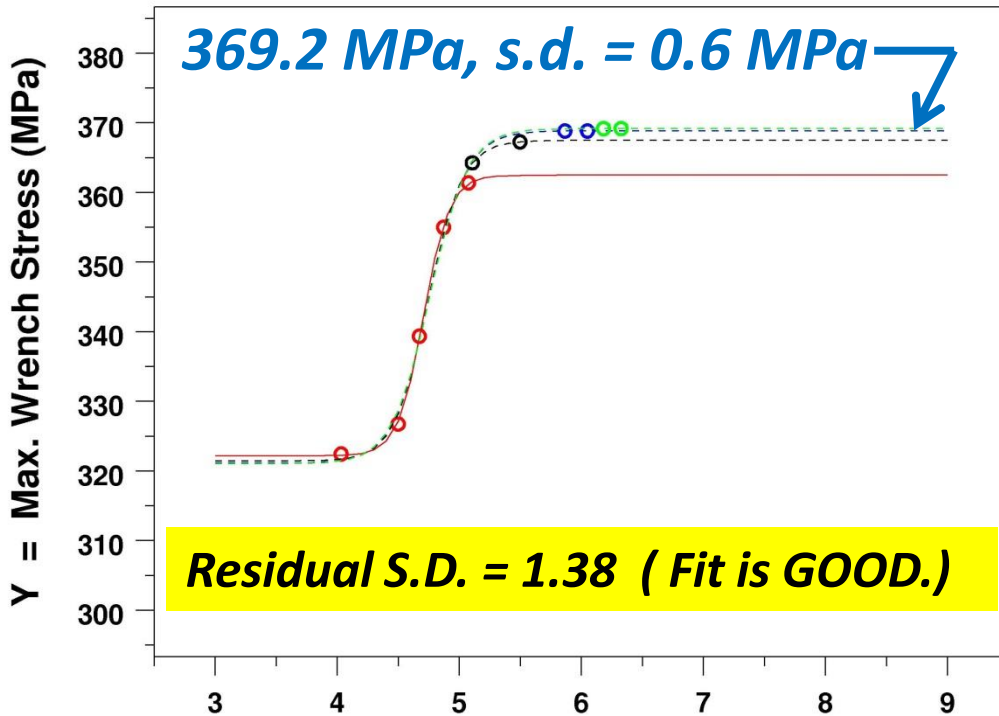
Messages Progress Log Table 2

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
10.000	369.72	5.0332E6
	369.61	5.9196E6
	369.71	6.9329E6

Max. Mises Stress = 369.71 MPa = 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

369.7 MPa

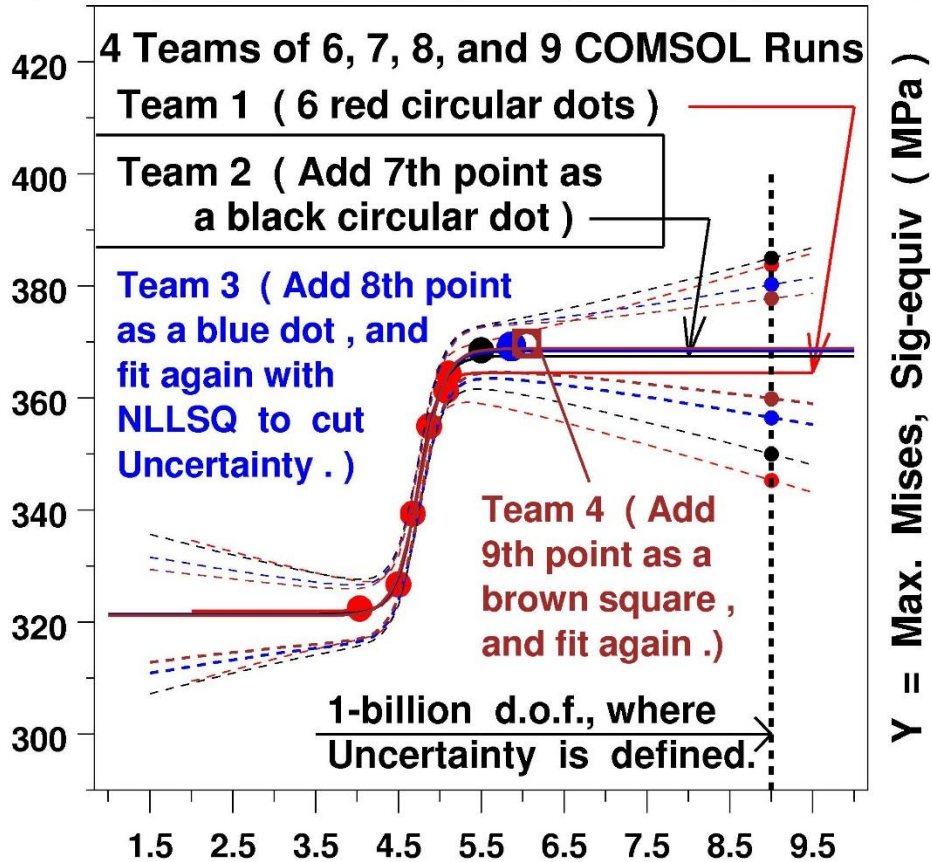
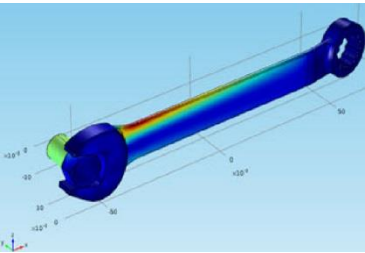
Ans. Max. Mises Stress at 95 % confidence level = (368.0, , 370.4 MPa)

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

A **2-metric** Verification of COMSOL Ex-1 (Wrench Max. Stress)

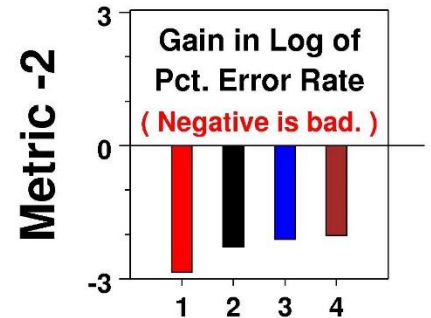
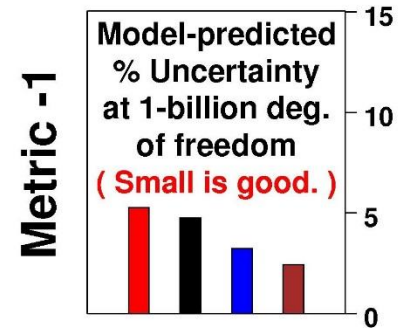
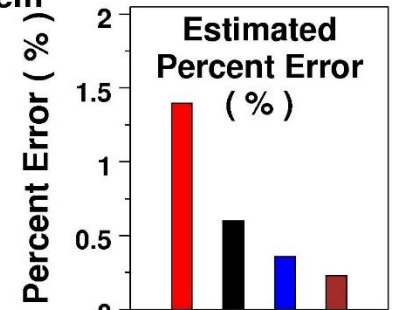
A 4-para. Nonlinear Least Squares (NLLSQ) Fit for a Wrench Problem

$$Y (\text{Stress}) = y_1 - L (\exp(-k (xx - x_0)) / (1 + \exp(-k (xx - X_0))))$$



$xx = \text{LOG}_{10}(X)$, where $X = \text{d.o.f. of Team 1 (red dot)}$,
 Team 2 (black dot), Team 3 (blue dot), and Team 4 (brown square).

By: Jeffrey T. Fong, N.I.S.T., Jan. 3, 2018.



1 = Team-1 (6 runs), 2 = Team-2 (7).
 3 = Team-3 (8 runs), 4 = Team-4 (9).

COMSOL Example-2: A Network of Blood Vessels.

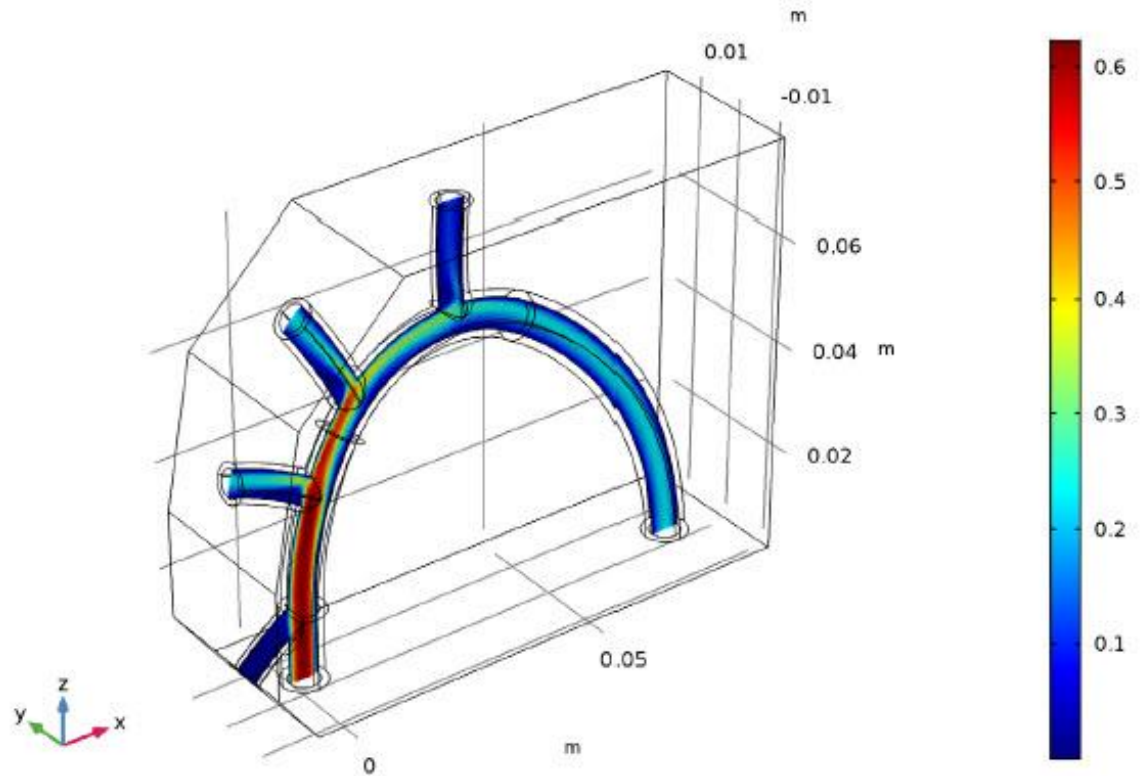
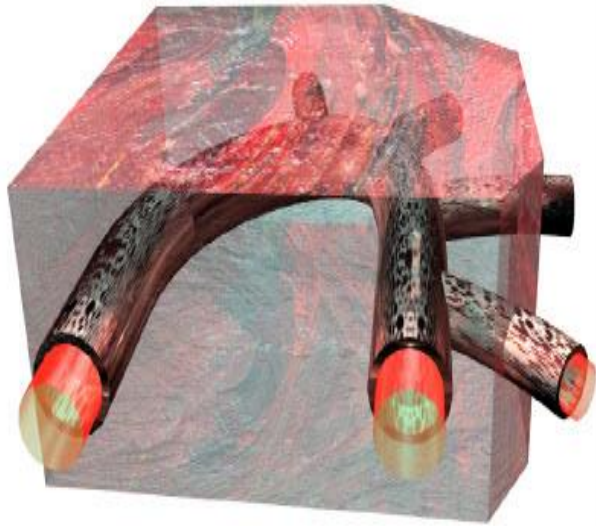


Figure 4: Velocity field in the aorta and its ramification (branching).

Metric V_{e-2} :

**Rel. Error Convergence Rate
at one billion DOF (10^{**9}).**

Definition of a

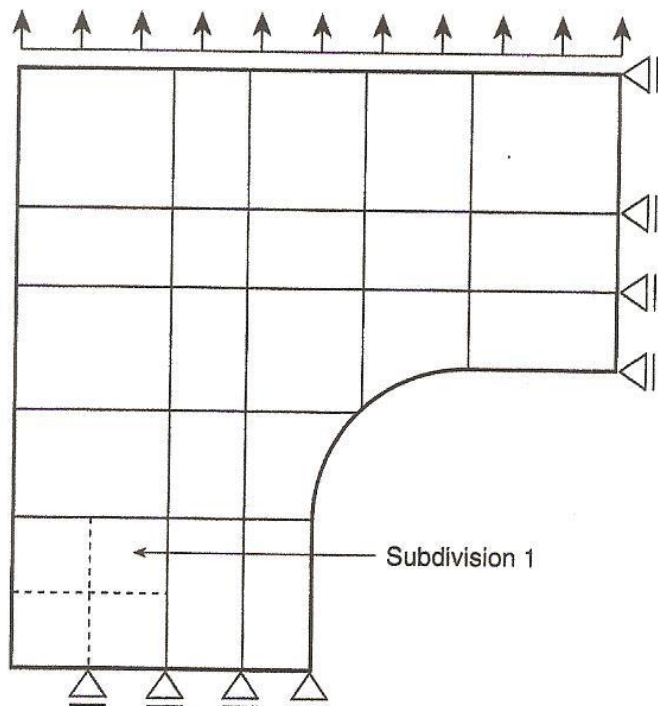
Relative Error Convergence (REC) Rate

Let $X_i = (d.o.f.)_i$, $X_{i+1} = (d.o.f.)_{i+1}$.

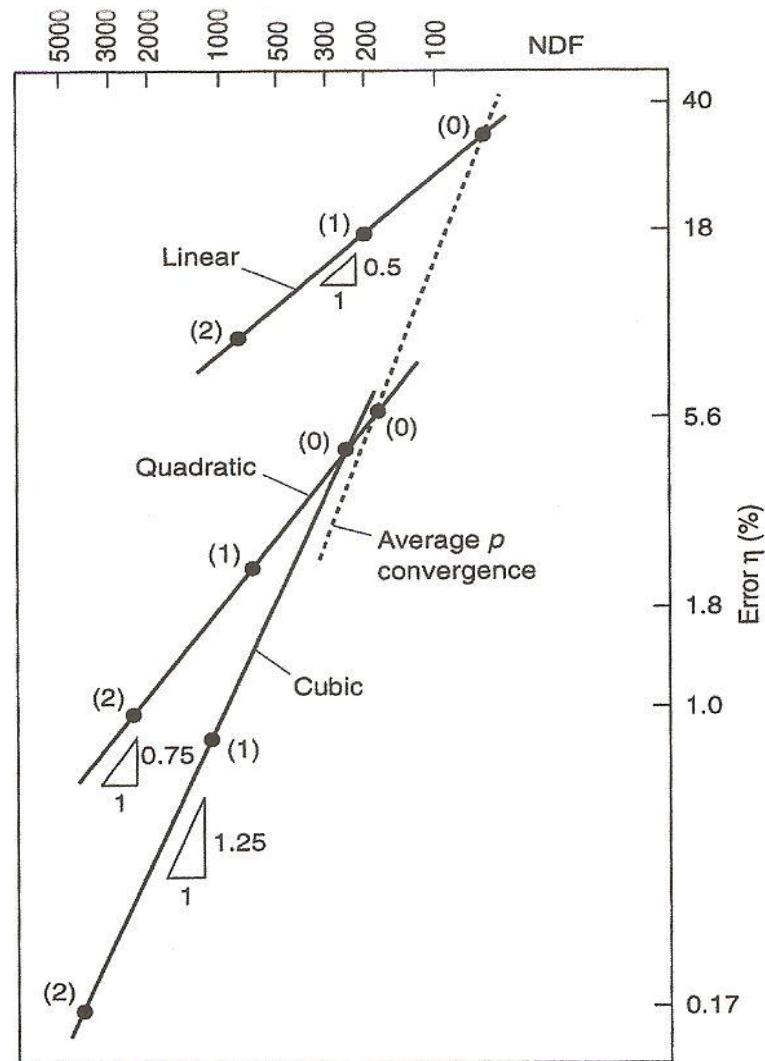
Let $x_i = \text{Log}_{10}(X_i)$, $x_{i+1} = \text{Log}_{10}(X_{i+1})$.

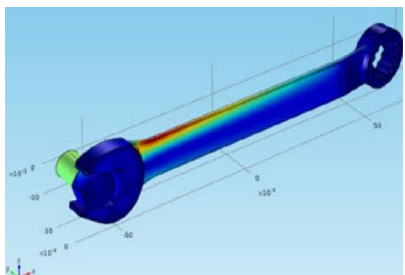
Let $(\text{Pct. Error})_{i+1} = 100 * (Y_{i+1} - Y_i) / Y_i$.

$(\text{REC Rate})_{i+1} = \{ (\text{Pct. Error})_{i+1} \} / (x_{i+1} - x_i)$.



Ref.: **Zienkiewicz and Taylor,**
2000, The Finite Element Method,
Vol. 1: The Basis, 5th ed., pp. 365-370.
Butterworth Heinemann (2000)

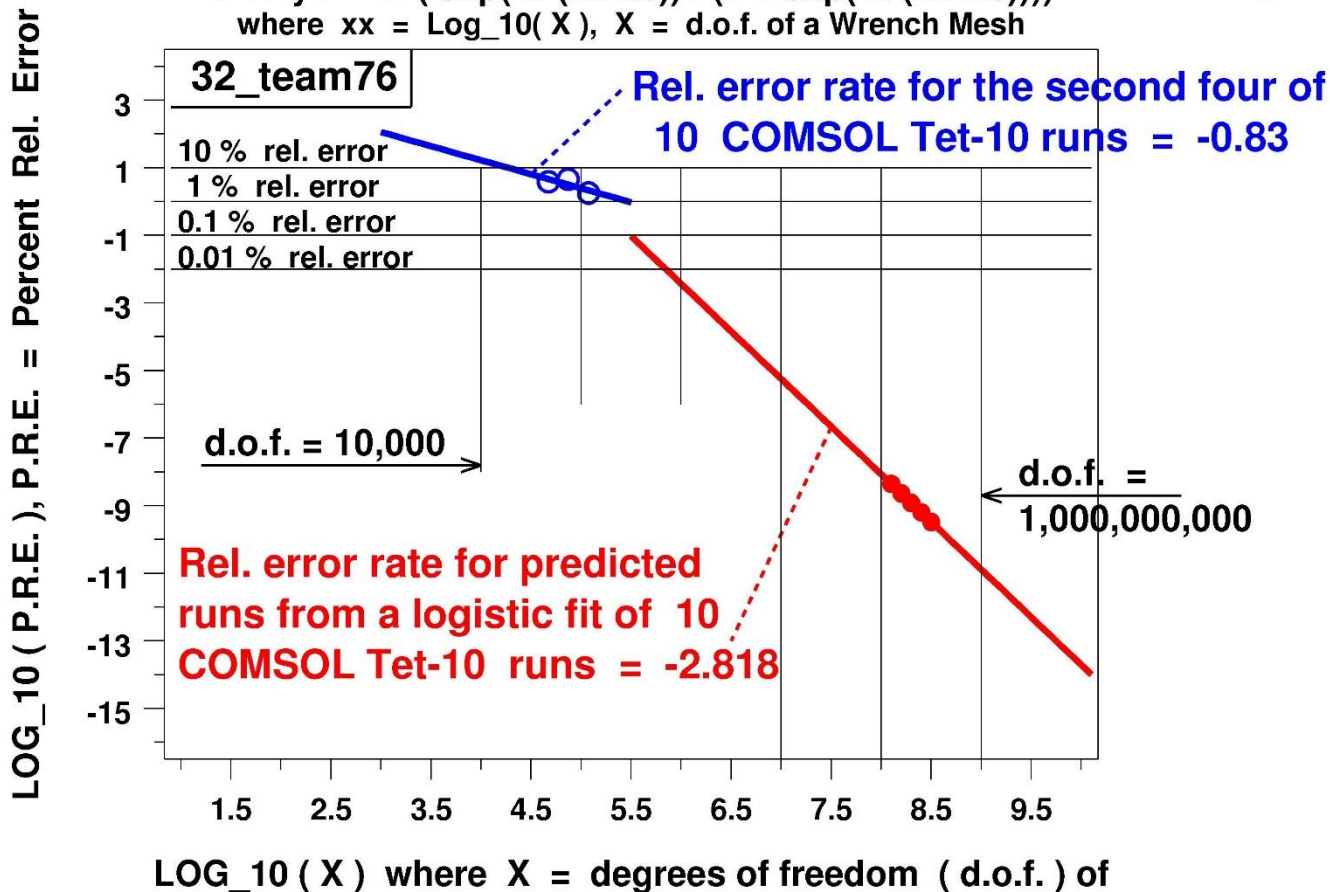




$$Y = y1 - L * (\exp(-k*(xx-x0)) / (1 + \exp(-k*(xx-X0))))$$

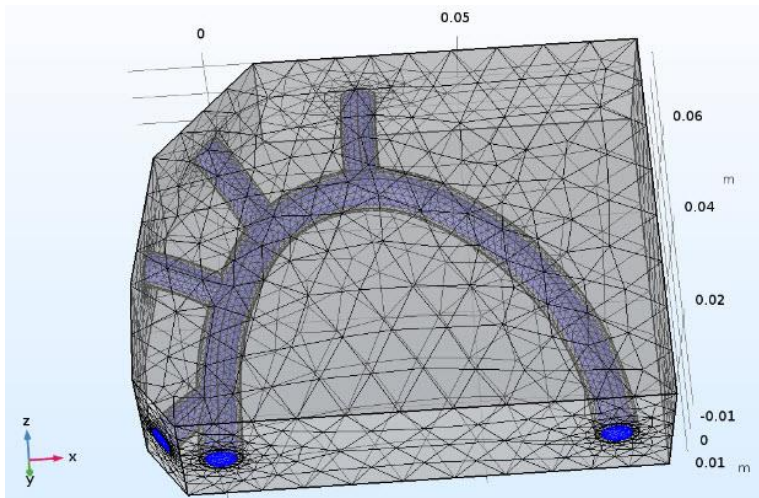
where $xx = \text{Log}_{10}(X)$, $X = \text{d.o.f. of a Wrench Mesh}$

3



P.R.E. Plot for second 4 of 10 COMSOL Tet-10 runs (blue circles) and Predicted (red dots) vs. Log₁₀ (X)
rerop4c.dp + 32_team76.dat

A 2-metric Verification of COMSOL Ex-2

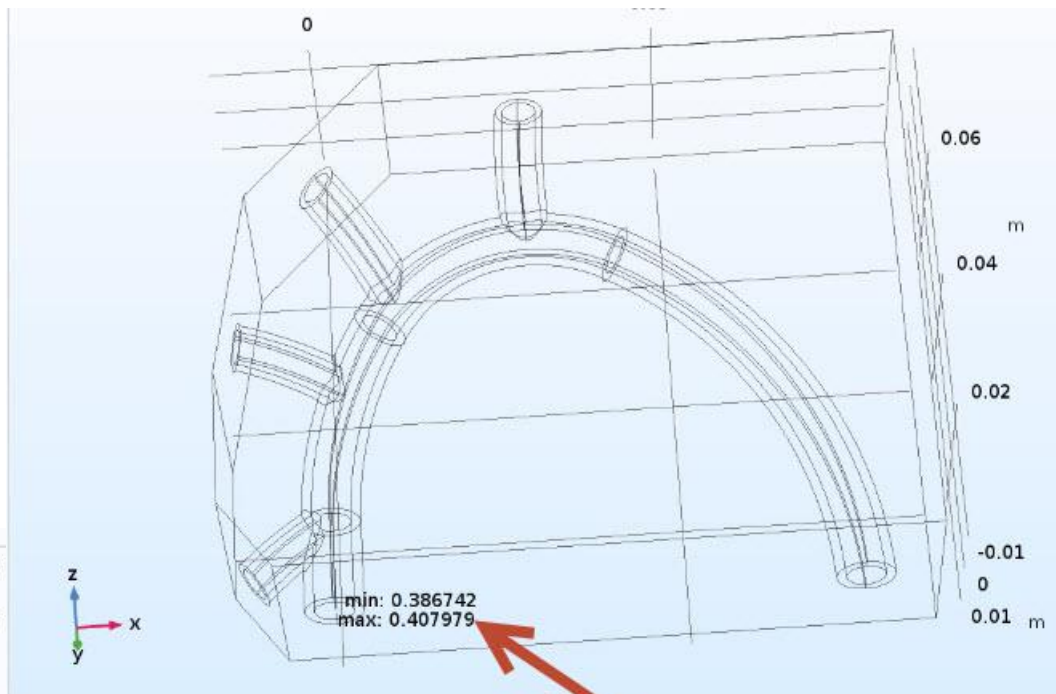


Saved file: C:\Lily\FongProject\Biomechanics\COMSOL_FSI_bloodvessel\COMSOL_bvresult\blood_vessel53a_normal.mph
 Complete mesh consists of 144156 domain elements, 16374 boundary elements, and 1929 edge elements.
 Saved file: C:\Lily\FongProject\Biomechanics\COMSOL_FSI_bloodvessel\COMSOL_bvresult\blood_vessel53a_normal.mph
 Number of degrees of freedom solved for: 60996 (plus 1 internal DOFs).
 Number of degrees of freedom solved for: 305241.
 Solution time (Study 1): 590 s. (9 minutes, 50 seconds)

305,241 dof

401aa before normal

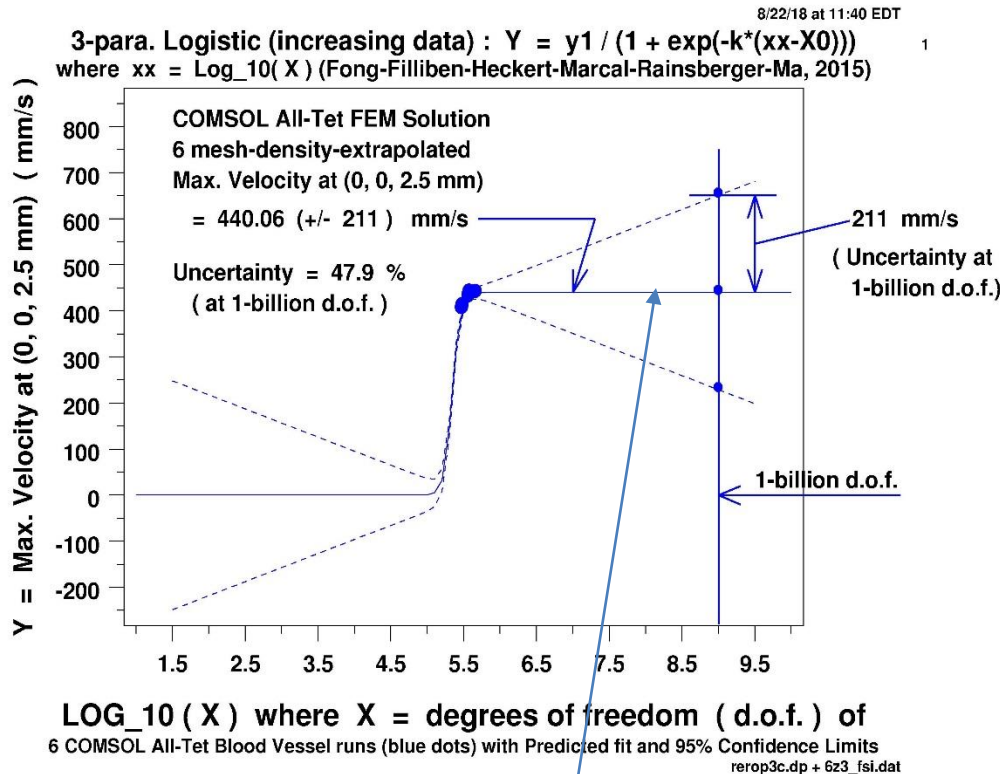
COMSOL Example Mesh
dof = 305,241



Messages Progress Log Maximum and minimum values 5

X	Y	Z	Velocity magnitude (m/s)
0.001	0	0.0025	0.38674231971308465
0	0	0.0025	0.4079790768007657

Velocity at (0, 0, 0.0025) = 408.0 mm/s



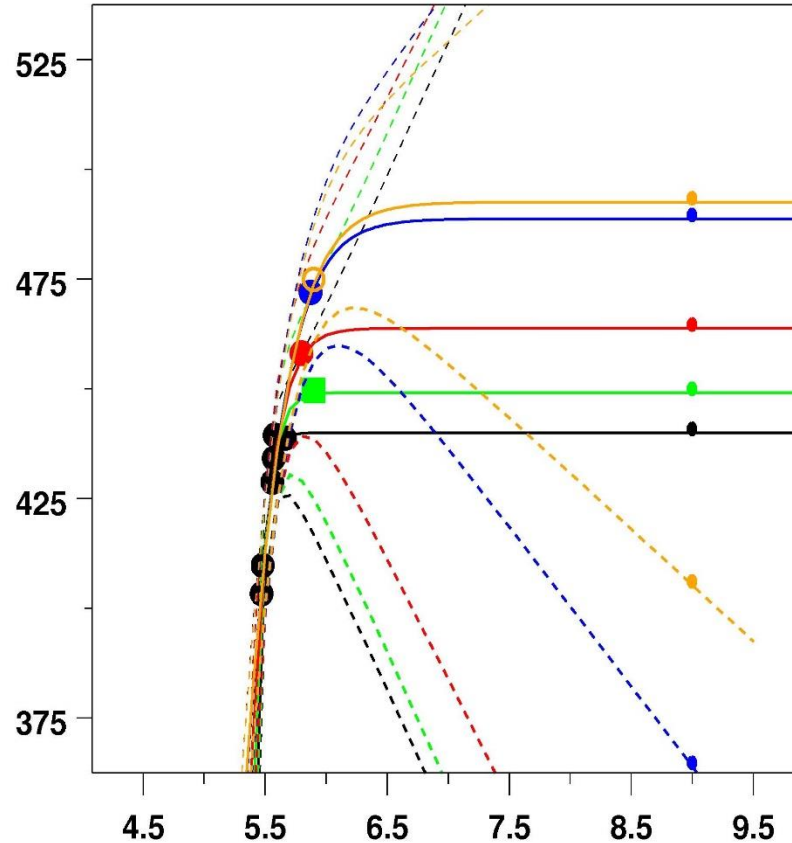
Velocity at (0, 0, 0.0025) Y (mm/s)	Degrees of Freedom (dof) X	Note: SF = Scale Factor
408.0 (?)	305,241	(COMSOL Example Mesh)
402.49	297820	(Modified COMSOL Mesh SF = 0.76)
408.94	303876	(Modified COMSOL Mesh SF = 0.75)
427.92	364184	(Modified COMSOL Mesh SF = 0.69)
433.30	374175	(Modified COMSOL Mesh SF = 0.68)
438.57	380617	(Modified COMSOL Mesh SF = 0.67)
437.92	462100	(Modified COMSOL Mesh SF = 0.63)
440.06	INFINITY	(β-parameter logistic function fit)

8/25/2018 at 00:29 EDT

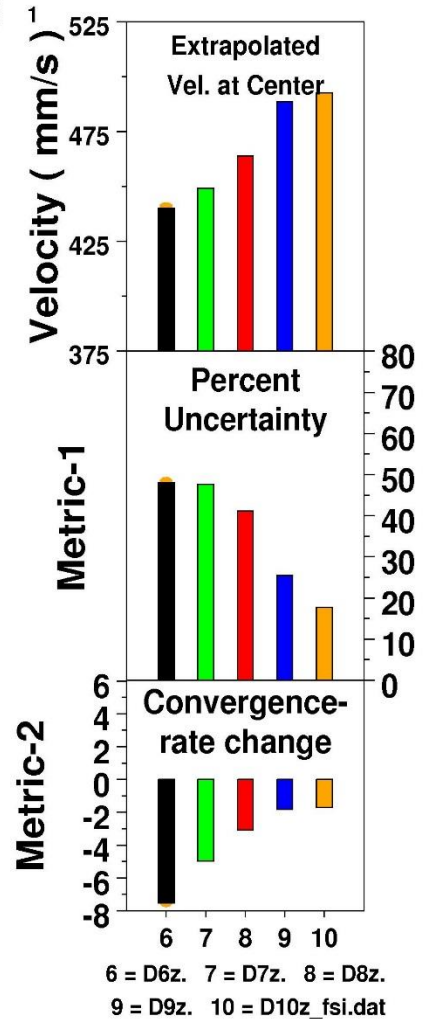
Velocity at (0, 0, 0.0025) Y (mm/s)	Deg of Freed. (dof) X
402.49	297820
408.94	303876
427.92	364184
433.30	374175
438.57	380617
437.92	462100
448.80	468598
456.45	513988
470.57	700972
475.11	802812

$$Y = y1 - L (\exp(-k (xx - x0)) / (1 + \exp(-k (xx - X0))))$$

where $xx = \text{Log}_{10}(X)$, $X = \text{d.o.f. of Blood Vessel Mesh}$



LOG₁₀(X) where X = d.o.f. of D6z (black dot), D7z (green square), D8z (red dot), D9z (blue dot), D10z (orange circle).
 fsi823e.dp +D6z +D7z +D8z +D9z +D10z_fsi.dat + fsi823b.dat

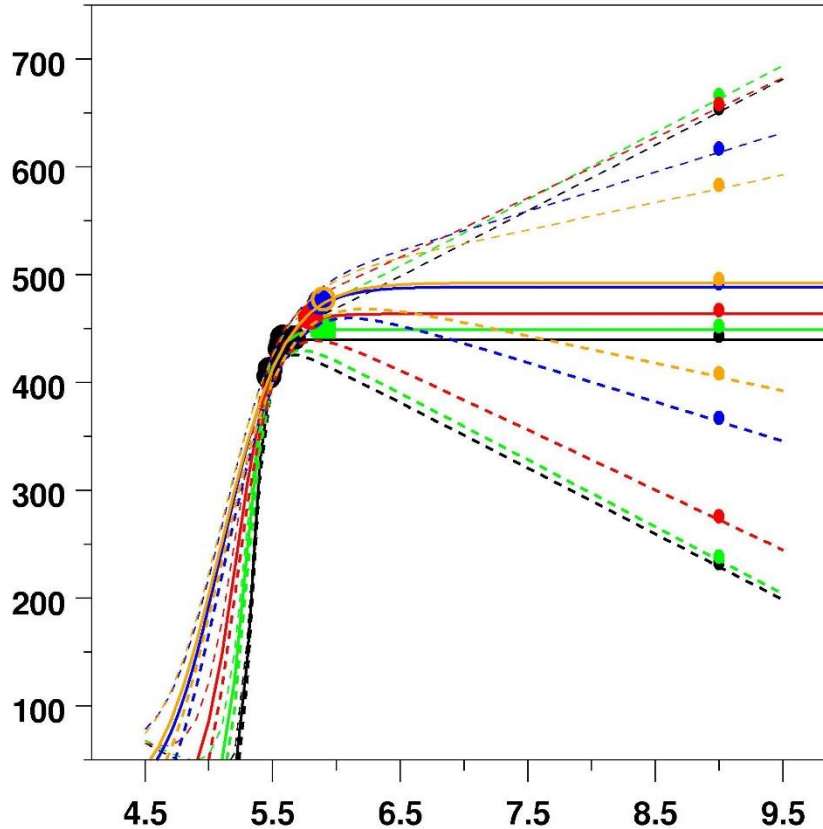


8/25/2018 at 00:25 EDT

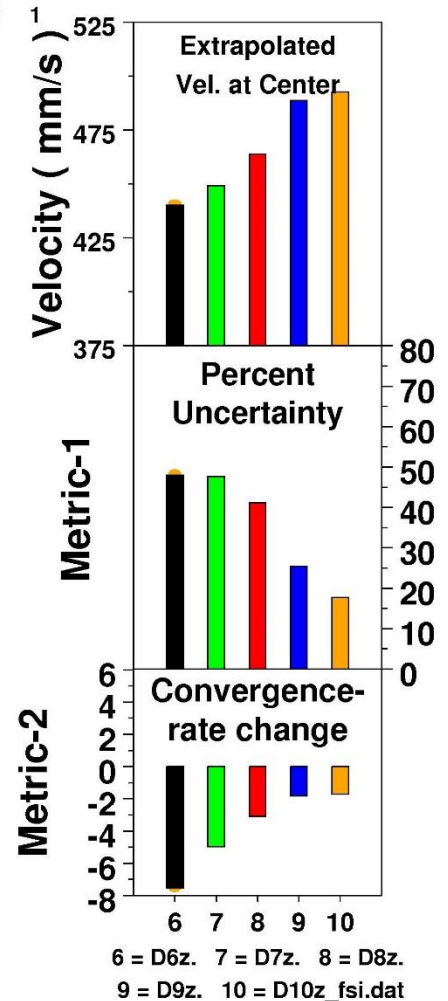
Y	X1
Asmpt. Velocity (mm/s)	PET No. of Points
440.06	6
449.18	7
463.82	8
488.79	9
492.59	10

$$Y = y1 - L \left(\frac{\exp(-k(xx - x0))}{1 + \exp(-k(xx - X0))} \right)$$

where $xx = \text{Log}_{10}(X)$, $X = \text{d.o.f. of Blood Vessel Mesh}$



LOG₁₀(X) where X = d.o.f. of D6z (black dot), D7z (green square), D8z (red dot), D9z (blue dot), D10z (orange circle).

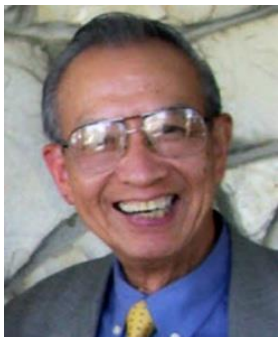


408.0 (before)
492.6 (after)
84.6 (17 % diff.)

Concluding Remarks .

1. An accurate estimate of **uncertainty** in FEM-based solution **is essential** in verification (Ve) and validation (Va) of the solution when FEM analysis is considered as a “**numerical experiment.**”
2. To estimate uncertainty of FEM results due to
 - (1) **element type** and **mesh density**,
 - (2) **mesh quality** (e.g., mean aspect ratio, standard error of Jacobians, etc.), and
 - (3) solution platform (FEM codes),a nonlinear least squares logistic fit method has been shown to yield FEM results extrapolated to **one billion degrees of freedom** with a measure of **uncertainty** and **Relative Error Convergence Rate** that are useful as metrics for assessing the accuracy of the FEM results.

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 150 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.”