Automation of electromagnetic simulation tools, parameter value extraction, and time-efficient design techniques for MKIDs and other devices

Cathal McAleer[a], Colm Bracken[a,b], Mario De Lucia[b,c], Eoin Baldwin[b,c], Jack Piercy[b,c], Oisin Creaner[b], Gerhard Ulbricht[b,c], and Tom Ray[b,c]

[a]Maynooth University, Department of Experimental Physics, Maynooth, Co. Kildare, Ireland
[b]Dublin Institute for Advanced Studies, 31 Fitzwilliam Place, Dublin 2, Ireland
[c]Trinity College Dublin, the University of Dublin,College Green, Dublin 2, Ireland

ABSTRACT

Superconducting detector technologies such as microwave kinetic inductance detectors (MKIDs), for example, offer photon-counting, spatio-spectral imaging without needing dispersive optics. State-of-the-art MKID instruments for the optical/infrared regime have up to 20,000 pixels, offering moderate energy resolution and simultaneous time resolution better than 1 microsecond. Given the relative ease with which MKIDs can be multiplexed to large arrays using frequency division multiplexing (FDM), megapixel arrays are fast approaching feasibility. However, the feature of the MKID that makes it inherently multiplexable through FDM, makes it impractical to simulate every one of the many thousand pixels. Given the unique geometry of each pixel in an MKID array, it becomes impractical to manually iterate through pixel model geometries before simulating each frequency sweep. We present a method of expediting the extraction of specific parameter values such as coupling-Q and resonant frequency from large data sets. The data sets herein involved parametric sweeps of capacitor geometry, with a frequency sweep performed for each geometry iteration. The EM software, Sonnet, was automated to simulate these parametric sweeps. We describe a python script that was developed to read-in the Sonnet output data, search the data, and output values of resonant frequency and corresponding capacitor geometry. A 2D planar MKID model was used for the example described in this paper, but the code can easily be adapted for use with other simulation tools. Useful applications of this python programme are described, for parameter value extraction and time-efficient designing of large-format MKID arrays. The programme is available on Github.

Keywords: MKID, superconductor, detector, frequency-division, LEKID, $Sonnet^{TM}$, coupling-Q, automation, Co-Planar Waveguide, Parameterization

1. MICROWAVE KINETIC INDUCTANCE DETECTORS

Within the astronomical community, the current preferred detectors for electromagnetic observations are, in terms of consumer demand, charged coupled devices (CCDs). These detectors allow for large formats, high quantum efficiency as well as low thermal noise. These semiconducting devices however are limited fundamentally due to their intrinsic bandgap (1.1eV for Si) and thermal noise source ($\sim 100K$) operating temperatures.[1] Signal readout within CCDs is also limited as faster readout speeds leads to higher noise level due to cell shifting, while too slow of a readout leads to errors caused by photon interactions with already charged cells during shifting. To avoid these limitations, the community has begun funding research into superconducting technologies.

First developed at Caltech and JPL, microwave kinetic inductance detectors (MKIDs) are a new competing, highly sensitive low-temperature detector technology with the advantageous property of being multiplexed into large arrays (up to 20,000 pixels) via frequency-division multiplexing (FDM), unlike other modern sub Kelvin detectors. MKIDs operate by detecting changes in surface impedance from photon interactions due to the kinetic inductance effect. Within a superconductive metal, energy is stored within the supercurrent which when reversed

Further author information: (Send correspondence to A.A.A.)
A.A.A.: E-mail: cathal.mcaleer@mu.ie, Telephone: +353 858495660

yields extra inductance, this is known as the kinetic inductance effect. These thin-film superconducting detectors utilize photon collisions occuring at the detectors surface and causing the seperation of the main charge carriers (Cooper pairs) to yield extra inductance. Copper pairs, according to BCS theory, are electrons that are bound together by the electron-phonon interaction, with binding energy $2\Delta \approx 3.5k_BT_c$, where T_c is the superconducting transition temperature, above which the material no longer acts as a superconductor.[2]
When seperated due to the increase in energy caused by the incident photon, charge carrier density within the superconductor decreases, increasing kinetic indutance according to the Drude model.

$$L_k = (\frac{m_e}{2n_se^2})(\frac{l}{A}) \tag{1}$$

The kinetic indutance of a superconducting wire in the Drude model is directly related to the length l, cross-sectional area A and charge carrier density n_s.[3] The change in a single pixels inductance can be observed by a change in resonant frequency and thus phase response, as MKIDs are modeled as a parallel LC circuit coupled to a single co-planar waveguide (microwave feedline). Up to 2,000 MKIDs have been demonstrated to be capacitively-coupled to a single feedline without significant crosstalk as shown on the DARKNESS spectrograph, which houses a 10,000 pixel (80x125) MKID array.[4]

$$\omega_0 = \frac{1}{\sqrt{LC}} \tag{2}$$

Figure 1 demonstrates both the kinetic inductance effect process as well as the expected read-out from a single pixel. By exploiting the LC circuits change in surface impedance and hence change in resonant frequency and phase, we can extract the measurement of the energy resolution (R$\sim$ 20–150) and arrival time (precision $\sim 1\mu s$) of individual incident photons with no false counts for X-ray and near-IR cases, while avoiding read noise and dark current typically seen in standard semiconductor technologies.[5]

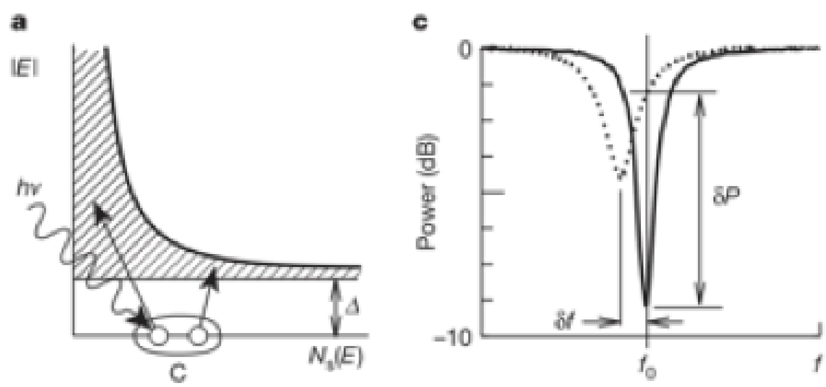

Figure 1. (Left) Showing the absorption of photons with energy $h\nu$ by the MKIDs superconducting film, exciting quasiparticles and lower charge carrier density. (Right) Demonstrates the readout of an MKID with photons incident on the film. During quasiparticle excitation, the resonant frequency changes (lowers) as shown in Eq.(2), showing a deviation from the driven resonance. The energy of the absorbed photon is determined by the degree of phase and amplitude shift. Source:[?]Mazin

The inherent resonant frequency is unique to a single MKID according to its specific geometry. In this way, large arrays of MKIDs are multiplexed using FDM by slightly altering the geometry of the pixel (namely the interdigitated capacitor geometry) during fabrication using lithography techniques.

2. EM SIMULATION SOFTWARE $SONNET^{TM}$

Currently, the method of designing and simulating geometries for specific resonant frequencies involves using the 3D planar full-wave electromagnetic (EM) simulation software $Sonnet^{TM}$. This program approximates a 2D model, sufficient for MKIDs due to their negligible thickness, and performs full-wave EM analysis of the two port circuit to produce a relatively accurate model of the resonator by solving Maxwell's equations.[6] Within the MKID community, simulations are performed on a single pixel design and a parameter sweep is executed to simulate a small amount of similar detectors while manually extracting resonant frequency, S-parameter values and Q-factor from the subsequent graphs. Publications to date have also described simulating every n^{th} resonator, where $10 < n < 100$, and basic interpolation methods are used to predict the resonance of each circuit. These processs however are not only extremely time consuming as the user must manually extract these values for each parameter by hand, with the Q-factor being estimated from the subsequent graphs, but in-accurate as it leaves room for large errors. Similarly, the number of parameter sweeps is dictated by the program package the user owns, possibly lowering data extraction effeciency.

Sonnet offer's three versions of its simulation package commercially, each with their own benefits and restrictions. Sonnet Professionall^{TM} allows for an unlimited amount of parameter sweeps, unlike other packages which only allow 1-3 sweeps. This can become challenging and limiting depending on your package when examining planar circuits over a large range of parameters, which is common place for MKID designers as stated above. However, this can be bypassed (to a certain extent) by driving Sonnet through a Python interface as demonstrated by D.Becerra-Pérez and J.E.Rayas-Sánchez and combined with the method described in this paper to automate parameter sweeps similar to the packages described above. For this paper, Sonnet Professionall^{TM} was employed as it offers the capability of unlimited parameter sweeps, ideal for automation of a large simulated data set. Sonnet can be calibrated to export a data file containing S, Y and Z parameters for all sweeps in either Touchstone, Cadence, Keysight MDIF or as Excel .csv formats. The work described below used the simulated S-parameter data for 27 unique MKID pixel geometries, exported to the .csv extension.

3. AUTOMATION OF DATA EXTRACTION FROM PARAMETER SWEEPS

3.1 SIMULATED MATERIAL PROPERTIES

This paper presents a method of extracting the exact resonant frequency, minimum S21 value and coupling Q-factor from a simulated data set from Sonnet^{TM} using Python code. Using the Sonnet Professionall^{TM} package, the MKID resonators, as shown in Figure 2., were constructed with a set kinetic inductance value of $5pH/sq$, two-port transmission line impedance $Z_0 = 50\Omega$ and ground plate of dielectric constant $\epsilon_{rel} = 11.8$. As these detectors are superconducting, they operate at temperatures below $1K$. While it is not possible to vary simulated temperature within the programme, Sonnet^{TM} allows the user to change the properties of the conducting metals, so the DC resistance (R_{DC}) and reactance (X_{DC}) of the conductor within the circuit was set to $0\Omega/sq$, modelling superconductor behaviour. The circuit itself is modelled after a Lumped Element Kinetic Inductance Detector (LEKID), consisting of an interdigitated capacitor (C) and an inductor (detecting island) with a double meander design, in order to cancel the electric-field produced within the island as well as to avoid crosstalk between pixels.[1]

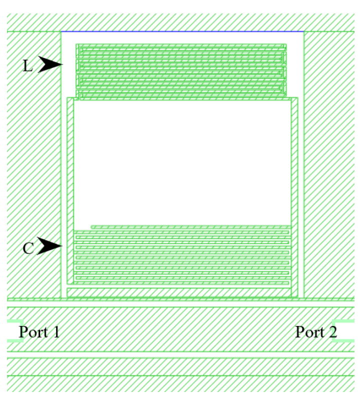

Figure 2. LEKID geometry simulated in Sonnet with interdigitated capacitor (C), double meander inductor (L), coupled to a two-port transmission line.

By parameterizing the length and number of interdigitated capacitor electrodes, a large range of resonant frequencies can be obtained, as demonstrated in literature and experimentally. The resonators simulated in this paper operated between 4GHz-7GHz.

3.2 EXPORTING SONNET SIMULATION DATA

A range of resonant frequencies were then selected according to the resonators unique geometry, with detector resonances seperated into groups according to the proximity of their resonant frequencies. Four groups were decided upon with 4 pixels ranging from 4GHz to 4.1GHz, 6 pixels ranging from 4.8GHz to 5GHz, 8 pixels ranging from 5.4GHz to 5.7GHz and 9 pixels ranging from 6.3GHz to 6.5GHz respectively. In order to accelerate the process of finding the correct interdigitated capacitor geometry for the selected resonant frequencies within each group, an anchored parameter sweep was performed on the length of a single electrode. Each parameter sweep was performed using the ABS sweep setting, sweeping a total of 10,000 unique frequencies with the default Q-factor accuracy setting ON. As stated in 2., Sonnet was programmed to exported all S-parameter data simulated for each sweep to a .csv file extension. This data file included all frequencies swept with the calculated magnitude and angle values from each port for a specific frequency.

3.3 METHOD OF AUTOMATION

Using the *csv* library in Python, the frequencies swept, parameter value and MAG[S21] columns were read into Python and stored in lists as float values. The .csv file contains this values in columns and repeats the structure of; comments, parameter title and data from each parameter swept, so all values within a single column (from all parameter sweeps) must be read into Python. Sonnet scans through more discrete frequencies using the Q-factor accuracy setting than the user inputted number of frequencies, preventing Python from ease of seperation between each parameter data set and thus a means of seperating each seperate parameter swept from the data set was required. This was accomplished by using Pythons *max* function as the data ends at the maximum (or final) frequency scanned and repeats the sequent pattern of comments, parameter title, data. Once each parameter sweep data set was seperated, the resonant frequency of the unique MKID could be easily found using Pythons *min* function to find the minimum S21 value, which corresponds to the resonators resonant frequency in the list, and printed out for the user. With this code, the specific length of the interdigitated capacitor electrode was chosen based on the extracted resonant frequency value.

3.4 USING AUTOMATION CODE TO EXTRACT REAL WORLD DATA

This program was then later used in deducing the kinetic inductance value of real MKID detectors, produced by DIAS[b] and modelled after the previously stated simulated geometries. The MKIDs consisted of a substoicheometric even layer of $TiN/Ti/TiN$ on Si wafers. The extraction of kinetic indutance was carried out by performing a parameter sweep on the kinetic inductance value of each detector in Sonnet initially and reading the .csv file produced into the Python code described. The simulated resonance closest to the experimental value was then selected and the kinetic inductance parameter for the simulated resonance was extracted. Table 1. demonstrates the values from both the tested and simulated MKIDs for group 4 containing 9 pixels. It should be noted that two of the tested MKIDs were not detected during testing and are referred to as "dead pixels". The postulated reasons for this include resonant frequencies being too close to one another, obscuring both signals or defects occuring during manufacture.

Once the average kinetic inductance per square($pH/\mu m$) for each group was esimated using Sonnet and the described method of automation, the capacitance and geometric inductance of the detectors was then calculated using the "L_k model" in Sonnet described by S.Doyle.[7]

Table 1. Extraction of kinetic inductance L_k using automation code for large simulated parameter sweeps. Group 4 resonators were found to have a mean L_k value of 7.963 pH/sq with $\sigma = 0.035$

Measured f_0 (GHz)	Simulated f_0 (GHz)	Extracted L_k (pH/sq)
5.1830502	5.181675	8.05
5.2070483	5.206825	7.97
5.2103982	5.211	7.96
5.2116286	5.2099	7.97
5.214266	5.21455	7.96
5.2160468	5.21625	7.96
5.2248198	5.22515	7.935
5.2254955	5.22575	7.94
5.2334954	5.23315	7.92

4. DEDUCING COUPLING QUALITY FACTOR FROM SONNET

Coupling Quality Factor (Q_c) is a critical factor in the production of all resonant circuits with a 2-port network. This factor describes how well the MKID couples to the transmission line.Q_c is defined as :

$$Q_c = 2\pi \frac{energy\ stored\ in\ resonator}{energy\ leak\ from\ port\ 3\ to\ port\ 1\ and\ 2\ per\ cycle} \tag{3}$$

Typically, the total quality factor of a resonat circuit is described as:

$$\frac{1}{Q_{tot}} = \frac{1}{Q_c} + \frac{1}{Q_i} \tag{4}$$

where Q_c denotes the coupling quality factor and Q_i denotes the internal quality factor.[?]
However, Sonnet is not capable of calculating a value for the internal Q_i as the quality of the dissipation in the load impedance of the transmission line goes to infinity within Sonnet. Thus, within Sonnet's simulation environment $Q_{tot} = Q_c$, and a value can still be extracted in order to deduce the quality of the MKIDs.
While Sonnet does not explicitly give the Q factor of a circuit, it does produce S-parameter data in the form of frequency sweep and S21 magnitude. By plotting both parameters against one another, we obtain the expected graph seen in most high-Q KIDs:

From this graph, the Q-factor can be deduced use the Full-Width Half-Maximum (FWHM) technique. However, Sonnet may only produce a single data point for the dip around the resonant frequency due to an inefficient amount of frequencies swept and thus Python can not calculate values that are not present within the dip. To avoid this, we propose interpolating the data points within the .csv file using Python's *scipy.interpolate* library. This allows the interpolate of data points within the dip, should we need them due to a lack of frequency points. Once interpolated, the new data set is then translated such that the middle of the curve intersects the x-axis (frequency). This is achieved using the previous *min* function to find the minimum S21 value at which resonance occurs as well as the first S21[MAG] value in the data set ($S21_{initial}$) to find the half-maximum. The interpolated curve is then transformed by:

$$\frac{(S21_{initial} + S21_{min})}{2} \tag{5}$$

This transformation then allows Python to find the two points on either side of the curve by solving for the roots of the curve (intersecting the x-axis) using the *sproot* function of Python's interpolation library. These two frequencies are then substracted in order to give the FWHM of the data set. Finally, the Q_c of the resonator is

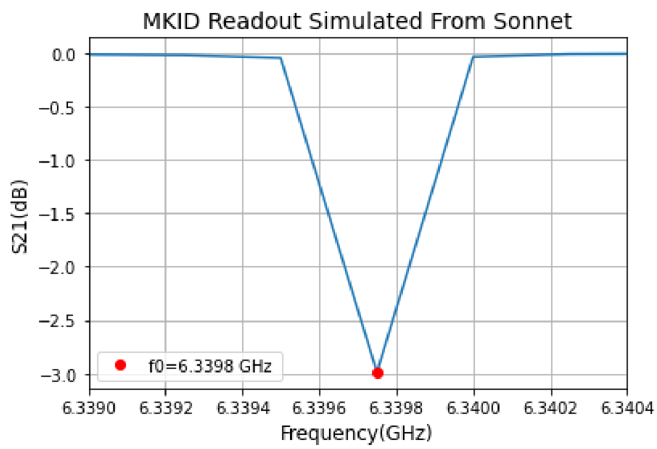

Figure 3. A typical frequency curve seen in MKIDs with a "dip" occuring at the resonant frequency of the resonator. This data was produced using Sonnet and due to a lack of discrete frequencies swept, has a linear trend, as opposed to the expected smoothing within the dip as shown in Fig.1.

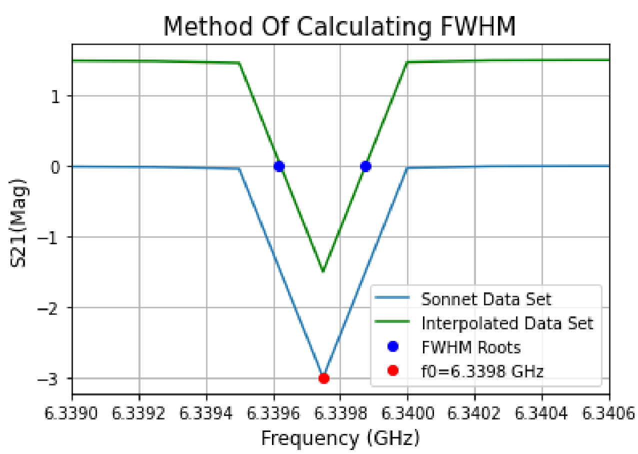

Figure 4. Demonstrating the method of calculating FWHM from a set of data exported from Sonnet. Firstly, the simulated data set (BLUE) is interpolated (GREEN) within Python and transformed by Eq.(5) such that the middle of the "dip" of the interpolated set now lies on the x-intercept (i.e. S21=0). Python's sproot function then finds the two points lying on the x-intercept and calculates the FWHM by substracting the roots from one another.

then calculated according to the equation:

$$Q_{tot} = Q_c = \frac{f_o}{FWHM} \tag{6}$$

5. CONCLUSION

Sonnet^{TM} offers an easy simulation tool for MKID geometries in order to predict resonant frequencies before manufacture but is limited in producing user specific data. MKID resonant frequencies are unique to their specific geometry and thus multiple intensive simulations using parameter sweeps must be carried out. This paper offers a programme that will allow users to extract resonant frequencies and Q-factor values of large parameter sweeps from a data file using Python. This is accomplished using only two main libraries; *csv* and *scipy.interpolate*. Resonant frequency of each parameter is extracted from indexing the minimum S21[MAG] in the data set while Q-factor is determined using the Full-Width Half-Maximum technique. Interpolation is performed to allow Q-factor extraction for data sets with insufficient discrete frequencies. It should be noted that within Sonnet, a minimum of 8000 discrete frequencies swept is required for a stable Q-factor calculation.

While this program was designed for automation of Sonnet data files, it is suggested that with small edits to the code, this program will also function with other EM simulation software's that produce external data sets for MKIDs. The program is available for free use on Github.com.[8]

REFERENCES

[1] Mazin, B., Bumble, B., Meeker, S., O'Brien, K., McHugh, S., and Langman, E., "A superconducting focal plane array for ultraviolet, optical, and near-infrared astrophysics," *Optics Express* **20**, 1503–1511 (2012). https://doi.org/10.1364/OE.20.001503.

[2] Day, P., LeDuc, H., Mazin, B., Vayonakis, A., and Zmuidzinas, J., [*A broadband superconducting detector suitable for use in large arrays*], Nature (2003). https://doi.org/10.1038/nature02037.

[3] Meservey, R. and Tedrow, P., "Measurements of the kinetic inductance of superconducting linear structures," *Journal of Applied Physics* **40**, 2028 (1969). https://doi.org/10.1063/1.1657905.

[4] Meeker, S., Mazin, B., Walter, A., Strader, P., Fruitwala, N., Bockstiegel, C., Szypryt, P., Ulbricht, G., Coiffard, G., and Bumble, B., "Darkness: A microwave kinetic inductance detector integral field spectrograph for high-contrast astronomy," *The Astronomical Society of the Pacific.* **130**, 988 (2012). https://doi.org/10.1088/1538-3873/aab5e7.

[5] McHugh, S., Mazin, B., Serfass, B., Meeker, S., O'Brien, K., Duan, R., Raffanti, R., and Werthimer, D., [*A readout for large arrays of Microwave Kinetic Inductance Detectors*], American Institute of Physics (2012). https://doi.org/10.1063/1.3700812.

[6] Sonnet Software, I., [*Sonnet User's Guide*] (May 2018).

[7] S.Doyle, [*PhD Thesis: Lumped Element Kinetic Inductance Detectors*], Cardiff University (2018).

[8] McAleer, C., "Sonnet automation programme for resonant frequency and q-factor extraction," (December 2021). https://github.com/scathalmca/Sonnet-Automation-Programme-for-Resonant-Frequency-and-Q-Factor-Extraction.