A COMSOL Analysis with Uncertainty Quantification (UQ) of a Prototype MRI Birdcage RF Coil (*)

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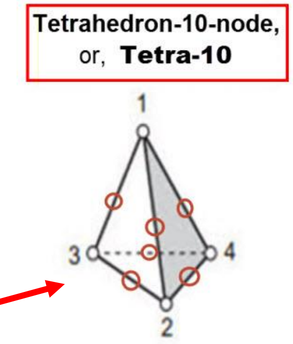
(*) Co-authored by Jeffrey Fong, James Filliben, Alan Heckert, Karl Stupic and Stephen Russek.

The Governing Equations.

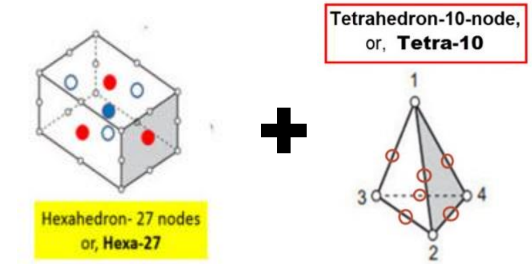
The Geometry of a Birdcage RF Coil.

The COMSOL Build for Two Meshes.



Mesh-1 (All Tetra-10, *automatic*).

Mesh-2 (Mixed Hexa-27 & Tetra-10).



Solution with *Uncertainty* for Mesh-1 and -2.

Concluding Remarks.

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The Governing Equations.

Maxwell's Equations:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$ Faraday

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$ Ampere

$$\nabla \cdot \mathbf{D} = \rho$$

$$\nabla \cdot \mathbf{B} = 0$$

Gauss

$$\nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t}$$ Continuity

(follows from Ampere and Gauss electric)

Constitutive Relations:

$$\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}$$ ϵ = permittivity (farads/meter)

$$\mathbf{B} = \mu_0 (\mathbf{H} + \mathbf{M})$$ μ = permeability (henrys/meter)

$$\mathbf{J} = \sigma \mathbf{E}$$ σ = conductivity (siemens/meter).

E: *electric field intensity,* [V/m]
D: *electric displacement* or *electric flux density,* [C/m^2]
P: *electric polarization vector ,* [C/m^2]
B: *magnetic flux density ,* [Wb/m^2]=[T]
H: *magnetic field intensity ,* [A/m]
M: *magnetization vector,* [A/m]
J: *current density,* [A/m^2]
ρ: electric charge density, [C/m^3]

- Only first two Maxwell's equations (Faraday and Ampere) are independent
- Gauss (electric and magnetic) equations follow from first two when supplemented by charge continuity
- Six equations (Faraday + Ampere) and six unknowns (E, H)

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The Governing Equations.

Frequency Domain Equations Solved in RF

Harmonic fields: $\mathbf{E}(\mathbf{r},t)=\mathbf{E}(\mathbf{r})e^{j\omega t}, \quad \mathbf{H}(\mathbf{r},t)=\mathbf{H}(\mathbf{r})e^{j\omega t}$

Faraday: $\nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t}$

Ampere: $\nabla\times\mathbf{H}=\mathbf{J}+\frac{\partial\mathbf{D}}{\partial t}$

$\xrightarrow{\frac{\partial}{\partial t}\to j\omega}$

$\nabla\times\mathbf{E}=-j\omega\mu\mathbf{H}$

$\nabla\times\mathbf{H}=\sigma\mathbf{E}+j\omega\varepsilon\mathbf{E}$

$\nabla\times\mathbf{E}=-j\omega\mu\mathbf{H}$

$\nabla\times\mathbf{H}=j\omega\varepsilon_c\mathbf{E}$

$$\varepsilon_c=\varepsilon-j\frac{\sigma}{\omega}$$

Wave Equation for **E**

$$\nabla\times \left| \frac{1}{\mu}\nabla\times\mathbf{E}=-j\omega\mathbf{H} \right. \Longrightarrow \nabla\times\left(\frac{1}{\mu}\nabla\times\mathbf{E}\right)=-j\omega\underbrace{\nabla\times\mathbf{H}}_{j\omega\varepsilon_c\mathbf{E}}$$

$$\nabla\times\left(\frac{1}{\mu}\nabla\times\mathbf{E}\right)-\omega^2\varepsilon_c\mathbf{E}=0$$

This is the equation solved in .emw

$$\varepsilon_c=\varepsilon-j\frac{\sigma}{\omega}$$

Once **E** is solved for, then **H** is calculated from Faraday: $\mathbf{H}=-\frac{1}{j\omega\mu}\nabla\times\mathbf{E}$

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The Governing Equations.

Energy density: $w = \frac{1}{2}\varepsilon|\mathbf{E}|^2 + \frac{1}{2}\mu|\mathbf{H}|^2, [J/m^3]$

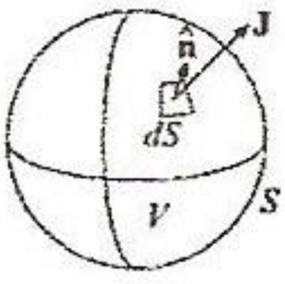
Poynting vector: $\mathscr{P} = \mathbf{E}\times\mathbf{H},\ [W/m^2]$

Rate of energy loss: $Q_{loss} = \mathbf{J}_{tot}\cdot\mathbf{E} + \mathbf{B}\cdot\frac{\partial \mathbf{H}^*}{\partial t}, [W/m^3]$

Energy conservation: $\frac{\partial w}{\partial t} + \nabla\cdot\mathscr{P} = -Q_{loss}$

$$-\oint_S \mathscr{P}\cdot d\mathbf{S} = \frac{d}{dt}\int_V w\,dV + \int_V Q_{loss}\,dV$$

Total power *entering* a volume V through the surface S goes partially into increasing the field energy stored inside V and partially is lost into heat



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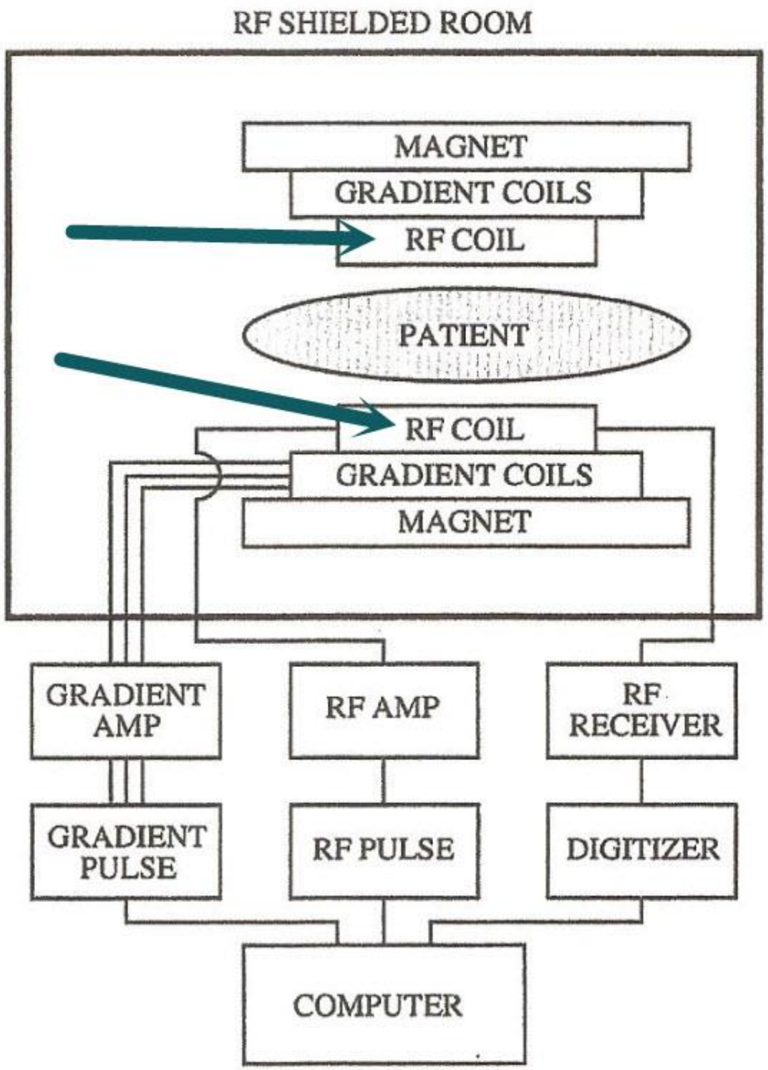
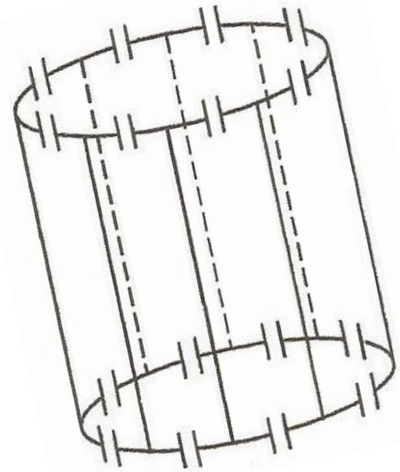
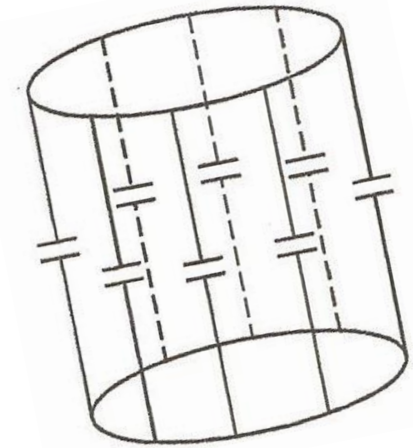
The Geometry of a Birdcage RF Coil.

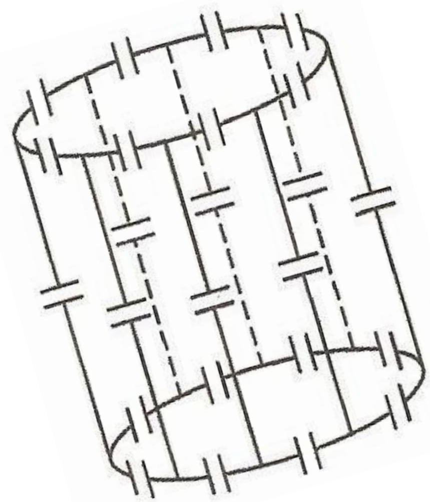




Highpass birdcage coil



Lowpass birdcage coil



Hybrid birdcage coil

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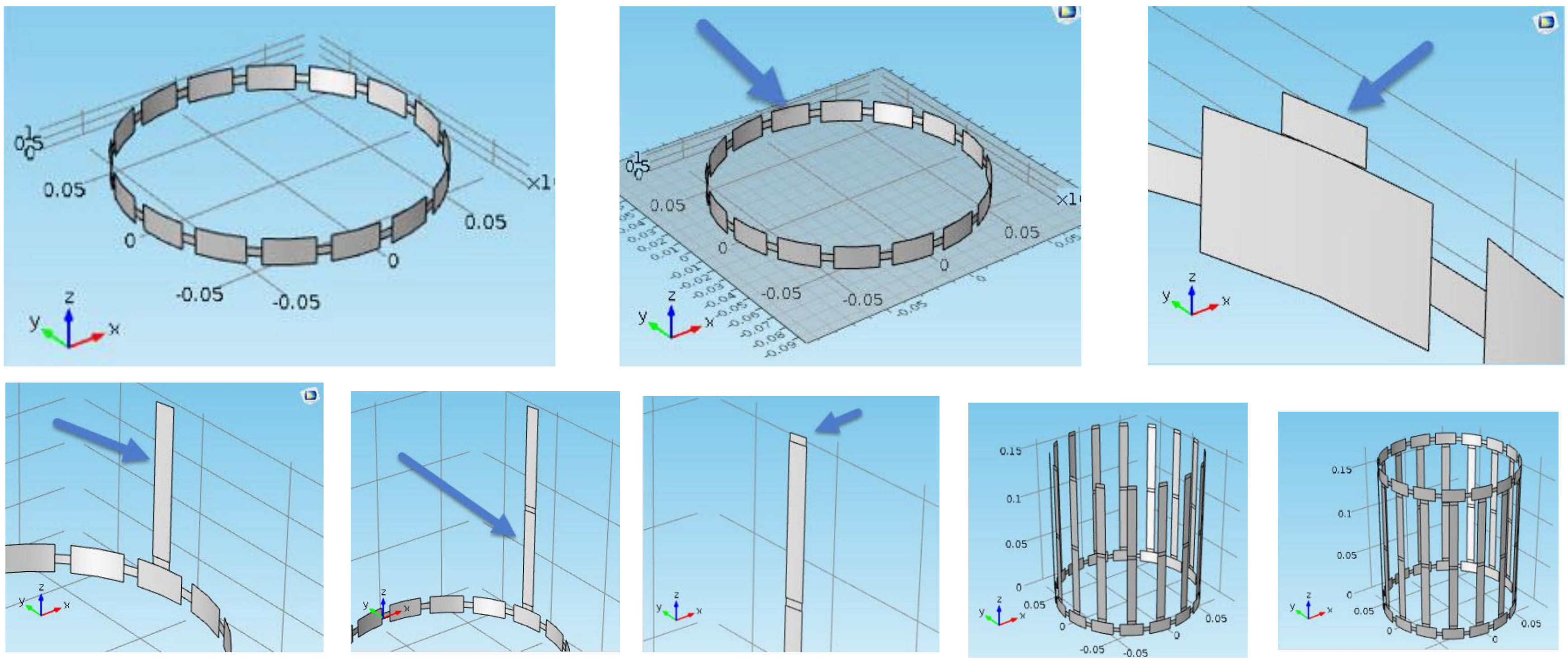
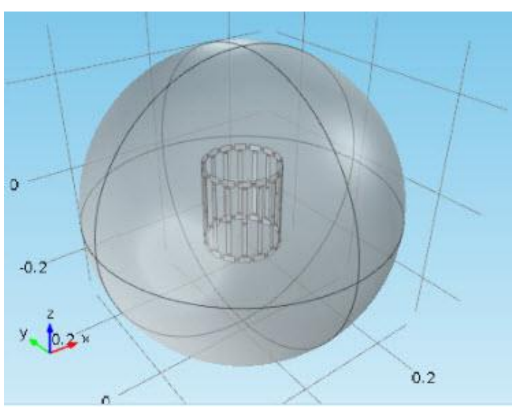
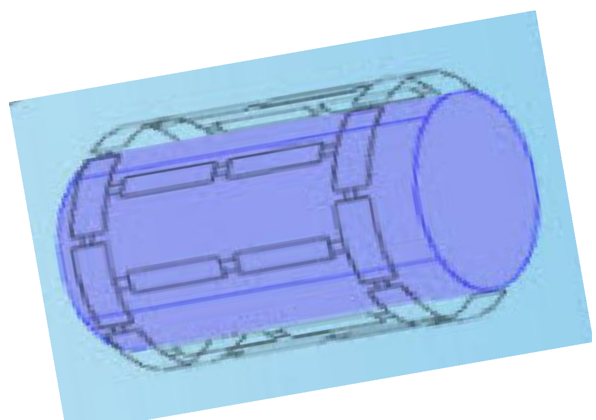
The Geometry of a Birdcage RF Coil.







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Mesh-1 (All Tetra-10, *automatic*).

- 2016_05_31b___RF_Lowpass_Coil_18.945_step_0.02
  - Global Definitions
    - Parameters
    - Materials
  - Component 1 *(comp1)*
  - Study 1: Nominal element size
  - Study 2_101a
  - Study 3__102a
  - Study 4____102b__refine_0.85
  - Study 5____102b2__refin_0.85
  - Study 6____102b3
  - Results
    - Data Sets
    - Derived Values
    - Tables
    - Electric Field (emw)
    - 1D Plot Group 3
    - 1D Plot Group 7: S11
    - Electric Field (emw) 1
    - S-Parameter (emw)
    - Electric Field (emw) 2
    - S-Parameter (emw) 1
    - Electric Field (emw) 3

For a parametric mesh design, we introduce a new parameter named "refine." For a typical run, we set refine to be 0.85.

Parameters

Name	Expression	Value	Description
bet2	5	5	small circular strip sector angle
bet3	6.4	6.4	short vertical strip sector angle
bet4	6.8	6.8	long vertical strip sector angle
L3	3.5[mm]	0.0035 m	short vertical strip length
L4	66.55[mm]	0.06655 m	long vertical strip length
N	16	16	number of legs
Ra	4*Rc	0.2912 m	radius of air domain
C	177[pF]	1.77E-10 F	port capacitance
V0	40[V]	40 V	excitation voltage
th	0.5[mm]	5E-4 m	coil thickness
CC	0.001[pF]	1E-15 F	
DD	0.001[pF]	1E-15 F	
Rw	0.9*Rc	0.06552 m	Inner water radius
Hw	1.2*Hc	0.20232 m	Inner water height
sig_water	0.1[S/m]	0.1 S/m	conductivity of water
eps_water	80	80	water permitivity
f0	50[MHz]	5E7 Hz	frequency_50
lam	c_const/f0/sqrt(eps_water)	0.67036 m	wave_length_50_water
z0	204.1[ohm]	204.1 Ω	lumped_port_imped_at_fr
fr	19.1[MHz]	1.91E7 Hz	resonance frequency
f1	18.727[MHz]	1.8727E7 Hz	lower freq at half z0
f2	19.4145[MHz]	1.9415E7 Hz	upper freq at half z0
Q	fr/(f2-f1)	27.782	Q-factor
el_size	lam/6	0.11173 m	min. element size to resolve wavelength
new_size1	el_size*refine	0.094967 m	
coil_elem_size	6[mm]*refine	0.0051 m	
diff	(3.9615-3.7832)/3.9615	0.045008	
refine	0.85	0.85	

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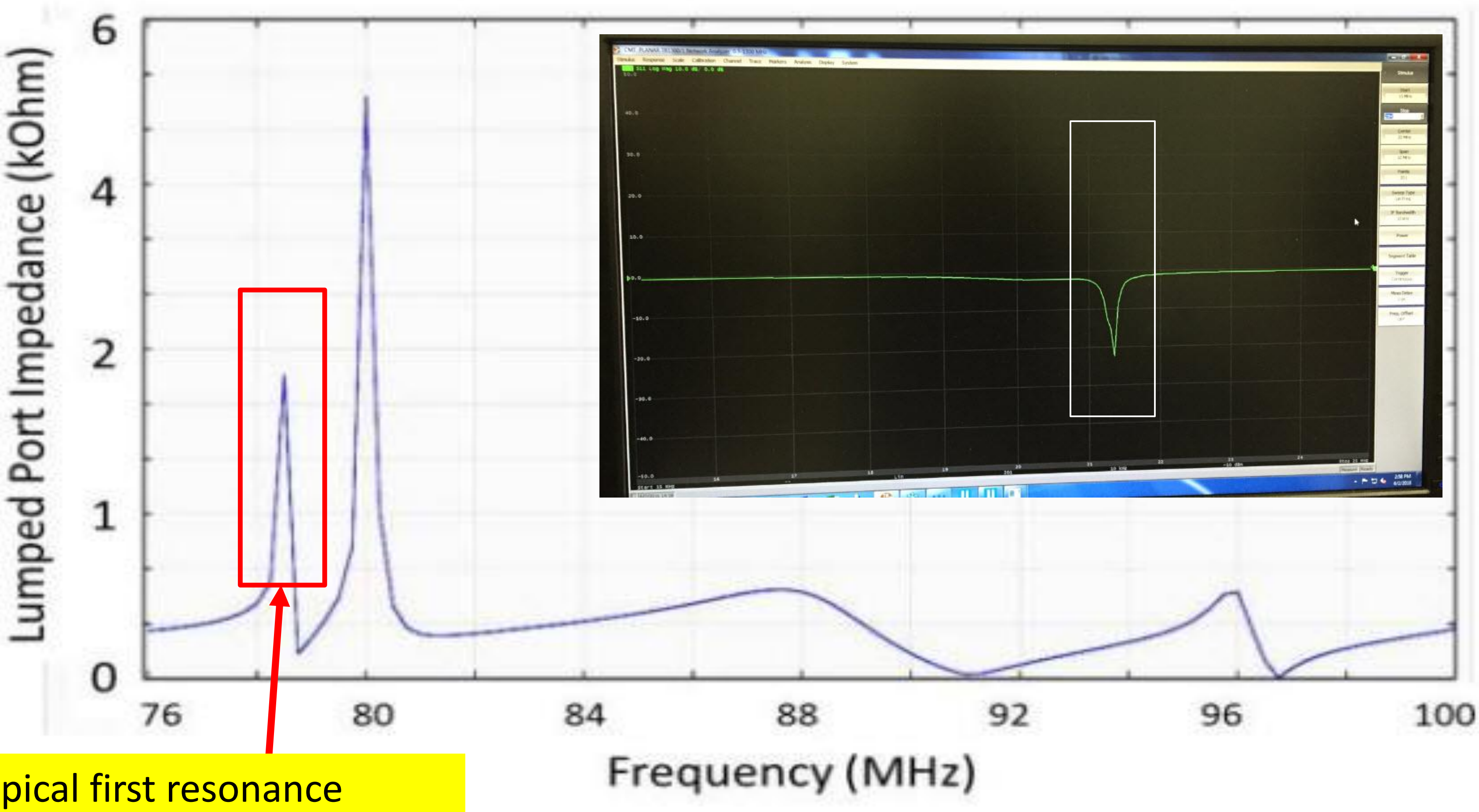
Mesh-1 (All Tetra-10, *automatic*).

Typical Analysis Results for Finding Resonance Frequencies



A typical first resonance frequency at about 77.2 MHz

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Mesh-1 (All Tetra-10, *automatic*).

For our first FEM modeling exercise with uncertainty quantification (UQ), we choose two basic mesh designs, namely, all-tetra, and mixed (about 90 % hex, and 10 % tetra).

For the all-tetra design, we chose to make 5 runs at refine = 0.95, 0.90, 0.85, 0.80, and 0.70. Typical results for two refine values, 0.90, and 0.70, are given on the right.

S11, a measurable parameter

All tetra, refine = 0.90

freq (MHz)	abs(emw.Zport_1) (Ω)	S-parameter, dB, 11 component (dB)
19	208.8483188602574 5	-3.743794980021971
19.002499999999998	208.8968447247037	-3.769320133084488 8
19.005	208.90478243559104	-3.7950100967473093
19.0075	208.87339085402255	[illegible]
[illegible]	208.80177762727385	[illegible]
[illegible]	208.68678760447125	-3.872732561855133
19.015	208.53330378386337	-3.8989093240703587
19.0175	208.33797275502667	-3.9252028172561095
19.02	208.1002166367731	-3.951678540395001

Max. impedance

S11 = - 3.79501 dB

All tetra, refine = 0.7

freq (MHz)	abs(emw.Zport_1) (Ω)	S-parameter, dB, 11 component (dB)
18.842499999999994	205.73600837159225	-3.629128483187789
18.845	206.01930496106016	-3.654397634785609
18.8475	206.25967500607823	-3.679908489165511 4
18.849999999999994	206.4655996744766	-3.705465512117087 6
18.8525	206.62808565600128	-3.731227753932406
18.855	206.7541345254009	-3.7570678989866724
18.857499999999998	206.83494111643256	-3.7831374858155793
18.86	206.87822464742388	-3.809269064145175
18.8625	206.87787773959104	[illegible]
[illegible]	206.83759279056358	[illegible]
[illegible]	206.7509627864563	-3.8887157268720642
18.869999999999997	206.62770746960373	-3.9154179921877184
18.8725	206.4623136997317	-3.942309089923546
18.875	206.2542967773596	-3.969333794498866

Max. impedance

S11 = - 3.80927 dB

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What is a

nonlinear least squares

logistic function fit ?

Ans. Pierre Francois Verhulst (1845)

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

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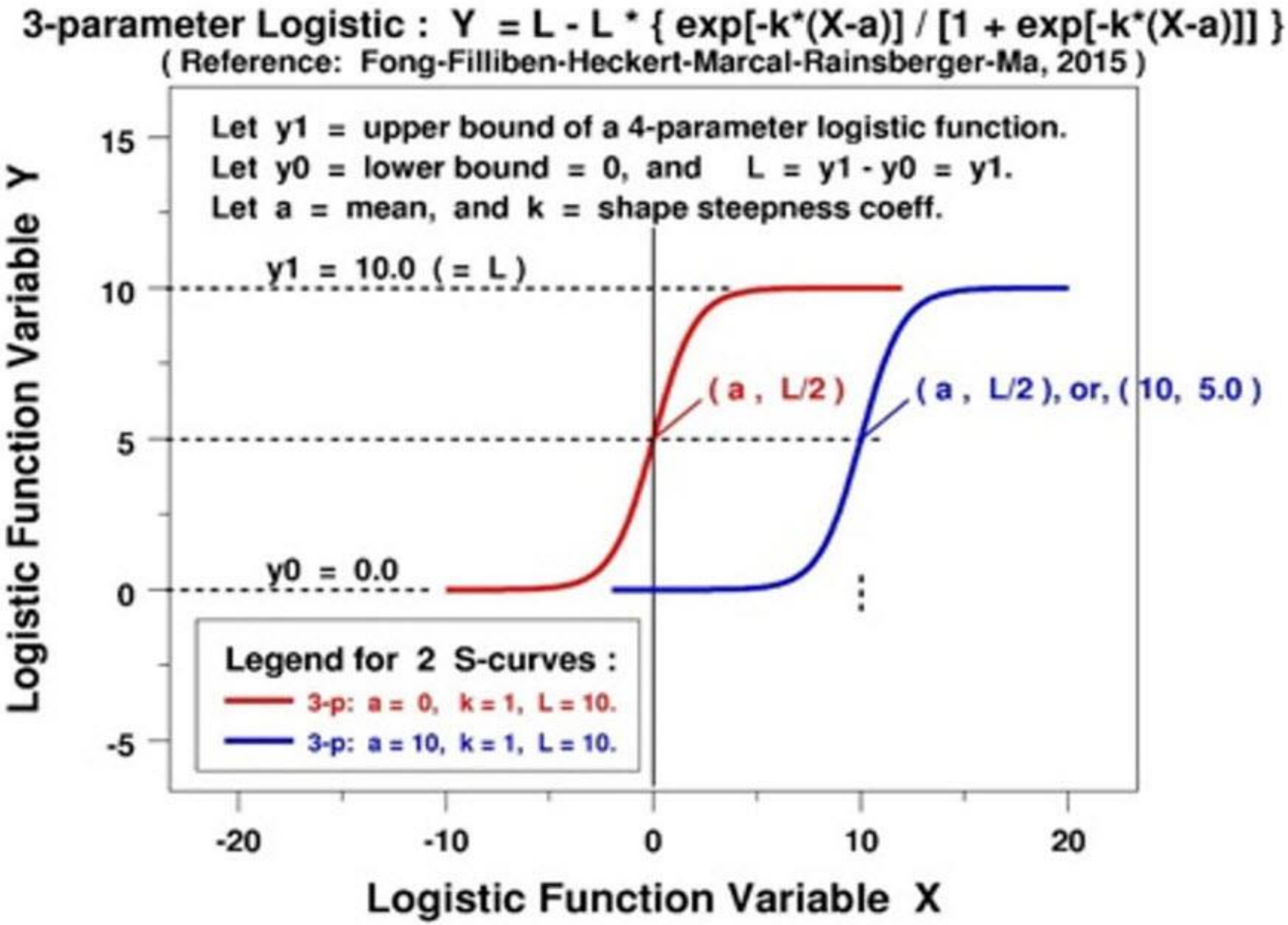
What is a logistic function ?



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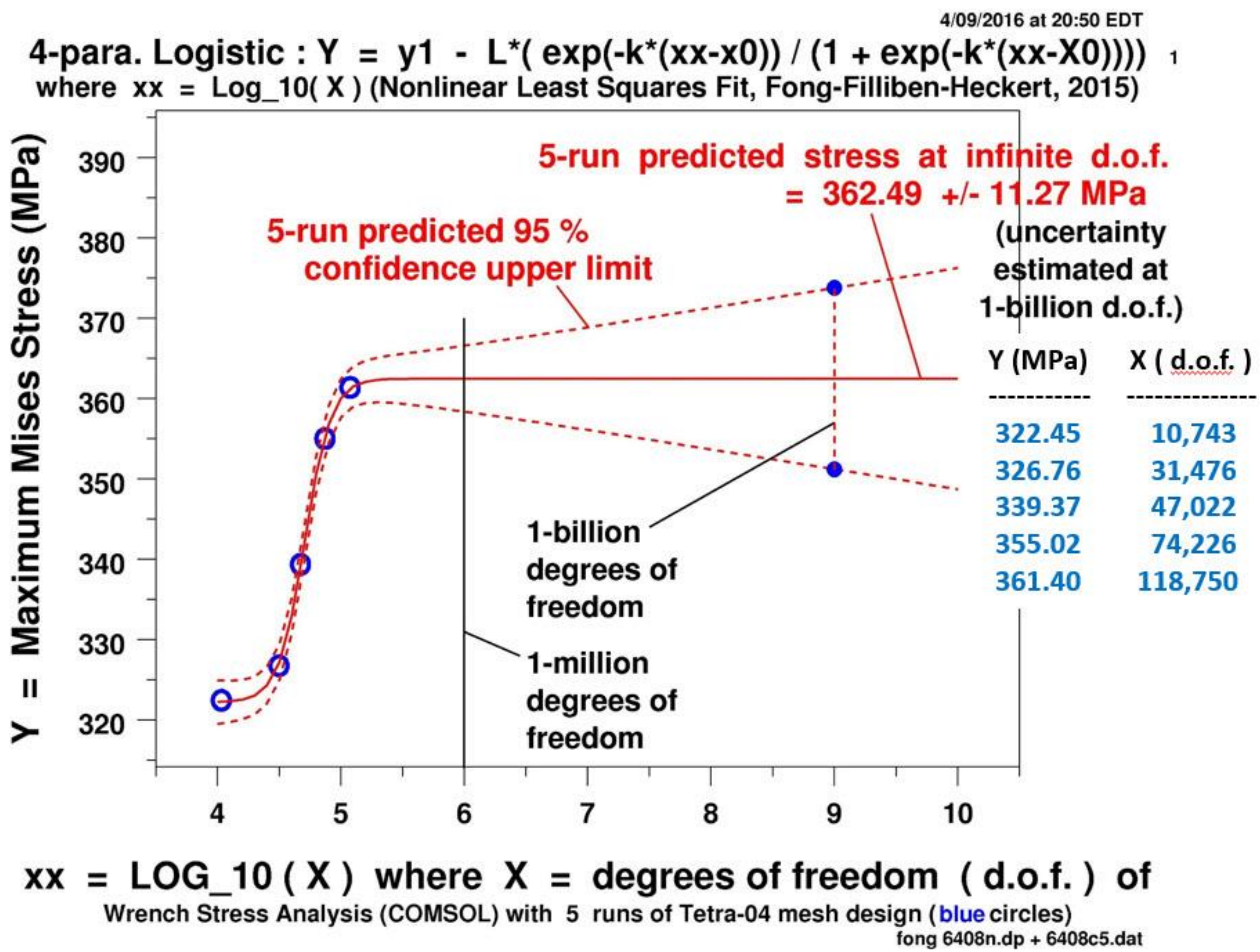
NLLSQ (Example 1. Wrench)



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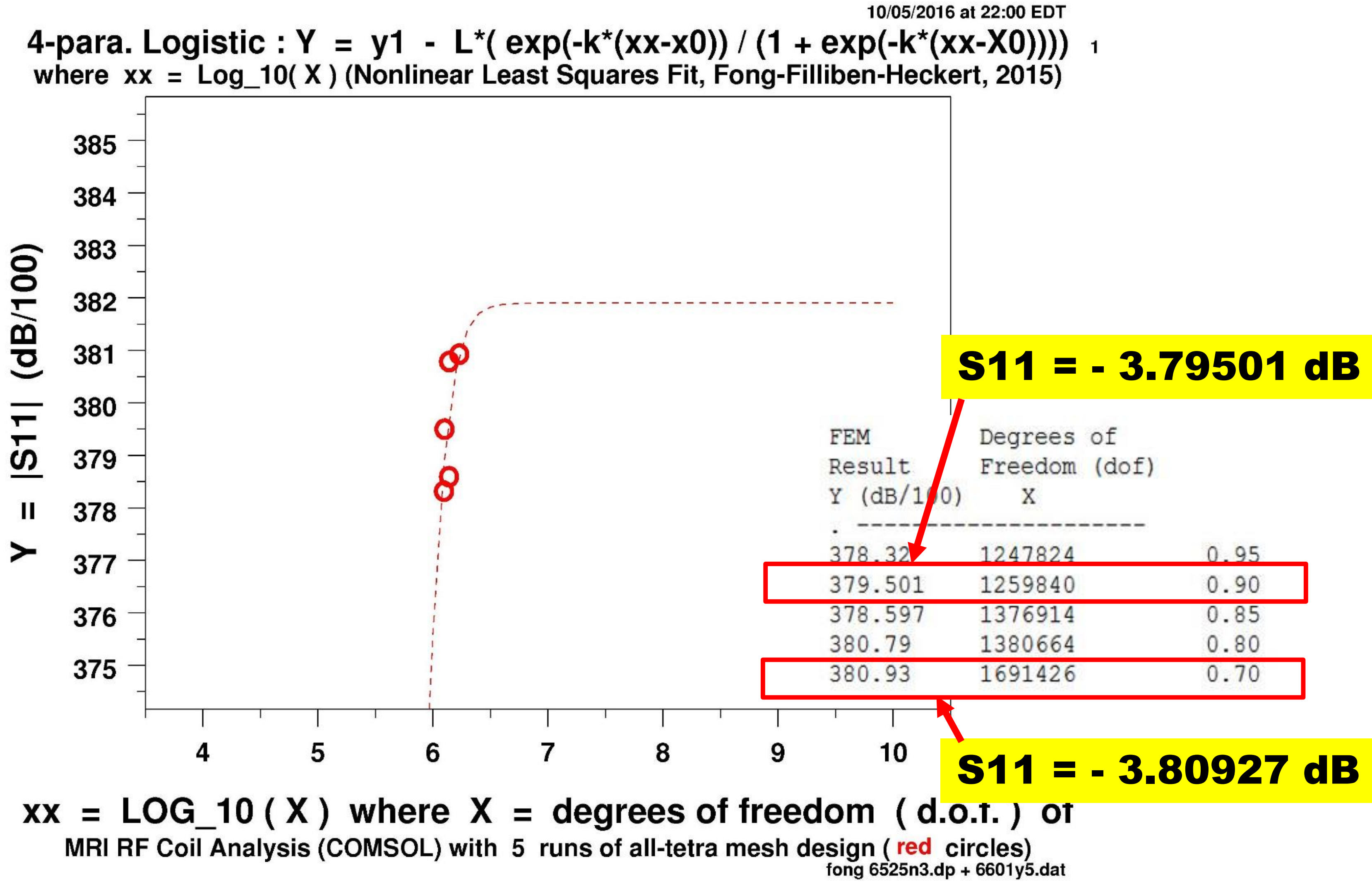
NLLSQ (Example 2. RF Coil-All tetra)



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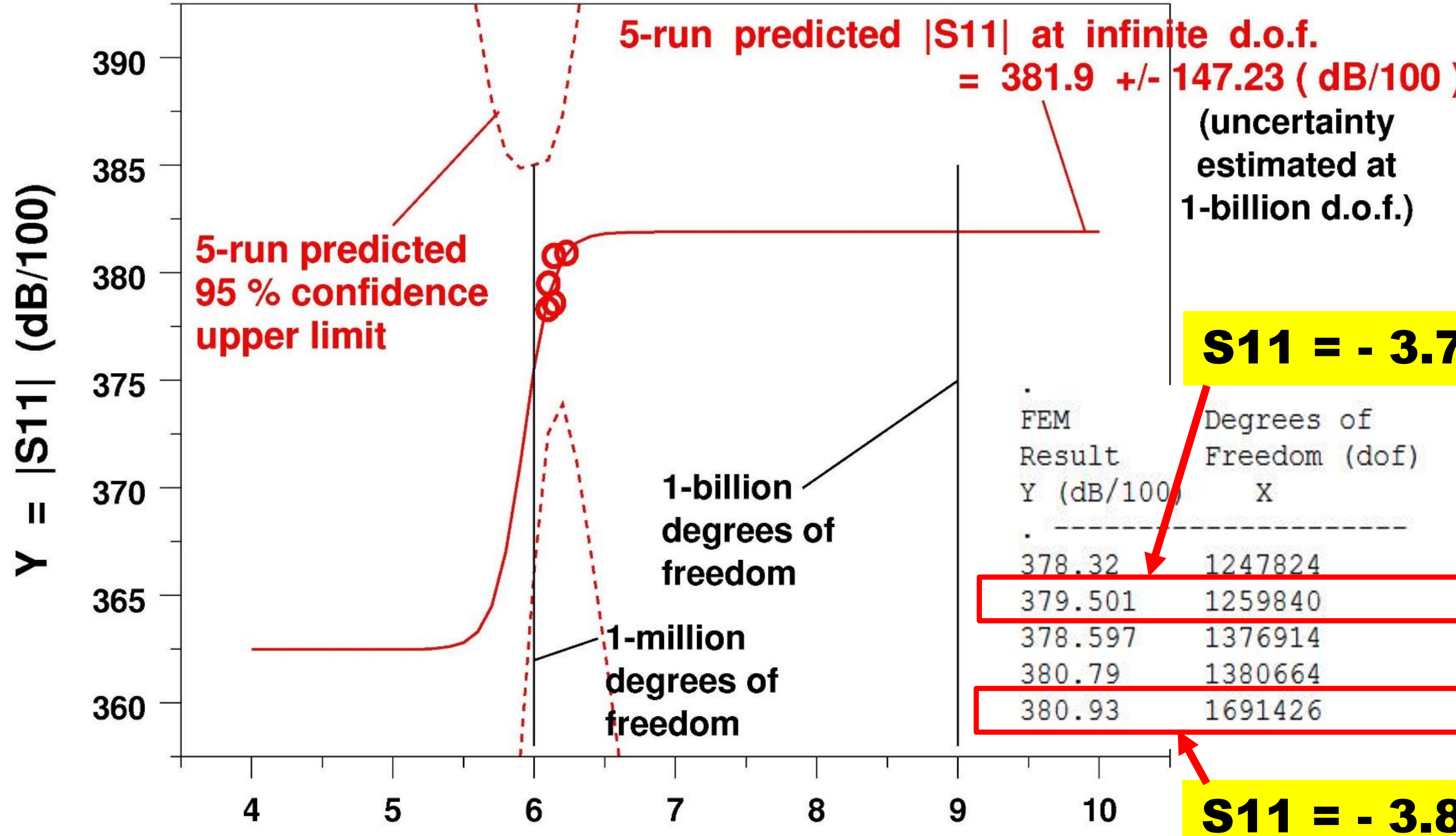
Mesh-1 (All Tetra-10, *automatic*).

6/02/2016 at 6:00 EDT

4-para. Logistic : Y = y1 - L*(exp(-k*(xx-x0)) / (1 + exp(-k*(xx-X0)))) 1
where xx = Log_10(X) (Nonlinear Least Squares Fit, Fong-Filliben-Heckert, 2015)



S11 = - 3.79501 dB

FEM Result Y (dB/100)	Degrees of Freedom (dof) X	
378.32	1247824	0.95
379.501	1259840	0.90
378.597	1376914	0.85
380.79	1380664	0.80
380.93	1691426	0.70

S11 = - 3.80927 dB

xx = LOG_10 (X) where X = degrees of freedom (d.o.f.) of
MRI RF Coil Analysis (COMSOL) with 5 runs of all-tetra mesh design (red circles)
fong 6525n2.dp + 6601y5.dat

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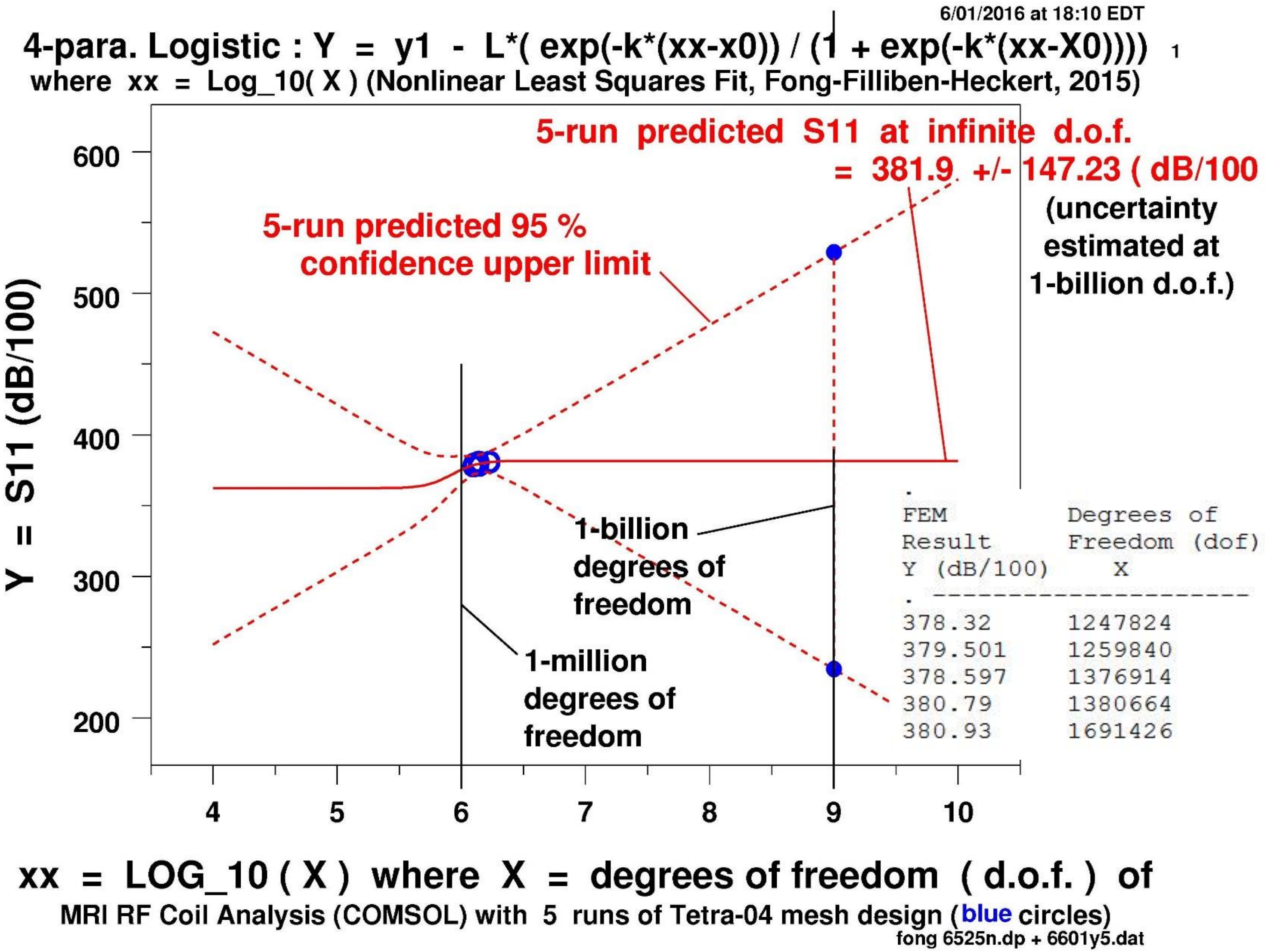
Mesh-1 (All Tetra-10, *automatic*).



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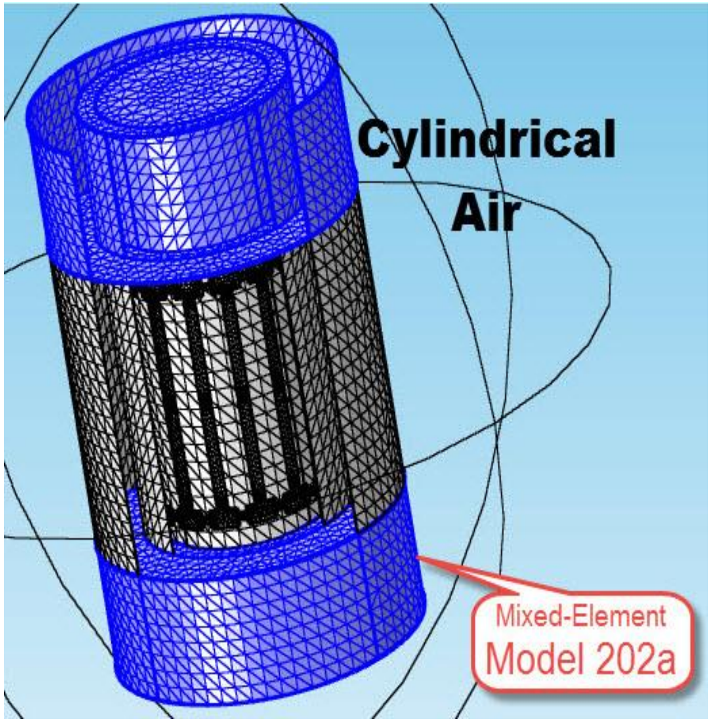
Mesh-2 (Mixed Hexa-27 & Tetra-10).



Results with sweep step **Δf=0.0025MHz**

refine	d.o.f.	Resonant (MHz)	S11, dB
1.0	366,804	18.5825	-4.6977
0.9	357.140	18.550	-4.6209
0.8	500,500	18.480	-4.6035
0.7	641,130	18.395	-4.5993
0.6	818,042	18.385	-4.5794
0.5	1,541,544	18.280	-4.4929

d.o.f. not smooth, DISCARD

refine = 1.0

freq (MHz)	abs(emw.Zport_1) (Ω)	S-parameter, dB, 11 c
18.5675	167.5117256368121	-4.541666878029899
18.57	167.6089499414505	-4.56741633987816
18.572499999999998	167.6912612243203	-4.593215307739826
18.575	167.75138023125416	-4.6191973049909025
18.5775	167.7954466988888	-4.6452399801370605
18.58	167.81783681210047	-4.671458766028917
18.5825	167.82397143870503	-4.697721376795229
18.585	167.80847162821925	-4.724159675417922
18.5875	167.77420830076792	-4.750717298600533
18.59	167.7205741390706	-4.777375239121876

refine = 0.9

freq (MHz)	abs(emw.Zport_1) (Ω)	S-parameter, dB, 11 c
18.535	170.60619960570068	-4.467244466482608
18.537499999999994	170.7126937761477	-4.492535083533854
18.54	170.79709903985378	-4.517996878745572
18.542499999999997	170.86437562537344	-4.543524673575717
18.544999999999998	170.9103278826809	-4.569207462844624
18.5475	170.93754690342865	-4.594953017355833
18.549999999999997	170.94202080485647	-4.620892645177169
18.5525	170.92931349620483	-4.646881181853474
18.555	170.89473976210573	-4.673014972544322
18.557499999999994	170.84044498471246	-4.699262389142246

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Mesh-2 (Mixed Hexa-27 & Tetra-10).

refine = 0.8

freq (MHz)	abs(emw.Zport_1) (Ω)	S-parameter, dB, 11 c
18.4725	170.5724311167183	-4.525864352508932
18.474999999999994	170.6327832032265	-4.551616006440511
18.4775	170.6716108003286 6	-4.577521081345017
18.48	170.69180621727514	-4.603516471311001
18.482499999999998	170.69066232244325	-4.629640852289745
18.485	170.67016522823252	-4.655876354784988
18.4875	170.628157518795	-4.682247391897374
18.49	170.5674711672644	-4.708726155498152
18.4925	170.48450675325503	-4.735349991705128
18.494999999999997	170.38296165323393	-4.762044131788831

refine = 0.7

freq (MHz)	abs(emw.Zport_1) (Ω)	S-parameter, dB, 11 cc
18.3825	170.23704061575592	-4.468536232065694
18.384999999999998	170.33687573249475	-4.494460969534298
18.3875	170.4176780218532	-4.520422373865811
18.39	170.4762371973736	-4.546631016069091
18.3925	170.51580685609602	-4.572924907852172 5
18.395	170.53399811332704	-4.5993308926209835
18.3975	170.53381867829094	-4.62580583165259
18.4	170.50966495263634	-4.652516611903125
18.4025	170.46751747769167	-4.679284636043822
18.404999999999998	170.40308274732632	-4.706223726266241

refine = 0.6

freq (MHz)	abs(emw.Zport_1) (Ω)	S-parameter, dB, 11 c
18.372500000000002	171.52455153345858	-4.449811397783272
18.375	171.61963576211897	-4.475491960891757
18.377499999999998	171.69613845218075	-4.501305600013004
18.380000000000003	171.7520877371454	-4.527188984430895
18.3825	171.78769317641454	-4.553223706678104
18.384999999999998	171.80130966447052	-4.579405034709617
18.387500000000003	171.79564847879826	-4.605669292501719
18.39	171.7667574256268	-4.632082566900425
18.3925	171.7185685643193	-4.658624905865834
18.395000000000003	171.6485198727767	-4.685292763371608

refine = 0.5

freq (MHz)	abs(emw.Zport_1) (Ω)	S-parameter, dB, 11 c
18.2675	175.22058038300148	-4.364404706749389
18.27	175.32209722141712	-4.38985381711027
18.2725	175.4010241486673	-4.415427669313403
18.275	175.45906989520614	-4.441121929932902
18.2775	175.4929368753370 8	-4.466990483057104
18.279999999999998	175.50661758390277	-4.492910375465279
18.2825	175.4966025262042	-4.518995406986013
18.285	175.46629783086277	-4.545152181921165
18.287499999999998	175.41227439648904	-4.571438124899577
18.29	175.33626742103075	-4.597863601040146

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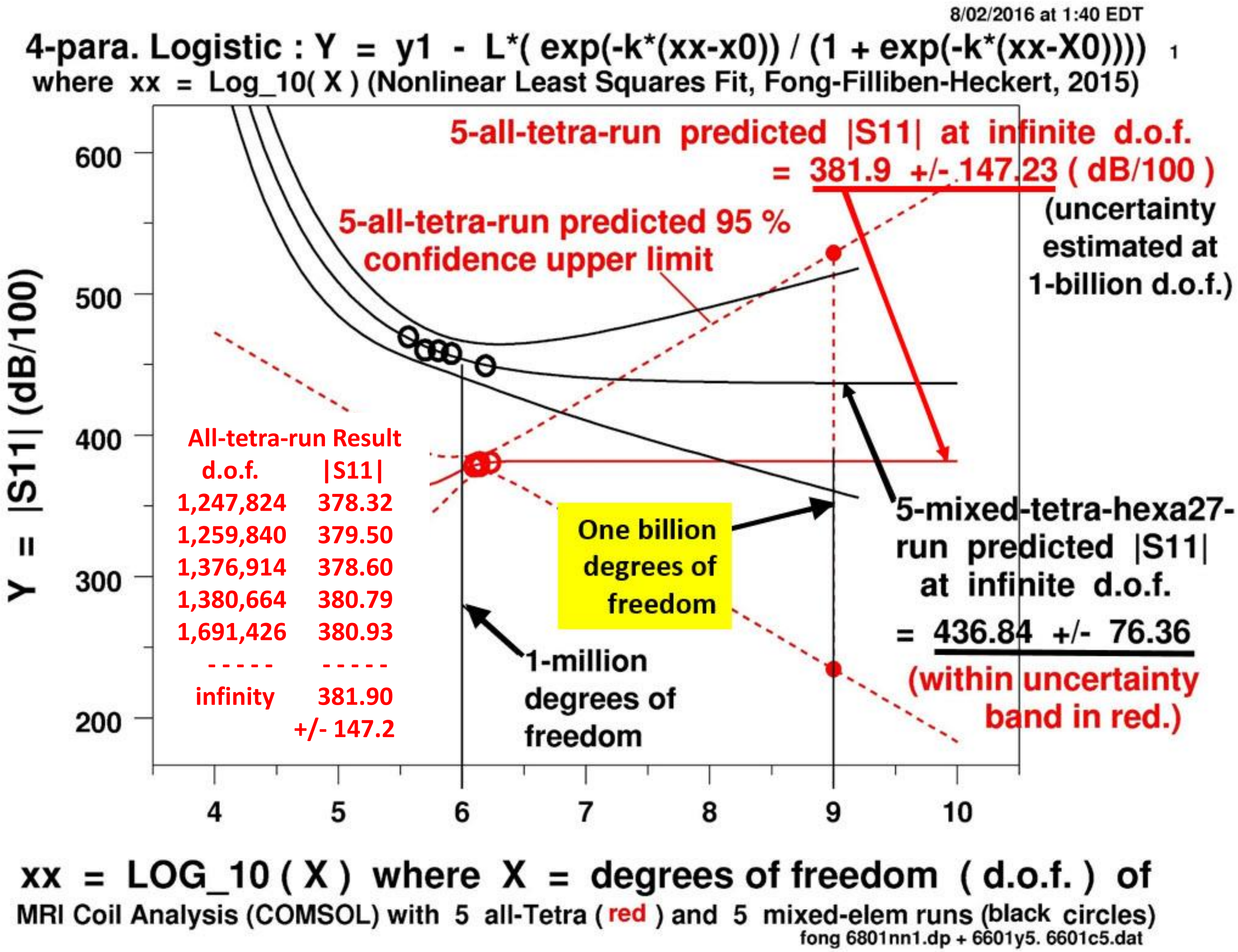
Solution with *Uncertainty* for Mesh-1 and -2

Mixed-tetra-and-hexa27-run Result

d.o.f.	|S11|
-------	---------
366,804	469.77
500,500	460.35
641,130	459.93
818,042	457.94
1,541,544	449.29
- - - - -	- - - - -
infinity	436.84 +/- 76.36



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Concluding Remarks.

1. An accurate estimate of **uncertaint**y in FEM-based solution **is essential** in verification (V1) and validation (V2) 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 (mean aspect ratio), 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 that is useful as a metric for assessing the accuracy of the FEM results.

3. For solving the resonance problem of an MRI birdcage RF coil, we chose to work with two mesh designs, **Mesh-1** (all tetra-10, automatic), and **Mesh-2** (mixed hexa-27 and tetra-10). After running **five** solutions of each mesh, and fitting each with a 4-parameter logistic function, the extrapolated S11 value to the infinite degrees of freedom and its uncertainty at one billion degrees of freedom for each mesh is given by

   Mesh-1: S11 = 3.82 dB (uncertainty, 38.6 %).
   Mesh-2: S11 = 4.37 dB (uncertainty, 17.5 %).

4. **We conclude, before making more runs to improve uncertainty in each mesh, Mesh-2 with less uncertainty is preferred over Mesh-1. Additional runs should be made using Mesh-2 to reduce uncertainty to less than 1 %. This is future work and on-going.**

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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.

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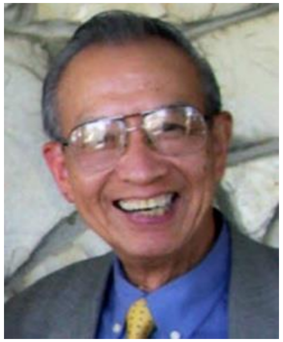
Speaker's Biographical Sketch



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."

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