Simulation of Superconducting Qubit Devices

Workshop on Microwave Cavities and Detectors for Axion Research

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Outline

- Definition of a qubit
- Non-linearity in superconducting qubits and Josephson junctions
- Cavity QED and Circuit QED
- Black box Circuit Quantization
- Types of Superconducting Qubits
- Physical realization of superconducting circuits
- Simulating RF components of qubits in COMSOL

Qubits

- A quantum “bit” or two level system / *effective* two level system with addressable energy levels
- In some cases, a qubit can be treated as a harmonic oscillator with non-linearly spaced levels
- Level spacing due to anharmonicity from non-linearity(ies), allows for designs that minimize leakage to higher excited states of the qubit(s)

Source of Non-linearity: Josephson Junction

- DC Josephson Effect – B. Josephson, 1962[1]
  - Non-zero periodic current, due to tunneling Cooper Pairs across an SIS (superconductor-insulator-superconductor) junction
  - The current varies periodically in the phase difference across the junction, acting as a macroscopic quantum variable
  - Josephson Current and Voltage Equations

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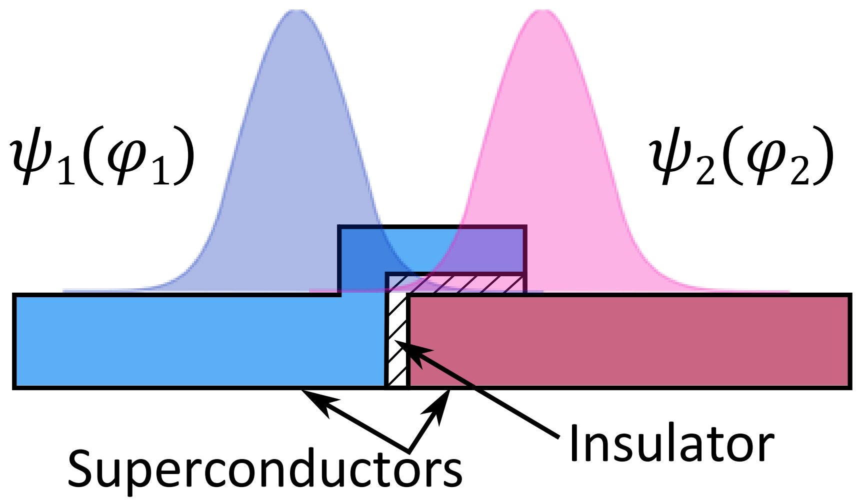
$$I = I_c \sin\varphi$$

$$V = \frac{\hbar}{2e}\frac{d\varphi}{dt} = \frac{d\phi}{dt}$$

$$\varphi = \varphi_1 - \varphi_2$$



[1] B.D. Josephson, Phys.Lett. **1**, 7 (1962)

IV Characteristics of Josephson Junctions

- The DC current in an SIS junction is given at zero temperature[2]

$$I_{\rm dc} = {\rm Im}\left\{j_2(\omega)\right\}, \quad I_{\rm dc} \sim {\rm sgn}(\omega) K_0\left(\left(\frac{x^2-1}{x^2-\delta^2}\right)^{1/2}\right), \quad x = \frac{|\omega|}{\Delta_1+\Delta_2}, \quad \delta = \frac{\Delta_1-\Delta_2}{\Delta_1+\Delta_2}$$

- where K_0 is the zero-th order modified Bessel function of the first kind, Δ_1, Δ_2 are the superconducting gap energies of the superconducting leads

[2] N.R. Werthamer, Phys. Rev. **147**, 255 (1966)

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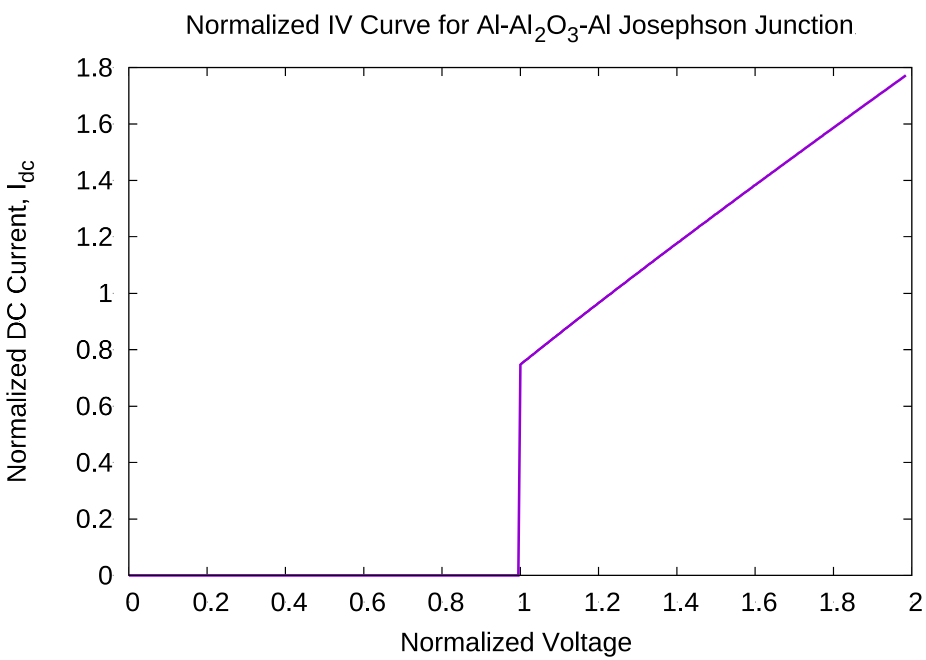

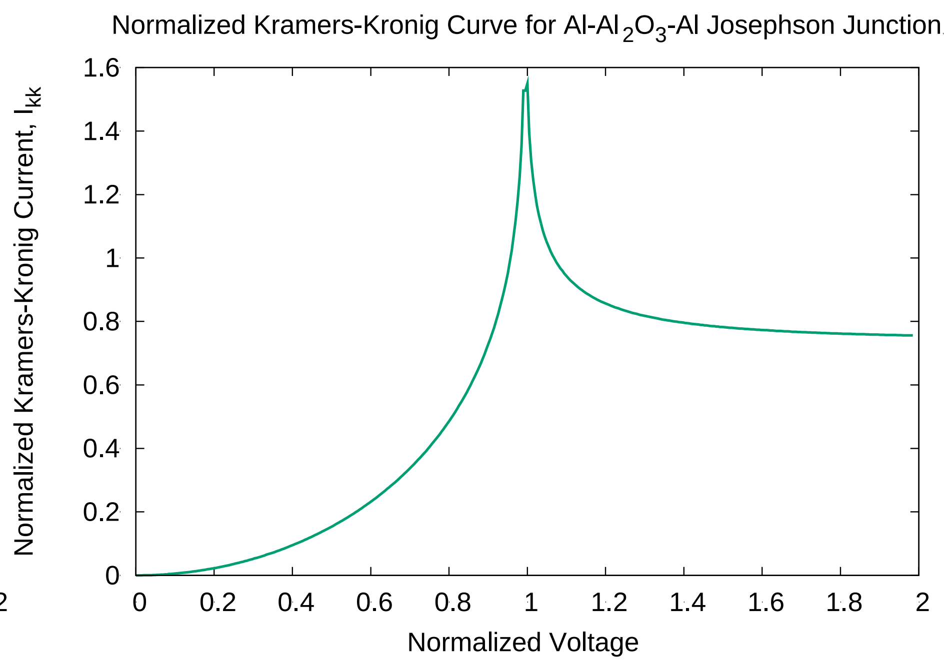

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Josephson Junction Circuit Model

- Josephson Junctions can be approximated by linear, passive circuit elements shunting a non-linear inductance L_J
  - RCSJ Model (Resistance and Capacitive Shunted Junction)[3]
  - Useful model for including simple non-linear behavior in classical simulations, e.g. COMSOL
  - From Kirchhoff's current law, the current flowing through each element in the circuit is given by

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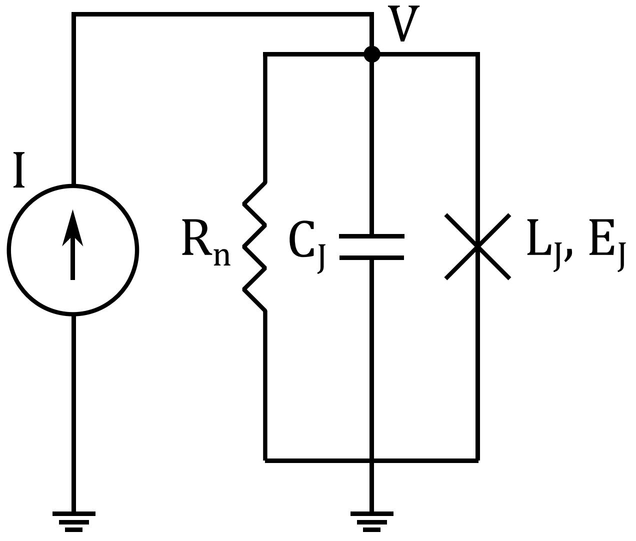
$$I = \frac{V}{R_n} + C_J \frac{dV}{dt} + I_c \sin(\varphi)$$



[3] D. I. Schuster, Circuit Quantum Electrodynamics. PhD thesis, Yale University, 2007.`

Circuit Quantum Electrodynamics (cQED)

- Use Josephson Junctions as a source of non-linearity to realize macroscopic quantum systems
- Borrow concepts from the optics community, e.g. cavity QED to implement familiar systems
- Atom in a resonant cavity is the most basic model

Cavity QED and Model Hamiltonians

- Cavity QED: two level atomic system trapped in a mirrored, high finesse resonant cavity
- Follows the Jaynes-Cummings Hamiltonian[3]

$$\hat{H} = \underbrace{\hbar\omega_r\left(\hat{a}^\dagger\hat{a} + 1/2\right)}_{\text{EM field quantization}} + \underbrace{\hbar\omega_a\hat{\sigma_z}/2}_{\text{spin-1/2 atom}} + \underbrace{\hbar g\left(\hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma_+}\right)}_{\text{atom-cavity interaction}}$$

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[4] R. J. Schoelkopf and S. M. Girvin, Nature, vol. 451, pp. 664–669, 02 2008.

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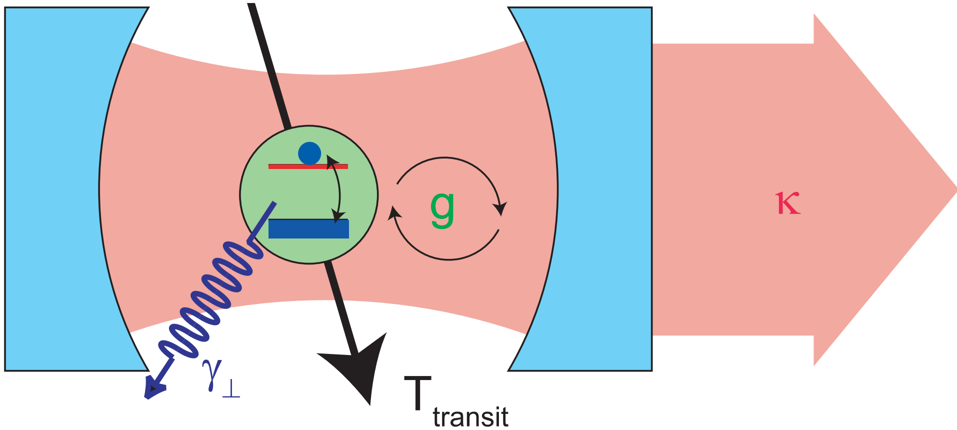
$2g = \text{Vacuum Rabi Frequency}$

$\kappa = \text{Cavity Decay Rate}$

$\gamma_\perp = \text{Transverse Decay Rate}$

$T_{\text{transit}} = \text{Time for atom to leave cavity}$



Atom trapped in a cavity with photon emission, atomic-cavity dipole coupling, and atom transit time shown[4].

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[4] R. J. Schoelkopf and S. M. Girvin, Nature, vol. 451, pp. 664–669, 02 2008.

Cavity QED and Circuit QED, from optics to RF

Cavity QED	Circuit QED
Two Level Atom	Artificial atom, truncated to two levels
High Finesse Cavity	High Q Cavity / Planar Resonator
Small transition dipole moment	Arbitrarily large transition dipole moment, e.g. strong coupling regime
$1/\kappa$, $1/\gamma$	T_1 , T_2

- Large dipole moment couples the qubit well to the cavity in superconducting qubits: coupling strength and energy levels are *tunable* by design or in situ

Cavity QED and Circuit QED, Device Comparison

Parameter	Symbol	Cavity QED[3]	Circuit QED[3, 5]
Resonator, Qubit Frequencies	$\omega_r, \omega_q / 2\pi$	~ 50 GHz	~ 5 GHz
Transition Dipole Moment	d / ea_0	~ 1	~ 10^4
Relaxation Time	T_1	30ms	60 µs
Decoherence Time	T_2	~1 ms	~10-20 µs

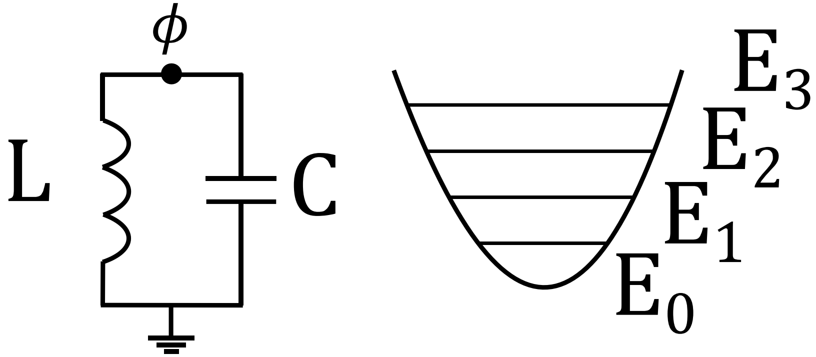
- Large dipole moment couples the qubit well to the cavity in superconducting qubits: coupling strength and energy levels are *tunable*
- Trapped atoms in cavities have *longer coherence times*, *not tunable*, weakly coupled to the cavity for measurement

[3] D. I. Schuster, Circuit Quantum Electrodynamics. PhD thesis, Yale University, 2007.
[5] H. Paik, et al., Phys. Rev. Lett. **107**, 240501 (2011)

Quantizing Simple Circuits

- Simplest model is an LC-resonator treated as a quantum harmonic oscillator with classical Lagrangian, Hamiltonian, and quantized operators[3]

$$\mathcal{L}(\phi, \dot{\phi}) = \frac{1}{2}C\dot{\phi}^2 - \frac{\phi^2}{2L}$$



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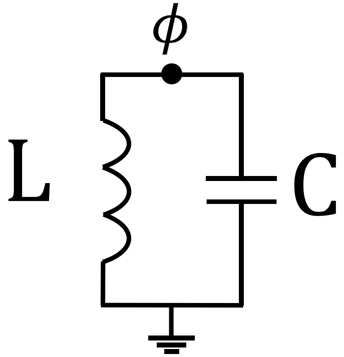

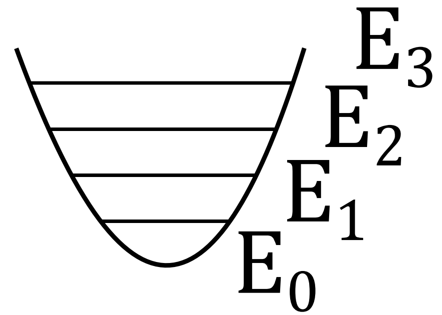

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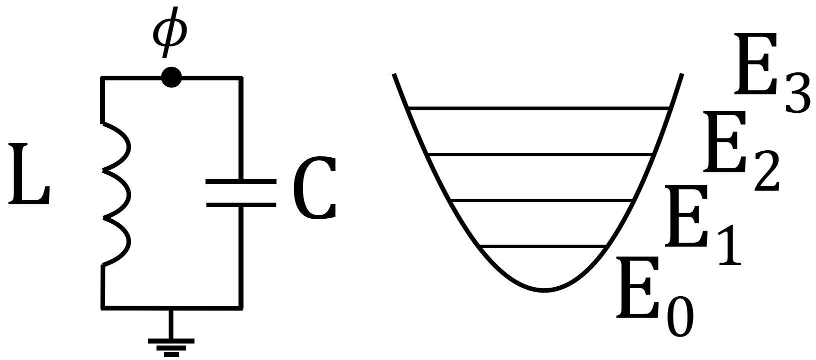
$$H \to \hat{H} = \frac{\hat{q}^2}{2C} + \frac{\hat{\phi}^2}{2L}, \qquad \left[\hat{\phi}, \hat{Q}\right] = i\hbar$$



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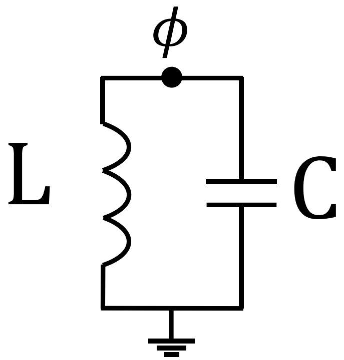

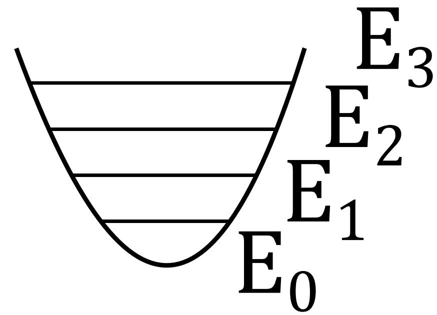

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$$\hat{\phi} = \sqrt{\frac{\hbar}{2\omega C}}\left(\hat{a} + \hat{a}^\dagger\right) \qquad \hat{q} = -i\sqrt{\frac{\hbar\omega C}{2}}\left(\hat{a} - \hat{a}^\dagger\right)$$

$$\omega^2 = 1/(LC)$$

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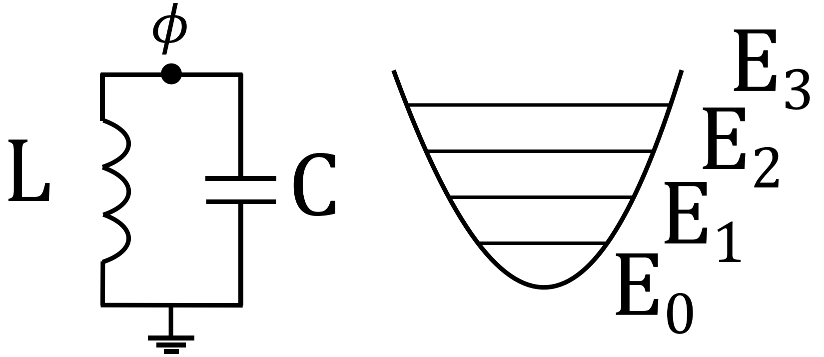

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$$\omega^2 = 1/(LC)$$

$$\Longrightarrow \hat{H} = \boxed{\hbar\omega\left(\hat{a}^\dagger \hat{a} + 1/2\right)}$$

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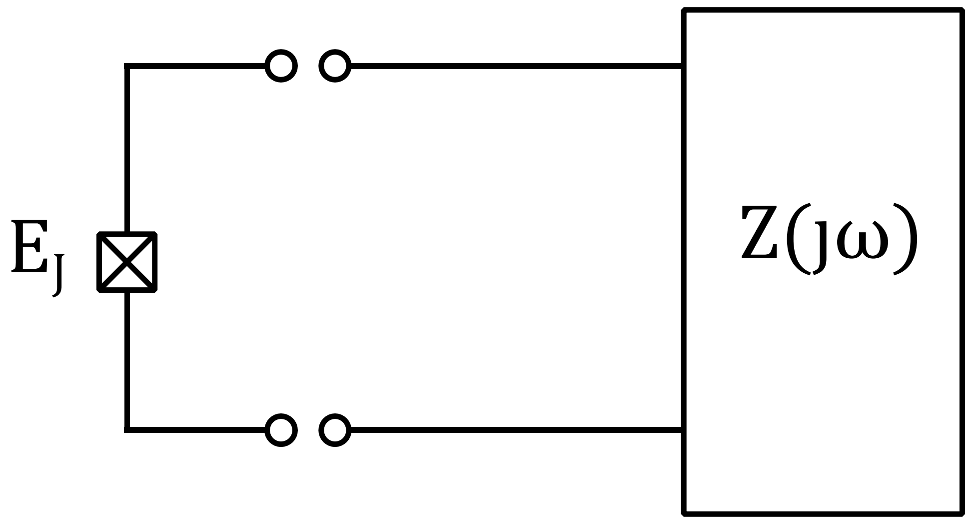
Black box Circuit Quantization

- Idea is to extract all linear components of the qubit and microwave circuitry by synthesizing an equivalent passive electrical network
- The network is obtained by computing the S-parameters of a device using FEM software (COMSOL, HFSS) and converting them to an impedance, Z (j!)

$$Z = (\mathbb{1} + S)(\mathbb{1} - S)^{-1}$$

$$\mathbb{1} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}$$



Black box Circuit Quantization—Vector Fit

- The impedance function is fit to a pole-residue expansion following the Vector Fit procedure, a least squares fit to a rational function of the form[6]

$$Z(s) \simeq \sum_{k=1}^{M} \frac{R_k}{s - s_k} + d + es$$

- From this form, there are two synthesis approaches with two quantization schemes
  - — Lossy Foster approach (approximate circuit synthesis)[7]
  - — Brune exact synthesis approach[8]

[6] B. Gustavsen et al., IEEE Tran on Power Delivery, 14(3):1052–1061, Jul 1999
[7] F. Solgun et al. Phys.Rev.B **90**, 134504 (2014)
[8] S. E. Nigg et al. Phys.Rev.Lett. **108**, 240502 (2012)

Black box Circuit Quantization—Lossy Foster

- Taking the constant term d = 0 and excluding the pole at s = 1 or setting e = 0 leaves the rational function with poles and residues R_k , s_k[7]

$$Z(s) = \sum_{k=1}^{M} \frac{R_k}{s - s_k}, \quad s_k = \xi_k + \jmath\omega_k, \quad R_k = a_k + \jmath b_k$$

- Expanding the k-th component of Z(s) in partial fractions and taking the low loss limit, »$_k$, b_k ¿ 1

$$Z_k(s) = \frac{R_k}{s - s_k} + \frac{R_k^*}{s - s_k^*} \simeq \frac{2a_k s}{s^2 - 2\xi_k s + \omega_k^2}$$

$$\Longrightarrow \boxed{Z_k(s) = \frac{\frac{\omega_k R_k}{Q_k} s}{s^2 + \frac{\omega_k}{Q_k} s + \omega_k^2}}$$

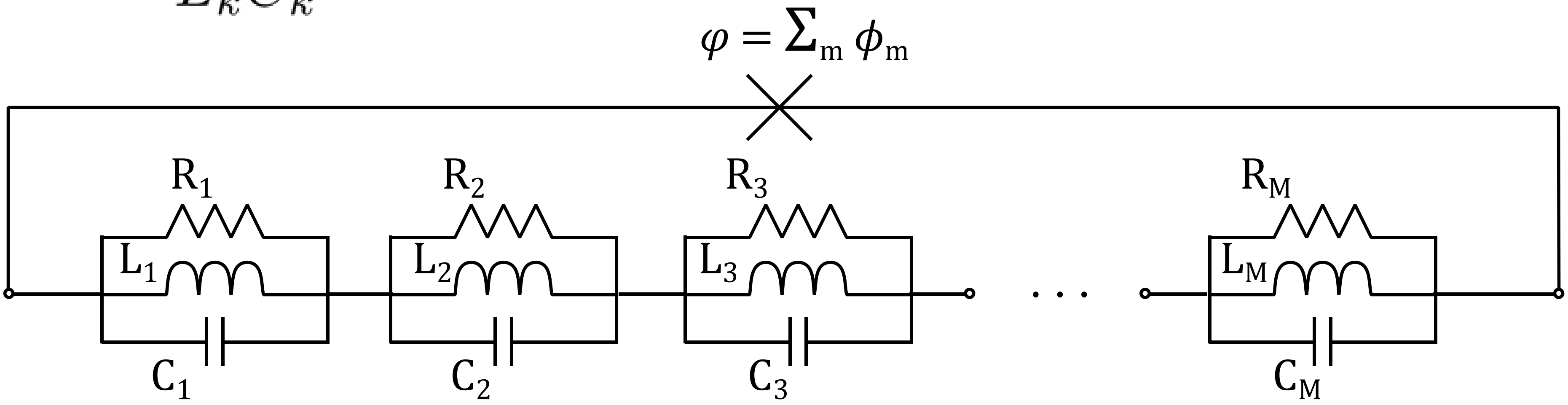
RLC Tank Circuit!

[7] F. Solgun et al. Phys.Rev.B **90**, 134504 (2014)

Black box Circuit Quantization—Lossy Foster

- Main result of the Lossy Foster treatment is a set of uncoupled harmonic oscillators as a series of RLC circuits
- Circuit elements in terms of the real and imaginary components of the poles and residues[7]

$$\omega_k^2 = \frac{1}{L_k C_k}, \quad Q_k = \omega_k R_k C_k = -\omega_k/2\xi_k, \quad R_k = -a_k/\xi_k$$



[7] F. Solgun et al. Phys.Rev.B **90**, 134504 (2014)
[9] J. Bourassa et al. Phys.Rev.A **86**, 013814 (2012)

Black box Circuit Quantization—Lossy Foster

- From the circuit elements, a lossless Hamiltonian is obtained by taking the limit $R_k \to 1\ 8_k$
- The LC circuits are quantized as harmonic oscillators giving the linear Hamiltonian[8]

$$\hat{H}_0 = \sum_{k=1}^{M} \hbar\omega_k \left(\hat{a}_k^\dagger \hat{a}_k + 1/2 \right)$$

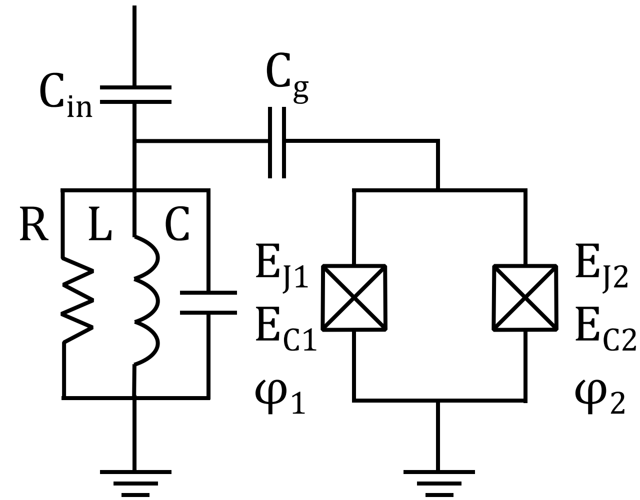
- A non-linear Hamiltonian accounts for the qubit and its coupling to the harmonic modes

$$\hat{H}_{\mathrm{nl}} = E_J \left(1 - \cos\hat{\varphi} - \frac{\hat{\varphi}^2}{2} \right), \quad \hat{\varphi} = \sum_{k=1}^{M} \sqrt{\frac{\hbar}{2\omega_k C_k}} \left(\hat{a}_k + \hat{a}_k^\dagger \right)$$

[8] S.E. Nigg et al. Phys.Rev.Lett. **108**, 240502 (2012)

Types of Superconducting Qubits: Charge Qubits

- Early Charge qubit – Cooper Pair Box (CPB)
  - Cooper pairs tunnel across the junction leading to a charge number operator
  - Typical implementations include a resonator that plays the role of a cavity
  - Hamiltonian in the charge basis for single Josephson junction[3]



$$\hat{H}_{\mathrm{CPB}} = 4E_C\left(\hat{N} - n_g/2\right)^2 + \frac{1}{2}E_J\sum_n\left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right)$$

  - "Split" CPB including RLC resonator and coupling[3]

$$\hat{H}_{\mathrm{CPB+RLC}} = \underbrace{4E_C\left(\hat{N} - n_g/2\right)^2}_{\text{CPB term}} + \underbrace{\frac{4E_C C_g\hat{V}\left(2V_g + \hat{V}\right)}{e}}_{\text{junction capacitance}} - \underbrace{\frac{4_C C_g\hat{V}\hat{N}}{e}}_{\text{RLC-CPB coupling}}$$

[3] D. I. Schuster, Circuit Quantum Electrodynamics. PhD thesis, Yale University, 2007.

Types of Superconducting Qubits: Charge Qubits

- Early Charge qubit – Cooper Pair Box (CPB)
  - Rotating wave approximation (RWA) and Jaynes-Cummings Hamiltonian
    - Approximate number and charge number operators as Pauli operators[3]

$$\hat{N} \approx \hat{\sigma}_z/2, \quad (|n\rangle\langle n+1| + |n+1\rangle\langle n|) \approx \hat{\sigma}_x$$

    - Expand voltage operator, V, apply RWA to coupling term and substitute the qubit plasma frequency, !$_p$ = $(L_J C_J)^{-1/2}$

$$\hat{V} = \sqrt{\frac{\hbar\omega_r}{2C}}\left(\hat{a} + \hat{a}^\dagger\right), \quad -\frac{4E_C C_g \hat{V}\hat{N}}{e} = 2\hbar g\left(\hat{a} + \hat{a}^\dagger\right)\hat{\sigma}_x$$

$$2\hbar g\left(\hat{a} + \hat{a}^\dagger\right)\hat{\sigma}_x \approx \hbar g\left(\hat{a}\hat{\sigma}_+ + \hat{a}^\dagger\hat{\sigma}_-\right)$$

$$\boxed{\hat{H}_{CPB+RLC} \approx \hbar\omega_r\hat{a}^\dagger\hat{a} + \hbar\omega_p\hat{\sigma}_z/2 + \hbar g\left(\hat{a}\hat{\sigma}_+ + \hat{a}^\dagger\hat{\sigma}_-\right)}$$

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**Reclaims Jaynes-Cummings Hamiltonian

[3] D. I. Schuster, Circuit Quantum Electrodynamics. PhD thesis, Yale University, 2007.

Types of Superconducting Qubits: Transmon

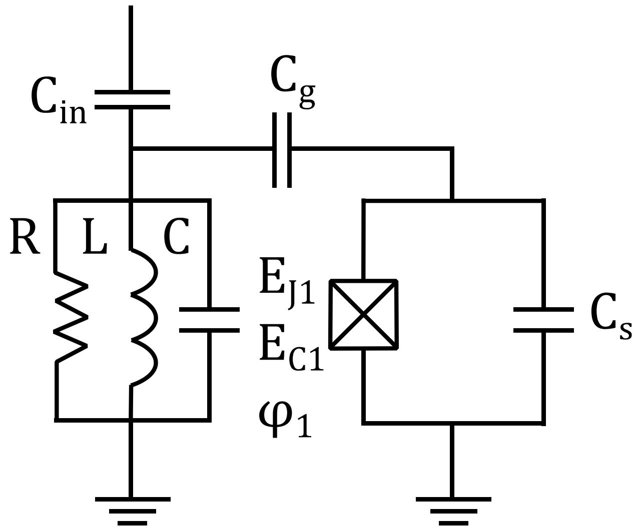
- Transmon, an improved charge qubit
  - Shunt capacitor reduces sensitivity to charge noise
  - Flatter energy levels, weakly anharmonic
  - Hamiltonian, qubit + resonator[3]

$$\hat{H}_{\text{trans}} = -4E_C \frac{\partial^2}{\partial\varphi^2} - E_J \cos(\varphi)$$

$$\approx -4E_C \frac{\partial^2}{\partial\varphi^2} - E_J \left(1 - \frac{\varphi^2}{2} + \frac{\varphi^4}{4!} + \mathcal{O}(\varphi^6)\right)$$

$$\varphi = \frac{1}{\sqrt{2}} \left(\frac{8E_C}{E_J}\right)^{1/4} \left(\hat{b} + \hat{b}^\dagger\right)$$

$$\hat{N} = \frac{1}{\sqrt{2}} \left(\frac{E_J}{8E_C}\right)^{1/4} \left(\hat{b} - \hat{b}^\dagger\right)$$



[3] D. I. Schuster, Circuit Quantum Electrodynamics. PhD thesis, Yale University, 2007.

Types of Superconducting Qubits: Transmon

- Transmon, an improved charge qubit
  - Hamiltonian in the energy basis, anharmonic oscillator[3]

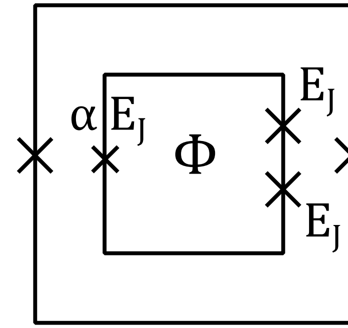
$$\hat{H}_{\mathrm{trans}} \approx \hbar\omega_p \left(\hat{b}^\dagger\hat{b} + 1/2\right) - \frac{E_C}{12}\left(\hat{b} + \hat{b}^\dagger\right)^4$$

  - Including resonator and coupling term follow a similar treatment as the CPB qubit
  - Kerr and cross Kerr terms may be included when expanding the fourth power in b

[3] D. I. Schuster, Circuit Quantum Electrodynamics. PhD thesis, Yale University, 2007.

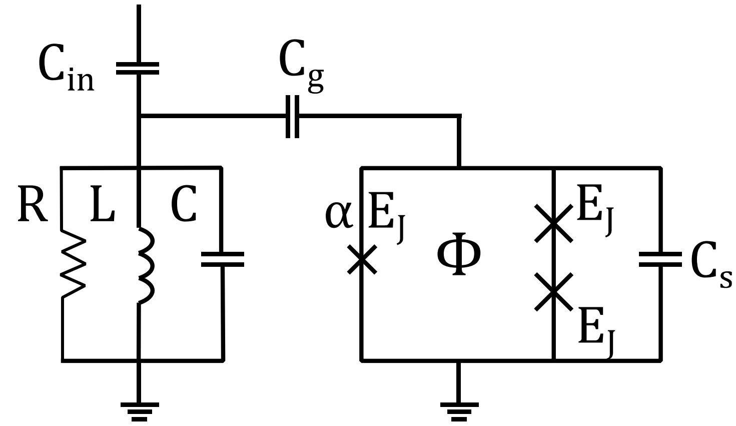
Types of Superconducting Qubits: Flux Qubits

- Flux qubit
  - Flux threading a loop is quantized; DC SQUID biases the qubit
  - Persistent current I_p forms in the superconducting loop
  - Hamiltonian, with fixed gap Δ[10, 11]



$$\hat{H} = I_p \Phi_0 \left(\Phi / \Phi_0 - (n + 1/2) \right) \hat{\sigma}_z + \hbar \Delta \hat{\sigma}_x$$

- Capacitively shunted flux qubit
  - Shunt the flux qubit with a large capacitor, similar to the transmon for charge qubits
  - Hamiltonian, with resonator[12]



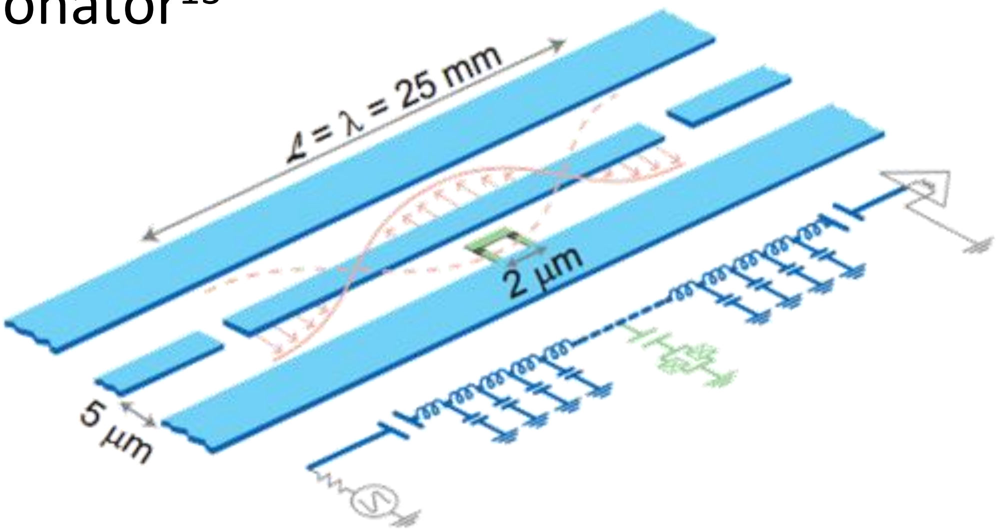
$$\hat{H} \approx \hbar \omega_q (\Phi_b) \hat{\sigma}_z / 2 + \hbar \omega_r \left(\hat{a}^\dagger \hat{a} + 1/2 \right) + \hbar \chi (\Phi_b) \left(\hat{a}^\dagger \hat{a} + 1/2 \right) \hat{\sigma}_z$$

[10] M.J. Schwarz et al. *New Journal of Physics* **15** (2013) 045001
[11] T.P. Orlando, Phys.Rev.B **60**, 15398 (1999)
[12] F. Yei et al, Nature Communications **7** (2016)

Physical Designs: CPW + CPB = Cavity + Atom

- Implemented as Josephson Junction capacitively coupled to transmission line resonator (coplanar waveguide, CPW)
  - Transmission Line Resonator ~ Cavity
  - 2D Planar or 3D cavity couples qubit to drive and readout
- Dipole moment, d , in terms of the magnitude of the applied voltage V_0 , CPW conductor width w , electric field magnitude E_0 , and coupling of the qubit to the resonator[13]

$$\hbar g = (ew)\,\frac{1}{w}V_0 = dE_0$$

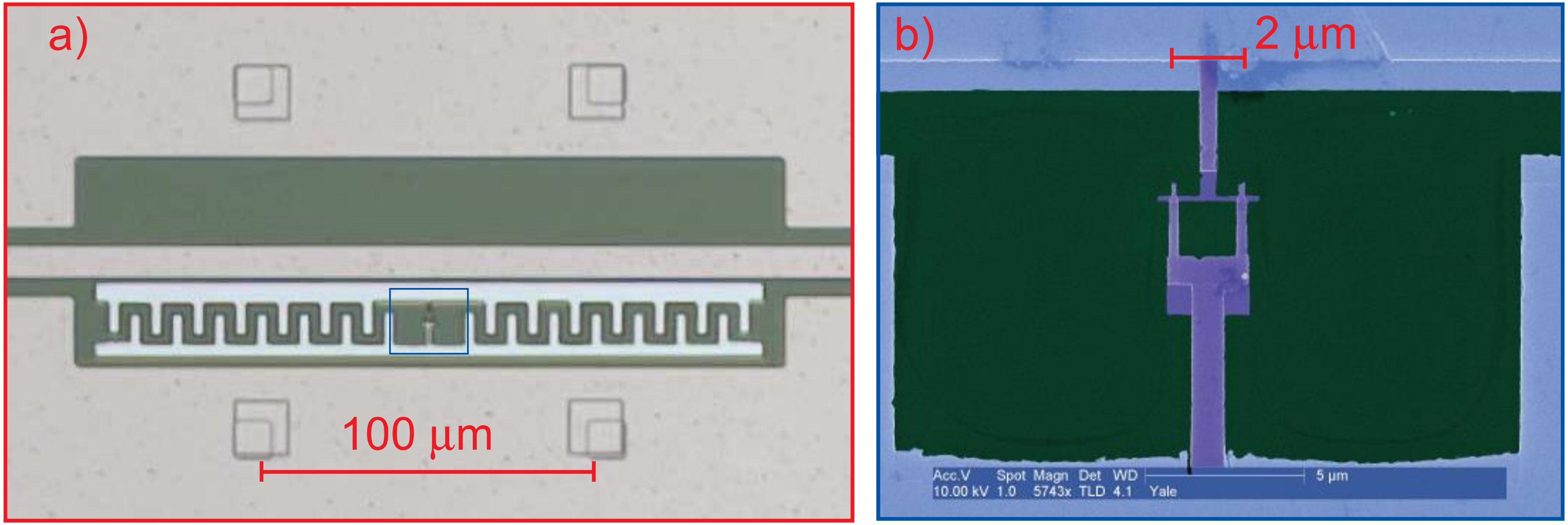


Coplanar waveguide resonator and lumped circuit[13]

[13] A. Blais et al., Phys. Rev. A **69**, 062320 (2004)

Physical Designs: Transmon

- Similar in design to CPB with the following modifications
  - Shunt capacitance implemented with an interdigitated capacitor or sufficiently large gap of exposed substrate between conductors



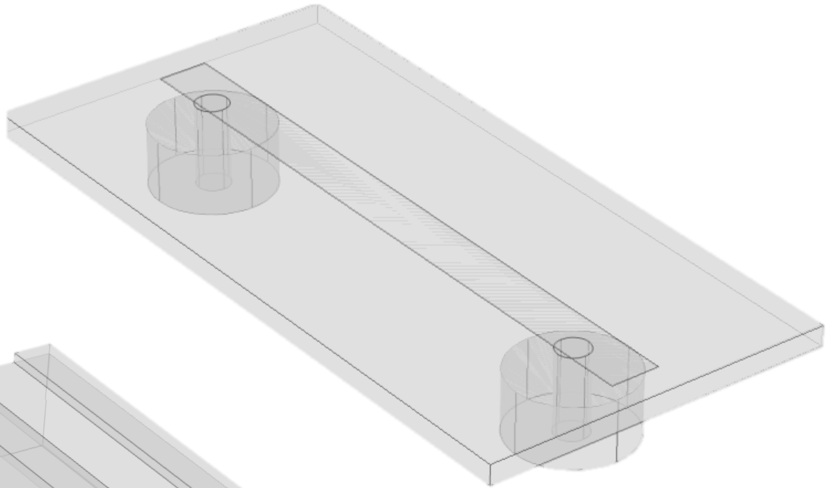
Micrograph of resonator and transmon reproduced from[3]

[3] D. I. Schuster, Circuit Quantum Electrodynamics. PhD thesis, Yale University, 2007.

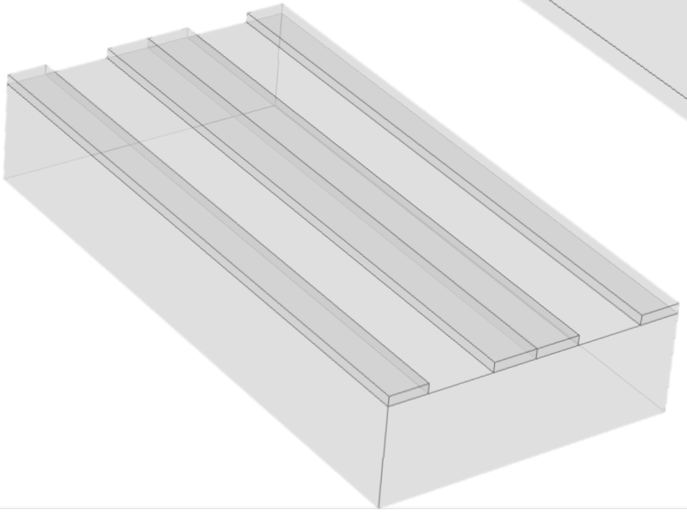
COMSOL RF Simulation Building Blocks

- Model systems used to develop more accurate descriptions of the microwave circuits that constitute a qubit
- Model Progression

1. Microstrip transmission line



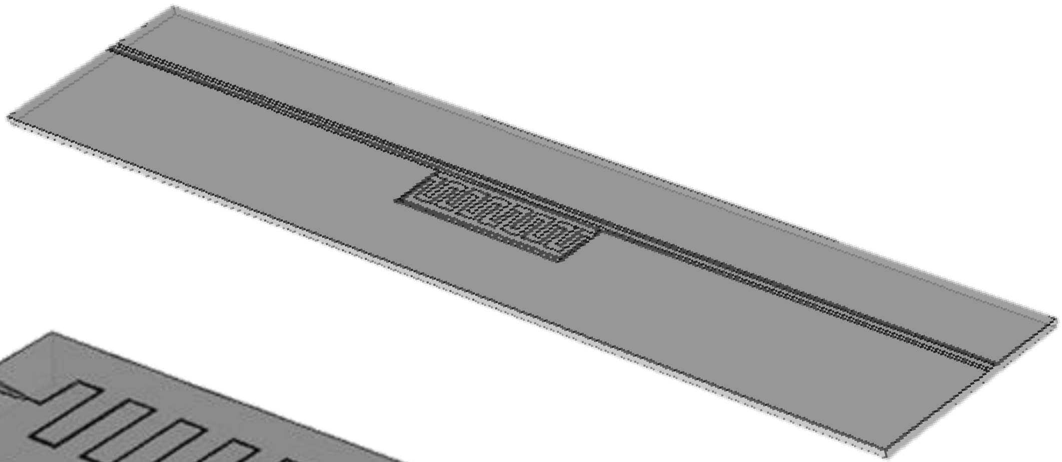
2. Coplanar Waveguide (CPW)



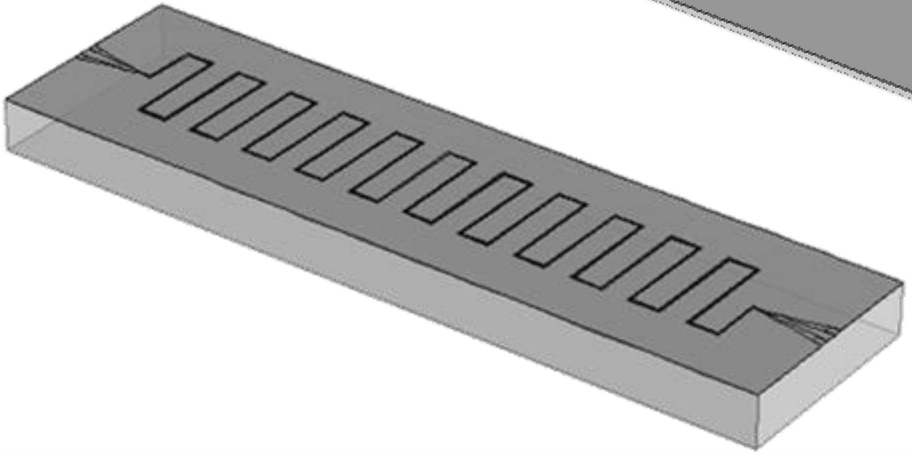
COMSOL RF Simulation Building Blocks

- Model systems used to develop more accurate descriptions of the microwave circuits that constitute a qubit
- Model Progression

1. Interdigitated Capacitor (IDC)



2. Meanderline resonator

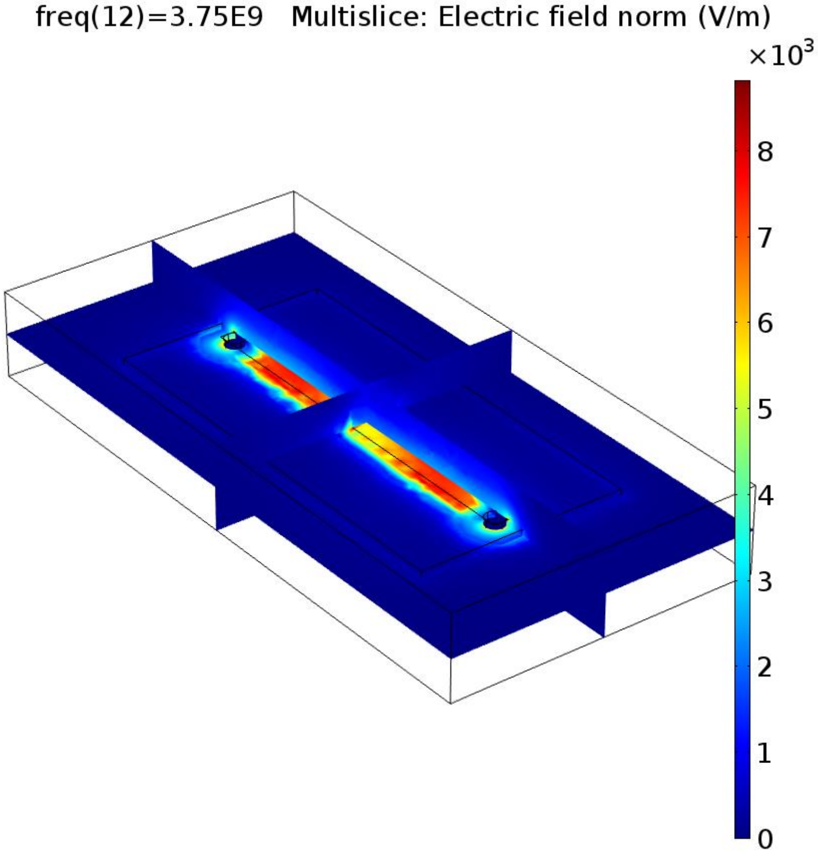


Microstripline Resonator

- Electric field norm and characteristic impedance, Z_0
- Characteristic impedance is given by

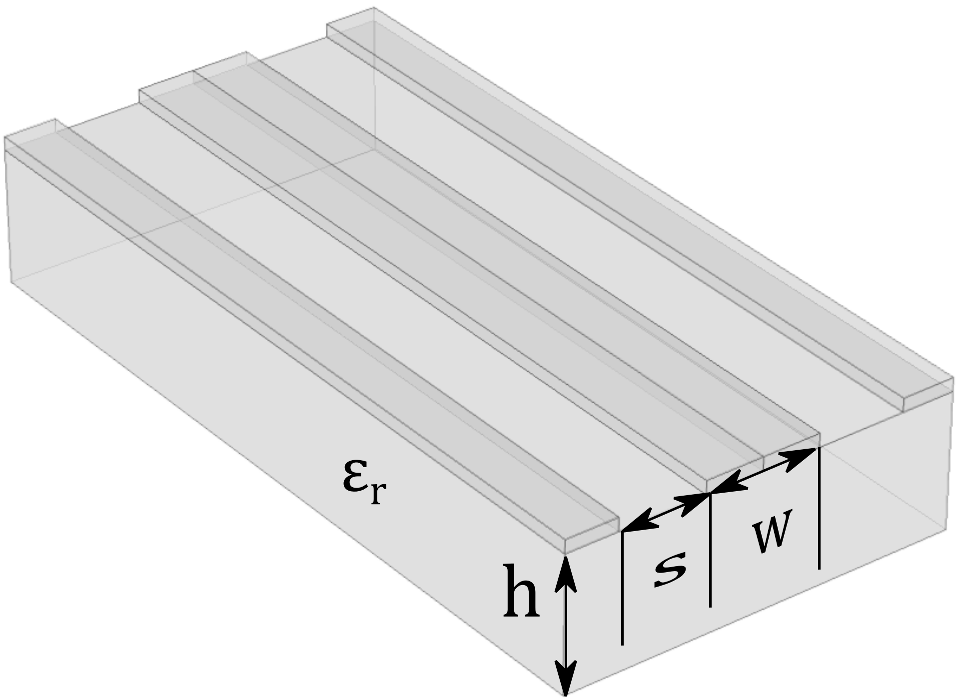
$$Z_0 = \frac{87}{\sqrt{\epsilon_r + 1.41}} \ln\left(\frac{5.98h}{0.8w + t}\right)$$

where h is the substrate thickness, t is the thickness of the microstrip, w is the width of the strip



Coplanar Waveguide

- Coplanar waveguide used as a resonant coupling structure, i.e. *cavity* with the qubit



- Characteristic Impedance from conformal mapping[14]:

$$\boxed{Z_0 = \frac{30\pi}{\sqrt{\epsilon_{\text{eff}}}} \frac{K(k_0')}{K(k_0)}}$$

$$\epsilon_{\text{eff}} = 1 + \frac{\epsilon_r - 1}{2} \frac{K(k_1)}{K(k_1')} \frac{K(k_0')}{K(k_0)}$$

$$k_0 = \frac{s}{s + 2w}, \quad k_0' = \sqrt{1 = k_0^2}$$

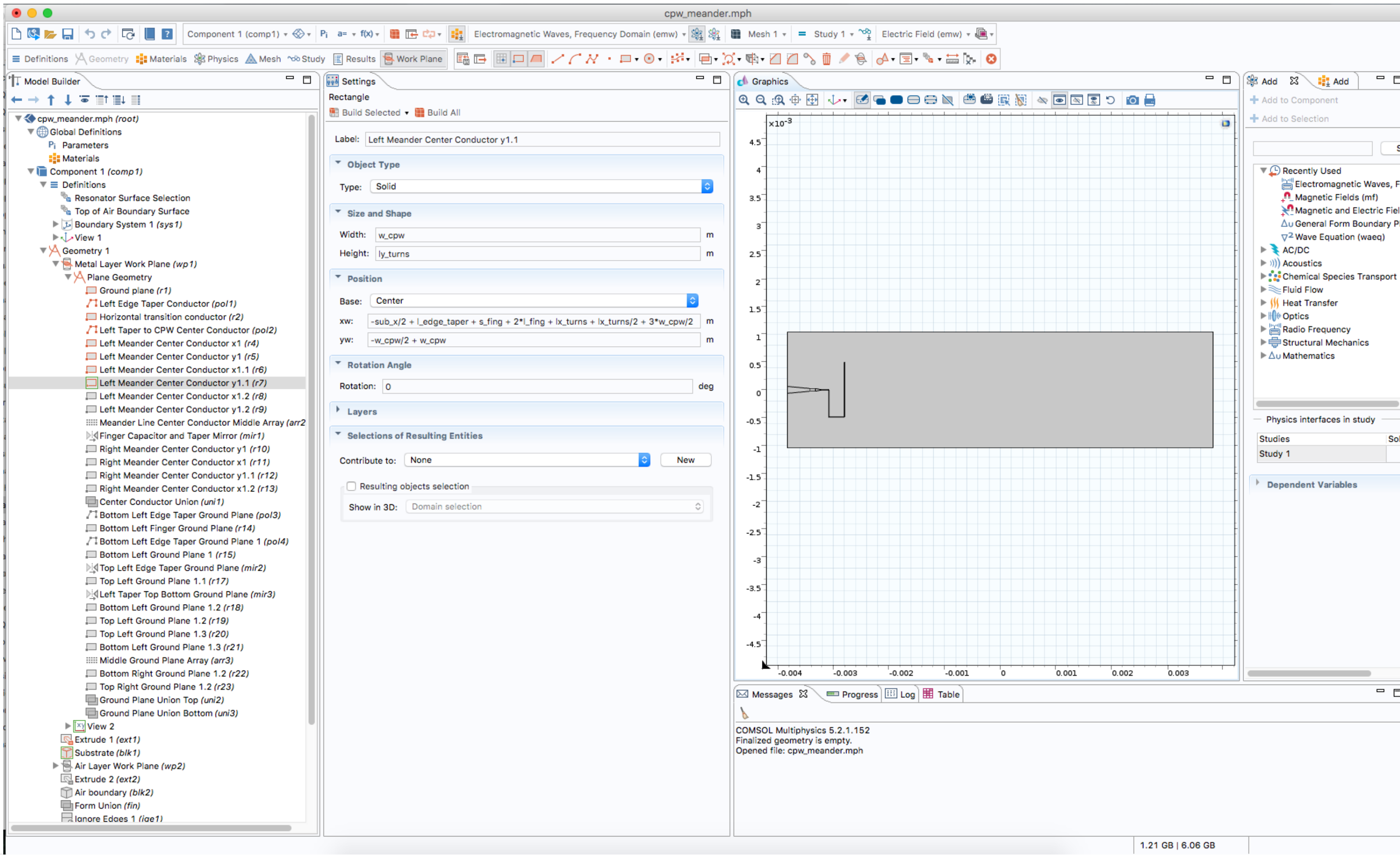
$$k_1 = \frac{\sinh(\pi s / 4h)}{\sinh(\pi(s + 2w)/4h)}$$

$$k_1' = \sqrt{1 - k_1^2}$$

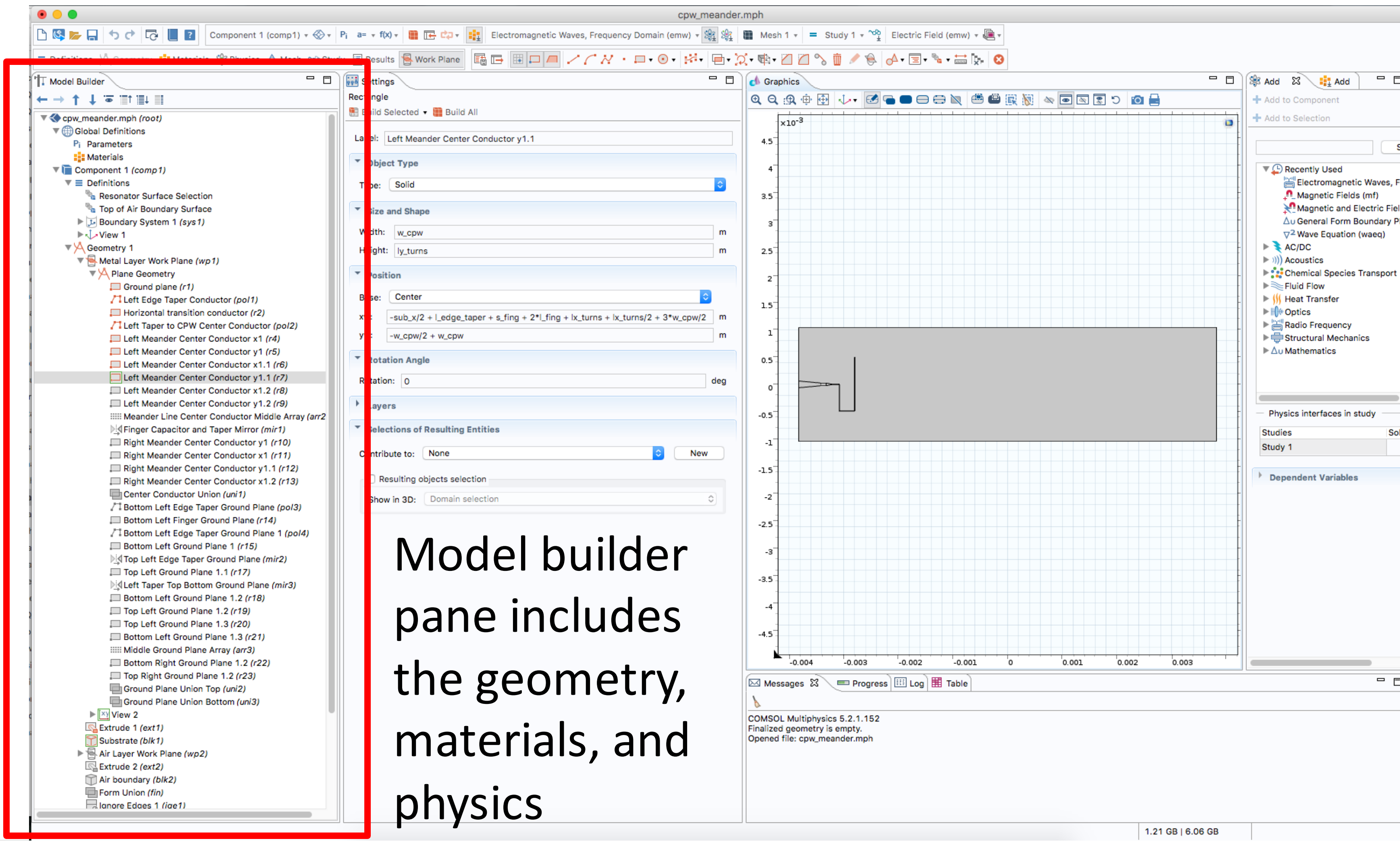
$$K(k) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - k^2 \sin^2\theta}}$$

[14] Rainee N Simons. Coplanar Waveguide Circuits, Components, and Systems, chapter 2. Wiley Series in Microwave and Optical Engineering. Wiley, 2001.

COMSOL RF Module Demo: Work planes

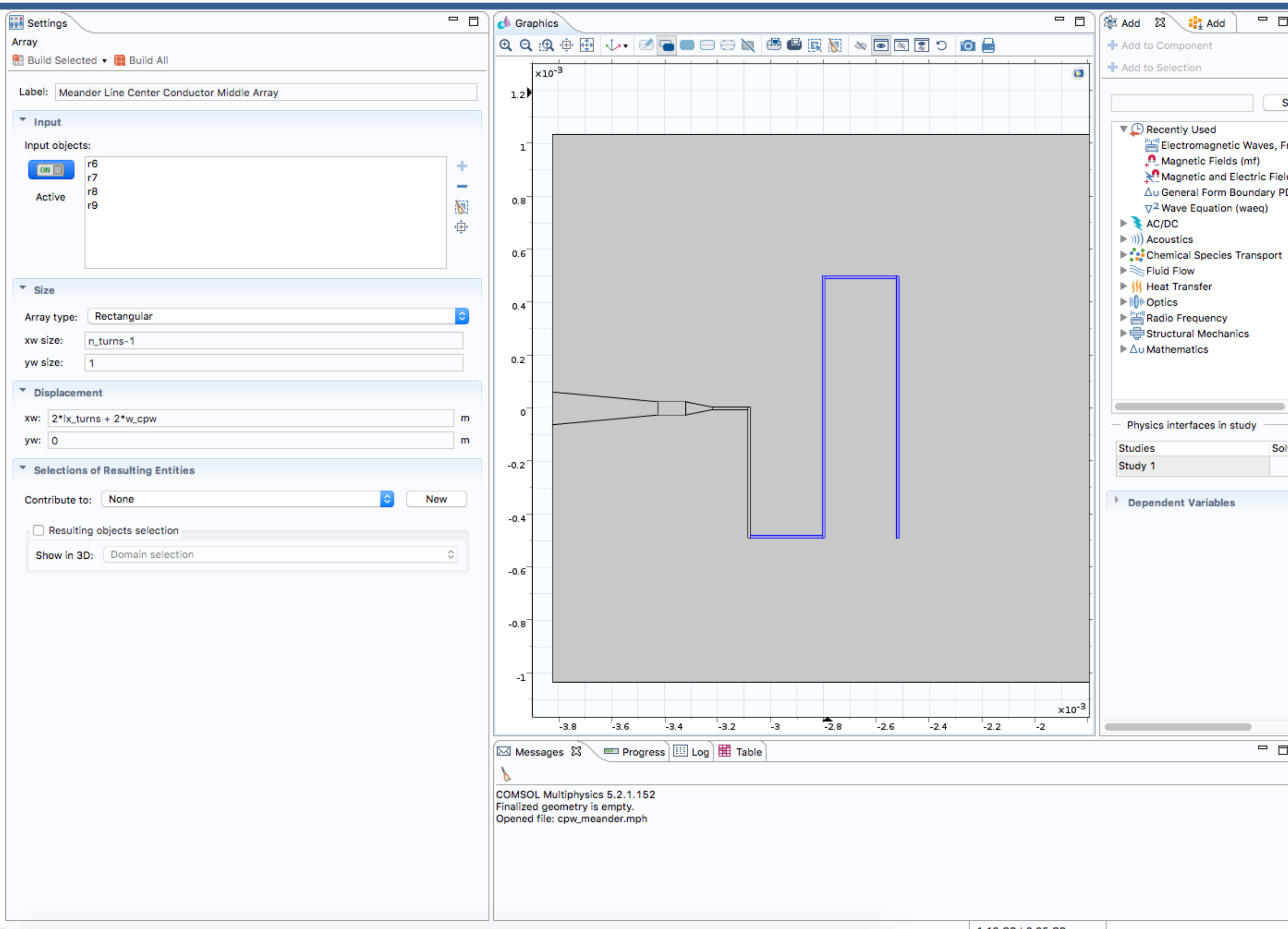


COMSOL RF Module Demo: Work planes

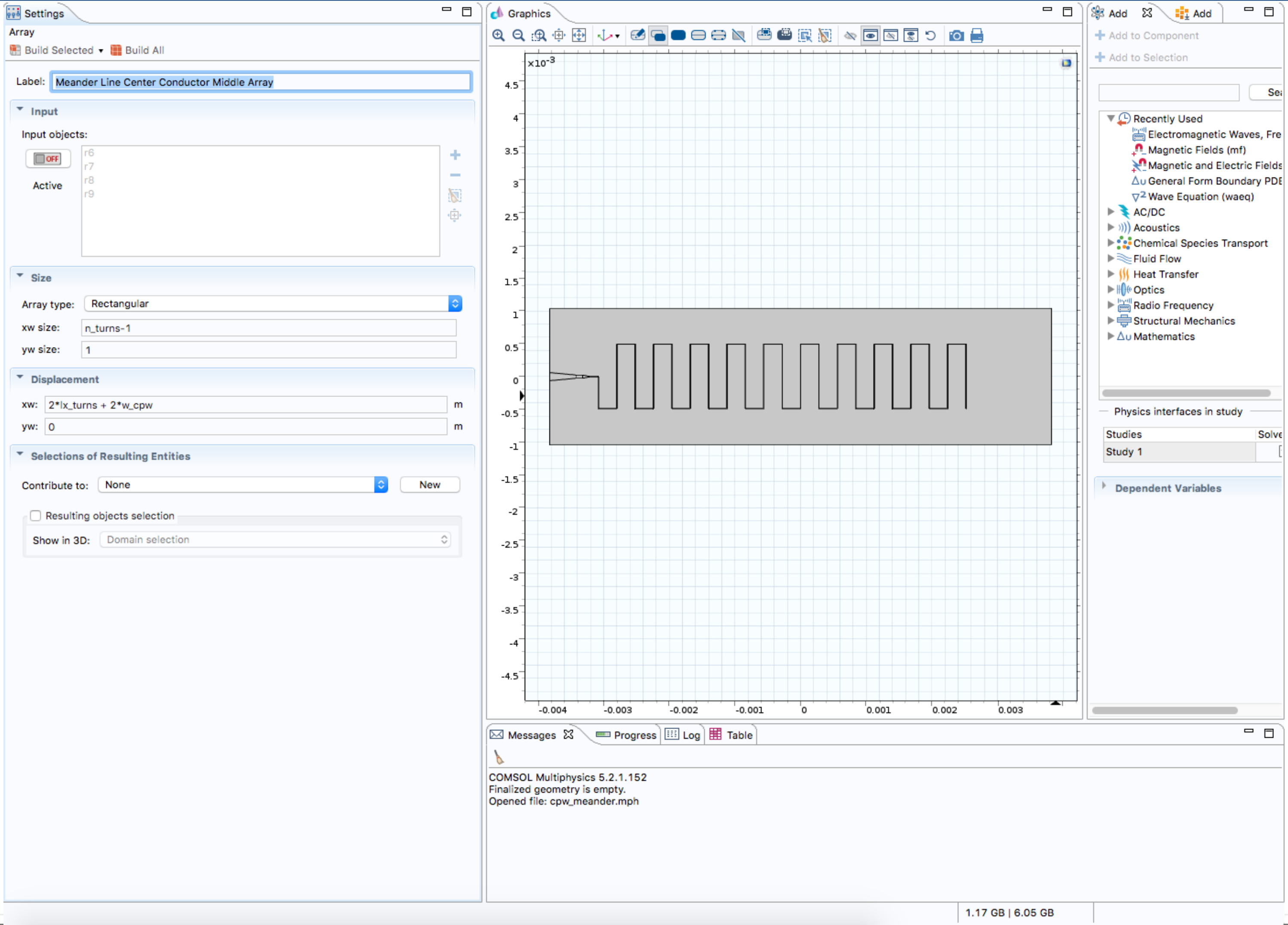


Model builder pane includes the geometry, materials, and physics

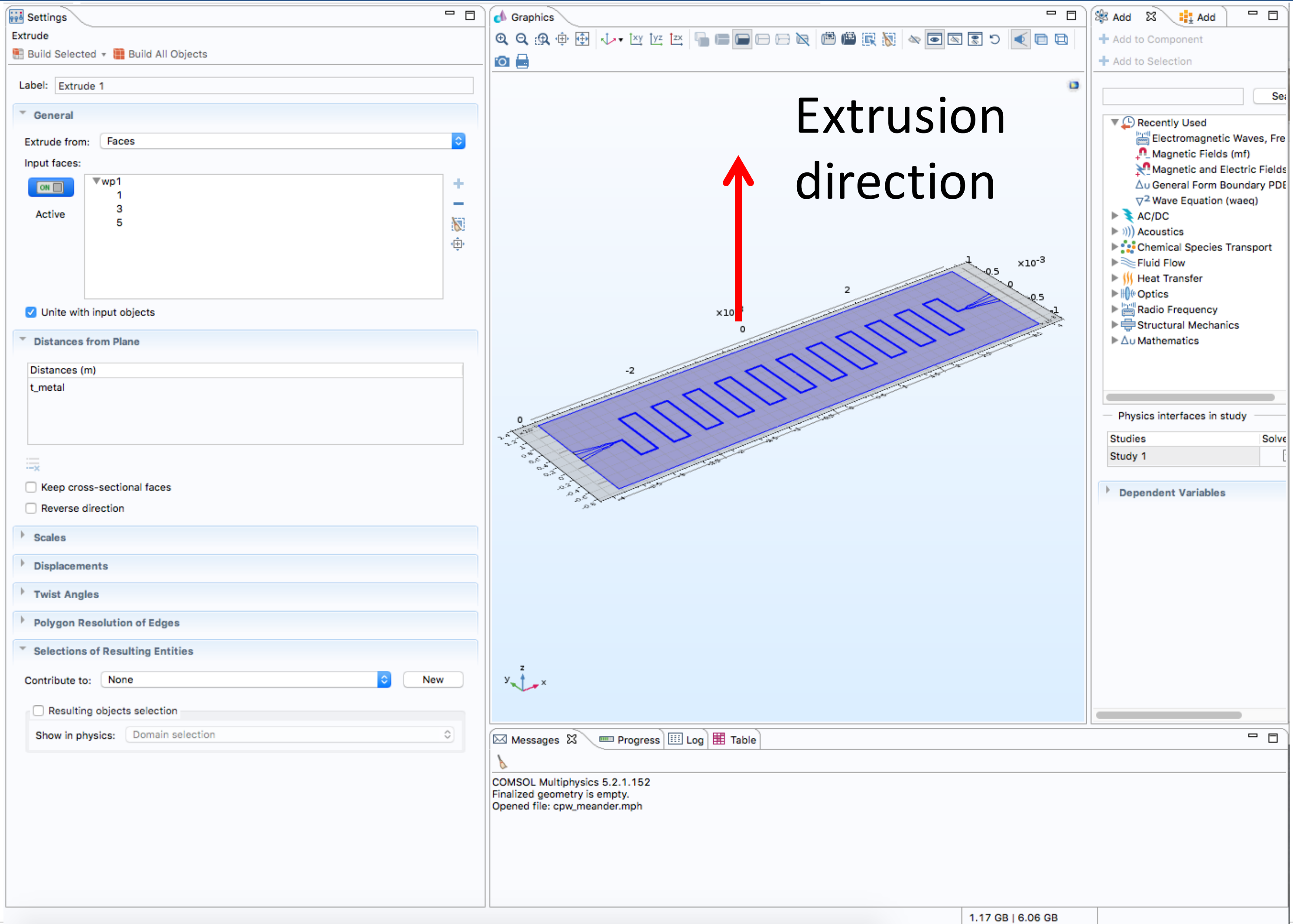
COMSOL RF Module Demo: Arrays



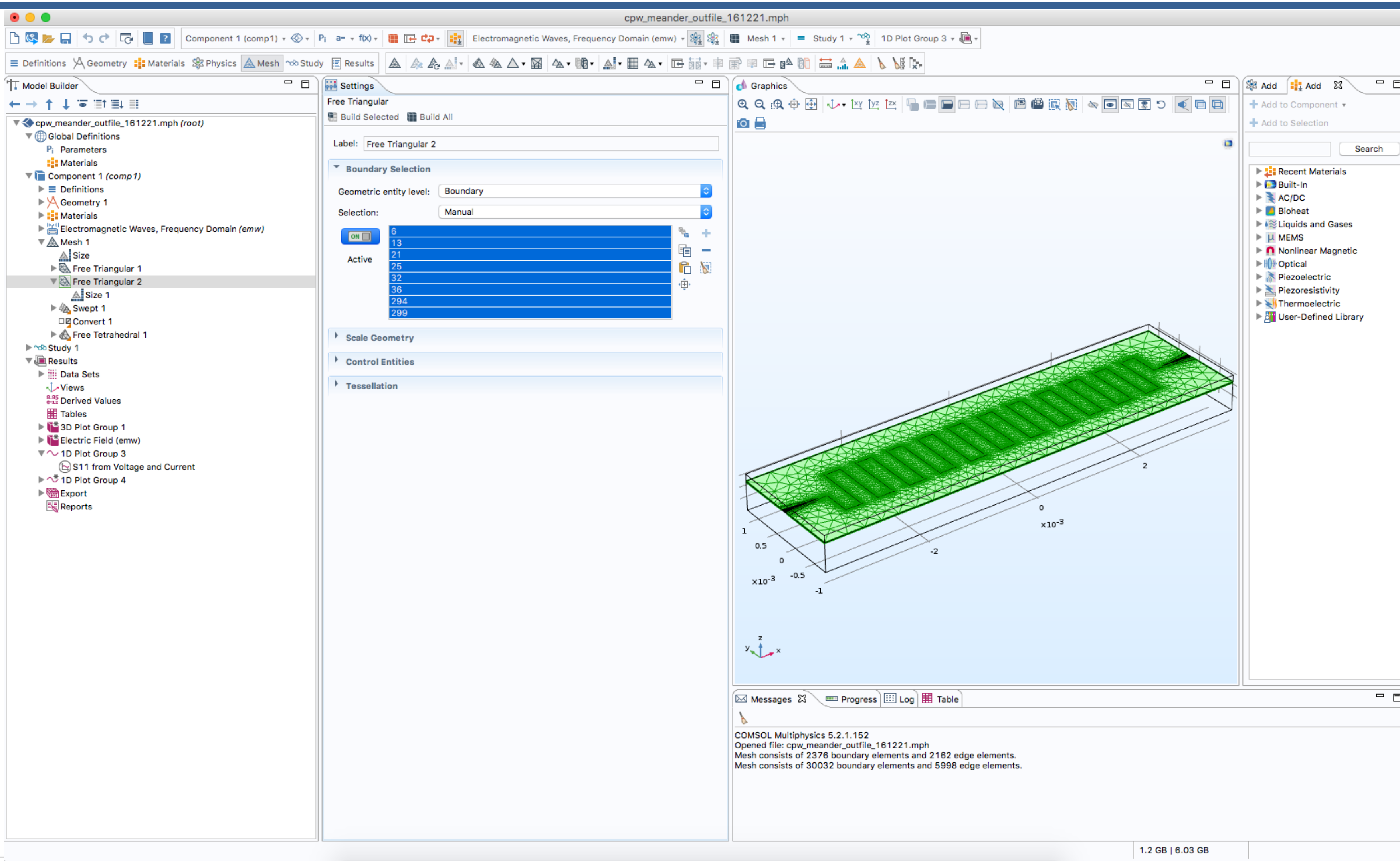
COMSOL RF Module Demo: Arrays



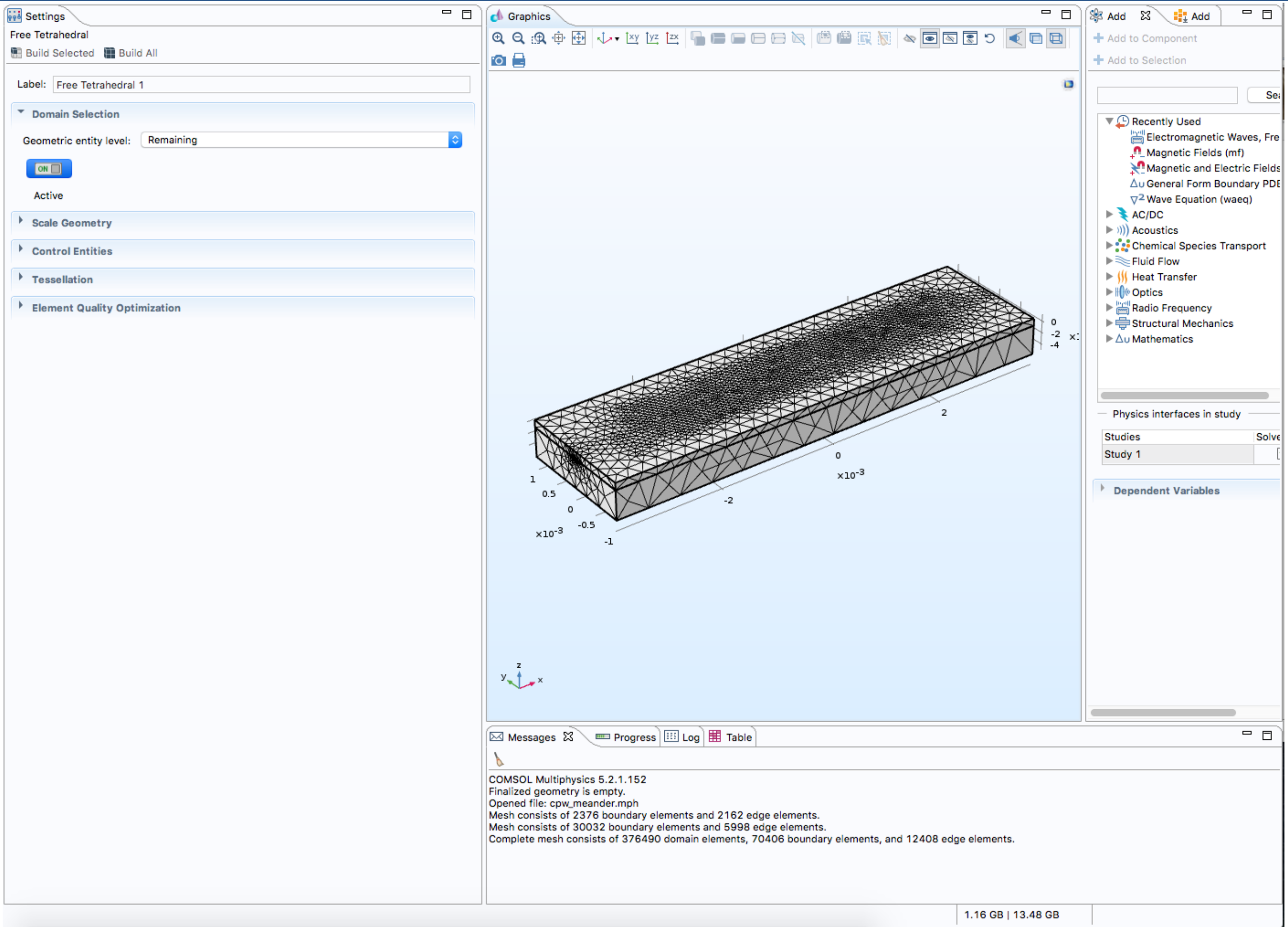
COMSOL RF Demo: Extrusions



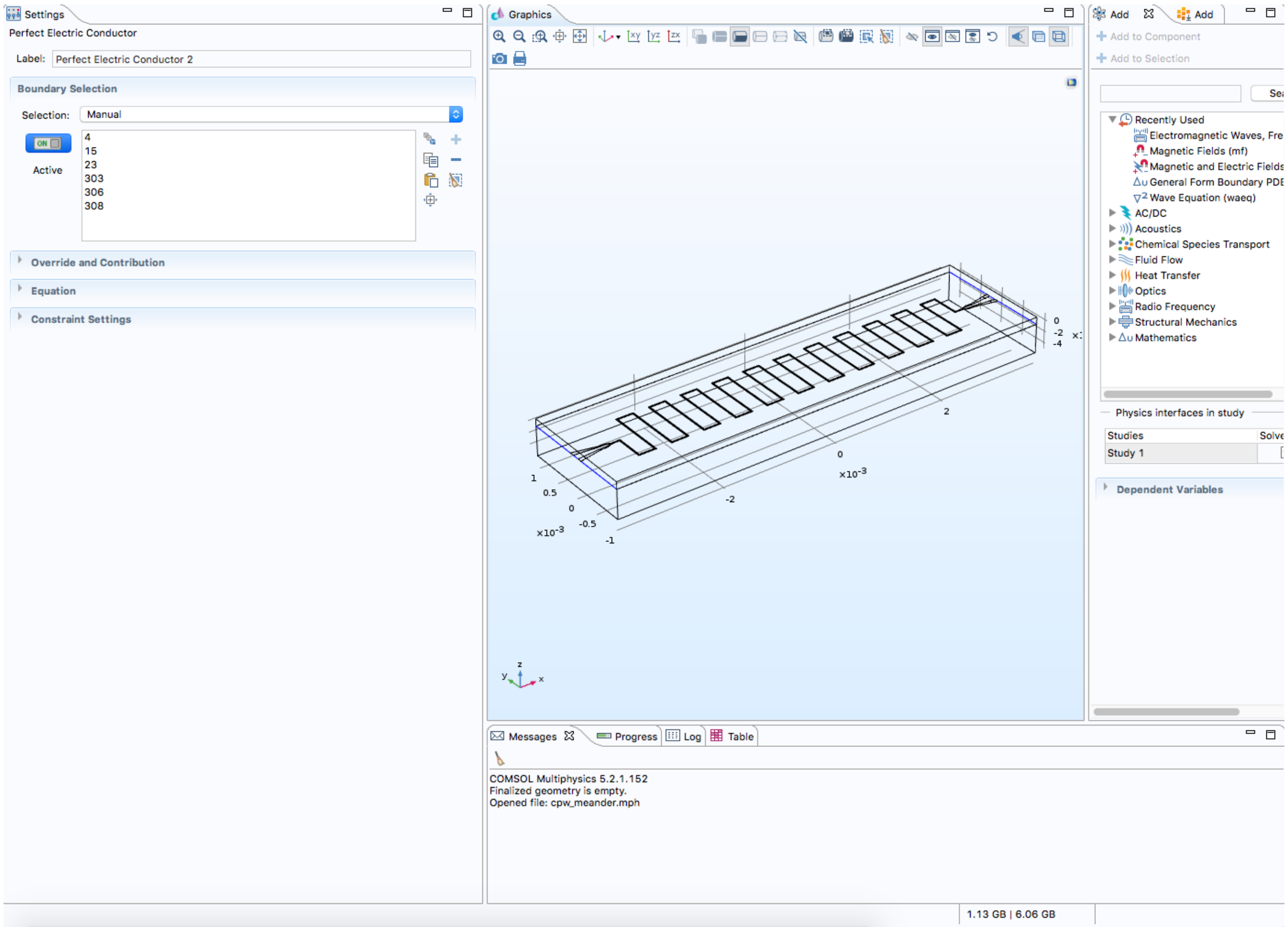
COMSOL RF Demo: Meshing



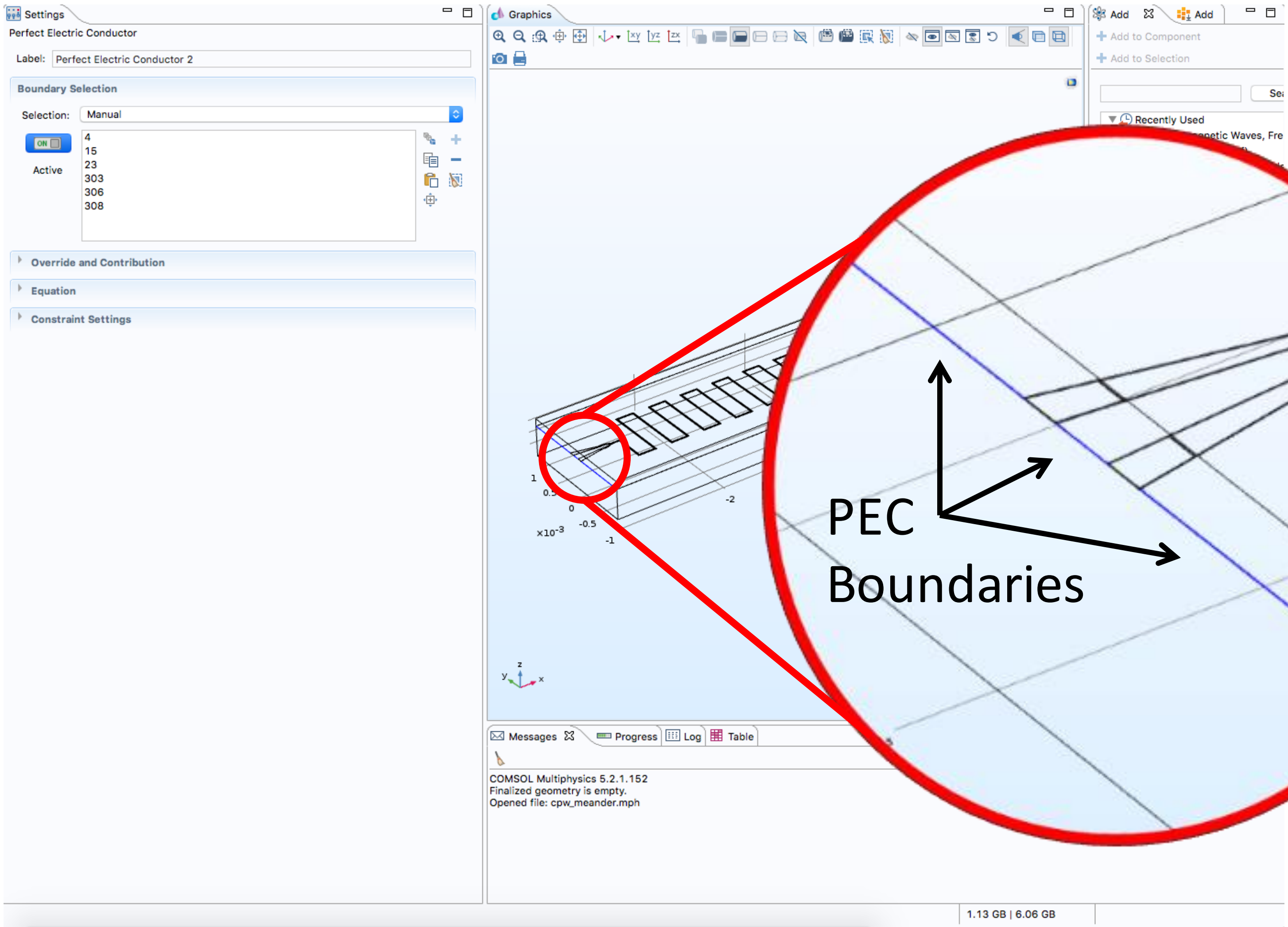
COMSOL RF Demo: Meshing



COMSOL RF Demo: Boundary Conditions, PEC

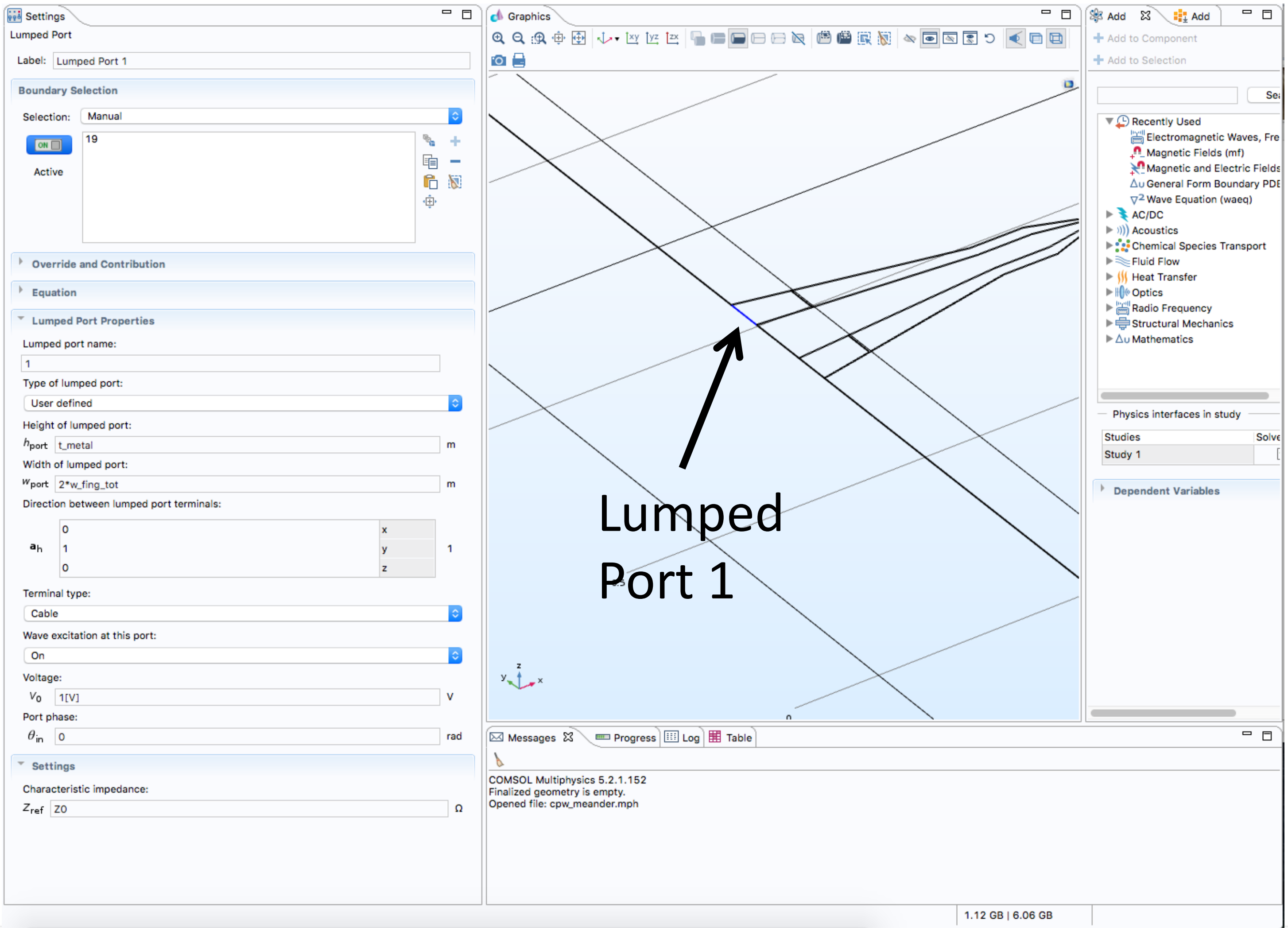


COMSOL RF Demo: Boundary Conditions, PEC

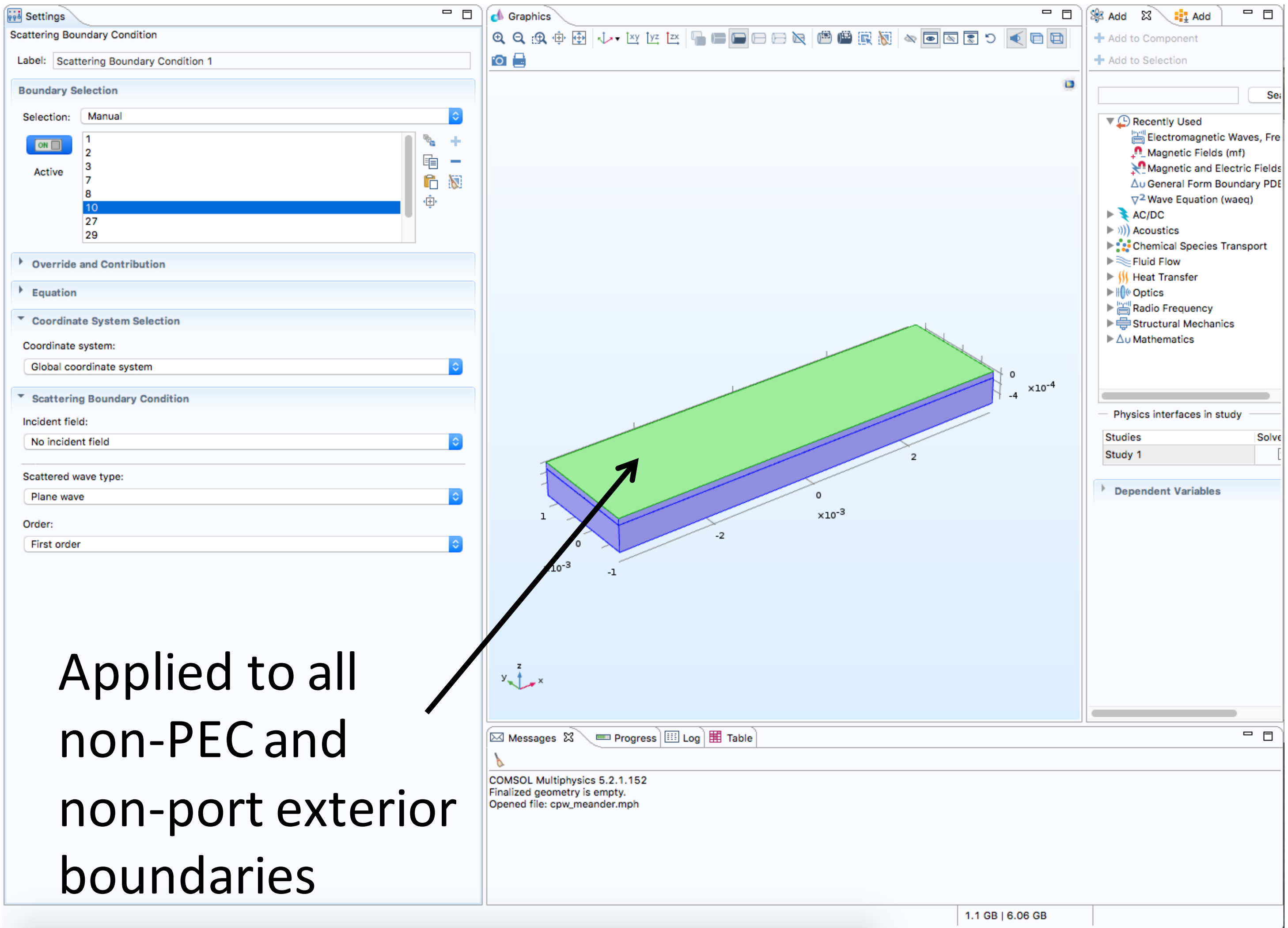


COMSOL RF Demo: Boundary Conditions, Ports

Terminal Settings →

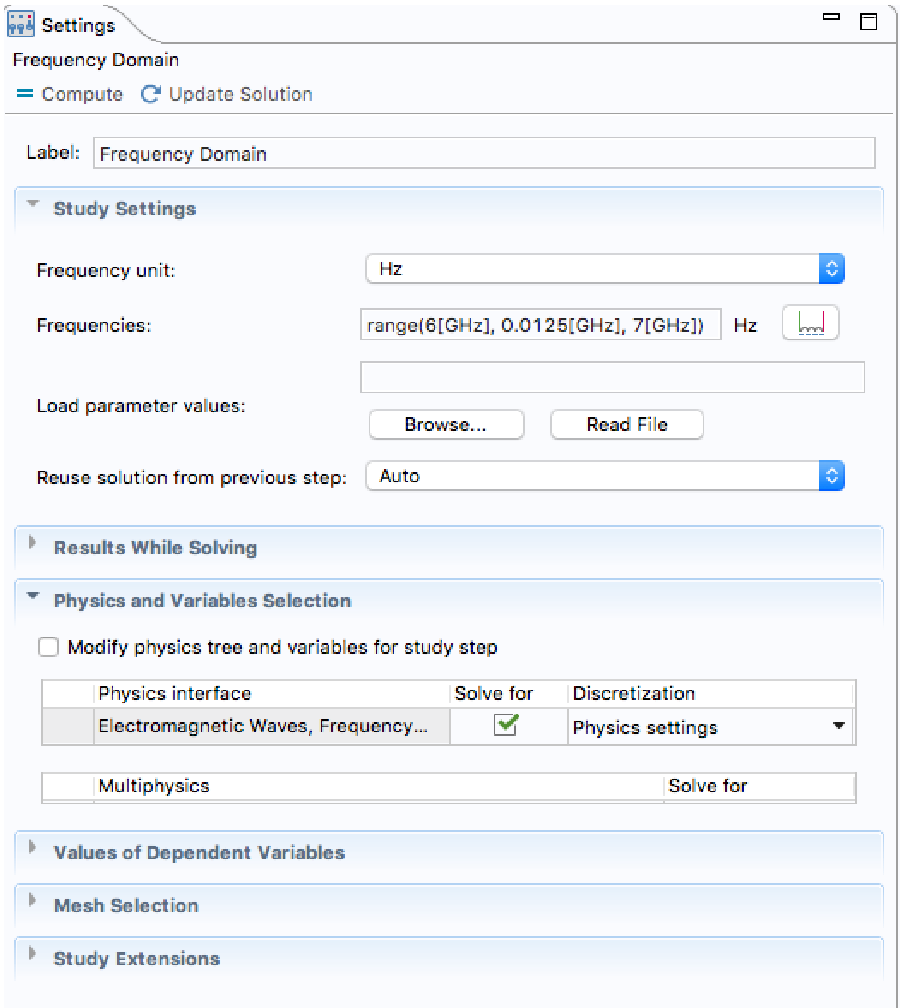


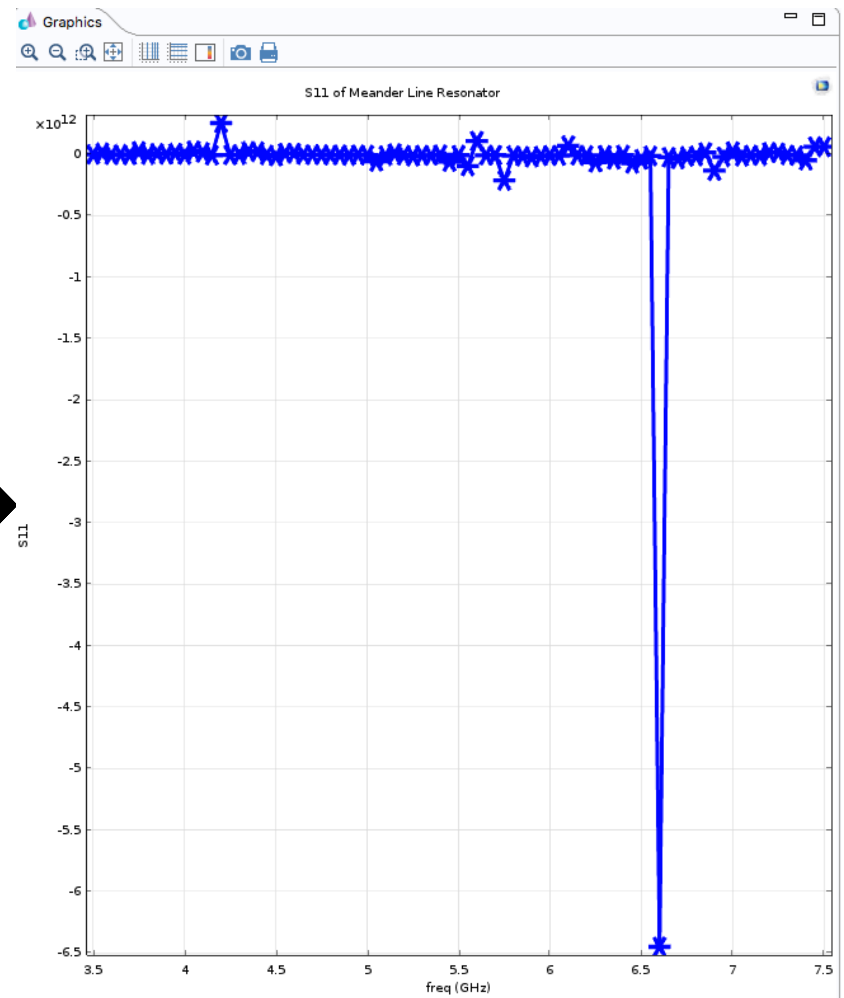
COMSOL RF Demo: Scattering Boundary Condition



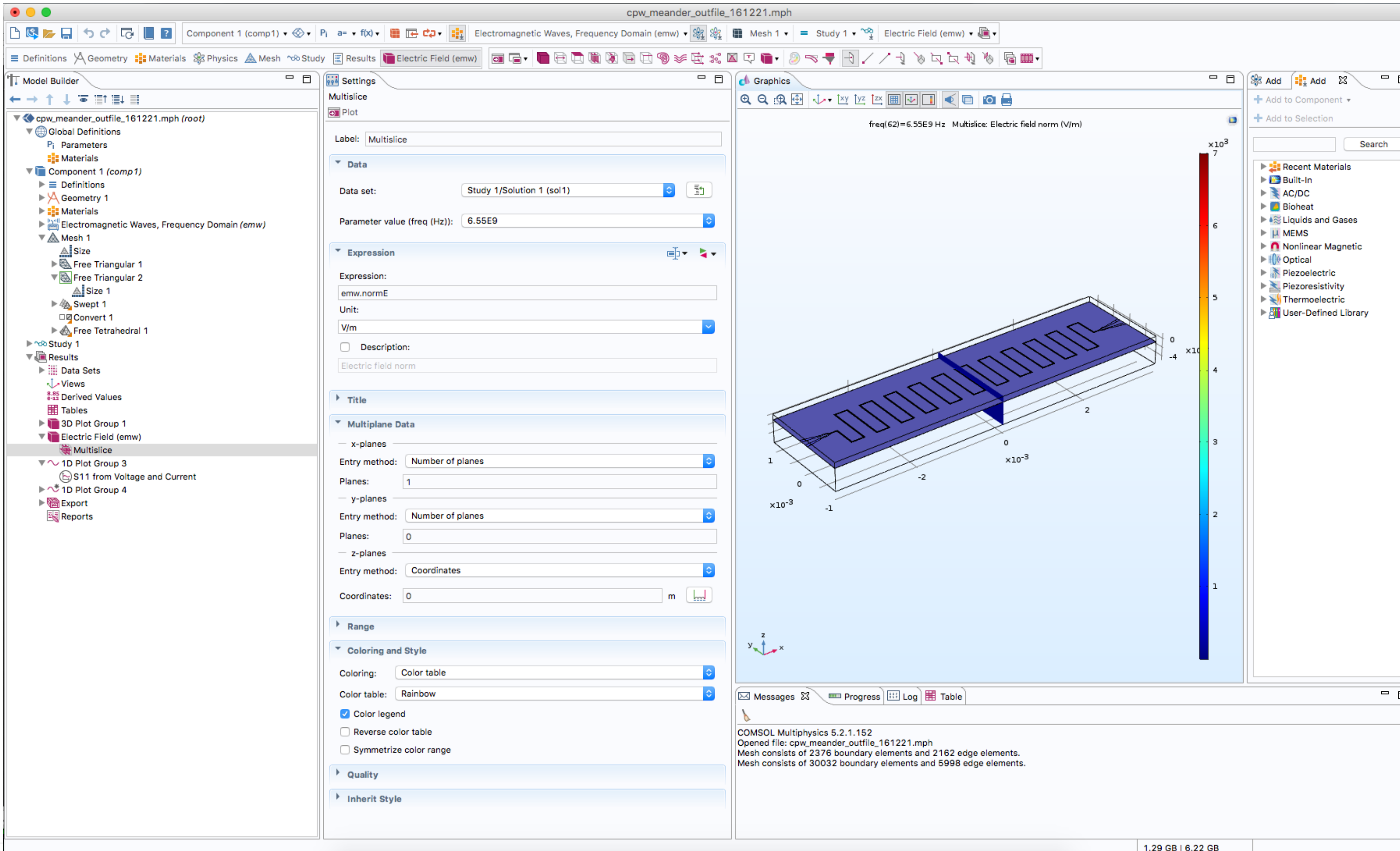
Applied to all non-PEC and non-port exterior boundaries

COMSOL RF Demo: Frequency Sweep

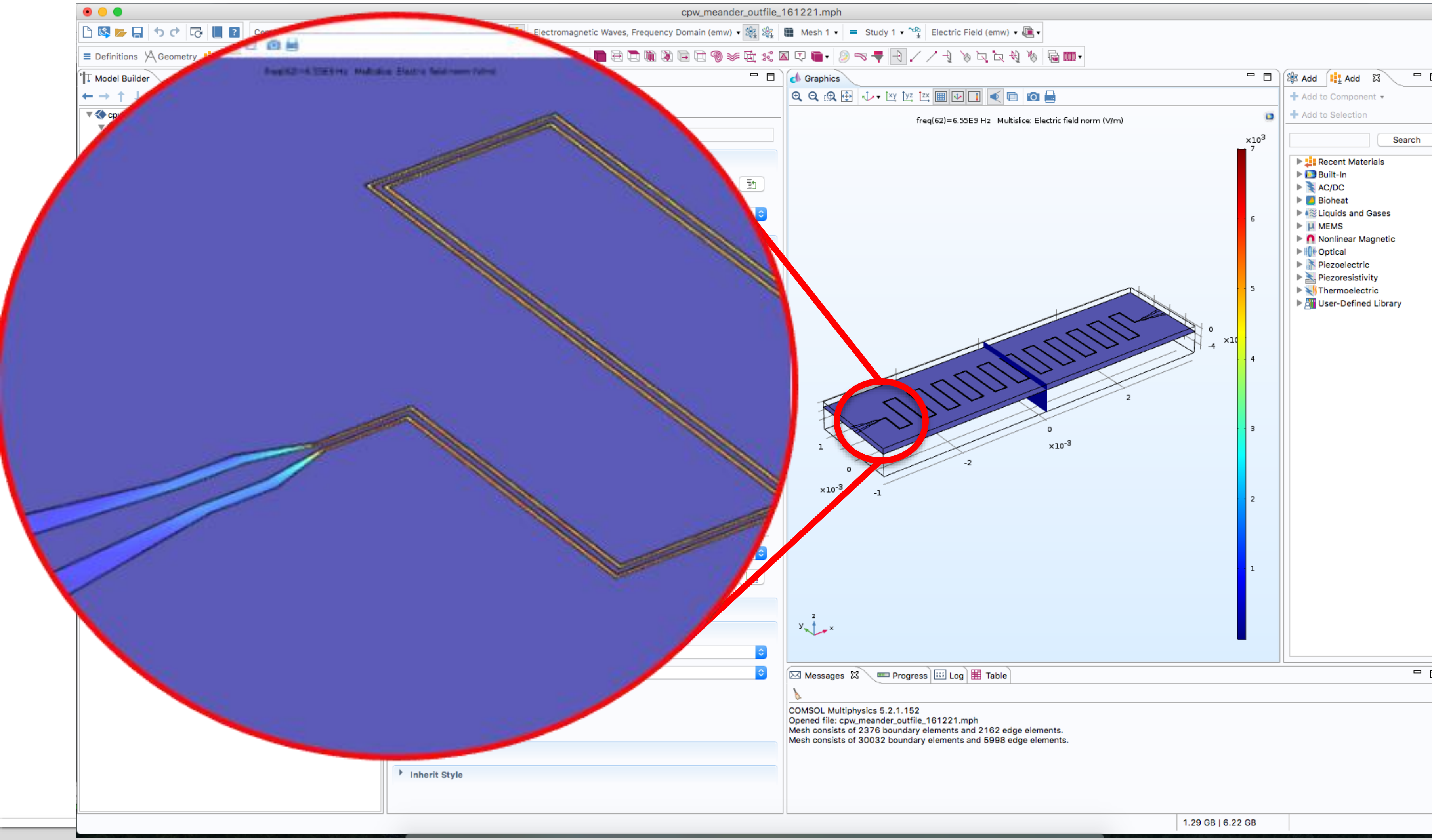




COMSOL RF Demo: E-Field Plot



COMSOL RF Demo: E-Field Plot



Closing Comments on cQED and COMSOL

- Superconducting qubits benefit from simple descriptions in cQED by through analogies with cavity QED
- Black box quantization provides a systematic method of quantizing the bulk features of devices as circuits
- COMSOL provides a simulation environment to model the classical geometric features of qubits

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- Jonathan DuBois, Eric Holland, Matthew Horsley, Vincenzo Lordi, Scott Nelson, Yaniv Rosen, Nathan Woollett
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Thank you—Questions