Modeling Nonlinear Behavior and 3D Geometrical Effects in Superconducting Quantum Interference Devices Containing Paramagnetic Elements

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Introduction
Low-temperature microcalorimetry has brought new physics to the problem of particle detection, enabling breakthrough energy resolution < 2eV at 6KeV, and ~40 eV at 100KeV [1]. This has brought powerful new capabilities to nuclear forensics, X-ray astronomy, and the characterization of materials and bio-materials, among other applications. Our experimental low-temperature physics group [2] is working to further improve the performance of low temperature microcalorimetry by developing non-dissipative temperature sensors based on the temperature dependence of paramagnetism.

As presently implemented [3], these “magnetic microcalorimeters” use a superconducting flux transformer to couple the change in magnetic flux into a “Superconducting Quantum Interference Device,” (SQUID). However, insufficient signal/noise in these devices creates a limitation for the achievable energy resolution. Our group is working on a new approach to improve signal strength by a factor of two, by eliminating the flux transformer and integrating the paramagnet and sensing coil directly into the SQUID loop itself.

SQUIDs are intrinsically nonlinear devices, relying on the interaction of two Josephson Junctions via a circuit network. Although their underlying physics is well-understood, they can exhibit complex and sometimes unexpected behavior. Thus, in any attempt to fundamentally alter their circuit topology, it is prudent to perform numerical simulations to validate new approaches before fabricating new microdevices. Our goals in this research project are to use numerical modeling to understand the impact of the SQUID on the paramagnet and vice-versa, and to determine if good SQUID performance can be obtained in this new type of device.

3D Geometrical Effects
The Problem: The sensing coil of the integrated device will carry part of the Josephson oscillation currents of the SQUID. Those currents are at high frequencies (1-100 GHz) and there is significant potential for deleterious eddy-current heating of the metallic paramagnet. We need to estimate the heating that will be seen in the integrated devices, including the effects of the 3D geometry of the paramagnet and coil, the skin depth of the paramagnet, and the London penetration depth of the superconducting coil.

Modeling Approach and Conclusions: We used 3D Finite-Element Modeling (FEM) of the sensing coil, paramagnet, and adjacent insulating and superconducting structures, with results checked wherever possible for consistency with analytical solutions. Heating of the paramagnet was estimated by using the sensing coil currents calculated by the SQUID simulations (next section) as an input to the FEM calculations.

Computational Approach and Conclusions: We were already using the commercial COMSOL FEM program to study 2D approximations of the problem. However, 3D FEM electromagnetic models require very large amounts of RAM and processing power. We were able to find an efficient solution by installing COMSOL on the poblano super-node at UNM’s Center for Advanced Research Computing. Poblano has 256GB of RAM, 32 CPUs and 32 FPUs.

COMSOL was installed and working on the super-node in just a few hours, and was able to hit almost 3200% CPU on Linux’s “top” utility while calculating solutions, showing that we could bring the full power of the machine to bear. Meshing efficiency, on the other hand, could be quite poor, but we found we could greatly reduce meshing time by artificially breaking up the geometry into more domains, which COMSOL could then mesh in parallel.
Simulating SQUID Internal Dynamics

The Problem: To fully assess the integrated device approach, we need to be able to calculate the Josephson oscillation current that passes through the sensing coil, and to perform extensive trade studies to optimize circuit parameters for good SQUID performance while minimizing Josephson oscillation current in the sensing coil, to minimize eddy-power heating of the paramagnet.

Modeling Approach and Conclusions: We developed in-house simulation software based on the lumped-element approach of Tesche and Clark [4]. Our approach incorporated two novel features to improve the accuracy and efficiency of the simulations. First, rather than a fixed-time-step integration scheme, Runge-Kutta with adaptive stepping was used to take advantage of modern supercomputing power. Second, rather than using random-number noise at fixed steps, we used continuous, bandwidth-limited white noise. On the super-node, this approach allowed us to simulate the nonlinear dynamics with high fidelity while still achieving sufficient simulation speed to perform the required parameter trade studies and the long runs required to estimate low-frequency noise.

Computational Approach and Conclusions: MATLAB was already available on the machines at the UNM Center for Advanced Research Computing, so we were able to capitalize on our existing code base. The SQUID simulations are compute-intensive but require only a few GB of RAM per job, and we were able to run at least 48 jobs in parallel on poblano without any swapping or apparent resource contention.

Summary
The calculations described here have shown that the integrated detector approach should be feasible, achieving eddy-power heating of the paramagnet <1 pW while staying with proven designs for the SQUID circuit elements. We also plan to test some new SQUID circuit element designs that these calculations have shown could drive the eddy-power heating down even further, for future applications. The large-RAM super-node has been an efficient and essential part of this research, allowing a group with little supercomputing experience to attack qualitatively new kinds of problems.

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References