



Design and simulations of transmon qubits in 3D cavities using Ansys and pyEPR

Energy participation ratio

- Energy participation describes how much inductive energy is distributed to element/junction j in mode m

- $H = H_{linear} + H_{nonlinear}$
 - ✓ $\varepsilon_j(\widehat{\varphi}_j) = \varepsilon_j^{lin}(\widehat{\varphi}_j) + \varepsilon_j^{nl}(\widehat{\varphi}_j)$
 - ✓ For one JJ: $\varepsilon_j(\varphi) = E_j[1 - \cos(\varphi)]$

- $H_{lin} = \sum_m (\hbar\omega_m a_m^+ a_m)$

- The nonlinear part will read

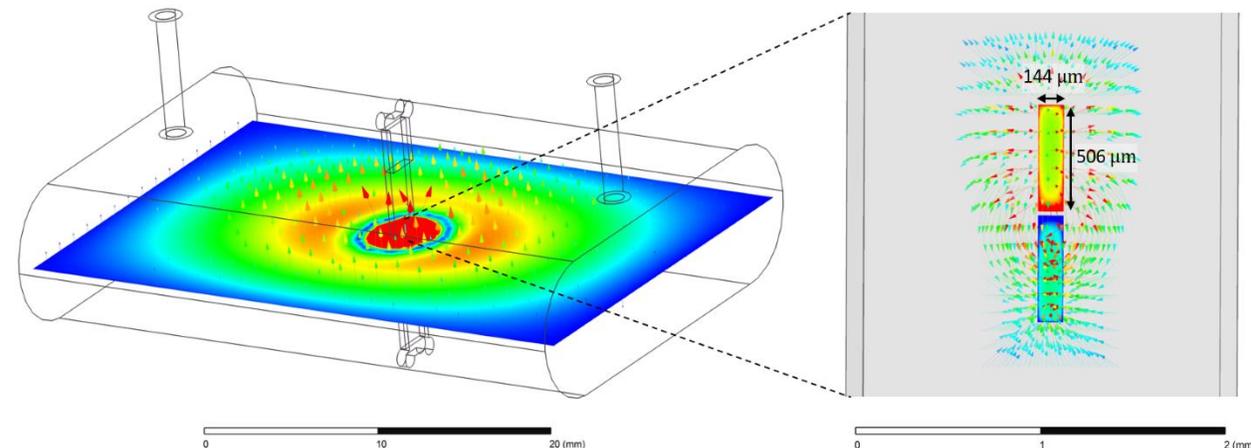
- ✓ $H_{nl} = \sum_{j=1}^J \varepsilon_j^{nl} = \sum_{j=1}^J E_j (c_{j3}\varphi_j^3 + c_{j4}\varphi_j^4 + \dots) \approx \sum_{j=1}^J E_j \sum_{p=1}^p c_{jp}\varphi_j^p$
 - ✓ $\varphi_j = \sum_{m=1}^M \varphi_{mj} (a_m^+ + a_m)$

- The EPR is defined as:

$$p_{mj} = \frac{\text{inductive energy stored in junction } j}{\text{Total inductive energy stored in mode } m}$$

- In terms of participation ratio, the flux zero-point fluctuations is:

$$\varphi_{mj}^2 = p_{mj} \frac{\hbar\omega_m}{2E_j}$$

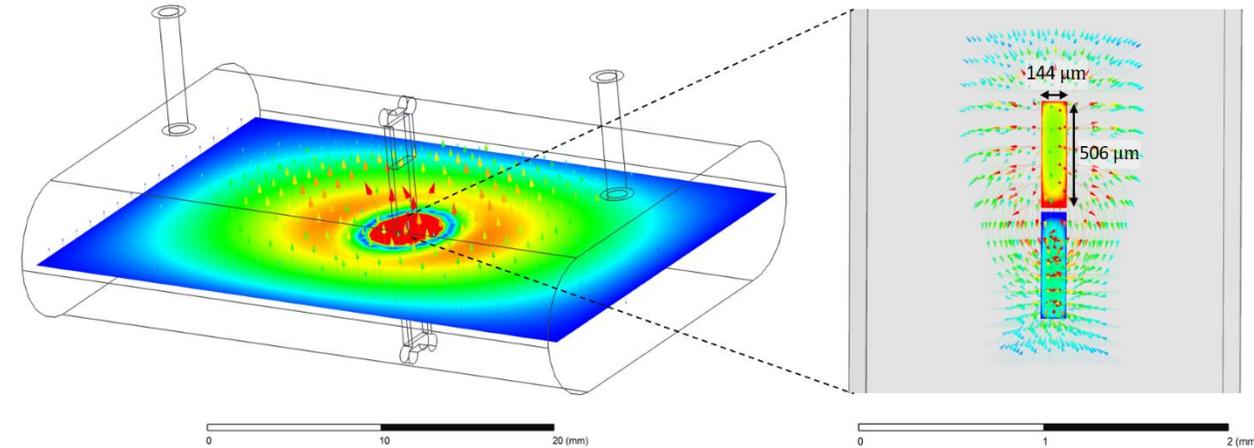


Appl. Sci. **2024**, *14*(4), 1478; <https://doi.org/10.3390/app14041478>

Energy participation ratio

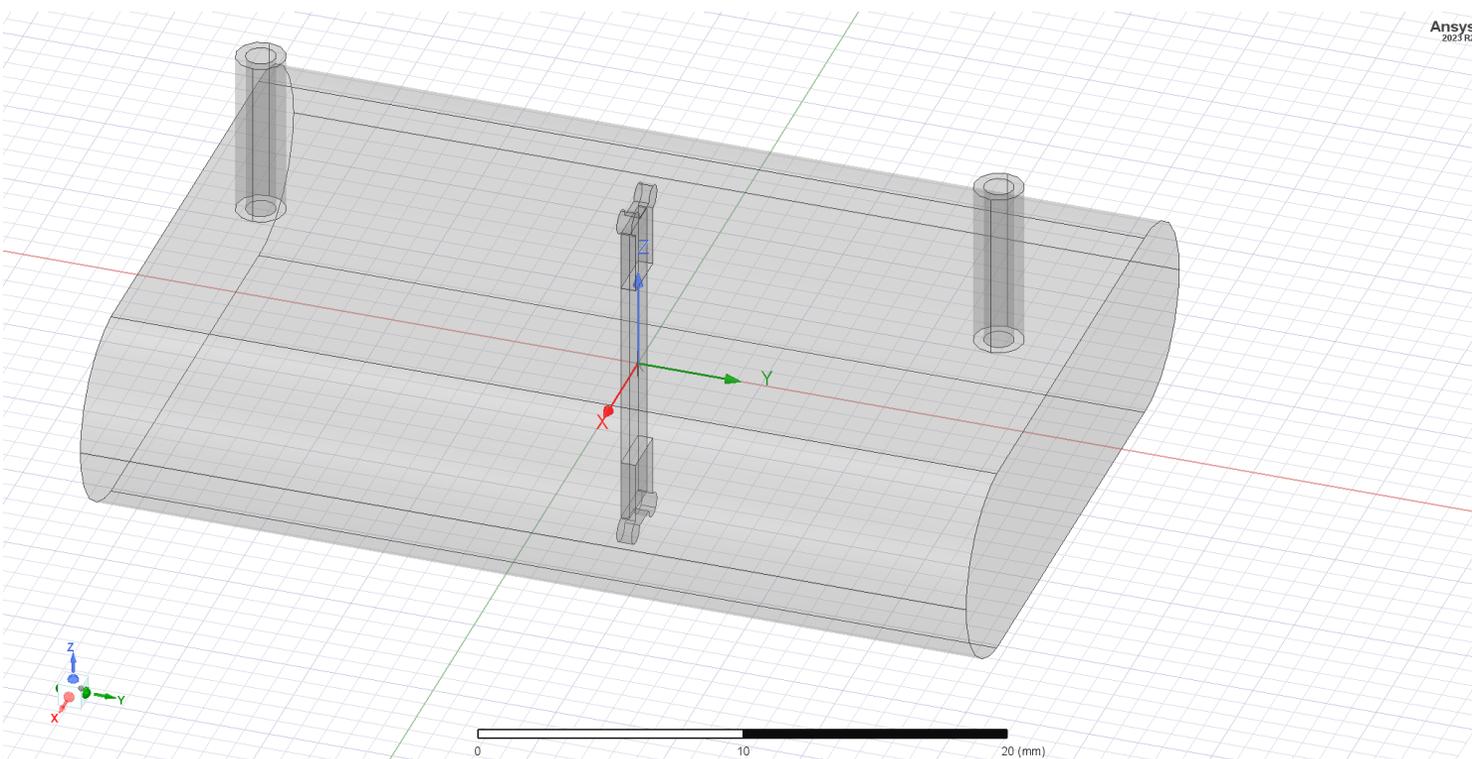
$$H = \sum_m \hbar \omega_m a_m^\dagger a_m - \hbar \left(\sum_{m=1}^M \Delta_m a_m^\dagger a_m + \frac{\alpha_m}{2} a_m^{+2} a_m^2 + \sum_{n \neq m} \chi_{mn} a_m^\dagger a_n^\dagger a_m a_n \right)$$

- Lamb shift : $\Delta_m = \sum_{n=1}^M \frac{\chi_{mn}}{2}$
- Anharmonicity : $\alpha_m = \frac{\chi_{mm}}{2} = \sum_{j=1}^J \frac{\hbar \omega_m^2}{8E_j} \rho_{mj}^2$
- Cross-kerr interaction : $\chi_{mn} = \sum_{j=1}^J \frac{\hbar \omega_m \omega_n}{4E_j} \rho_{mj} \rho_{nj}$

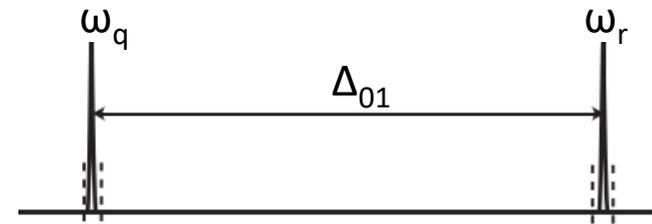


Appl. Sci. **2024**, *14*(4), 1478; <https://doi.org/10.3390/app14041478>

Qubit in 3D cavity



Dispersive regime



$$H_{JC} = (\omega_r - \frac{\chi_{12}}{2} + \chi\sigma^z)a^\dagger a + \frac{1}{2}(\omega_q + \chi_{01})\sigma^z,$$

$$\chi = \chi_{01} - \frac{\chi_{12}}{2} \quad \chi_{ij} = \frac{g_{ij}^2}{\Delta_{ij}}$$

$$\Delta_{01} = \omega_q - \omega_r \quad \omega_q = \omega_{01}$$

Parameters

Mode frequencies (MHz)

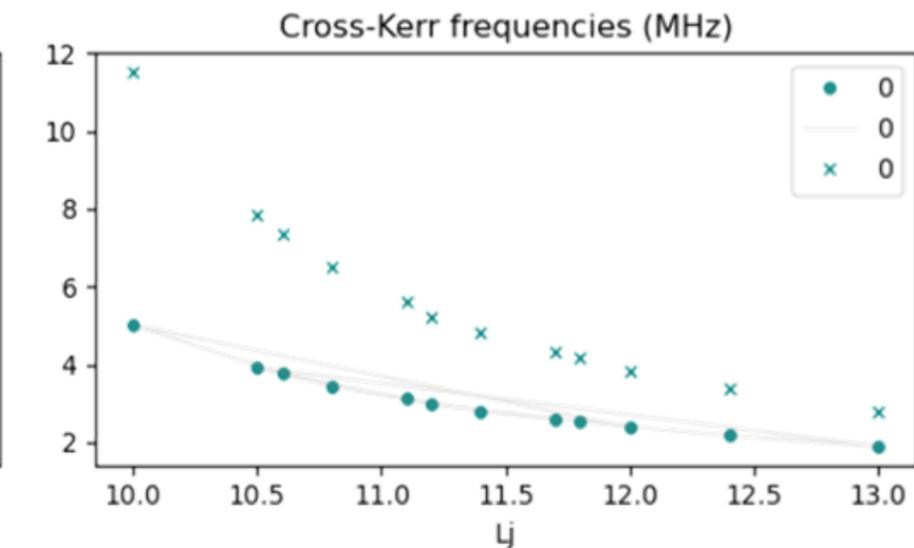
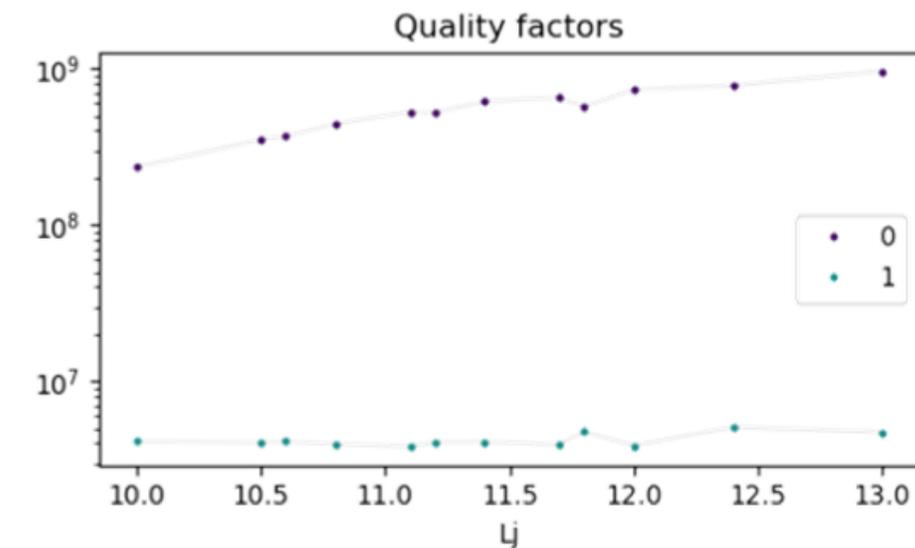
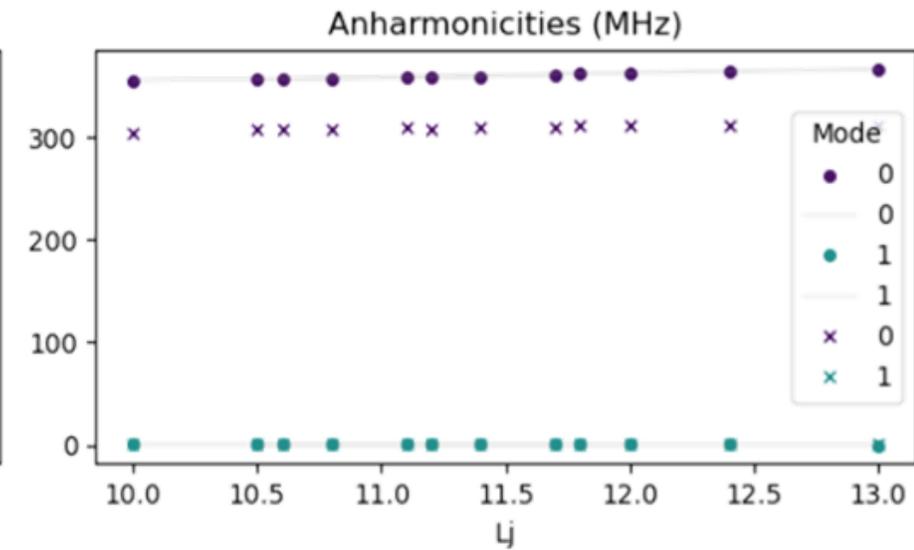
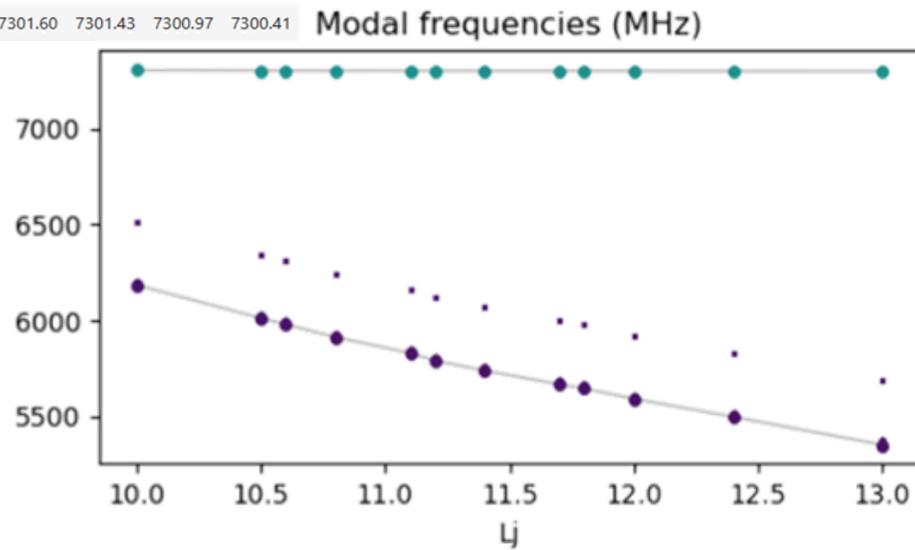
Numerical diagonalization

Lj	10.0	10.5	10.6	10.8	11.1	11.2	11.4	11.7	11.8	12.0	12.4	13.0
0	6184.01	6012.22	5979.44	5913.40	5829.95	5790.54	5739.04	5666.95	5645.63	5591.64	5497.71	5351.71
1	7305.05	7303.48	7303.16	7302.84	7302.29	7302.21	7301.90	7301.55	7301.60	7301.43	7300.97	7300.41

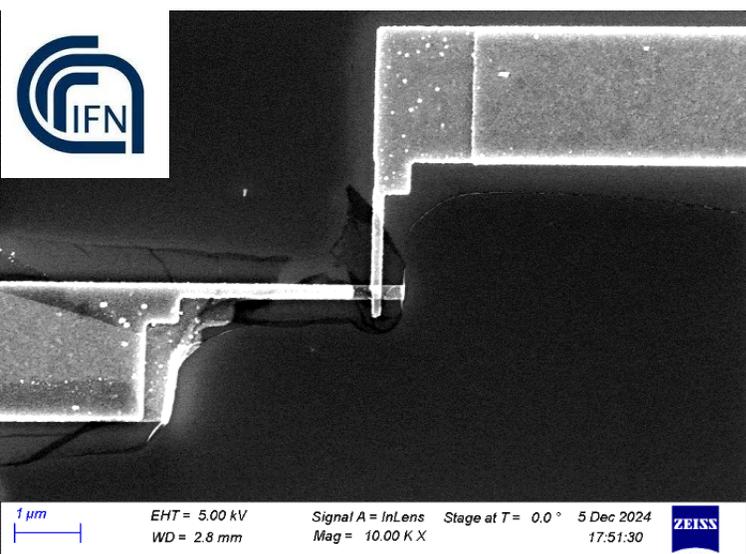
Kerr Non-linear coefficient table (MHz)

Numerical diagonalization

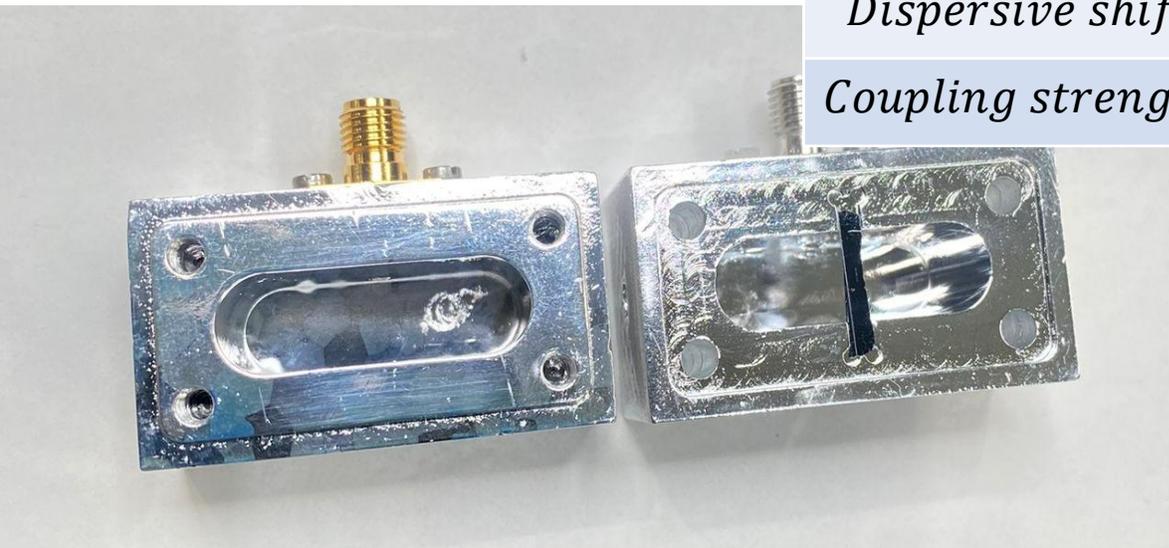
Lj		0	1
12.0	0	363.20	2.38e+00
	1	2.38	5.18e-03
10.0	0	356.02	5.01e+00
	1	5.01	2.64e-02
10.6	0	357.38	3.75e+00
	1	3.75	1.40e-02
11.2	0	358.12	2.97e+00
	1	2.97	8.42e-03
11.8	0	362.81	2.53e+00
	1	2.53	5.90e-03
12.4	0	365.37	2.17e+00
	1	2.17	4.20e-03
13.0	0	366.42	1.89e+00
	1	1.89	3.14e-03
10.5	0	357.19	3.92e+00
	1	3.92	1.54e-02
10.8	0	357.50	3.45e+00
	1	3.45	1.16e-02
11.1	0	359.24	3.12e+00
	1	3.12	9.31e-03
11.4	0	359.41	2.81e+00
	1	2.81	7.43e-03
11.7	0	361.75	2.59e+00
	1	2.59	6.19e-03



Measured data vs simulated



Parameters	Measured ($\frac{1}{2\pi}$ MHz)	Simulated ($\frac{1}{2\pi}$ MHz)	Error $e = (s - m)/s $
Qubit frequency ω_q	5740	5739.04	0.0167%
bare cavity frequenc	7252	7436	2.40%
Anharmonicity α	353	359	1.67%
Capacity C	54.87 fF	53.94 fF	1.73%
Detuning Δ	1510	1696.96	11.01%
Dispersive shift χ	1.2	1.405	14.29%
Coupling strength g	90 (from χ_{01})	94.33	4.59%

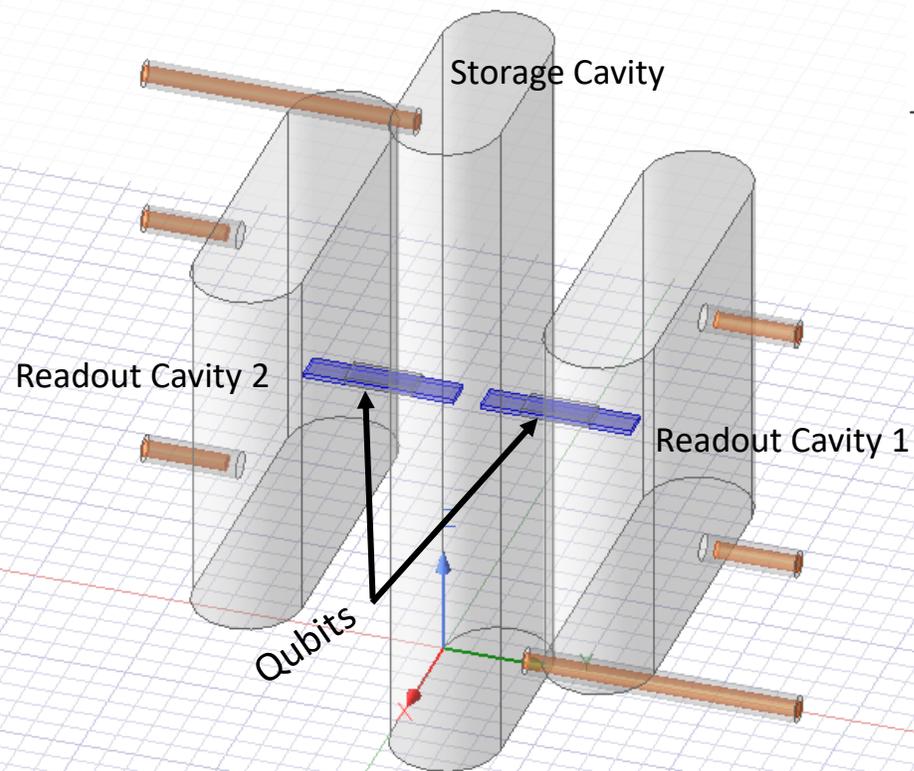


$$\chi = -\frac{g^2}{\Delta} \frac{E_c/\hbar}{\Delta - E_c/\hbar}$$

Experimental data validated the simulations values within a few percent

Two qubits -- 3 cavities

Ansys
2023 R2

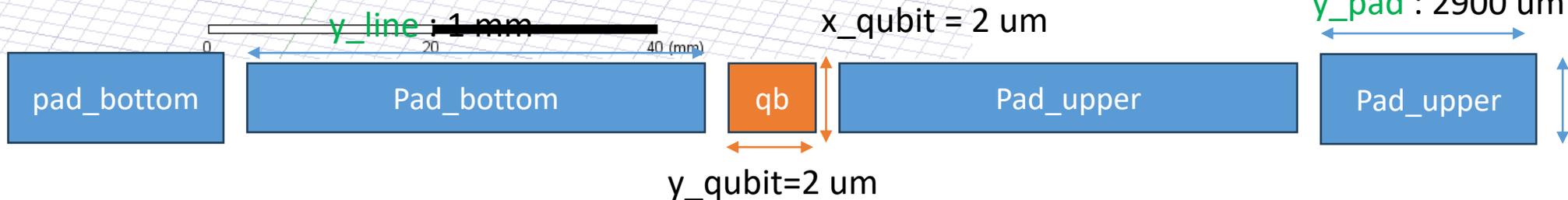
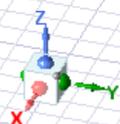


$$\hat{H}_{eff} = \frac{1}{2}\hbar\omega_{q1}\sigma_1 + \frac{1}{2}\hbar\omega_{q2}\sigma_2 +$$

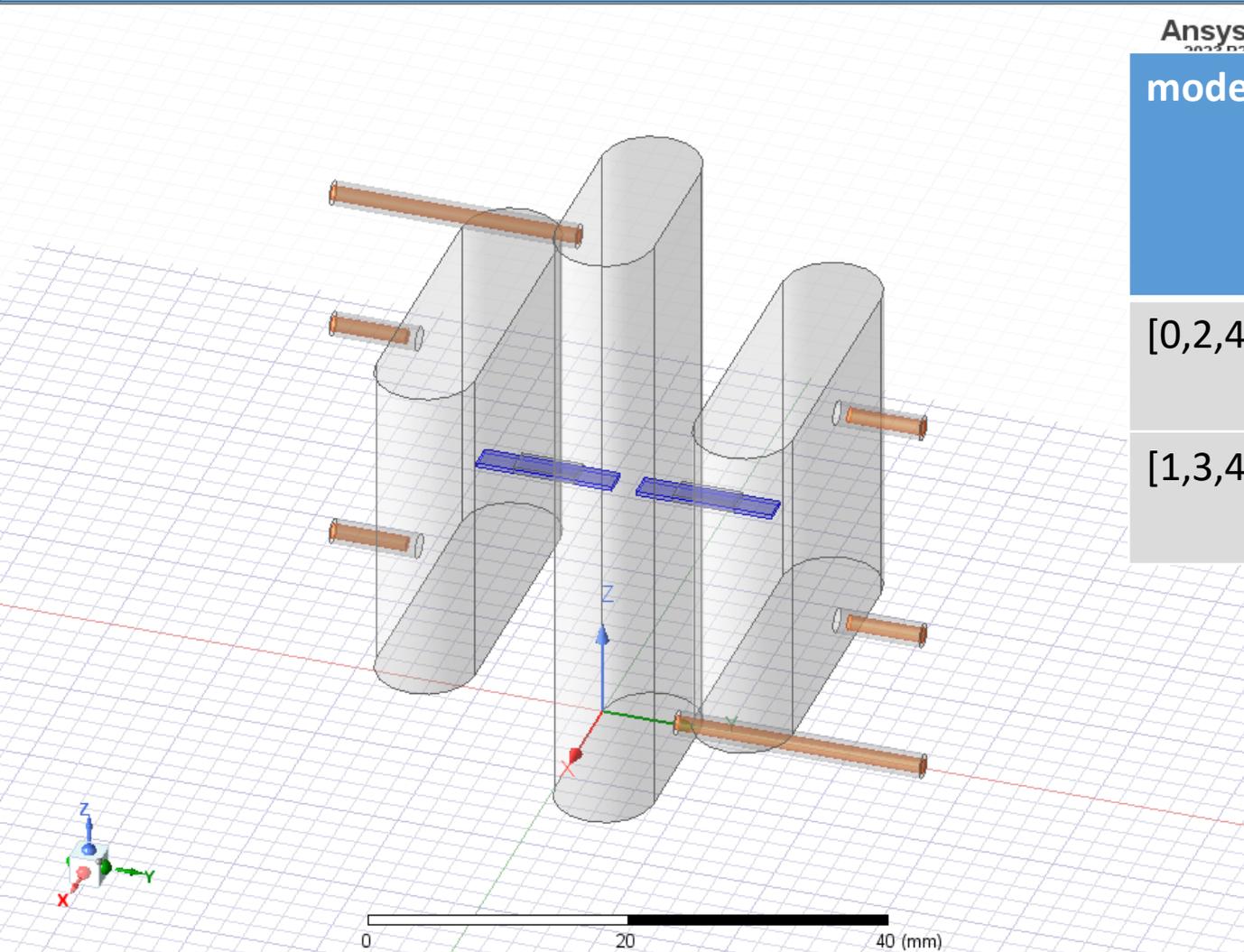
$$+(\hbar\omega_{r1} + \hbar\chi_1^{r1}\sigma_1 + \hbar\chi_2^{r1}\sigma_2) \hat{a}^\dagger \hat{a} + (\hbar\omega_{r2} + \hbar\chi_1^{r2}\sigma_1 + \hbar\chi_2^{r2}\sigma_2) \hat{c}^\dagger \hat{c} +$$

$$+(\hbar\omega_s + \hbar\chi_1^s\sigma_1 + \hbar\chi_2^s\sigma_2) \hat{b}^\dagger \hat{b} + \hbar J(\sigma_1^- \sigma_2^+ + \sigma_2^- \sigma_1^+)$$

$$L_{j1} = L_{j2} = 10 \text{ nH}$$



Two qubits -- 3 cavities



Ansys

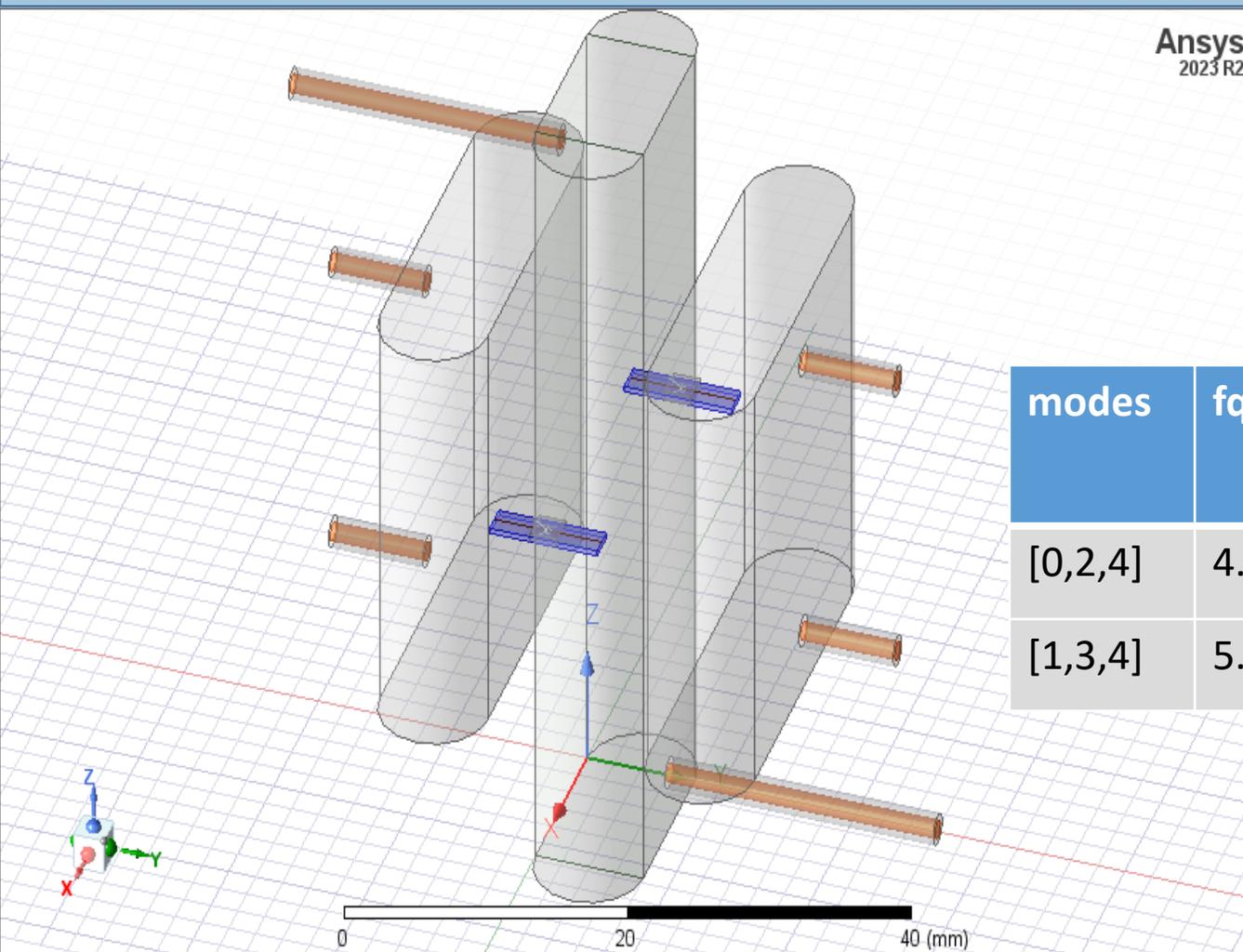
modes	f _q [GHz]	g ₀₁ 1° [MHz]	g ₀₁ 2° [MHz]	α [MHz]	χ 1° [MHz]	χ 2° [MHz]
[0,2,4]	4.91	18.15	48.98	62.80	0.12	0.62
[1,3,4]	4.98	47.12	49.80	69.67	0.78	0.65

Modes 0 & 1: Qubits 1 & 2

Modes 2 & 3: Readout cavities 1 & 2

Mode 4 : storage cavity

Two qubits -- 3 cavities



$$L_{j1} = 11 \text{ nH}$$

$$L_{j2} = 9 \text{ nH}$$

modes	f _q [GHz]	g ₀₁ 1° [MHz]	g ₀₁ 2° [MHz]	α [MHz]	χ 1° [MHz]	χ 2° [MHz]
[0,2,4]	4.61	52.33	57.82	119.97	0.87	0.79
[1,3,4]	5.01	53.50	56.91	104.11	1.01	0.84

Modes 0 & 1: Qubits 1 & 2

Modes 2 & 3: Readout cavities 1 & 2

Mode 4 : storage cavity

Both qubits are detuned and separated from each other by a distance dz

NEXT ???



Optimization of the two qubits device is in progress



Fabrication will follow as well

