SQuADDS: A Validated Design Database and Simulation Workflow for Superconducting Qubit Design

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SQuADDS

Motivation

In a typical superconducting quantum lab, researchers will simulate designs, fabricate, test, and then iterate on the simulation parameters until the simulations converge to experimental results. The eventual working designs and simulation parameters are often held as “secret sauce” and not shared with the community. This presents a major barrier to entry for new groups, as fabrication and measurement runs are costly and time-consuming. Even for well-established groups it can be challenging to move to a new device type or geometry, as simulation parameters that worked for one style of device may not work for another. The purpose of the SQuADDS project is to remove this barrier**.**

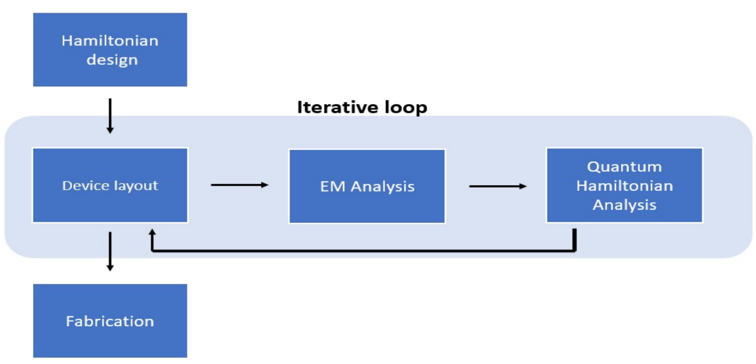

Figure 1: A typical iteration based workflow used in superconducting quantum device design and fabrication

Introducing **SQuADDS**

SQuADDS is a software tool that aims to streamline the journey from the Hilbert space to the cleanroom.

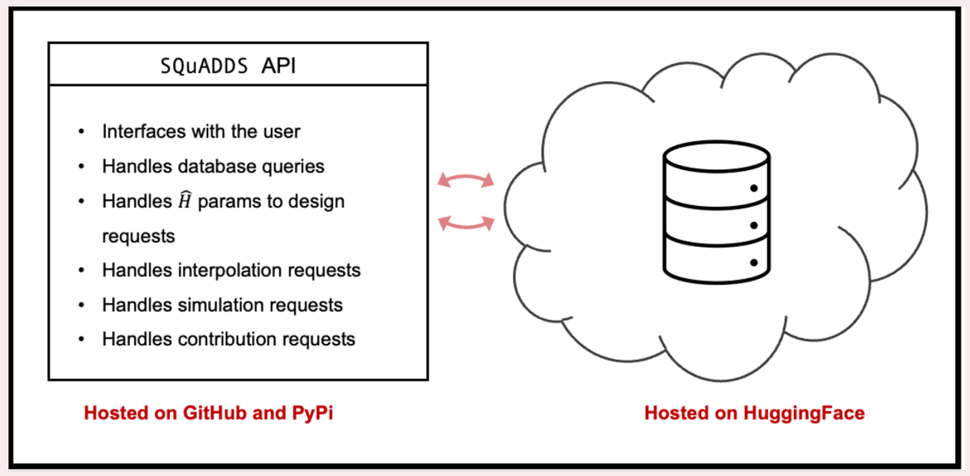

Figure 2: The SQuADDS toolkit comprises a python package and associated HuggingFace dataset

SQuADDS provides access to an open-source database of dense pre-simulated designs and accurate simulation results that provide a “single shot” workflow to simplify the entire design process.

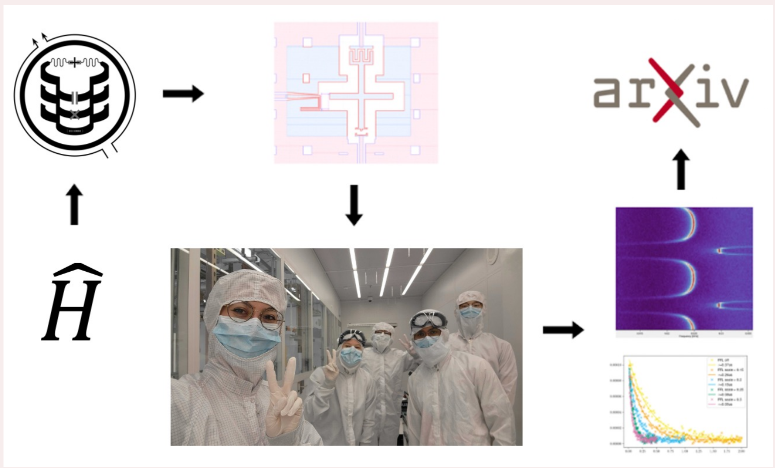

Figure 3: A workflow using SQuADDS for design generation

arxiv/2312.13483 | lfl-lab.github.io/SQuADDS | SQuADDS/SQuADDS_DB | LFL-Lab/SQuADDS

Building the SQuADDS Database

The goal of SQuADDS is to create a database that serves as a lookup table, providing superconducting quantum device designs for queried Hamiltonian parameters. To build this database, we start by measuring Hamiltonian parameters from real devices. We began with a chip fabricated by the SQUILL foundry program, featuring six Transmon qubits, each coupled to its own quarter (half)-wave CPW resonator. We perform two key characterization measurements: punchout, which provides the resonator frequency (ω_r) and linewidth (κ), and qubit spectroscopy, which measures the qubit transition frequency (ω_q), anharmonicity (α), and coupling rate (g). We simulate the device designs using FEM solvers like ANSYS, which provide capacitance matrices, eigenfrequencies and Quality factors. From these results, we derive equations from circuit QED (in the non-RWA regime) to compute the Hamiltonian parameters from simulation outputs.

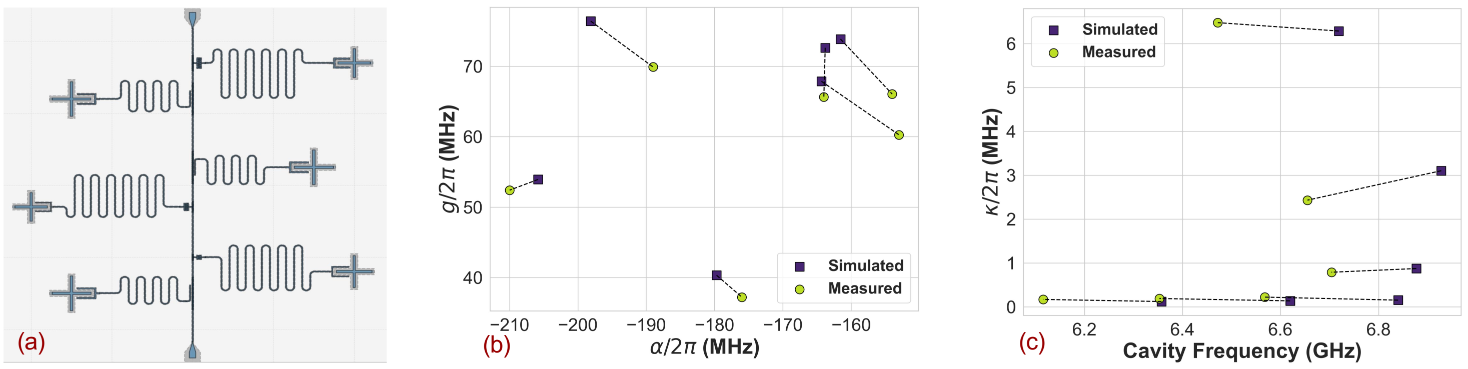

Figure 4: a), SQUILL Foundry chip containing six devices (rendered in Qiskit Metal), b), the error between measured and simulated g and α for these six devices, and c), the error between measured and simulated ω_r and κ

Next, we refine the hyperparameters of the simulations (mesh size, tolerance, etc.) to develop a robust simulation pipeline that converges to the experimental results. Using this procedure, for the devices shown we achieve RMS errors of 4.1%, 16.9%, 10.4%, and 3.0% for α, κ, g and ω_r. In the final step, we perform local sweeps in the design space, leveraging combinatorial growth with modular units to explore numerous device geometries. This ensured the simulation pipeline's robustness and generated a wide range of Hamiltonian parameters, enriching the database for accurate "best guess" predictions.

Designs Available	Simulation Results Type	Components
Measured: 11 Pre-simulated: ~ 5e6	Capacitance Matrices, Eigenmode frequencies and Quality Factors	Xmons, half and quarter wave CPWs, dissipators, couplers

Table 1: Status of the SQuADDS Database as of July 2024

Accessing the SQuADDS Database

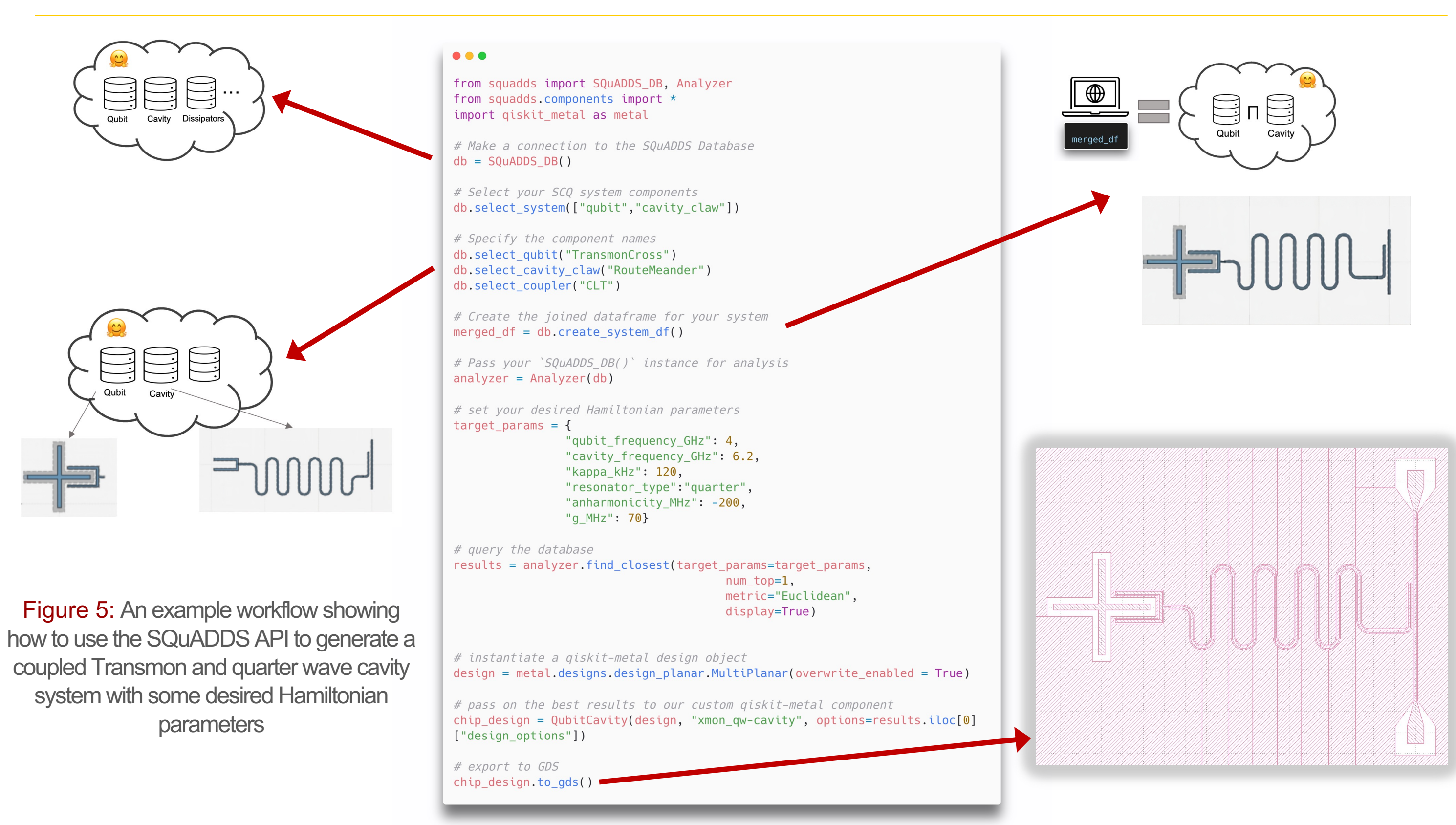

Figure 5: An example workflow showing how to use the SQuADDS API to generate a coupled Transmon and quarter wave cavity system with some desired Hamiltonian parameters

Beyond the Database

SQuADDS has a feature that provides users a “best guess” design for their target Hamiltonian parameters using a physics-informed interpolation algorithm.

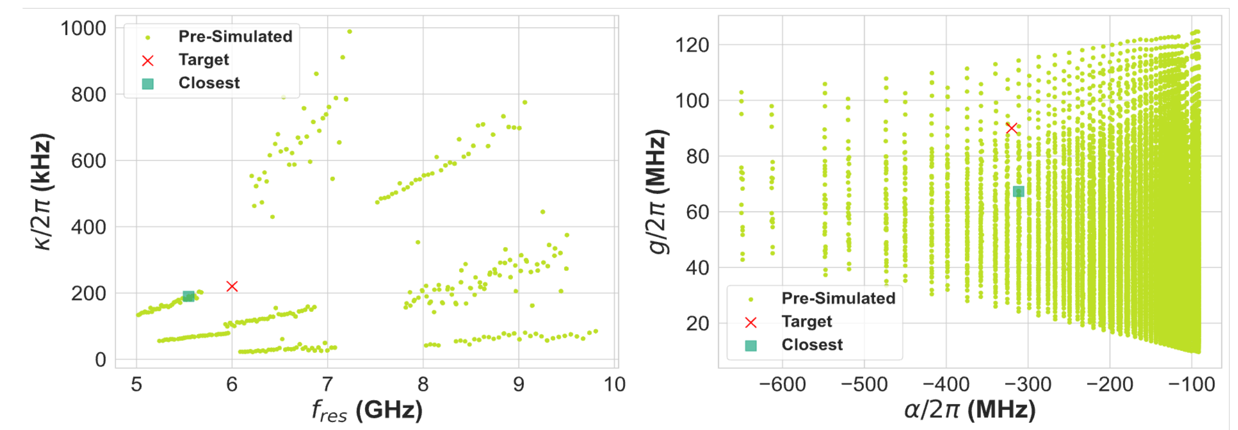

Figure 6: Visualization of quarter-wave cavity simulation data points and user desired target points (marked as x) in Hamiltonian space

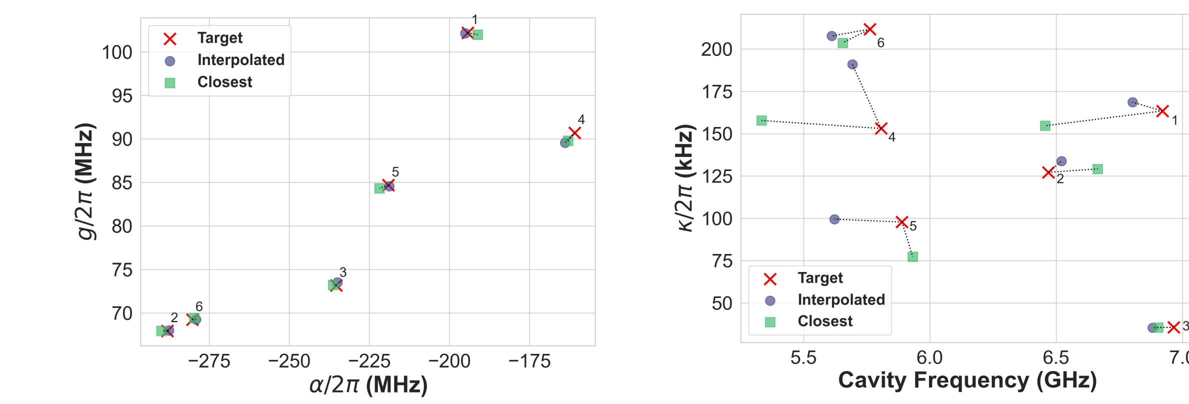

Figure 7: α, κ, g and ω_r with 6 target points (x) compared to the best pre-simulated points (●) and interpolated designs (■)

Design No.	$\Delta g(\%)$	$\Delta\alpha(\%)$	$\Delta\kappa(\%)$	$\Delta f_{res}(\%)$	$\Delta f_q(\%)$	$\max_{\{\xi_i\}}(\xi, \Delta\xi)$
1	0.05	0.42	3.17	1.71	0.38	$(f_r,\ 6.70\%)$
2	0.05	0.16	5.24	0.81	0.12	$(f_r,\ 3.02\%)$
3	0.49	0.16	0.70	1.20	0.12	$(f_r,\ 0.89\%)$
4	1.27	1.87	24.78	1.96	0.04	$(f_r,\ 8.15\%)$
5	0.16	0.12	1.67	4.54	0.10	$(\kappa,\ 20.91\%)$
6	0.02	0.42	1.92	2.62	0.23	$(\kappa,\ 3.82\%)$

Table 2: RMS percentage differences from the target values for the interpolated points in the α, κ, g and ω_r space

Community Contributions

There are many exciting developments going on within the SQuADDS community. Here are some of the highlighted contributions:

- Adding support and data for fluxonium (Andersen Lab @ Delft, Pechenezhskiy Group @ Syracuse), Schuster-style qubits (Schuster Lab @ Stanford) and Trimons (LFL @ USC) to the SQuADDS database
- Integration (with simple API) of AWS Palace as a drop-in replacement for Ansys (LFL @ USC, SQD Lab @ EQUS)
- Development of Machine Learning (ML) models to scale the nature and scope of physics-informed interpolation algorithms (LFL @ USC)
- Using SQuADDS database for various ML solutions to to accelerate superconducting qubit design (Fermilab, UW, PNNL, NUS)

Acknowledgments

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