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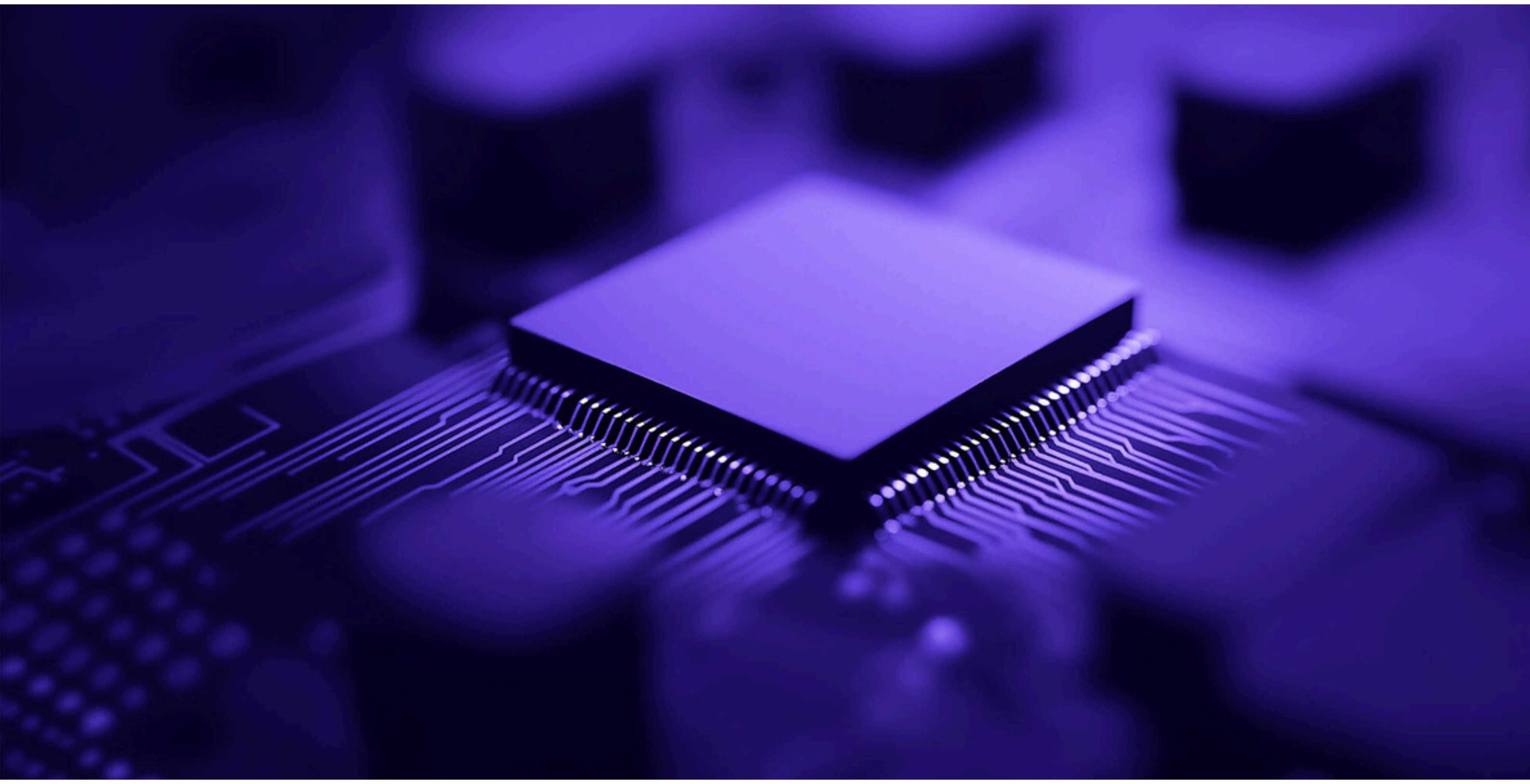

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Estimation of composite material properties using an inverse approach with Quanscient Allsolve

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Abstract

Accurate material characterization is fundamental to achieving reliable computational simulations, particularly in systems involving composite or anisotropic materials. Traditional experimental methods for material property estimation are often time-consuming, costly, and limited in scope. As engineering applications grow increasingly complex, there is a growing demand for more efficient and accurate alternatives. Inverse problems provide a powerful framework for estimating unknown material properties by minimizing discrepancies between simulated and experimental data. This approach shifts the focus from direct measurement to iterative optimization using computational models.

This paper presents a methodology for estimating material properties through inverse simulations using Quanscient Allsolve, a cloud-native, multiphysics simulation platform. The study focuses on a practical case involving a JEDEC-standard printed circuit board (PCB), in which an API-driven optimization loop is employed to minimize the residual error in eigenfrequency predictions.

The workflow integrates finite element analysis (FEA) with gradient-based optimization techniques from SciPy, achieving material properties that closely match those reported in the literature.

The results demonstrate a high degree of correlation between simulated and experimental data, validating the proposed methodology and highlighting the computational efficiency afforded by cloud-native parallelization.

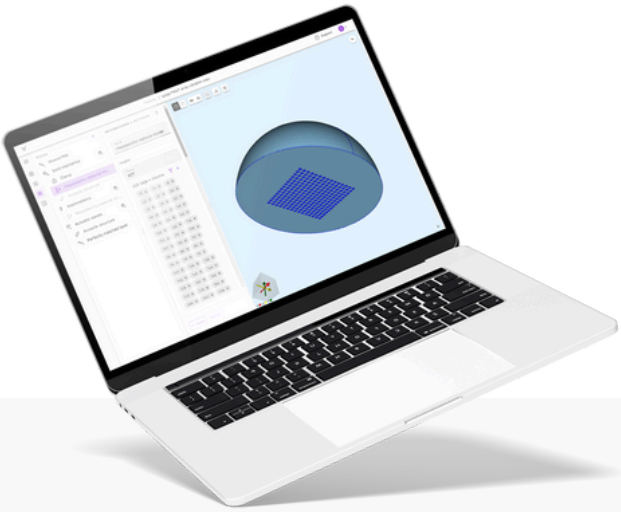
This paper underscores the relevance of inverse simulation techniques for material characterization and illustrates the potential of automated, cloud-based workflows in engineering simulations.

Keywords — Inverse problem; material property estimation; Finite Element Method (FEM); cloud computing; PCB simulation; multiphysics modeling; automated optimization

Introduction to Quanscient Allsolve

The cloud-based multiphysics simulation platform Quanscient Allsolve was used for all simulations featured in these case studies.

Learn more at quanscient.com ⟶



Quanscient Allsolve

- A cloud-based FEM multiphysics simulation platform
- Developed by Quanscient, a company established in 2021 in Tampere, Finland
- Built upon the open-source solver *Sparselizard* developed by our CTO, **Dr. Alexandre Halbach**

Trusted in both industry and academia

UK Atomic Energy Authority · Infineon · MIT Massachusetts Institute of Technology · Proxima Fusion · imec · Paul Scherrer Institut PSI

Introduction to inverse problems for material property optimization

The mechanical behavior and reliability of systems such as printed circuit boards (PCBs) are heavily influenced by the properties of their constituent materials. Characterizing these materials is essential for constructing accurate computational models, particularly when using finite element analysis (FEA) to simulate mechanical or vibrational responses.

Traditional experimental methods, while effective, are resource-intensive and frequently impractical for high-throughput or early-stage design applications. As a result, computational methods for estimating material properties have gained prominence. These methods are especially useful in systems composed of complex, layered, or anisotropic materials where direct measurement is challenging.

Challenges about estimation of material properties

Experimental Constraints: The need for controlled environments, specialized equipment, and multiple iterations makes experimental characterization laborious.

Resource Demands: Physical testing consumes significant time and financial resources, especially in prototyping stages.

Complexity of Material Behavior: Materials such as composites exhibit directionally dependent properties that are not easily captured using standard characterization techniques.

Motivation for simulation

To address the limitations of conventional experimental approaches, inverse problem-solving presents a viable computational alternative. In this context, the estimation of material properties is formulated as an optimization problem wherein simulation outputs are compared to experimental data, and material parameters are adjusted iteratively to minimize the discrepancy.

Quanscient Allsolve, with its automated, API-driven workflow and cloud-based architecture, provides an ideal environment for implementing such a methodology.

The objective of the simulation presented herein is to demonstrate the feasibility and accuracy of this approach using a packaged PCB model subjected to modal analysis.

Material property optimization
Methods and models

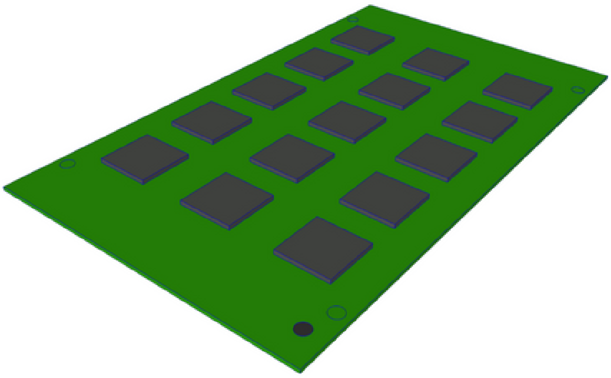


Fig.1: CAD model of the standard packaged PCB.

Simulation methodology

The study employs an inverse simulation approach to estimate unknown material properties through iterative optimization. The methodology involves defining initial material parameters, performing eigenmode analyses, and minimizing the residual error between simulated and experimental eigenfrequencies.

The following procedural components were employed:

Finite Element Modeling: The PCB was modeled as an anisotropic material characterized by three independent elastic constants. The mounted packages were modeled as isotropic materials.

Optimization Framework: A gradient-based optimization algorithm from the SciPy library was used to iteratively refine the material parameters.

Simulation workflow

The simulation began by defining initial material properties for the PCB and package structures. Using Quanscient Allsolve, an eigenmode analysis was performed to determine the system's natural frequencies. The simulated eigenfrequencies were then compared to experimentally obtained values, and the residual error was calculated. This residual served as the input for updating the material parameters through a gradient-based optimization algorithm. The process was repeated in an iterative loop until the convergence criteria were satisfied.

Material property optimization
Methods and models

Simulation setup

The test case involved a JEDEC-standard drop test PCB with dimensions of 132×77×1 mm^3. The board included a 3×5 full array of 13×13 mm packages. The goal was to estimate the equivalent material properties of the PCB and its mounted components by minimizing the discrepancy between simulated and experimental eigenfrequencies.

The simulation was designed to estimate the unknown material properties of the PCB and the mounted packages with sufficient accuracy to align simulation results with experimental modal data. To achieve this, an iterative optimization approach was used to minimize discrepancies between simulated and measured eigenfrequencies.

This optimization process was automated using Quanscient Allsolve's API, allowing for efficient integration with external libraries and minimizing the need for manual adjustments. The API-based workflow ensured repeatability and scalability throughout the process.

he workflow comprised several sequential steps designed to iteratively minimize the discrepancy between simulation and experimental results. Initially, material parameters for the PCB and package structures were defined based on approximate or literature-based values. These parameters were then used to set up and execute an eigenmode analysis using Quanscient Allsolve, which calculated the system's natural frequencies.

Following each simulation, the resulting eigenfrequencies were compared against corresponding experimental data to evaluate the accuracy of the current material model. The discrepancy, or residual error, between the two datasets was computed and used to inform the update of material parameters. This process (simulation, comparison, residual calculation, and parameter update) was repeated in an automated loop using a gradient-based optimization algorithm until convergence criteria were met. The automation and cloud-native nature of the platform significantly accelerated the process and ensured consistency across iterations.

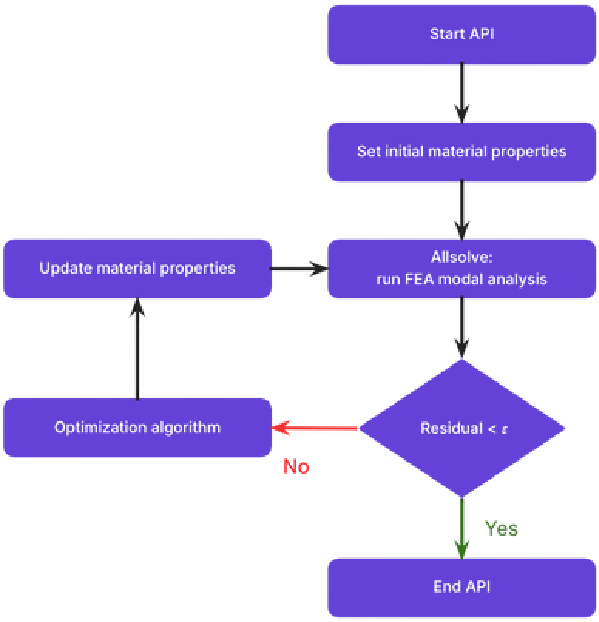


Fig. 2: API optimization workflow.

Material property optimization
Results and discussion

The optimization routine converged after 85 iterations, resulting in a 5.7% relative residual error. This outcome indicates a high degree of fidelity between the simulated and experimental eigenfrequencies.

Accuracy of Estimation

The optimized material properties were in close agreement with values reported by Lee et al. [2], with minor deviations attributed to modeling simplifications, such as the exclusion of the accelerometer mass.

Reduction in Manual Effort

The API-driven workflow enabled automation of the entire optimization process, reducing manual intervention and ensuring consistency.

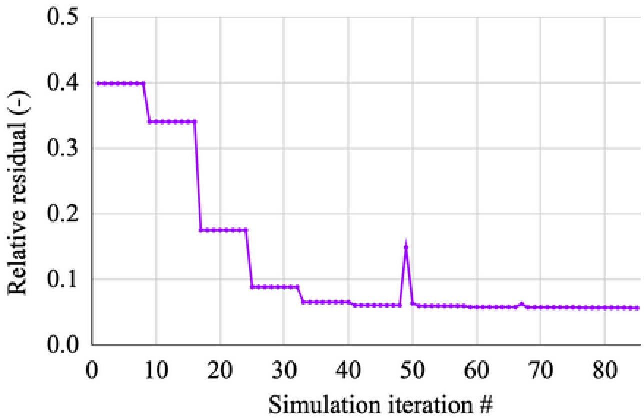


Fig. 3: Iterations of the material properties.

Property		Initial	Optimized (present work)	Lee et al. [2]
PCB	E_b (GPa)	15.50	9.48	9.42
	G_b (GPa)	6.46	3.00	3.12
	ν_b (-)	0.20	0.20	0.25
	ρ_b (kg/m^3)	1910	2100	2050
Package	E_p (GPa)	28.00	19.51	20.00
	ν_p (-)	0.35	0.41	0.4
	ρ_p (kg/m^3)	1810	1850	1840

Table 1: Comparison between initial and optimized material properties.

Material property optimization
Results and discussion

Validation of Simulation Results

Simulated eigenfrequencies were found to be within ±16% of experimental measurements. Mode shapes were qualitatively consistent with both experimental data and previously published finite element analysis results.

Modelling Assumptions

Discrepancies in mode shapes and eigenfrequencies were primarily due to simplifications such as the use of gradient-based optimization (prone to local minima) and omission of certain physical elements in the simulation model.

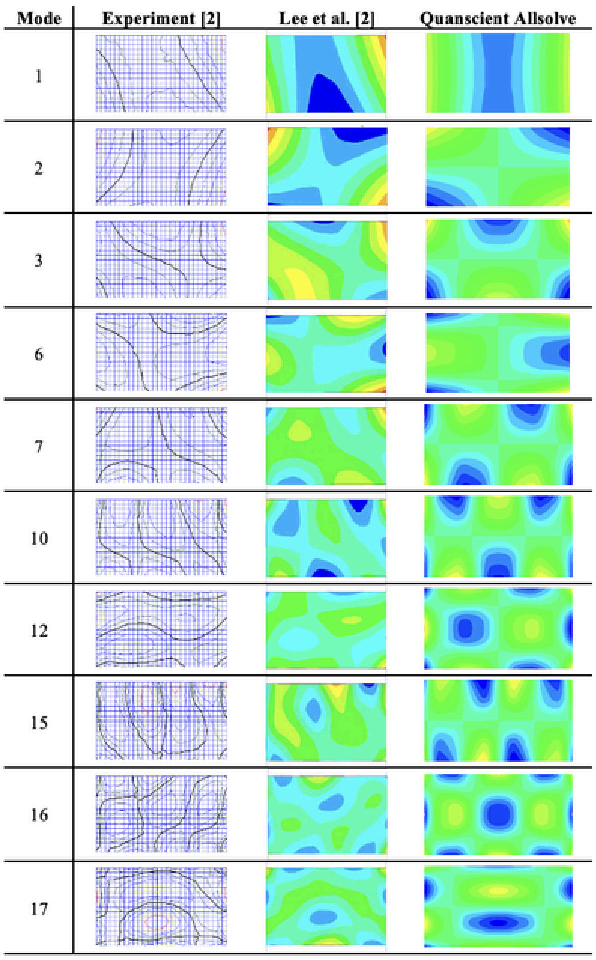


Fig. 4: Comparison of selected modes with experimental modal analysis and finite element analysis from Lee et al. [2]. The deviations in mode shapes are attributed to neglecting accelerometer mass and use of simple gradient-based optimization, leading to a local optimum rather than a global one.

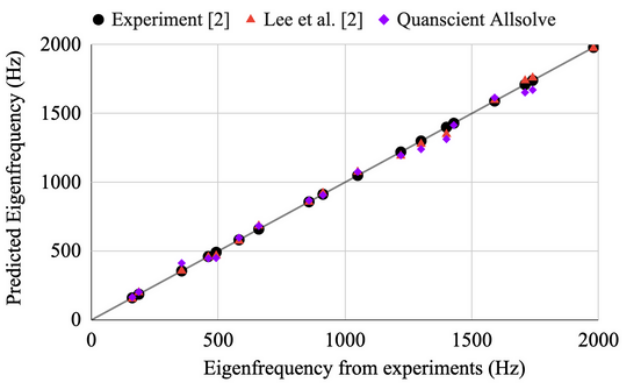


Fig. 5: Comparison of predicted eigenfrequencies with experimental measurements.

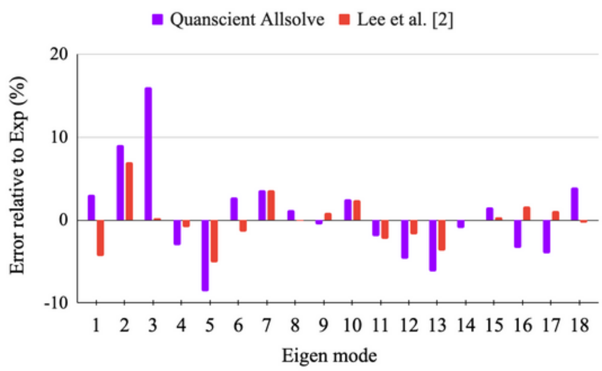


Fig. 6: Error relative to experimental values of eigenfrequencies.

Material property optimization
Conclusion

1

The **methodology presented** in this study demonstrates the utility of inverse simulation techniques for estimating material properties in composite systems. These techniques **offer an efficient alternative** to experimental approaches, particularly **when dealing with complex, layered, or anisotropic materials** where direct characterization is difficult or infeasible.

2

Quanscient Allsolve, with its cloud-native infrastructure and API-first architecture, **provides a powerful platform** for deploying such inverse modeling workflows. Its parallel computing capabilities and integration with optimization libraries enable the automation of time-consuming processes, leading to **faster iterations and higher consistency** in simulation outcomes.

3

The case study involving a packaged PCB serves as a proof-of-concept for broader engineering applications. By integrating cloud computing with automated optimization, the approach showcased in this study represents a meaningful **advancement in simulation-driven design and analysis**, offering increased accuracy and significant time savings.

Material property optimization
Key takeaways

- Inverse problems help estimate material properties by minimizing the difference between simulations and experimental data
- With an API-driven workflow, Quanscient Allsolve automates this process, reducing manual work and speeding up optimization
- Quanscient Allsolve runs simulations in the cloud with parallel computing, significantly reducing processing time
- The optimized material properties closely matched experimental data, improving simulation reliability in this case example
- Printed circuit boards (PCBs) are one example where this approach might be useful, but the method itself is very general and can be applied to other complex material systems

Get in touch

Learn more and request a demo at
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Material property optimization
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