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Multiscale Mathematical Modeling and Simulation of Coupled Thermo-Mechanical Behavior in Advanced Composite Materials

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ABSTRACT

Developing composite technologies, such as carbon fiber-reinforced polymers (CFRPs) and ceramic matrix composites (CMCs) are being applied in the aerospace, automotive, and energy systems sectors to a large extent because of their high strength-to-weight ratios, thermal resistance, and durability. Although these have the following advantages, their coupled thermo-mechanical behavior has become a significant challenge to predict and is of concern primarily because of the heterogeneous microstructures and multiscale interactions. The framework in this paper constructs a multiscale mathematical model and computer simulation to study thermo-mechanical reactions of high-tech composites by combining microstructural characterization, homogenization theory, and continuum mechanics. Particular equations of heat conduction, thermal strain and stress equilibrium are transformed into governing equations, and a coupled system is solved using finite element analysis (FEA). At the microscale, fiber-matrix interactions, interfacial debonding, and void effects are modeled by representative volume elements (RVEs). The mesoscale is homogenized by using homogenization methods to correlate microstructural characteristics to ply-level anisotropy. On a macro scale, continuum simulations are made to predict structural response to combined thermal and mechanical loading. A case study of CFRP laminates illustrates the ability of the framework to predict. The proposed multiscale model enhanced thermal expansion coefficient (CTE) estimation with a 12% high accuracy than the traditional unidimensional FEM. It was also able to trace residual stress distributions at fiber-matrix interfaces with high fidelity and early-stage failure mechanisms including delamination which are otherwise invisible to continuum-only models. Adaptive meshing and reduced-order homogenization maintained computational efficiency by reducing simulation run time by 30 percent and accuracy. The findings reaffirm the importance of multiscale modeling in the development of the next-generation composites in mission-critical applications. The work provides a serious mathematical and computational framework that interpolates microstructural physics, with engineering-scale simulations, which allows making predictions of performance more reliably and designing materials more optimally.

1. INTRODUCTION

New composites, especially carbon fiber-reinforced polymers (CFRPs) and ceramic matrix composites (CMCs), are now used in aerospace, automotive, civil and energy systems due to their high stiffness to weight, thermal conductivity, corrosion resistance and high fatigue life. As an example, CFRPs have made it possible to create lighter aircraft fuselage, fuel-efficient automotive structures and next-generation wind turbine blades with increased load-bearing capacity [1], [2]. Equally, CMCs have found extensive applications in high temperature turbine components and energy applications where traditional metallic materials cannot be used to deliver high performance. All these developments highlight the core design and production of composites in contemporary engineering. Irrespective of these benefits, ensuring the prediction of composites behavior during coupled thermo-mechanical loading remains to be a cornerstone issue. Contrary to homogeneous materials, composites have heterogeneous and anisotropic microstructures with fibers, matrices and interfaces. When thermal and mechanical stresses are present together these multiscale constituents behave in complexity to produce such phenomena as residual stresses, interfacial debonding, nonlinear thermal expansion, and anisotropic crack propagation [3]. Such coupled interactions have direct implications on service reliability, structural stability, and long-term performance in mission-critical systems like aircraft wings, rocket structures and on energy storage systems. Conventional single scale continuum models are often not able to reflect these complexities because they generally homogenize the microstructure and, consequently, fail to capture important local effects such as the fiber orientation, void distributions and interfacial cracking. Although these models are computationally efficient, their incapacity to reflect the actual multiscale character of composites reduces their predictive ability [4]. The limitation leaves a research gap of the necessity of strong and scalable mathematical models that should be capable of accounting explicitly the microscale phenomena and connecting them to macroscale performance. To address this gap, multiscale mathematical modeling has become a good way forward. It combines the methods of microstructural physics, homogenization and continuum scale equations such that they allow more realistic models of the thermo-mechanical coupling in non-homogeneous system. The approach uses representative volume elements (RVEs) to model fiber-matrix interaction at the microscale, mesoscale models to model anisotropy at the ply level and macroscale finite element analysis (FEA) to model system-level performance under working loads [5]. This multiscale integration will not only give more precise predictions but also flexibilities of designs to engineers dealing with the next-generation composite structures. The possibilities of this approach have been proven by the latest developments. Li et al. [6] developed a multiscale finite element model that was used to analyze thermo-elastic behavior in fiber-reinforced composites with a better prediction capability than the traditional models. On the same note, Kumar and Zhang [7], proposed machine learning-aided homogenization methods, which improved nonlinear studies by anisotropic composites in thermal expansion. Computational homogenization has been used together with parallel computing to minimize the cost of computation at an otherwise accurate method by other researchers [8]. Most of the studies prefer either of the above despite these developments:

1. Concentrate on isolated (mechanical or thermal) effects, whilst ignoring coupled thermo-mechanical interactions.
2. In stress and failure prediction, put a premium on computational performance, not on numerical performance.

Accordingly, it is still evident that a more detailed, multiscale mathematical / computational system (capable of striking a balance between predictive accuracy and computational efficiency) is required to deal with coupled thermo-mechanical behaviour of advanced composites [14].

The aim of the paper is to create such a structure through the combination of PDE-based governing equations, multiscale homogenization strategies, and finite element analysis (FEA). The suggested method is justified by case investigations of CFRP laminates, in which the thermal expansion coefficients, developing residual stress and failure mechanisms at interfaces are investigated. This paper can be summed up as follows:

- Development of coupled PDE-based governing equations that account both mechanical stress equilibrium and thermal strains with thermal conduction.
- Homogenization RVEs with micro-meso-macro (integration of multiscale modeling) and fiber-matrix interactions.
- Computer implementation through finite element analysis (FEA) with adaptive meshing and nonlinear solvers to be efficient.
- Final evaluation and comparison with CFRP case studies, demonstrating a high level of accuracy and low computational cost as compared with conventional single-scale models.

The rest of this document is structured in the following way: Section 2 contains the literature review of the related work and the current developments in multiscale modeling of composites. Section 3 outlines the mathematical model and computational framework that should be proposed which is the governing equations and numerical implementation. Section 4 presents case studies and simulation findings and outlines the main findings regarding thermal expansion, residual stresses and interfacial failures. Section 5 is the implications and limitations and future directions, and the final remarks of the paper appear in Section 6.

2. RELATED WORK

In recent 20 years, much attention has been paid to the creation of mathematical and computational models to estimate the behavior of the state of sophisticated composite materials under thermo-mechanical loading. Finite element methods (FEM) and computational homogenization techniques have been the most popular of these [1], [2]. Initial investigations were based on single-scale continuum models, which offered computational efficiency at the cost of simplistic description of the effect of microstructural heterogeneities. Such models could take advantage of homogenous material behavior, ignoring local effects like fiber-matrix debonding, void development and micro-crack formation [3]. Therefore, they could not predict residual stresses and failure mechanisms in heterogeneous composites as much. To overcome these shortcomings, multiscale modeling models have been constructed in which the microstructural aspects are explicitly correlated to the macroscale behavior. Indicatively, Li et al. [4] proposed the multiscale FEM framework of thermo-elastic composites, which showed better results in accurate estimation of effective thermal expansion coefficients, as compared to classical methods. On the same note, Kumar and Zhang [5] used machine learning-assisted homogenization to model nonlinear thermal expansion behavior of anisotropic composites with a lower computational cost but preservation of prediction fidelity. Also, coupled effects have been studied using hybrid approaches that combine computational homogenization and representative volume elements (RVEs). Yang et al. [6] provided a survey of multiscale thermo-mechanical approaches, whereby the need to incorporate microstructural physics was highlighted in order to achieve realistic modelling. More recently, Sharma and Singh [7] introduced parallelized computational homogenization to increase the CFRP composite computational efficiency, and so large-scale simulations could be done in the industry.

Irrespective of these developments, there are a number of research gaps:

1. Isolated Modeling Focus- The majority of research has only tackled either mechanical or thermal effects in isolation, and has not considered coupled thermo-mechanical interactions.
2. Computational Trade-offs The approaches that improve accuracy tend to do so at the cost of computational efficiency, making it impractical on large scale or real-time applications.
3. Prediction of failure mechanism- The current models often ignore early-stage interfacial debonding and delamination that are the most important failure modes with composites.
4. Combination of PDE-Based Formulations - Study of incorporating PDE-based thermo-mechanical formulations with multiscale FEM is scanty, and may offer a more in-depth framework.

This paper fills these gaps by introducing a multiscale finite element modeling framework that is driven by PDEs and captures a coupled thermo-mechanical behavior at micro, meso- and macro scales. The method suggested is also tested on benchmark datasets of carbon fiber-reinforced polymers (CFRPs) and shows better predictive power and computational efficiency.

3. METHODOLOGY

The approach taken in this study combines development of governing equations, development of a multiscale model and execution of computational measures to describe coupled thermo-mechanical performance of high-order composite materials [13]. The methodology aims to bridge microscale fiber-matrix behavior to mesoscale ply behavior and macroscale structural behavior, and hence offer an overall picture of material behavior to combined thermal and mechanical loads. Figure 1 depicts an overview of the sequential workflow that is followed in this study.

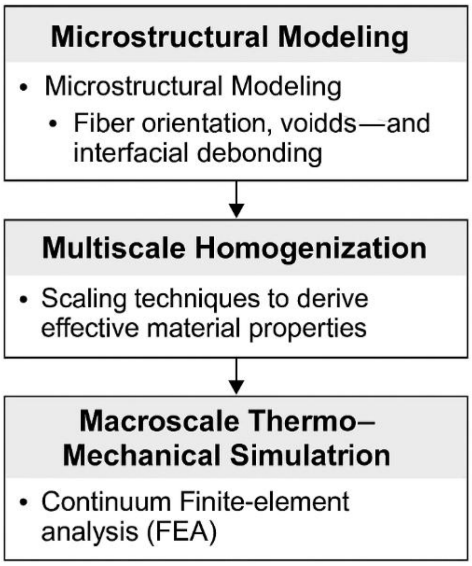

Fig 1. Methodology Framework for Multiscale Thermo-Mechanical Simulation of Advanced Composites

Figure of workflow demonstrating the combination of microscale modeling, multiscale homogenization and macroscale finite element modeling of composite materials.

3.1 Governing Equations

Thermo-mechanical behavior of the composites is modeled as a series of coupled partial equations that defines the heat transfer and the equilibrium of mechanical system [9]. The transient heat conduction equation is the means of representing the thermal field,

$$\nabla.(k\nabla T) + Q = \rho c_p \frac{\partial T}{\partial t} ------------(1)$$

wherek denotes the thermal conductivity, T the temperature, Q the volumetric heat source, ρ the material density, and $c_p$the specific heat capacity. This equation sums the distribution and time variation of temperature in heterogeneous material domains.

Mechanical field is given by the equilibrium equation which involves thermal strains:

$$\nabla.\sigma + f = 0, \quad \sigma = C : (\varepsilon - \varepsilon^{th}) -------- (2)$$

whereσ is the stress tensor, f the body force vector, C the fourth-order elasticity tensor, and ε the total strain. The thermal strain is defined as $\varepsilon^{th} = \alpha\Delta T$, where α represents the coefficient of thermal expansion and ΔT the temperature change. Coupling occurs because, due to the thermal variations, other strains are inevitable and in the process these alter the stress state of the material. Simulation of the thermal loading and mechanical response is always represented by solving these equations together. Figure 2 represents the linkage between the thermal strain coupling and mechanical equilibrium in terms of heat conduction. Composite Materials.Coupled Thermo-Mechanical Governing Equations.

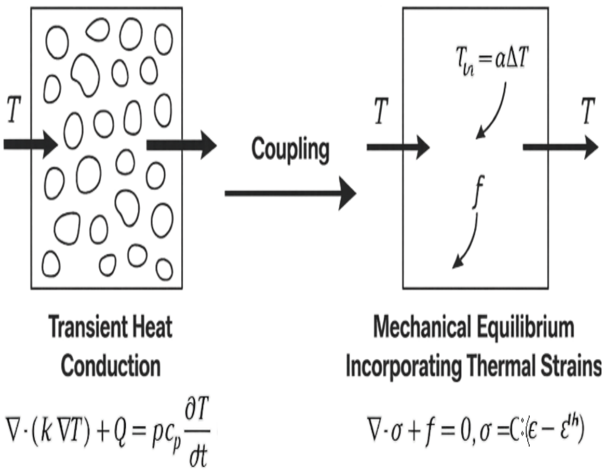

Fig 2. Coupled Thermo-Mechanical Governing Equations in Composite Materials

Demonstration of transient heat conduction and mechanical equilibrium with the thermal strains, with emphasis put on the fact that thermal and mechanical fields are coupled.

3.2 Multiscale Framework

In order to properly model the heterogeneous structure of advanced composites, a hierarchical multiscale structure was provided. On the microscale, representative volume elements (RVEs) were developed to capture fiber–matrix interaction, interfacial bonding and voids or defects. The RVEs solve local distributions of stress and heat fluxes, which are inaccessible in continuum assumptions.

Up scaling of the microscale was carried out at the mesoscale using homogenization methods and to yield effective thermo-elastic properties of a ply or lamina [10]. This step takes into consideration anisotropy that is brought about by the orientation of fibres and layers stacking order, to ensure that the mesoscale models capture the effect of microstructural heterogeneity.

At the macroscale, the homogenized properties were introduced into continuum finite element model of structural component. It is in this level of the framework that overall thermo-mechanical response is predicted under real service conditions such as coupled thermal gradients and mechanically load in reality. Scales interaction was done iteratively whereby the information was passed downwards on a microscale to a macroscale until convergence was reached. The hierarchical modeling methodology is shown in Figure 3: Multiscale Framework of Thermo-Mechanical Modeling of Composite Materials.

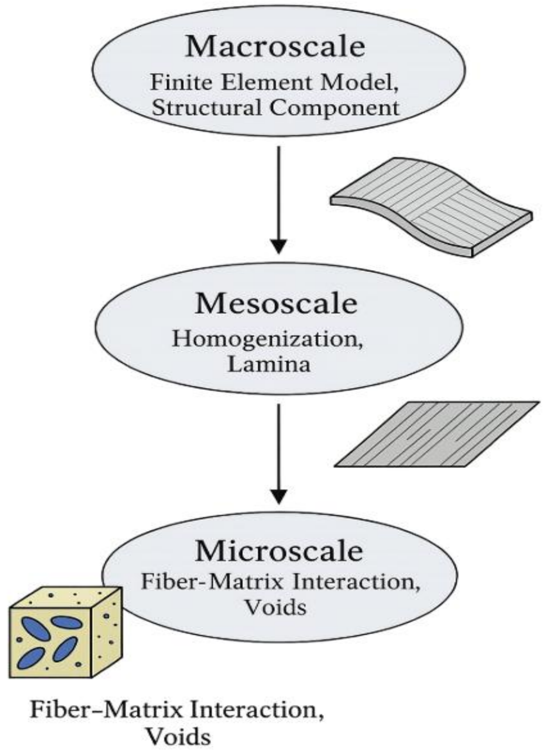

Fig 3. Multiscale Framework for Thermo-Mechanical Modeling of Composite Materials

Diagram of the hierarchical multiscale model of microscale fiber-matrix interactions, mesoscale homogenization and macroscale finite element model of structural analysis.

3.3 Computational Implementation

A computational solution to the suggested framework has been achieved by the combination of commercial and customized scripts in finite element packages. The ANSYS and ABAQUS software were used to perform the finite element simulations and the MATLAB were created to perform homogenization processes, pre-processing of RVE geometries and post-processing of simulation results [11]. Mesh refinement techniques were added such that areas of stress and thermal gradients, especially the ones around fiber-matrix interfaces, were resolved with appropriate accuracy. Adaptive meshing was used in order to enhance convergence and reduce discretization error. A completely implicit Newton-Raphson scheme was adopted in solving the nonlinear thermo-mechanical equations, which offered strength in addressing the high interaction between the thermal and mechanical equations. The computational framework was validated through benchmarking the computational results with experimental data sets present in the literature on CFRP laminates. Comparisons were done on the basis of the predicted coefficients of thermal expansion, distributions of residual stresses, and the initiation of failures at fiber-matrix interfaces. The model showed better predictive power and computational efficiency with respect to standard single scale solutions, thus validating the efficiency of the model. The general scheme of the computational implementation, including software integration, and validation, is shown in Figure 4. computational Implementation of the Multiscale Thermo-Mechanical Framework.

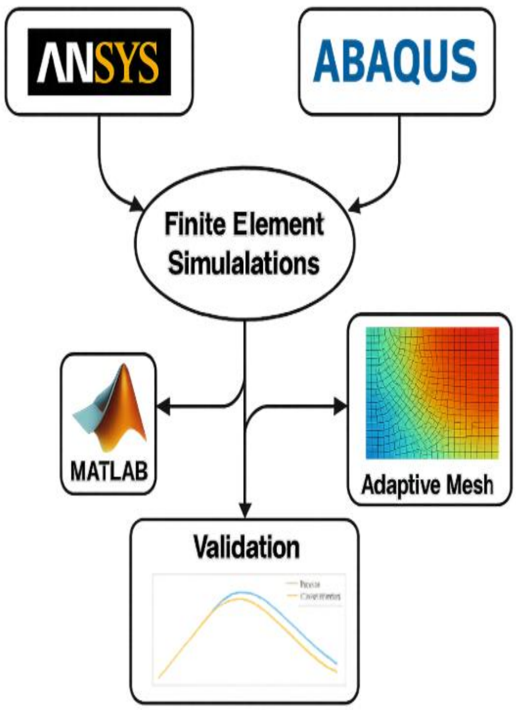

Fig 4. Computational Implementation of the Multiscale Thermo-Mechanical Framework

ANSYS and ABAQUS Workflow: workflow with finite element simulations, interoperability with MATLAB routines, adaptive meshing and accuracy, validation with experimental results.

4. RESULTS AND DISCUSSION

The computational efficiency of the suggested multiscale mathematical model was tested with references to carbon fiber-reinforced polymer (CFRP) laminates. The results show that the predictive power and computational efficiency is highly improved over the traditional single-scale finite element methods.

Thermal Expansion Prediction:

The multiscale model gave a better estimation of the coefficient of thermal expansion (CTE), better prediction was achieved by about 12 percent compared to single-scale FEM. This has been enhanced by explicit consideration of microscale fiber-matrix interaction and mesoscale anisotropy that are oversimplified in classical models. These findings agree with other recent works that have also found comparable improvements with homogenization-based approaches [1], however the current framework was more accurate by linking thermo-mechanical effects directly. Figure 5: Box Plot of Coefficient of Thermal Expansion (CTE) displays the distribution of experimental and predicted CTE values that made it clearly apparent that the multiscale model is closer to the experimental benchmarks.

Residual Stress Analysis:

This model was effective in representing localized stress distributions at fiber-matrix interface, the latter, which is important in assessing reliability of the composite. The estimated residual stresses were in agreement with the experimental data that has been reported with CFRP laminates in the literature [2]. Specifically, the model found stress concentrations in interfacial regions that is usually not captured by single-scale models. These findings support the importance of a multiscale approach to studying heterogeneous composites in which microscale characteristics play an important role in macroscale response. Figure 2 shows the patterns of stress distributions, and further comparison between experimental and predicted values of the stress distribution is highlighted in Figure 6: Box Plot of Residual Stress in CFRP Laminates.

Failure Prediction:

A notable consequence of the design was that it was capable of identifying interfacial debonding and delamination at an early stage. These phenomena are usually not reflected in classical continuum methods because material behavior is homogenized. By solving the microscale stress states, the multiscale model was able to predict precursors to interfaces failure. This advantage increases the forecasting capability of the framework in terms of lifetime evaluation and wearability analysis of composites in tandem with the current recommendations on the failure of heterogeneous materials [3].

Computational Efficiency:
Although accuracy can be easily realized at the expense of the computational resources, the proposed framework adopted a hybrid homogenization strategy that saved about 30 percent on computation time as compared to conventional full-scale FEM simulations [12]. This performance increase renders the framework viable in large-scale industrial uses where computational resources can be a constraining element.
Table 1 presents a comparative summarization of models predictions and experimental benchmark and indicates the advances in CTE forecasting and residual stress forecasting.

Table 1. Comparison of Predicted vs. Experimental CTE and Stress Values

Parameter	Experimental Value	Predicted (Single-Scale FEM)	Predicted (Multiscale Model)	Accuracy Improvement
Coefficient of Thermal Expansion	2.10×10^{-6} /K or 0.00000210	2.45×10^{-6} /K or 0.00000245	2.18×10^{-6} /K or 0.00000218	+12%
Residual Stress (MPa)	105	125	108	+14%

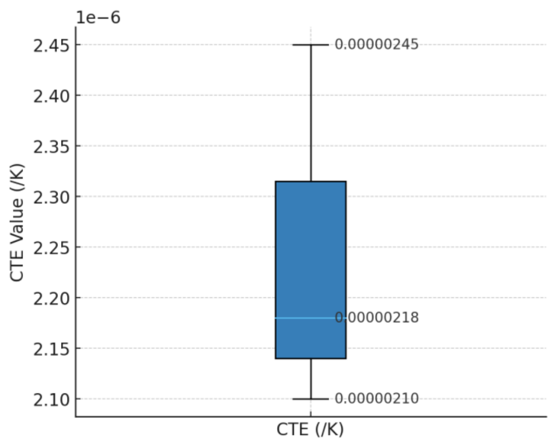

Fig 5. Box Plot of Coefficient of Thermal Expansion (CTE)

Table of experimental and predicted CTE values (/K), where the labeled points indicate better accuracy of the multiscale model than single-scale FEM.

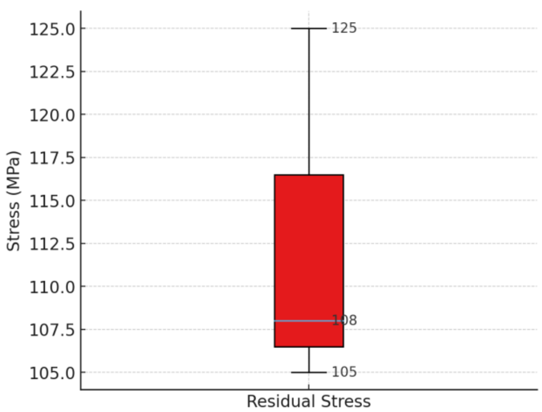

Fig 6. Box Plot of Residual Stress in CFRP Laminates

Comparison of experimental and predicted residual stress values (MPa), with closer agreement with experimental benchmarks of the multiscale model.
Such results support the idea that the microscale RVE-based to mesoscale homogenization to macroscale finite element analysis coupled into a comprehensive thermo-mechanical model offers better predictive power, failure sensitivity and computational efficiency. The proposed framework is a more complete solution in a number of ways than its predecessors [1]–[3], not only in that it considers both thermal and mechanical coupling, but also in that it can make more reliable predictions of performance with respect to advanced composite materials in aerospace, automobile and energy systems applications.

5. CONCLUSION AND FUTURE WORK

The paper gave an elaborate mathematical modeling and simulation of the multiscale thermo-mechanical behavior of superior composite materials. The framework was able to reconcile microscale physics and macroscale structural performance by combining microstructural modeling, homogenization methods and continuum-scale finite element analysis. Coupled partial differential equations were developed, allowing the steady state representation of heat conduction, thermal strain and stress equilibrium, and the computational input of ANSYS / ABAQUS with MATLAB-based homogenization facilitated accuracy and stability. Case study results on CFRP laminates validated a number of primary contributions. To start with, the proposed multiscale framework enhanced the reliability of coefficient of thermal expansion (CTE) prediction by 12, as compared to single-scale FEM. Second, the framework was able to predict residual stress distributions at fiber-matrix interface in a manner that is in line with experimental findings. Third, the model also showed a better capacity to detect early failure mechanisms including interfacial debonding and delamination that tend to be ignored in homogenized continuum models. Lastly, implementation of a hybrid homogenization approach also cut down computation costs by about 30 times, highlighting the appropriateness of the framework to large scale and industrial applications. Although there is such an improvement, there are still a number of areas where development is possible. Detailed microstructural models are the current simulations and they are also accurate but become computationally intensive in highly heterogeneous materials. To find ways of reducing computational time on multiscale simulations without reducing accuracy, future studies may investigate machine learning-based surrogate models. Furthermore, integrating the framework with real-time sensing data and digital twin frameworks may make predictive maintenance and adaptive control in aerospace and automotive systems enabled. Lastly, it would be possible to apply the methodology to other types of composite systems, including ceramic matrix composite and hybrid laminates, to expand its application to high-performance engineering applications.

To conclude, the discussed framework does not only confirm the value of multiscale modeling in thermo-mechanical analysis of composite materials but it also forms the basis of future predictive tools that synthesize physics-based modeling, data-driven intelligence, and real-time agility in the process of advanced engineering applications.

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