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AFRL-UNIVERSITY COLLABORATIVE CENTER IN STRUCTURAL SCIENCES

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14. ABSTRACT The 2013-2020 AFRL-University Collaborative Center in Structural Sciences (CCSS) is a four-university collaborative team from The Ohio State University, University of Illinois, Arizona State University, and Johns Hopkins University. The overarching goal of the CCSS was to collaborate with the AFRL/RQ Structural Sciences Center to provide methods and expertise to assess the state of a representative high-speed structural configuration. The CCSS was formatted such that there are three complementary research thrusts: a) Adaptive Multi-Scaling; b) Damage-Integrated Reduced-order Models; and c) Continuum Damage Models. Research projects within each thrust area were brought together through Integration Projects, and the methodology and results were transitioned to AFRL researchers. The CCSS enabled collaborative, multidisciplinary, DoD-relevant research for 17 PhD and Master's students, and 5 postdoctoral researchers.						
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1. INTRODUCTION

1.1.Motivation and Goal

The aerospace technical community - the U.S. Air Force in particular - is currently seeking advanced aerospace systems; the development of which is severely limited by uncertainties and knowledge gaps in structural analysis and life prediction, and where overcoming these challenges necessitates close interaction between multiple disciplines [1-5]. Of specific interest are vehicles and components subjected to combined, extreme environments, which leads to the coupled action of severe combined loading conditions. The design/development challenges originate from the tight interaction between dynamic fluid, thermal, and structural physics along with limited allowable conservatism in structural design so as to maintain mission responsiveness [1-3]. Relevant applications are any platforms with embedded engines and ultra-high-speed flight platforms.

Within this context, the goal of the 2013-2020 AFRL-University Collaborative Center in Structural Sciences (CCSS) was to provide methods and expertise to assess the state of a representative high-speed structural configuration.

1.2.Background and Technical Challenges

Historically, structural design and life forecasting has relied on a time-phased superposition of worst-case loads identified from discrete operating points on a trajectory. However, compliance of a structure combined with thermal and damage progression lead to *path-dependence* of the structural response and life over significant portions of a flight trajectory [2,3]. That is, the structural behavior depends on material properties that are functions of the evolving temperature field throughout a mission, and the accumulation of damage during both the mission and the life of the platform. Simultaneously, the fluid-based loads depend on the structural behavior through evolving surface displacements and temperature. Thus, the environment loadings (aerothermodynamic, thermal, acoustic, etc.) and the structure are mutually coupled, and dependent on the prior operational history of a platform. These complex and coupled features of the problem cast significant doubt on the ability of current practices to reliably define the true response and life of structures operating in extreme environments for extended periods of time [2,3]. Thus, as depicted in Figure 1.1, the successful development of advanced aerospace systems necessitates simultaneous consideration of nonlinear, multi-scale (in space and time) energy transfer between the physics associated with the environment, structure, and material. That is, one must consider the intrinsically coupled multi-scale, multi-physics by understanding and managing small-scale phenomena - e.g., transmission of fluid-loads through turbulent boundary layers, or micro-mechanical response of a structure involving plasticity and crack nucleation - that interact with responses over large spatial and temporal scales - e.g., response of a structural component/system over a generic trajectory and/or operational life.

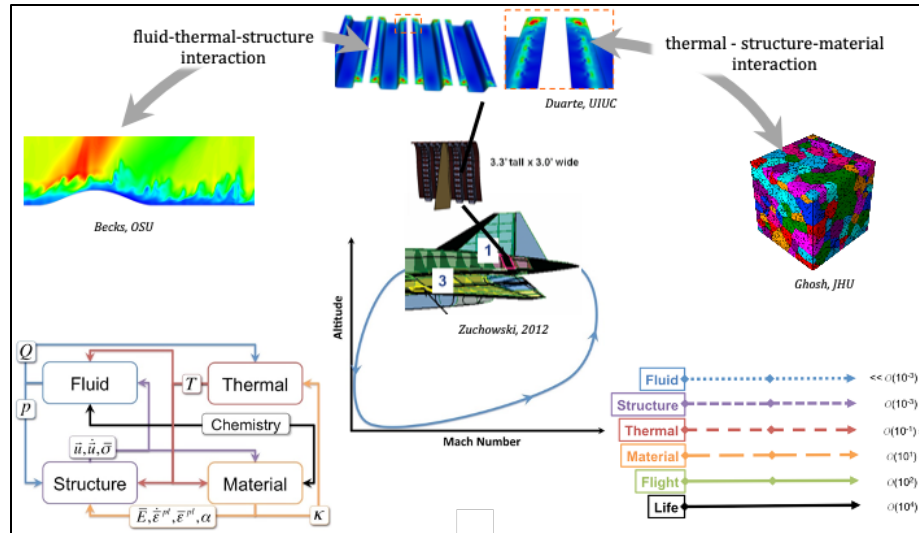


Figure 1.1: Complexity of Structural Response Prediction in Combined, Extreme Environments

As depicted in Figure 1.2, the status quo approach of progressing multi-physics simulation capabilities through either improved modeling fidelity with limited multi-discipline interactions or improved coupling fidelity using substandard models. However, in order to enable a *structural-scale “Digital-Twin” simulation framework*, both must advance synergistically through improved understanding of the structurally relevant physics and interactions, and development of numerical techniques capable of managing the multi-scale nature of the problem.

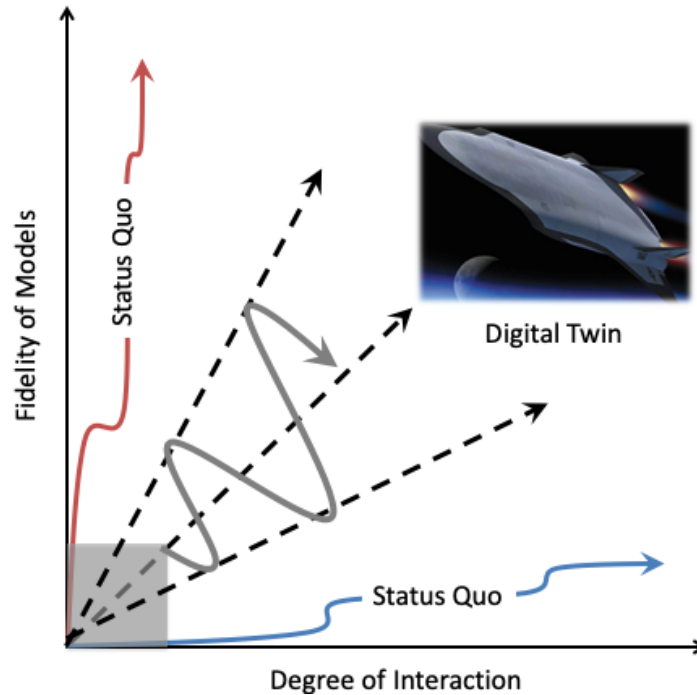


Figure 1.2: Required Paradigm Shift in Multi-physics Simulation of Combined Environment Structures

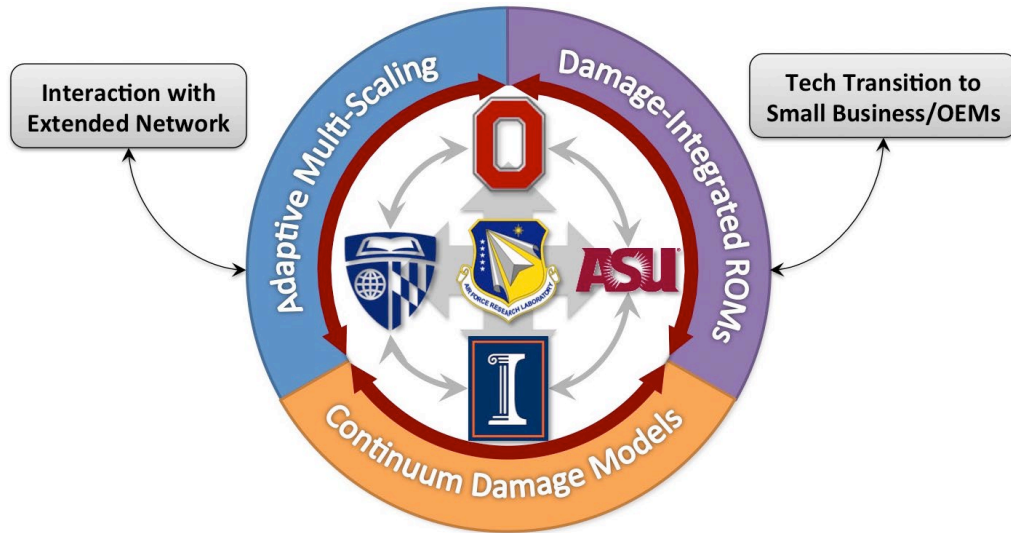
2. Overview of the Collaborative Center

The foundational vision of the CCSS was to engage in tight collaboration between the academic partners, the in-house AFRL/RQ Structural Sciences Center team. Engagement was also emphasized with the extended collaborative network that the AFRL/RQ Structural Sciences Center has established, as well as technology transition to small business/OEMs.

This started with a 3Day pre-kickoff technical interchange meeting between the academic partners and the in-house AFRL/RQ Structural Sciences Center; which lead to the joint establishment of the overarching goal stated above “**to provide methods and expertise to assess the state of a representative high-speed structural configuration**” and the identification of three core thrust areas:

1. adaptive, spatial and temporal, multi-scaling strategies for long duration path-dependent combined-environment structural simulation;
2. damage-integrated, structural-thermal reduced-order-models for realistic structural components;
3. continuum-level, constitutive and material damage evolution models.

Consistent with our objective of collaboration was immediate recognition that a *necessary* condition for significant advancement of the state-of-the-art in structural simulation in combined, extreme environments is *interlocked progression* within the three above thrust areas.



AFRL-University Collaborative Center in Structural Sciences
Capture the Physics | Expand Knowledge | Enable Discovery

Figure 2.1: AFRL-University Collaborative Center in Structural Sciences (CCSS)

2.1.Academic Team

Considering the technical needs and challenges highlighted above, the following individuals were selected to lead the academic contributions of each partner institution based on their subject matter expertise:

- **Jack McNamara**, The Ohio State University (OSU), Principal Investigator
 - Computational Methods for Fluid-Structural and Fluid-Thermal-Structural Interactions
 - Reduced Order Modeling
- **Armando Duarte**, University of Illinois Urbana-Champaign (UIUC), Co-Investigator
 - Computational Mechanics and Methods
 - Generalized Finite Element Method for Multiscale Multi-Physics Structural Analysis
 - Computational Fracture Mechanics
- **Marc Mignolet**, Arizona State University (ASU), Co-Investigator
 - Computational/Theoretical Structural Dynamics
 - Uncertainty Quantification
 - Thermo-Structural Reduced Order Models
- **Somnath Ghosh**, Johns Hopkins University (JHU), Co-Investigator
 - Computational Mechanics of Materials
 - Multi-Scale Modeling of Mechanical Behavior/Failure of Materials
 - Structural-Material Interactions

A schematic of the technical focus areas of each academic partner to the collaborative center and contributions toward the stated goal of coupled structural state prediction of representative high-speed structural components is shown in Figure 2.2. Ohio State focused on the advancement of relevant fluid models and co-simulation of multi-physics; UIUC focused on efficient multi-scale thermo-structural analysis; ASU focused on nonlinear structural-thermal reduced order models (ROMs); and JHU focused on material constitutive behavior and damage evolution. A more detailed summary of these overall contributions is provided next for each academic partner.

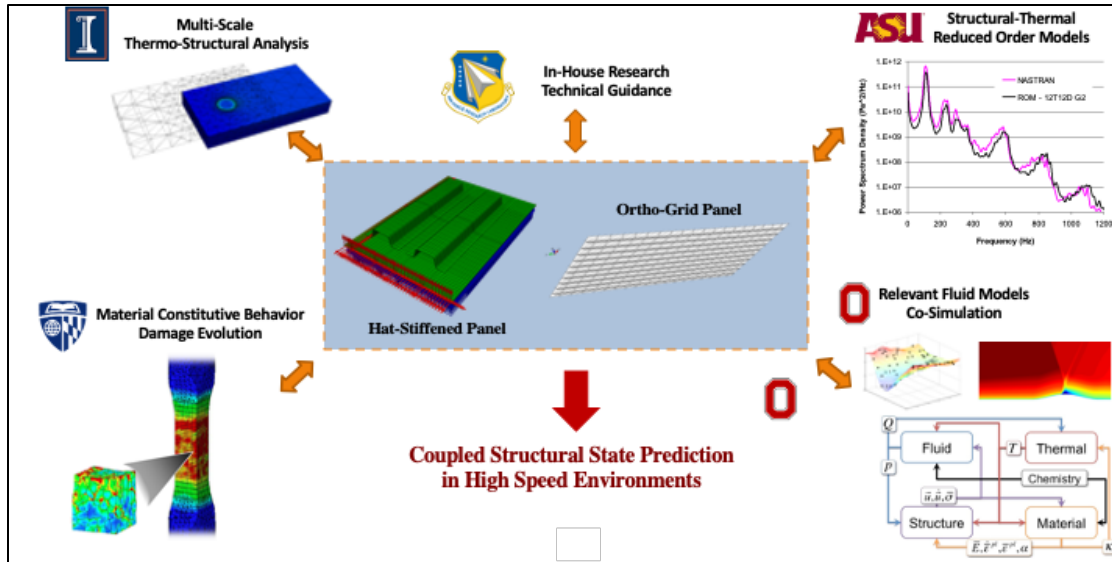


Figure 2.2: Schematic Depicting the Technical Focus Areas of Each Academic Partner Towards the Overall Goal of the CCSS

2.1.1. The Ohio State University (OSU)

As highlighted in the introduction and depicted in Figure 1.1, coupled interactions between the operational environment and the structure are an important consideration in the accurate response prediction. As depicted in Figure 2.3, addressing these issues requires co-simulation of numerical solvers for fluid-thermal-structural-material interactions and the ability to capture the pressure and heat loads induced by a highly complex flow environment. Challenges involve developing interfaces between different solvers for the fluid, thermal, structural, and material; efficient and accurate time-stepping algorithms for the disparate characteristic time scales of each field; and the identification and modeling of the relevant flow features for prediction of coupled loads.

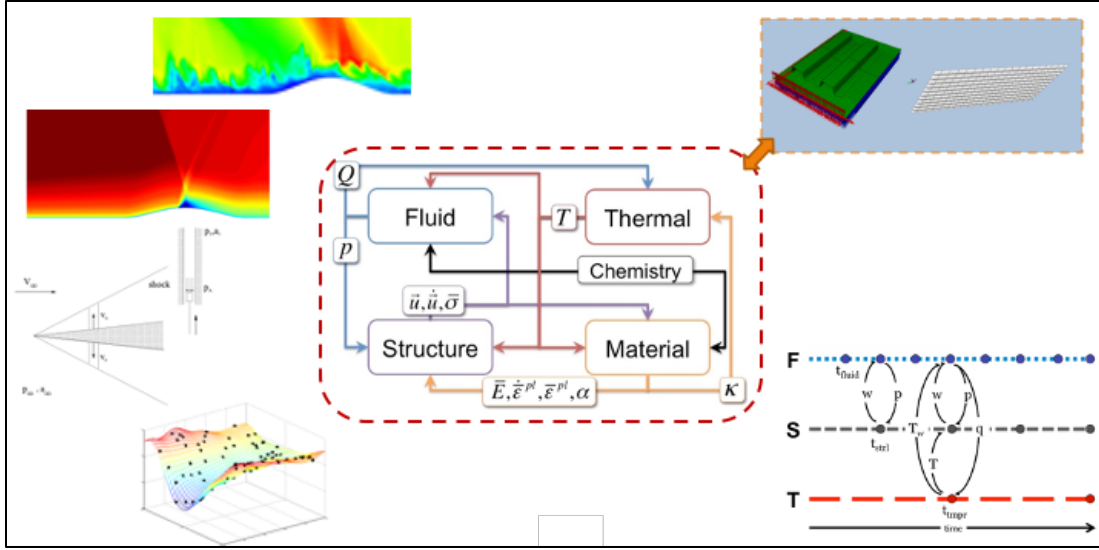


Figure 2.3: Technical Contributions to the CCSS by OSU for the Development of Relevant Fluid Models and Co-simulation Frameworks

2.1.2. University of Illinois, Urbana-Champaign (UIUC)

Successful design and development of reusable high-speed aircraft necessitates revolution in structural analysis capabilities. This is rooted by the need to simultaneously address the unavoidable requirement for optimal weight structural systems and the resulting extreme environment that such a structural system must repeatedly survive. Achievement of this requires consideration of multiscale and multi-physics aspects in the structural analysis, where there are strong two-way linkages between the structural-scale response, and non-linear, time-dependent localized responses around spot welds, fractures, sharp thermomechanical gradients, etc.

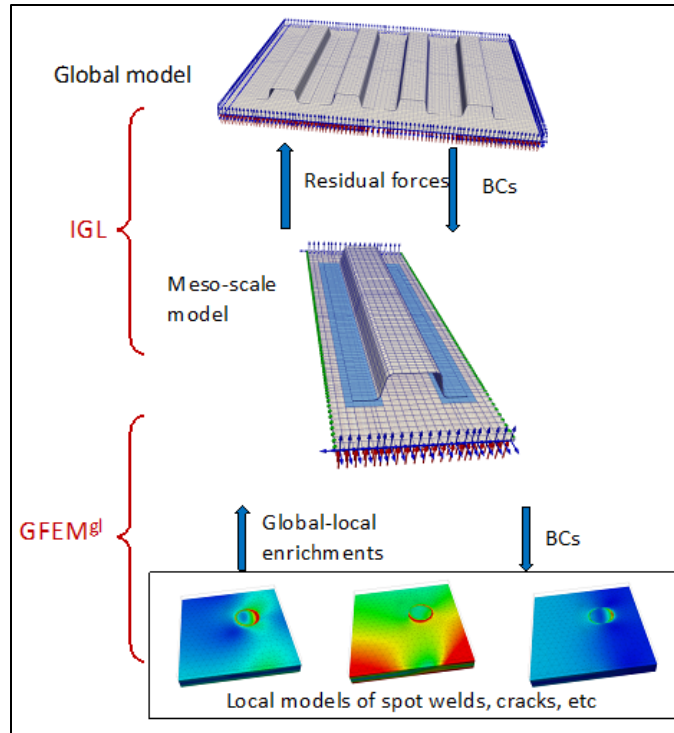


Figure 2.4: Technical Contributions to the CCSS by UIUC for the Development of Multiscale Multi-physics Structural Analysis Frameworks

2.1.3. Arizona State University (ASU)

Both accurate prediction strategies and computational efficiency are critical to enable the long duration, e.g., of the order of hours of real time, analyses that are required especially for fatigue/damage assessment. Structural-thermal ROMs have shown great potential to address the computational efficiency requirements. However, challenges exist to render these ROMs fully predictive, robust, and applicable to a broad set of configurations. These include the a priori selection of the basis functions – both structural and thermal; maintaining this basis small enough to ensure computational efficiency even as the structural complexity increases; and accurately identifying the ROM coefficients on which the accuracy of the prediction is dependent.

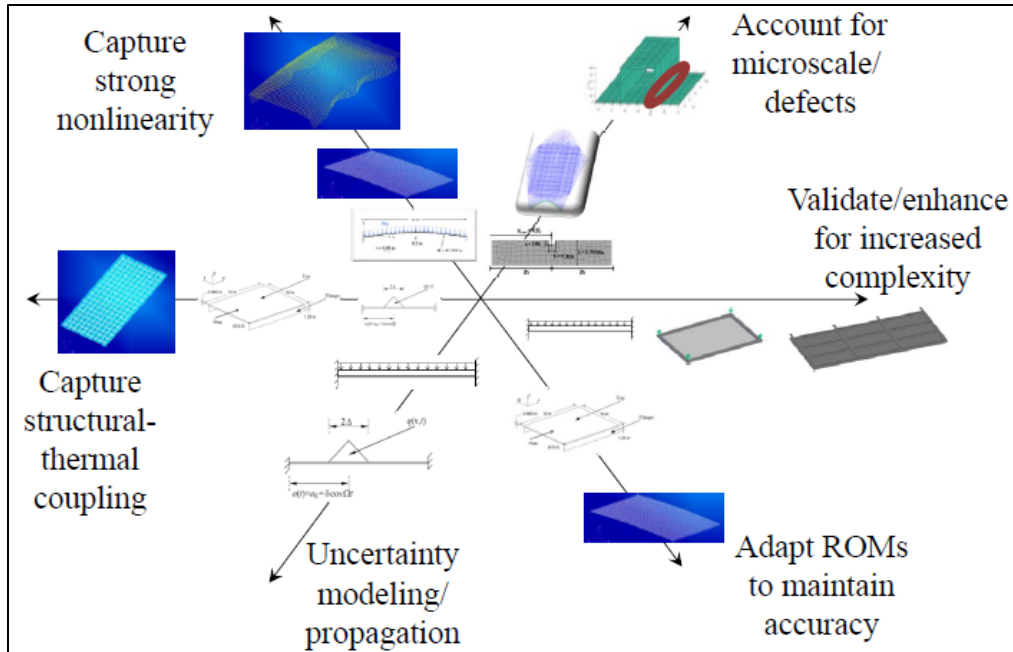


Figure 2.5: Technical Contributions to the CCSS by ASU: 6-dimensional Focus of Structural-Thermal ROM Research

2.1.4. Johns Hopkins University (JHU)

Physics-based material constitutive models are needed for high-fidelity structural analysis to accurately predict microstructure dependent response at the structural scale. Incorporating microstructural details in structural simulations entails a hierarchical multi-scale framework that uses a detailed micromechanical model to develop a reduced order constitutive model. Challenges in this task include identifying how the macroscopic response depends on microstructure, calibrating the relationship between continuum material properties and different microstructural features and incorporation of constitutive models in commercial codes for integration with structural analysis frameworks.

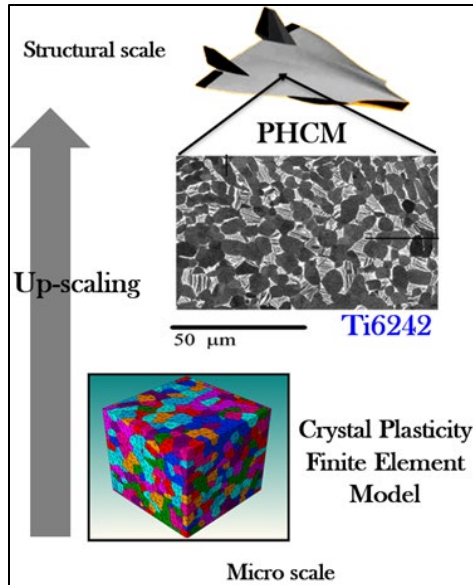


Figure 2.6: Technical Contributions to the CCSS by JHU for the Development of Microstructure Sensitive Material Constitutive and Crack Nucleation Models

2.2. Collaboration Strategy

As noted, multi-faceted collaboration between academic partners, in-house AFRL/RQ Structural Sciences Center Researchers, and the broader technical community were foundational to the CCSS. This was achieved through several aspects, including:

- cooperative planning and advising on projects between different sub-groups;
- regular scheduled and unscheduled Technical Interchange Meetings (TIMs);
- hosting three “Advances in Structural Sciences” conferences to showcase progress to stakeholders and an Executive Advisory Board;
- co-advising of students;
- summer research by students/faculty onsite at the AFRL/RQ Structural Sciences Center;
- capstone integration efforts

As noted above, upon the initiation of the CCSS in Spring of 2013, a 3Day “Pre-Kickoff” meeting was scheduled between the in-house AFRL/RQ Structural Sciences Center and the four academic co-investigators (McNamara, Duarte, Mignolet, and Ghosh). This brainstorming session focused on identifying:

- key knowledge gaps in the state-of-the-art for high-speed structural sciences;
- broad research thrusts that address the above knowledge gaps;
- the overarching center goal;
- sub-groups consisting of both academic co-investigators and AFRL/RQ Structural Sciences Center in-house researchers based on interest areas and subject matter expertise relevant to the knowledge gaps and research thrusts.

2.3. Specific Research Thrusts

As noted, one of the key outcomes of our initial pre-kickoff brainstorming session was the identification of three core research thrusts along with a plan for transition in order to reach our goal of advancing the methods and expertise to assess the state of a representative high-speed structural configuration. This is graphically depicted in Figure 2.8, where an important milestone was transition of accomplishments from the core research thrusts into integration efforts. The core research thrusts (A, B, and C) align along subject matter expertise (SME), while the integration research thrust (I) aggregates advancements within each into a more comprehensive framework.



Figure 2.8: Research Thrusts Identified in Order to Close Critical Knowledge Gaps and Enable Material-informed Structural State Evolution Prediction

Project proposals were cooperatively developed by both lead academic investigators and AFRL/RQ Structural Sciences Center researchers. The project proposals were then circulated amongst the broader team for feedback and refinement as needed, prior to discussion and evaluation by the Technical Steering Committee.

Each project proposal consisted of roughly two-pages of content containing the following information:

- Research Thrust Area
- University Lead and Co-investigators
- AFRL Co-Investigators
- Staffing requirement: Graduate Student or Post-Doc
- Why is this task important?
- What needs to be done?
- How is this related to other aspects of CCSS?
- References

An additional important aspect for success on integration projects was pre-planning for the primary staff person on the project to spend time at each of the different institutions involved. In both projects, the staff person spent onsite time at partner institutions in order to develop a familiarity with the tools being assimilated, and to develop the interfaces needed for implementation. A catalog of all projects, along with page location within this report, is provided in Table 2-1.

Table 2-1: Catalog of CCSS Projects

Category	Title	Page #
A: Adaptive Reduce Order Models		
A.1	Enhancements/Adaptation of Structural-Thermal ROMs	15
A.2	Enhancement and Refinement of CFD Surrogates	27
A.3	Nonlinear Reduced Order Modeling of a Hat-Stiffened Panel	37
A.4	Nonlinear Reduced Order Modeling of a Structure Exhibiting Strong Nonlinearity	45
A.5	Nonlinear Reduced Order Modeling of a Curved Shell under Combined Thermal and Mechanical Loads: Comparison with Experiments	59
B: Adaptive Multi-Scaling		
B.1	Linking Solid and Dimensionally Reduced Models	71
B.2	Linking Polycrystalline and 3D Solid Models	79
B.3	Spatial Multi-Scaling in Reduced Order Models (ROMs)	82
B.4	Temporal Multi-Scaling	93
B.5	Extraction of Stress Intensity Factors of Three-Dimensional Fractures in Anisotropic Materials	103
C: Adaptive Material Constitutive/Damage Modeling		
C.1	Micromechanical Deformation, Creep and Crack Nucleation Model Development	109
C.2	Continuum Level Homogenized Models for Deformation and Creep	118
I: Integration		
I.1	Generalized Finite Element Method Integration w/ CFD Surrogates and Continuum Damage Modeling	140
I.2	Response of a Built-up Structure to Localized Loadings	148

3. COLLABORATIVE CENTER PROJECT OVERVIEW AND RESULTS

This section highlights each project within the three core thrust areas:

- A: Adaptive ROM
- B: Adaptive Multi-Scaling
- C: Adaptive Material Constitutive/Damage Modeling

3.1.A: Adaptive ROMs

3.1.1. A.1: Enhancements/Adaptation of Structural-Thermal ROMs

CCSS Personnel: Yuting Wang (Ph.D. student), Raghavendra Murthy (postdoc), Marc Mignolet

AFRL Personnel: J.J. Hollkamp, R. Perez, S.M. Spottswood

Period of Activity: 1/2014-10/2017

ROMs have been introduced in the past for the prediction of the displacement field and temperature distributions of high-speed vehicles as accurate and computationally expedient alternatives to using full finite element model (FEM) approaches. Moreover, early validations of these concepts have been successful but have also pointed to three specific challenges that the present investigation addressed. The first one of these is the large number of basis functions and thus coefficients that are necessary in structures with relatively high modal density, such as stiffened panels. The second identified challenge was the systematic definition of a thermal basis that leads to a good capture of not only the temperature distribution but also of its effects on the structural response. The final challenge was the expedient determination of the ROM capacitance and conductance matrices as the temperature distribution changes when the specific heat and thermal conductivity depend on temperature. The first and third of the above issues affect the computational efficiency while the second one relates to the accuracy of the predictions. All three challenges were successfully addressed without modifying the core features of the ROM but rather complementing them with novel basis selection strategies and a capacitance/conductance matrices computation strategy.

This effort was sub-divided into three components that were identified as potential showstoppers in early ROM based efforts. These three components are:

A.1.1: Improvement of the structural ROM methodology for complex multi-bay structures;

A.1.2: Computationally efficient determination of the temperature field dependent thermal ROM conductance and capacitance matrices;

A.1.3: Definition of a rational thermal basis appropriate for the coupling with the structural ROM.

The background for these three separate efforts and the achievements made within the funded period are described in the ensuing sub-sections.

A.1.1. Improvement of the Structural ROM Methodology for Complex Multi-bay Structures

Motivation and Background:

One of the core challenges of structural ROMs is the large number of stiffness coefficients, and thus the computational efficiency of the method, when the basis becomes large. Indeed, the number of these stiffness coefficients increases as the fourth power of the number of modes, i.e., as $M^4/6$, where M is the number of structural modes. This observation has led to the consideration of sparse ROMs where only a limited number of coefficients are retained, e.g., see [6,7].

A well noted structural configuration that has a high density of modes, including modes with close frequencies, are stiffened panels owing to the partial decoupling that the stiffeners induced. For example, the 9-bay panel introduced in [8], see Figure 3.1, for which a large (85 modes) ROM was first developed in [9], has 50 natural frequencies in the band [0,350]Hz but a flat plate of the same dimensions and boundary conditions but without the stiffeners would have only 8 of them (see [10]). On this basis, and given the importance of stiffened panels in aircraft, a dedicated effort was focused on modifying the ROM methodology to lead to an effective decrease in the number of modes necessary and thus to an increase in computational efficiency.

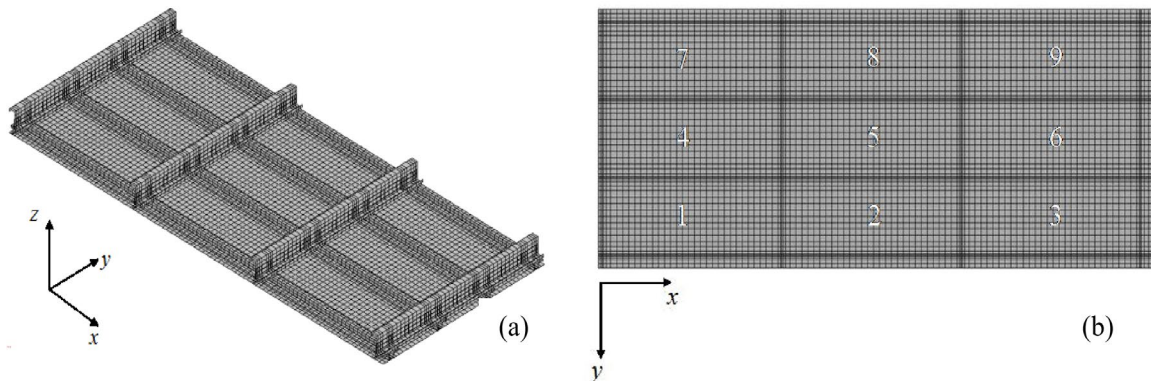


Figure 3.1: FEM of 9-bay Fuselage Sidewall Panel, (a) Isometric View, (b) Top View from [8]

Achievements:

The present effort led to the formulation of *component centric ROMs* which are ROMs that provide a good prediction of the response in a specified component of the stiffened structure, e.g., one of the bays in the 9-bay panel, but not of the entire structure. However, all components of the structure can be treated in this manner and thereby achieve the response prediction for the entire structure. By focusing only on a part of the structure, nonlinear component centric ROMs have a smaller number of modes, typically 40% less, and accordingly require a much smaller computational effort, around 10-15%, than a ROM predicting the response of the entire structure. This saving is maintained even if every component of the structure must be predicted because the component centric ROMs corresponding to different components can be run in parallel to each other as they are independent. It is important to note that component centric models did not exist in linear

vibration problems. Thus, the present effort has not only contributed to nonlinear ROMs development but also linear vibration theory.

Strategy:

The starting point of the formulation of component centric ROMs is the recognition that the modal response of a particular component is very similar for a series of modes of the entire structure but scaled differently as is demonstrated in Figure 3.2 for the 9-bay panel of Figure 3.1.

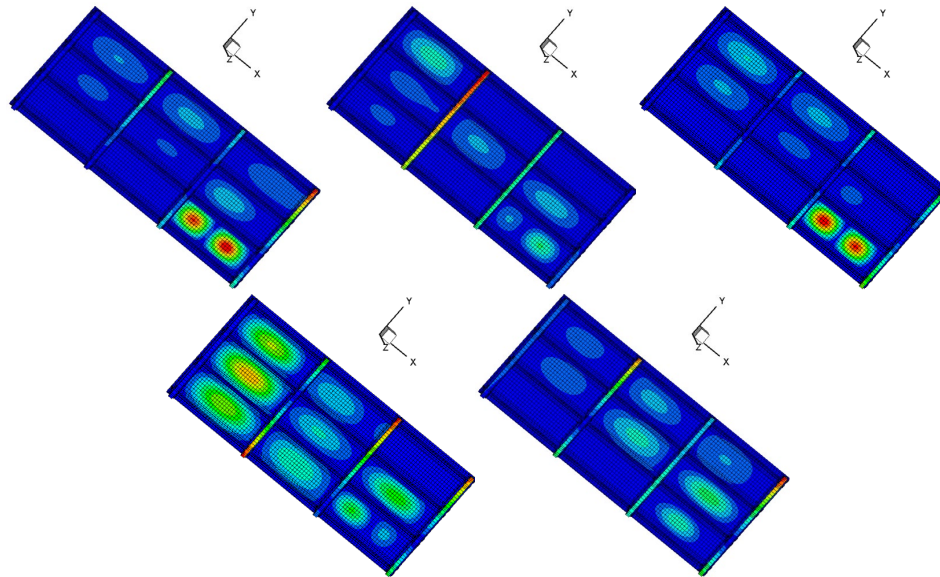


Figure 3.2: Contour Plots of the Norm of Displacements for Linear Modes 8-12 (in Order (a)-(e)) in the Band [127,136] Hz, Dark Blue/Red Zones Correspond to the Lowest/Highest Values

Moreover, note that the frequencies of these modes are close to each other, 127.48 Hz, 129.01 Hz, 130.43 Hz, 132.00 Hz, and 135.43 Hz. Then, the response of these 5 modes can be “lumped” together as if the 5 modes had identical frequencies. In that case, a rotation of these modes could then be carried out to have *only one mode* responding in the component of interest. Clearly, how these modes are lumped is different in different bays and thus lumping cannot be achieved for the entire structure. The reduction of the number of modes necessary for the component centric ROMs is due to the above lumping but also the elimination of certain modes that do not respond significantly in the component of interest.

In the context of linear structures, the above discussion is sufficient to produce component centric ROMs. For structures in the nonlinear regime, it is necessary to account in the component centric ROMs for the nonlinear coupling between any mode kept and the modes that are lumped onto it. This issue was resolved in [10] by a “closure” strategy, approximating the coupling terms by a single term involving only the generalized coordinates of the mode kept.

Results:

Shown in Figure 3.3 and Figure 3.4 are the power spectra of the transverse response of the center of bays 1 (in a corner) and 4 (along one side in the middle) induced by an acoustic excitation of OASPL equal to 144 dB that is uniform in space and varying in time as a bandlimited white noise excitation in the frequency range [0,350] Hz. It is clearly seen that the component centric ROMs (“ROM, modes lumped”) lead to predictions that are close to those of the 74-mode one which models the entire structure. Also shown on these figures are the predictions from ROMs in which the modes lumped in the previous ones are simply eliminated. That prediction is clearly worse than when the modes are lumped, even though the computational cost will be the same.

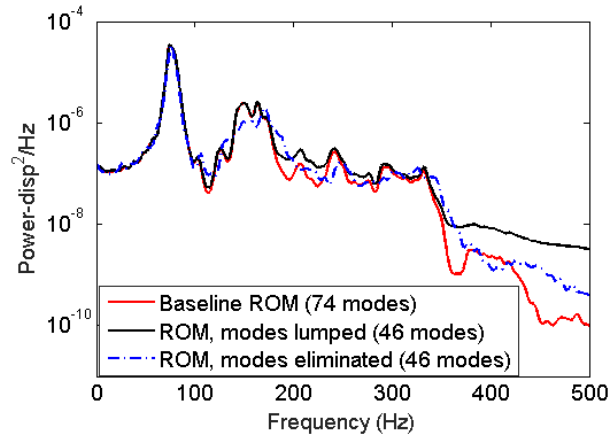


Figure 3.3: Power Spectral Density of the Transverse Response of Bay 1 Center

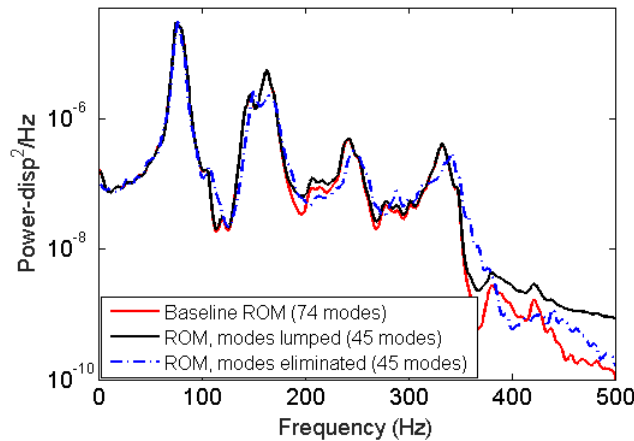


Figure 3.4: Power Spectral Density of the Transverse Response of Bay 4 Center

Additional results at different excitation levels and for all bays are presented in [10] together with a comprehensive discussion of a stiffened beam exhibiting similar features.

A.1.2. Computationally Efficient Determination of the Temperature Field Dependent Thermal ROM Conductance and Capacitance Matrices

Motivation and Background:

In the first formulation of coupled structural-thermal ROMs [11], it was assumed that the properties of the structure, i.e., elasticity tensor, coefficient of thermal expansion, specific heat, and conductance were independent of temperature. However, this is clearly not the case, especially not when the temperature increases are large as would be expected for high speed vehicles. The temperature independence approximation was however acceptable in that paper as the focus was on developing the coupling effect in the model.

A follow-on paper [12] extended the model to include linear variations with local temperature of the elasticity tensor and coefficient of thermal expansion, which represent good approximation of the physical behavior of most materials until they soften catastrophically. Including such variations was shown in [12] to lead to linear stiffness terms that are cubic with respect to the temperature generalized coordinates (vs. linear for temperature-independent properties). Moreover, the quadratic and cubic stiffness coefficients were found to be linear with respect to these thermal generalized coordinates (vs. constant for temperature independent properties). Thus, the consideration of the temperature dependence in the elasticity tensor and coefficient of thermal expansion leads to a significant increase in the number of coefficients to be identified.

In parallel with [12], it was also noted that the specific heat and thermal conductivity depend on temperature. Unfortunately, this dependence is often more/much more complex than linear, e.g., see Figure 3.5. While polynomial approximations of these functions would be appropriate, they would lead to conductance and capacitance matrices that are similar polynomials of the thermal generalized coordinates. So, if the conductivity is a monomial of degree p of the local temperature, then any of the components of the $\mu \times \mu$ ROM conductance matrix would be a homogenous polynomial of degree p of the μ thermal generalized coordinates τ_i , i.e., would contain order of μ^p terms. The entire conductance matrix would then include order of μ^{p+2} terms which would be very large for reasonable values of μ and p .

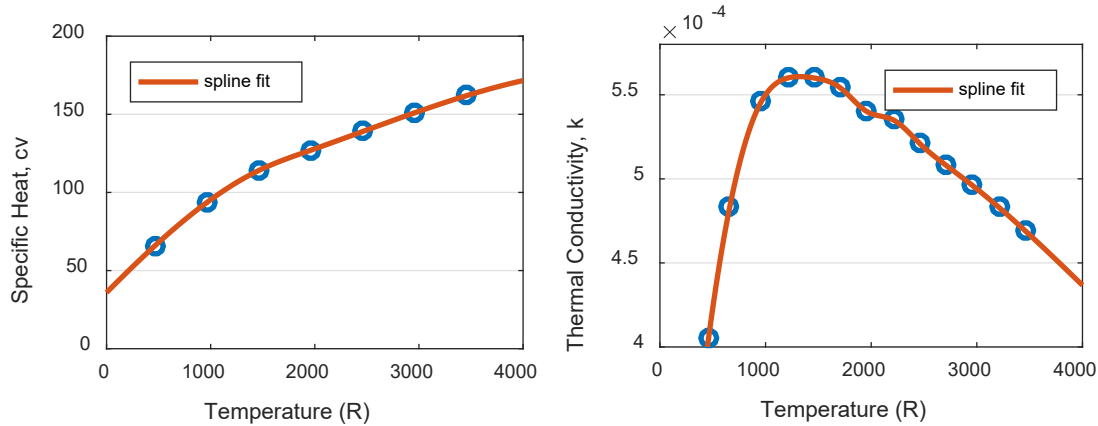


Figure 3.5: Temperature Dependence of Panel Thermal Properties, Specific Heat (left), and Thermal Conductivity (right) Including Spline Interpolant for Advanced Carbon-carbon 4

This issue was encountered in [13],[14] and was sidestepped by rebuilding at each time step the ROM capacitance and conductance matrices from the FEMl with the temperature distribution of that time step. This effort was possible in the problem considered there as all elements of the

thermal FEM were of identical dimensions and properties. In general, however, this approach is not acceptable. Recently, an approach was introduced [15] to model the capacitance and conductance matrices but the computational effort notably increases with increasing number of thermal modes.

Achievements:

An alternative approach was formulated to obtain a compact representation of the ROM conductance and capacitance matrices in terms of the thermal generalized coordinates. Moreover, this representation is applicable regardless of the form of the temperature dependence of the specific heat and thermal conductivity. This representation effectively removes the last hurdle in considering temperature dependent properties in the structural-thermal ROMs and enables an efficient computation of the temperature distribution.

Strategy:

The approach followed here is based on the expectation/assumption that high temperature distributions on a panel in high speed flight will be dominated by a constant temperature. That is, the temperature difference between two points on the panel in flight will be small in comparison to the average temperature rise of the panel in flight vs. at rest on the ground. Then, for clarity of presentation, it will be assumed that the uniform temperature is the first thermal basis function and T_0 will denote that temperature/generalized coordinate. Then, the elements of the conductance and capacitance matrices can be expressed primarily as a nonlinear function of T_0 in which the other thermal generalized coordinates τ_j will have a small effect. Accordingly, for each value of T_0 in the expected range of interest, a Taylor series expansion can be performed with respect to the τ_j to find the first order and, as necessary, the second order corrections of each of the capacitance and conductance matrices elements. Experience has shown that second order corrections are only necessary for a very limited number of generalized coordinates. Nevertheless, if all of them are taken, the number of parameters to evaluate for each capacitance or conductance matrix element is of the order of $n_0 \mu^2$ where n_0 denotes the number of selected values of T_0 used to discretize the temperature domain.

Results:

The above methodology was validated on the coupled structural-aerodynamic-thermal problem discussed in [13],[14], [16] and relevant to the panel shown in Figure 3.6.

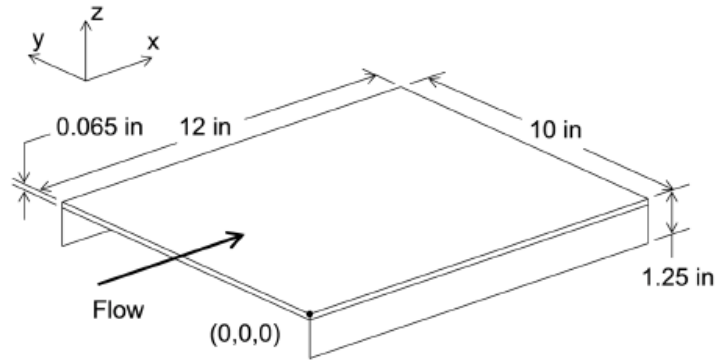


Figure 3.6: Representative Panel for Structural-aerodynamic-thermal Interaction [16]

Then, shown in Figure 3.7, are norm errors of the ROM capacitance and conductance matrices obtained by projection from the full FEM and by the above perturbation approach using the quadratic terms. Clearly, the approximation is excellent. Based on this matching, a fully coupled aero-thermal-structural simulation was run for the full trajectory of the panel using the perturbation scheme to compute the temperature-varying thermal properties during the simulation. The fully coupled structural response of the panel computed this way, see Figure 3.8, was found to match closely the one obtained by the methods from [13] with spline interpolation indicating that the perturbation scheme does indeed provide accurate modeling of the temperature-varying thermal properties for the propagation of the structural response through its coupling with the temperature field.

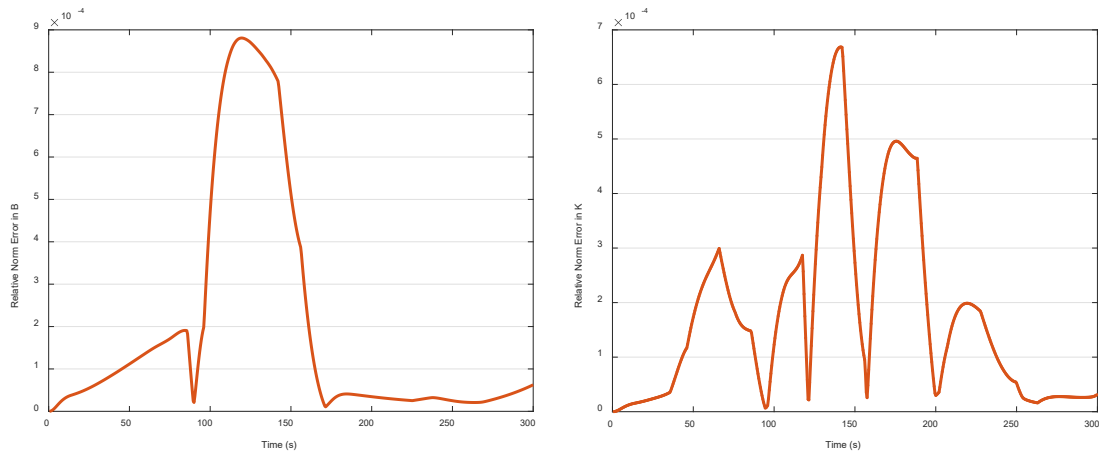


Figure 3.7: Relative Norm Error vs. Time for ROM Capacitance (left) and Conductance (right) Matrices Modeled Using the Perturbation Approach

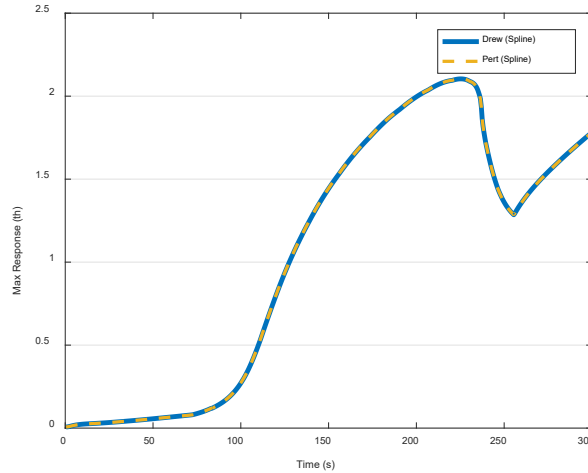


Figure 3.8: Evolution of Maximum Panel Deformation vs. Time – Baseline vs. Perturbation Solution Using Spline Interpolation for Thermal Conductivity and Specific Heat

A.1.3. Definition of a Rational Thermal Basis Appropriate for the Coupling with the Structural ROM

Motivation and Background:

Basis selection is a critical aspect of ROMs: if the basis is not appropriate to represent the solution, the prediction cannot be accurate. For the structural alone problem, this selection appears well in control, the selection of linear and dual modes appears to be appropriate for most problem (see discussion of project A4 for a counter example involving local buckling). For the thermal only problem, the situation is not as clear. The use of eigenvectors of the heat conduction as suggested in [11] provides a baseline set of modes but higher order eigenvectors may be closely spaced depending on boundary conditions (see [63] for discussion) and thus the convergence of the basis may be slow. This feature is in fact associated with the possible localization of the temperature in which case this field will be strongly dependent on the heat flux, not the geometry/material properties of the structure.

Accurate prediction of temperature is particularly important because of its strong effect on the structural response. This observation has led to the question of whether it is possible to define temperature distributions to which the structural response is particularly sensitive. These distributions, referred to below as optimum thermal modes, would be critical components of the thermal basis which would be included as a first set of thermal basis functions in any structural-thermal coupled problem.

Achievements:

Two sets of thermal basis functions that optimally affect the structural response were defined and determined from the structural ROM of the heated structure. These modes lead to a maximum of the coupling between the temperature and specified, i.e., dominant, structural modes. One set of modes is derived by considering the coupling through the thermal loading while the other maximizes the coupling terms in the linear stiffness matrix. It is found that these modes correspond

to the distributions of the linear and nonlinear stress induced in the structure when it deforms along the dominant structural modes considered.

The optimum thermal modes are not expected to represent a complete set of thermal basis functions as one can devise temperature distributions with little effect on the structural response. However, the effects of such distributions on the stresses as well as on the possible convection with the surrounding air is of importance. Recognizing that fact, a second set of thermal basis functions was introduced to capture these effects.

Strategy:

As discussed in [11], temperature affects a structural ROM through new terms arising in the linear stiffness matrix as well as a thermal loading term appearing on the right-hand-side, i.e., as an external excitation. Using the mathematical expressions for these terms derived in [11], it was first shown that the temperature field optimizing the thermal loading of a particular structural mode is in fact proportional to the stresses induced in the structure when it responds linearly in that mode. It is similarly found that the temperature field optimizing the thermally induced linear stiffness matrix element ij is proportional to the nonlinear stress induced when the structure deforms along a combination of the modes i and j . These temperature distributions are thus functions of the structural model only.

Note that these tentative temperature distributions will not in general satisfy the thermal boundary conditions, more specifically the Dirichlet ones (imposed temperatures), and thus are not acceptable as such. A second phase of the computation rectifies this issue and proceeds as follows. Using the finite element capacitance and conductance matrices of the structure without imposed boundary conditions, the fluxes that would give rise to these temperature distributions are determined. Then, these fluxes are reimposed on the structure with the correct boundary conditions and the resulting temperature distributions are obtained. These are referred to as enhanced stress distributions. Owing to the large number of these functions, which can be as many as the number of structural modes squared for those arising from the linear stiffness matrix, a proper orthogonal decomposition is next carried out and its leading eigenvectors are the desired optimal thermal modes.

The optimum thermal modes described above capture the temperature effects on the structure well. However, they do not completely capture the temperature distribution because they are solely focused on the coupling of the temperature field with the structural problem. Hence, thermal enrichment modes need to be added to the basis to complete the representation of the temperature field and more specifically capture the effects of the applied fluxes. If these are known or can be estimated, the corresponding temperature distribution can be used as a starting point to get the enrichments. Specifically, these enrichments would be constructed by carrying out a proper orthogonal decomposition (POD) on the residuals of projection on the optimum thermal modes of the temperature distributions. If the fluxes result from fully coupled structural-aerodynamic-thermal computations, it is proposed here to utilize the temperature distributions obtained from coupled fluid-thermal analyses conducted over a statically deformed panel, more specifically deformed along its dominant linear modes to reduce the computational effort.

Results:

The determination of the optimum thermal modes and enrichments was demonstrated on three structures: a heated beam, the panel in Figure 3.6, and the orthogrid panel shown in Figure 3.9. The panel was subjected to aero heating on its top (the flat skin) while radiation was imposed as a nonlinear boundary condition on the bottom (orthogrid side). No flux boundary conditions were imposed everywhere else.

To demonstrate the optimum thermal modes, consider the first structural linear mode which is shown in Figure 3.10. Then, the resulting original and enhanced linear and nonlinear stress distributions are shown in Figure 3.11. These computations were repeated here for all 58 modes of the structural basis. In practical applications, this process would only be accomplished for the dominant structural modes but it was of interest here to look at the comprehensive set. The large number of enhanced stress distribution was then reduced through 2 POD efforts, one for the linear stresses and another for the nonlinear ones. The first 12 and 10 eigenvectors of the linear and nonlinear stress POD problems, respectively, were retained for a first thermal basis of 22 modes, see Figure 3.12 for the corresponding eigenvalue plots.

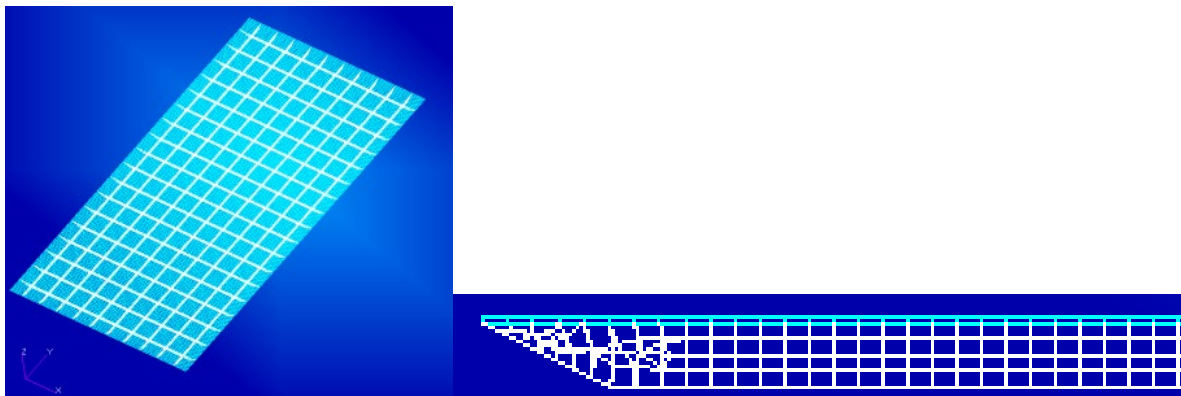


Figure 3.9: FEM of the Orthogrid Panel, Overall (left), Cross-section (right)

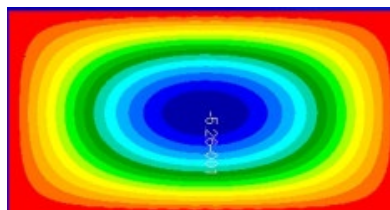


Figure 3.10: First Structural Linear Mode of the Orthogrid Panel

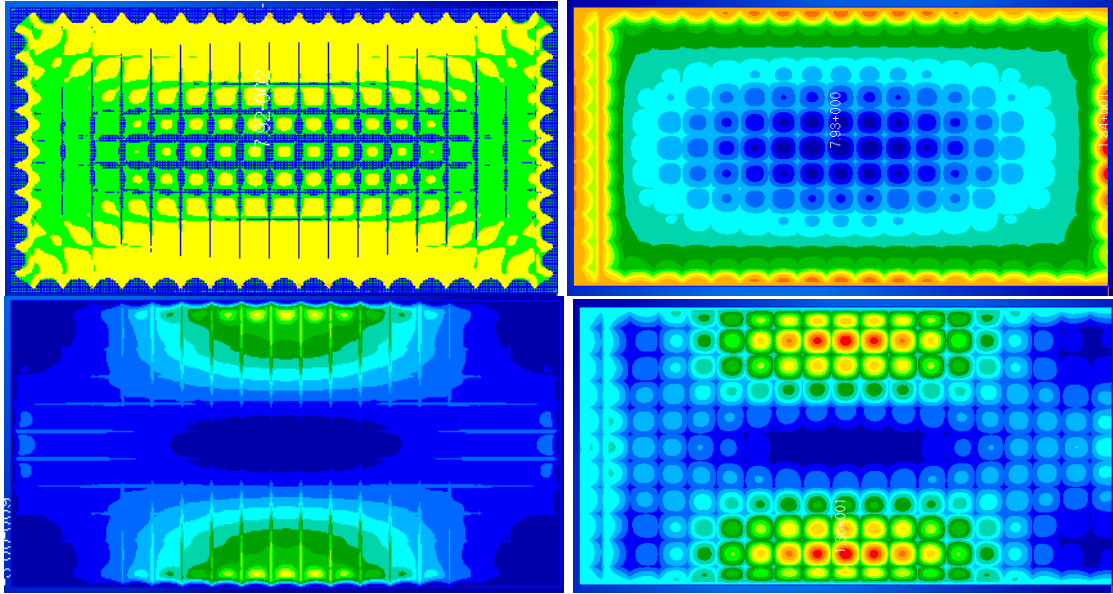


Figure 3.11: Original Linear (upper left) and Nonlinear (bottom left) Stress Distributions Corresponding to the First Mode with Enhanced Versions of Distributions (upper and bottom right, respectively)

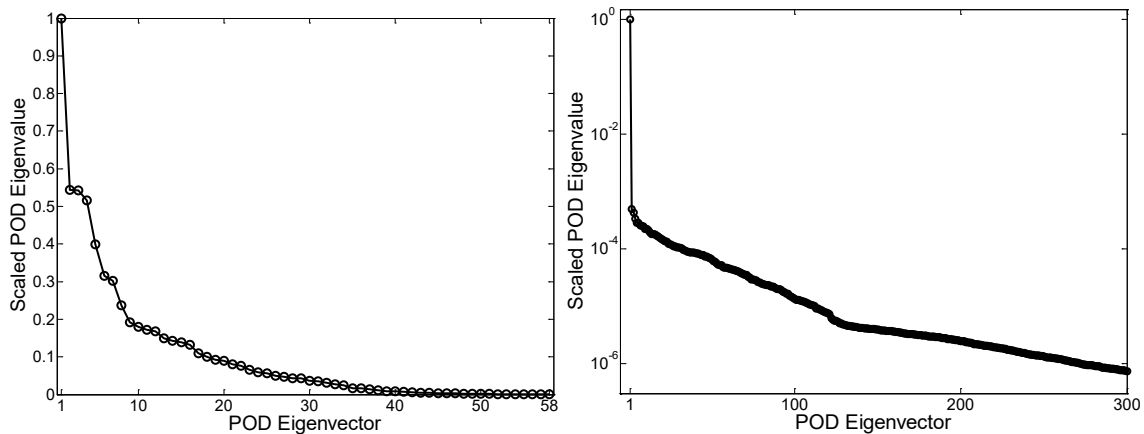


Figure 3.12: Eigenvalues of the POD of the Set of Linear (a) and Nonlinear (b) Enhanced Stress Distributions

Enrichments to the 22 optimum thermal modes were next sought based on an aerodynamic-thermal computations over the deformed panel. In these computations, the aerodynamic forces and aerodynamic heating were determined using piston theory and the Eckert reference enthalpy approach. Moreover, static displacements were imposed proportional to the first 8 linear modes and their combinations with peak displacements of 2 and 4 thickness both into and away from the flow. A total of 15 statically deformed panels were thus considered and the coupled aerodynamic-thermal analysis was carried out until a steady temperature distribution was reached. Each of the

resulting temperature distributions was then projected on the 22 optimum thermal modes and the uniform temperature distribution added as 23rd basic basis function.

The ensemble of 30 residuals from this projection effort was then treated by POD to extract enrichments needed to accurately capture them and, hopefully, the temperature distribution resulting from the fully coupled aerodynamic-structural-thermal analysis. Specifically, the first 9 POD eigenvectors were retained and added to the previous 23 thermal modes to form a 32-mode thermal basis.

The validation of this basis was achieved using results from the fully coupled structural-aerodynamic-thermal in static/steady conditions for a Mach 7 flow with 500 K, 800 K, and 900 K radiation temperatures. The structural and thermal problems were solved using the Nastran FEM and solution 153. The aerodynamic solver was as described earlier, i.e., piston theory and Eckert reference enthalpy approach. Then, the heat fluxes obtained in these full computations were imposed on the thermal ROM corresponding to the 32-mode basis and the resulting temperatures were compared to those from the full computations. This comparison is shown in Figure 3.13: the agreement between Nastran and the ROM is found to be excellent with norm errors for the 500 K radiation temperature case equal to 1.3% and for the 800 K radiation temperature case equal to 0.45%. An ensuing structural validation was also carried out in which the Nastran and ROM predicted temperatures were imposed on the structural FEM and an almost exact match of the displacements was obtained. These results fully support the construction of the thermal basis grounded in the optimum thermal modes.

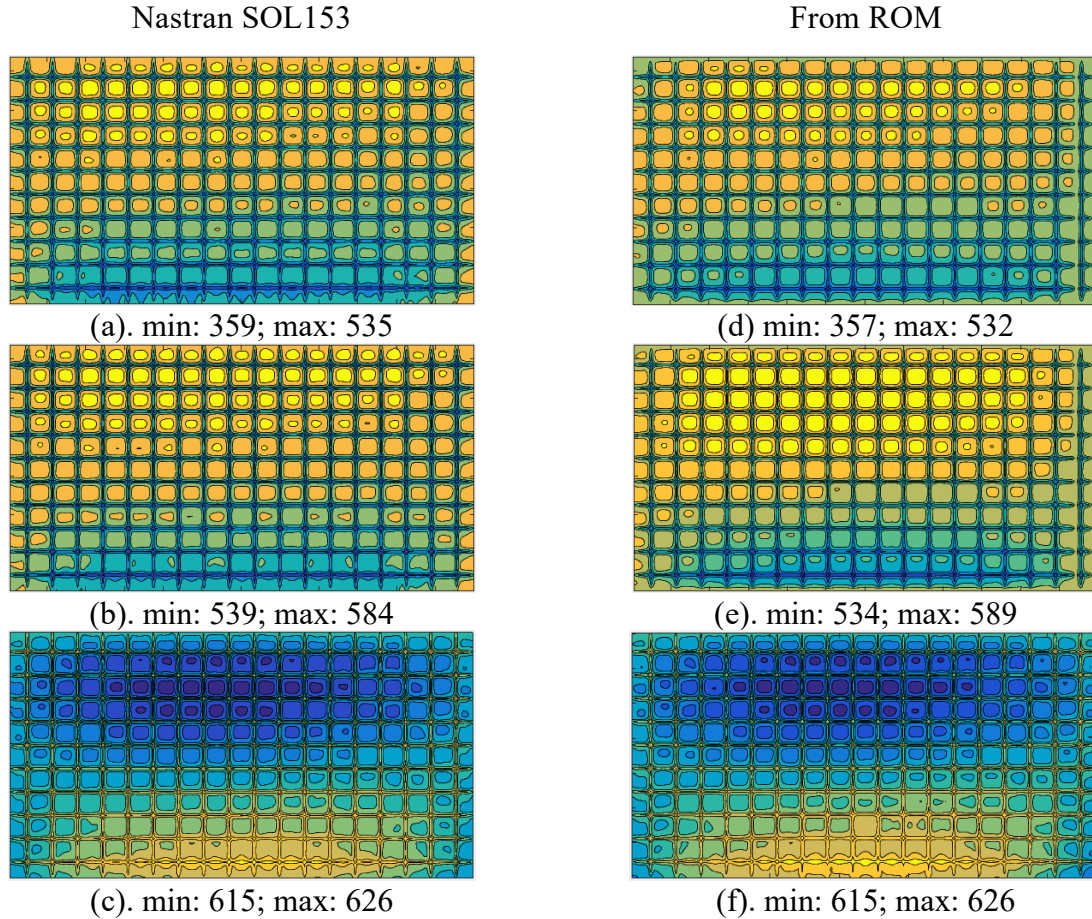


Figure 3.13: Steady-state Prediction of Nastran Thermal Solution SOL153 at (a) 500 K, (b) 800 K, and (c) 900 K vs. Steady-state Prediction of Thermal ROMs at (d) 500 K, (e) 800 K, and (f) 900 K

3.1.2. A.2: Enhancement and Refinement of CFD Surrogates

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Period of Activity: 7/2013 – 12/2019

Sufficiently accurate and expedient modeling of loads induced by the operational environment is critical for the development advanced high-speed platforms. However, the presence of complex flow physics, including strong inviscid-viscous interactions, impinging shock waves, and three-dimensionality pose a significant challenge to the fielding of such platforms. This only increases as the desire to minimize weight tends to increase structural compliance, resulting in the potential for path-dependent loading conditions and deformed configurations that evolve over long-durations. While computational fluid dynamics (CFD) provides high accuracy solutions, computational costs limit application for loads prediction online with the structural response analysis. In contrast, historical engineering-level approximations are efficient, but lack broad

accuracy. These issues have motivated the development of CFD surrogates that harness the predictive accuracy of high-fidelity models while retaining the computational efficiency needed for online predictions [30-32]. While a significant body of work has demonstrated the capabilities of the CFD surrogate method to bridge these gaps, open questions remain regarding the viability of the approach for shock-dominated environments and systems with high-order structural response. This project seeks to address these questions through the identification and development of required improvements. Specific tasks included characterizing the accuracy of the CFD surrogate method approach for aeroelastic loads prediction in the presence of shock impingements and the development of modeling strategies to account for arbitrary structural deformation.

Methodology:

A schematic of the different field problems and coupling mechanisms is shown in Figure 3.14. Note that the pressure (p) and heat flux (q) act as loads to the structural and thermal fields, while the surface displacement and velocity act as feedback mechanisms that alter the fluid response. CFD surrogate representations of the pressure and heat flux are shown in Figure 3.15 for the enhanced framework developed with this project.

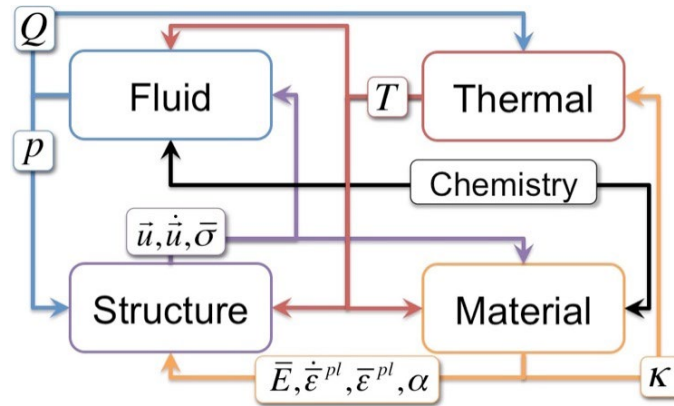
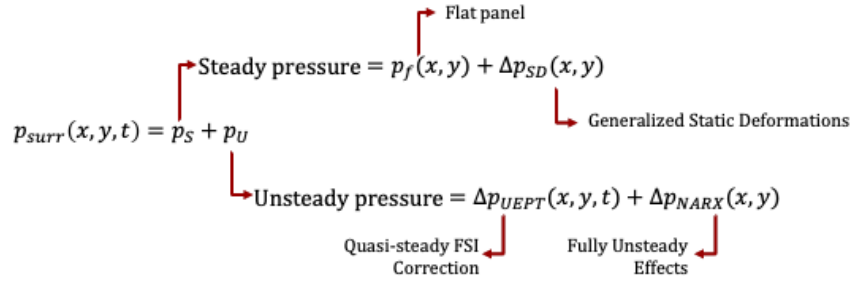


Figure 3.14: Field Problems and Corresponding Coupling Mechanisms to Enable Structural Response Prediction in Extreme Environments

Here the unsteady pressure is broken into two main components: a steady pressure component and an unsteady pressure component. The steady pressure component is composed of a data-driven model that computes the local pressure of the undeformed surface and a data-driven correction to capture deviations from the undeformed pressure due to static surface displacements. For the undeformed surface, spatial variations occur due to three-dimensionality, boundary layer displacement, shock impingements, etc. The unsteady pressure also has two components. The first is an “enriched piston theory” correction. This is based on a local piston theory representation, where the local flow quantities required for the piston theory model are extracted from the CFD surrogate over the undeformed surface. The purpose of this component is to capture perturbations to the surface pressure due to surface motion. For conditions where quasi-steady flow theory is valid, this term is all that is needed for an unsteady pressure model. However, in cases where quasi-steady flow theory breaks down the last correction is added to incorporate a Nonlinear Autoregressive network with exogenous inputs (NARX) model for full unsteady flow effects.

Pressure:



Heat flux:

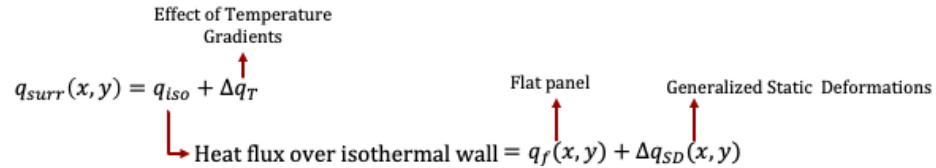


Figure 3.15: Enhanced CFD Surrogate Framework for Robust Online Prediction of Fluid Pressure and Heat Flux Loads Coupled to Thermo-structural Response

Similar to the pressure, the heat flux is also broken into sub-components. The first component is the heat flux model that predicts the heat flux based on pointwise surface temperature values. This component is constructed from CFD solutions with isothermal boundary conditions. This component is analogous to the steady pressure model and is similarly broken into two parts: 1) an undeformed model and 2) a model that corrects for static surface displacements. Note that because this model only incorporates pointwise surface temperature, a correction is needed to capture surface temperature gradients [31].

Application: Shock-Induced Panel Flutter

An important step for transitioning CFD surrogate methods for broad use is demonstration of accuracy and robustness in complex loading conditions that cannot be captured using engineering level approximations. One such problem is the shock-induced panel flutter problem, which is schematically depicted in Figure 3.16. Shock-induced panel flutter is a relatively newly identified aeroelastic instability first identified by Visbal [33, 34] and subsequently studied in [35, 36]. The aeroelastic instability of the panel is known to be sensitive to impingement location, shock strength, cavity pressure, and relative panel stiffness to aerodynamic loading (non-dimensional dynamic pressure). Classical engineering models do not naturally capture the impinging shock wave, nor do they include features associated with the shock-boundary layer interaction.

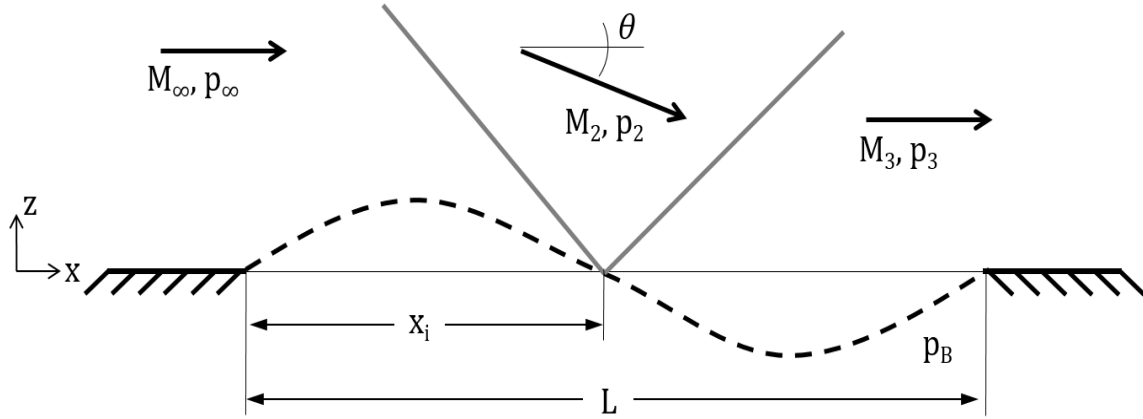


Figure 3.16: Schematic of a Skin Panel Response to Shock Impingement in 2D Flow [33]

Sample results are shown in Figure 3.17 for the non-dimensional panel displacement at the 75% chord location and the Strouhal number (non-dimensional frequency) as a function of non-dimensional dynamic pressure (λ). These results indicate that the CFD surrogate model accurately captures the flutter onset, both super-critical and sub-critical responses, and the frequency response for these shock strengths. This indicates that the model captures both the relevant physics and coupling mechanisms for this problem. Furthermore, the CFD surrogate model represents a significant computational speed up compared to the actual CFD, in this case the surrogate model required 6 minutes of computational time to compute the aeroelastic response on one processor compared to 17 days for the CFD model using 55 processors.

These results demonstrate the powerful capabilities of CFD surrogate models. However, a critical consideration when using reduced models is in the identification of limits of applicability. The results in Figure 3.17 are generated using only the enriched piston model to capture unsteady fluid-structural coupling. A detailed study on this was carried out for this project in the context of shock boundary layer interactions. In particular, the focus was on the introduction of shock-induced separation which was observed to break down the quasi-steady nature of the flow due to viscous dominated hysteresis with surface deformation and motion not captured by the inviscid piston model. This results in a phase shift in the generalized aerodynamic forces and inaccurate response predictions. Aeroelastic flutter responses for this latter case are shown in Figure 3.18. Here, increasing the shock strength increases the size of the separation bubble at the shock foot, breaking the ability of the enriched piston model to accurately model the generalized aerodynamic forces.

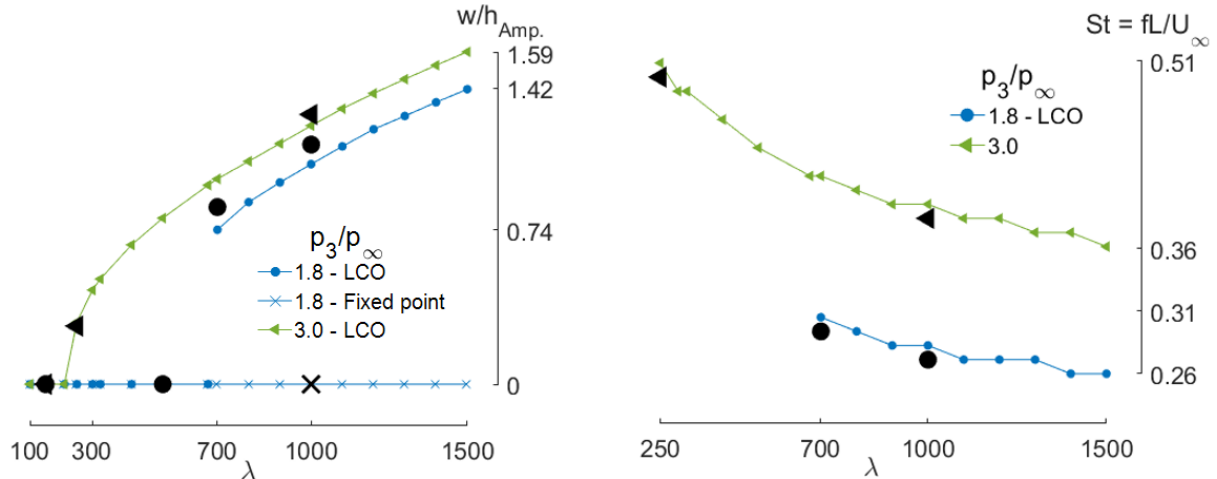


Figure 3.17: Variation in Non-dimensional Panel Displacement and Stouhal Number for Panel Subject to Different Strength Shock-impingements with Symbols Corresponding to CFD flow model & Lines Corresponding to CFD Surrogate

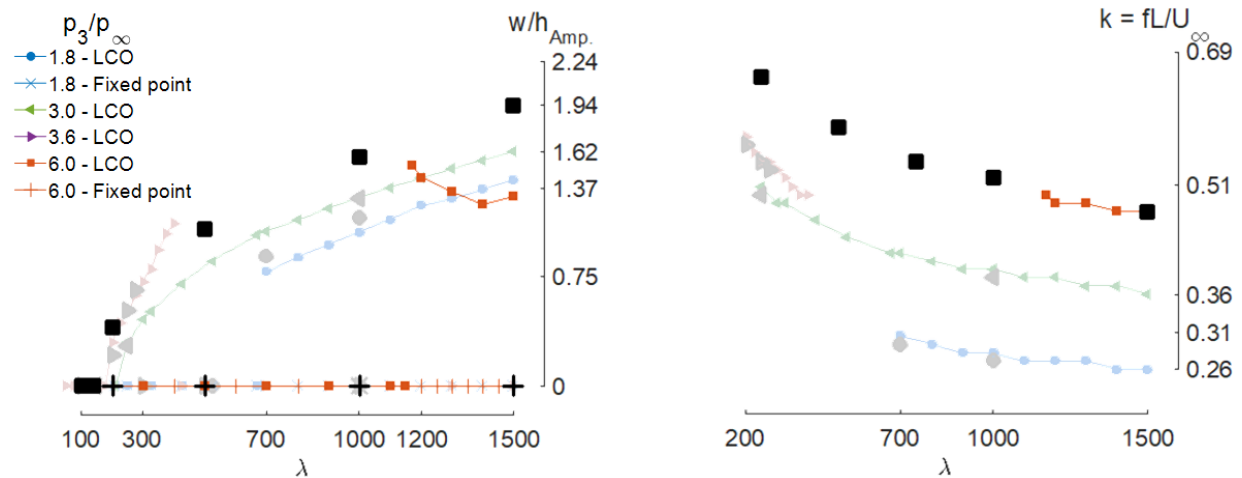


Figure 3.18: Variation in Non-dimensional Panel Displacement and Stouhal Number for Panel Subject to Different Strength Shock-impingements with Symbols Corresponding to CFD flow model & Lines Corresponding to CFD Surrogate

A detailed study into this behavior was undertaken in order to both understand the interaction of surface deformation with and develop a CFD surrogate model that can capture it. In the first part, surface deformation was propagated through the governing equations following work by Toubert and Sandham [37, 38]. This yielded the following proportionality that identifies the fundamental mechanisms by which surface displacements drive pressure gradients and separation [38]:

Definitions

- ε - Distance from LE to separation
- M_∞ - Freestream Mach number
- w'' - Curvature
- $\dot{w}'$ - Spatial gradient of velocity

$$LHS\left(\frac{\partial \varepsilon}{\partial t}, \varepsilon\right) \propto \frac{-1}{M_\infty} \left(w'' + \frac{\dot{w}'}{u_\infty} \right)$$

Here, the size of the separation bubble is proportional to the surface curvature and streamwise gradient of nondimensional surface velocity. This proportionality explains the phase shift introduced in the generalized aerodynamic loads due to phase shifts between velocity and displacement.

Additional study on this phenomenon identified separation length of roughly 4% of the panel length to correspond with the breakdown in quasi-steady flow theory. Below this value, quasi-steady flow theory was a sufficient approximation for accurate aeroelastic response prediction in the presence of shock impingements. Beyond this threshold, an additional correction is needed for stronger unsteady flow effects. This is shown in Figure 3.19 below, where there is a significant shift in the quantities shown beyond 4% separation length relative to panel length. As a point of reference, for the results shown in Figure 3.18, the separation length is 20% of the panel length for a shock ratio of 6.0.

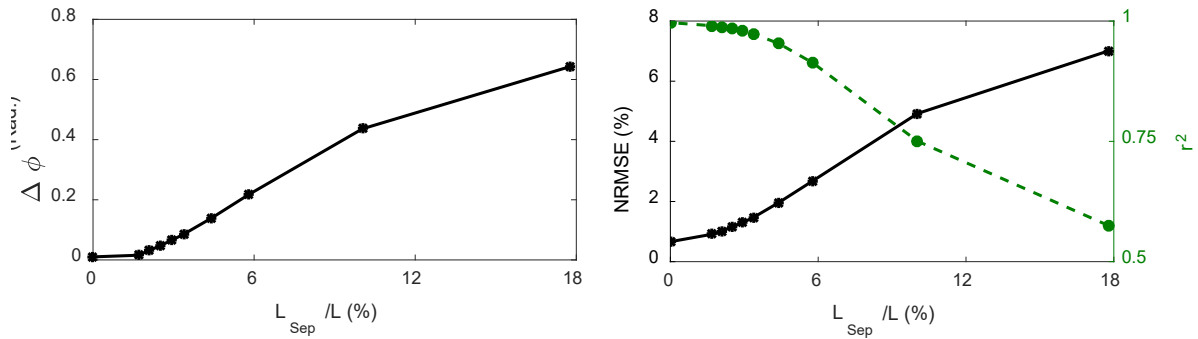


Figure 3.19: Phase Shift (left) and Error in Generalized Aerodynamic Forces (right) as Percent of Non-dimensional Shock Induced Separation Length

Updated results are shown in Figure 3.20 to correct for this behavior by adding a NARX model for strong unsteady flow effects introduced by the shock induced separation. While this correction requires additional training from using unsteady CFD solutions, the online cost is not measurably impacted.

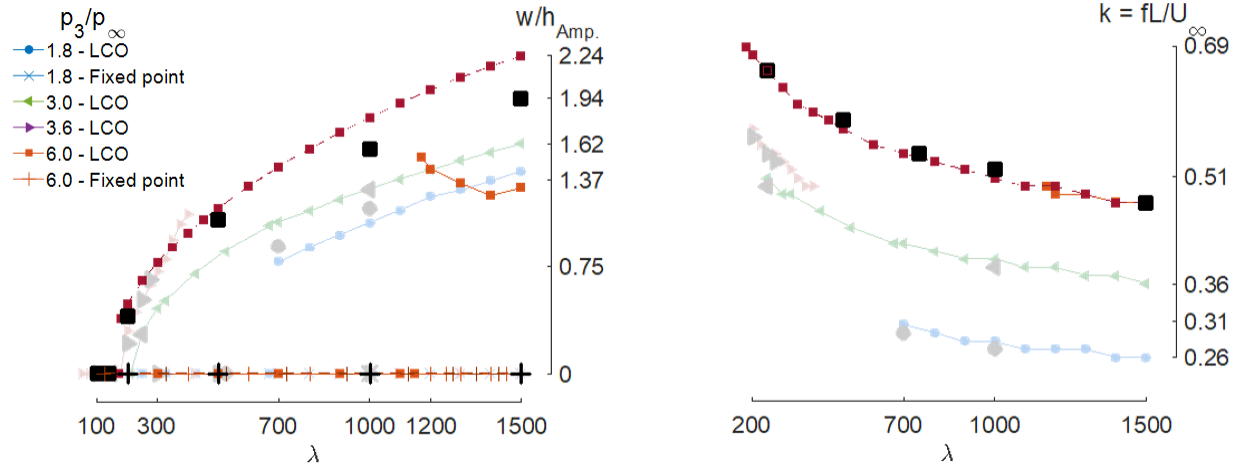


Figure 3.20: Updated Variation in Non-dimensional Panel Displacement and Stouhal Number for Panel Subject to Different Strength Shock-impingements with Symbols Corresponding to CFD flow model & Lines Corresponding to CFD Surrogate - Surrogate is Augmented with a Correction Using a NARX Model for Unsteady Effects Induced by Shock-induced Separation

Detailed discussion on this work is provided in Refs. [38] - [40].

Application: Aerothermoelastic Response of a Built-up Structural Panel with High-Order Deformation

As noted above, one of the challenges with CFD surrogates prior to this research project was robust and efficient handling of high-order surface deformation. Since CFD surrogates often have a data-driven element in order to facilitate online use of CFD data, there are inherent input-output models needed (e.g., kriging interpolants or neural networks). This requires identification of input parameters. The status quo approach is to parameterize structural deformation in terms of modal coordinates, with the assumption that a relatively few number of modes are dominant in the structural response. While this is generally true for simple structures, built-up structural systems can have a high number of modes within frequency bands relevant to the loads. While different types of modal decompositions are possible, these typically require a high degree of a priori knowledge of the expected structural response. Thus, this project sought to develop a more general set of input parameters to mitigate the need for a priori assumptions.

The first step in this process was to identify from the governing equations the dominant set of parameters. These were identified through study of viscous-inviscid interaction formulations, and yielded the following parameter sets:

$$\Delta p_{SD}(x, y) = p_s(x, y) - p_f(x, y) = F_1 \left[T_w, Z', p_f, \int_0^x p_f dx, \Delta p_{S,EPT}, \int_0^x \Delta p_{S,EPT} dx \right]$$

$$\Delta q_{SD}(x, y) = q_{iso}(x, y) - q_f(x, y) = F_2 \left[T_w, q_f, p_s, \int_0^x p_s dx \right]$$

where T_w is the wall temperature, Z' is the surface slope, p_f is the surface pressure on an undeformed plate, p_s is the pressure on a plate with static deformation, $\Delta p_{S,EPT}$ is the static pressure correction predicted using CFD enriched piston theory, and q_f is the surface heat flux on an undeformed surface. Also, the integral expressions are carried out streamwise and capture upstream effects, which are important when a boundary layer is present on the surface.

The next step was generating a set of CFD flow solutions to develop a data-driven model for the corrections above. An advantage in this case is that the training data is pointwise, where each flow solution generates a number of surface points to train on. See for example Figure 3.21, where 80 CFD solutions on a 201 x 201 surface mesh produces approximately 3 million training points. This large amount of data was leveraged by developing an adaptive sampling strategy to minimize the number of training points required to produce an accurate representation of surface deformation effects. This is schematically depicted in Figure 3.22. A significant advantage of selecting the above parameters and implementing the adaptive sampling strategy was an order of magnitude reduction in the offline costs of training the models.

Using this procedure, the method was tested on an orthogrid panel developed by the Boeing company [2,4] and shown in Figure 3.23. Structural dynamic analysis by the ASU group demonstrated that over 30 free vibration modes were within a 1 KHz frequency band, which is typically the cutoff used for dynamic loading. Furthermore, the use of POD on responses generated using broadband excitation up to 1 KHz required 15 modes for sufficient reconstruction of the displacement.

The newly developed approach was compared against several different approaches for fluid-thermal-structural analysis, listed in Table 3-1. The first row represents the industry standard for computing the fluid loads, where the pressure and heat flux are independent of deformation and a linearized model for fluid-thermal heat transfer is used. The second row uses basic engineering models for capturing the coupled pressure and heat flux loads. The last row represents the reference solution, carried out using RANS CFD coupled to the thermo-structural response for the pressure and heat flux loads. The remaining two rows are the CFD surrogate using the different approaches for incorporating static structural deformation: 1) modal coordinates of POD modes generated from response data to random loading of the panel; 2) ASD is the generalized model described above. The results from this study are shown in Figure 3.24 - Figure 3.26. The uncoupled model does the worst of all cases, missing many of the important gradients in the loads and response. The basic models do a reasonable job, albeit substantially over-predicting surface temperatures. The POD and ASD approaches are generally comparable in accuracy. However, the ASD approach requires fewer a priori assumptions to generate and also an order of magnitude less training data to construct the model. Comparing surface contours, the ASD approach is indistinguishable from the CFD generated response yet requires 4 orders of magnitude lower computational time. For complete details on this approach, refer to Ref [41].

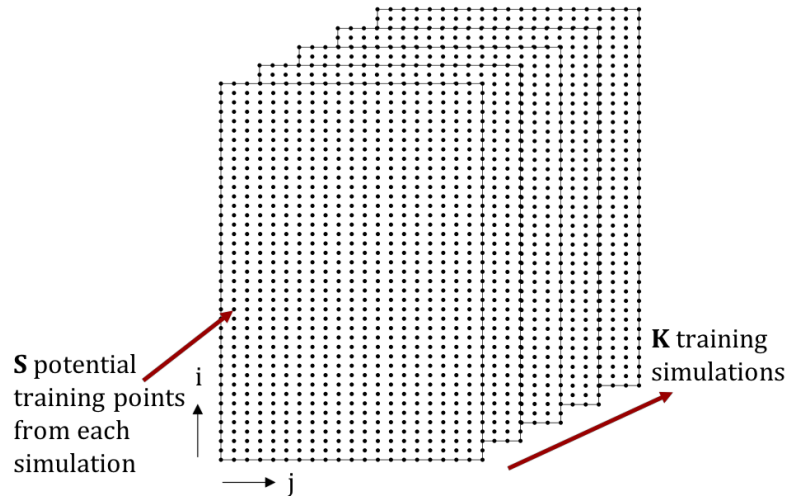


Figure 3.21: Depiction of Training Data Generated for Pointwise Models of Surface Data with Each Dot Representing a Potential Training Point

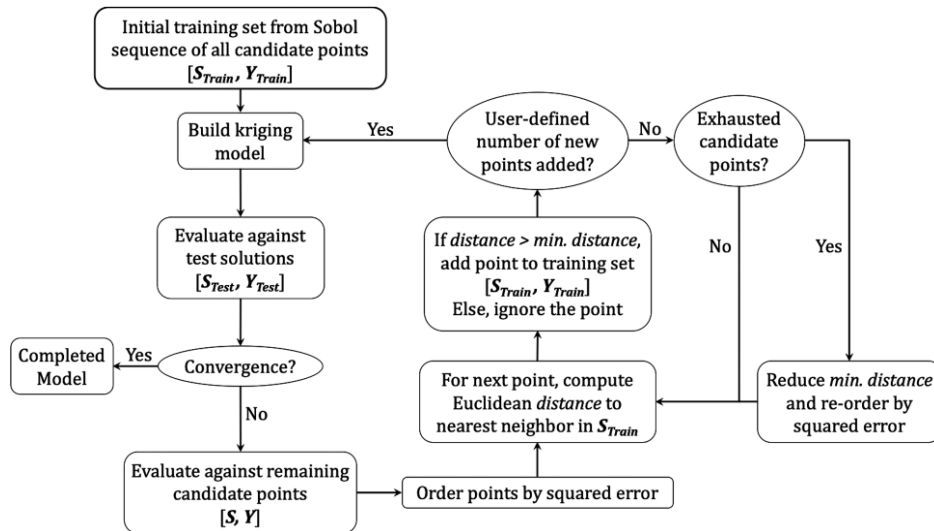


Figure 3.22: Adaptive Sampling Procedure for Minimizing the Number of Training Points

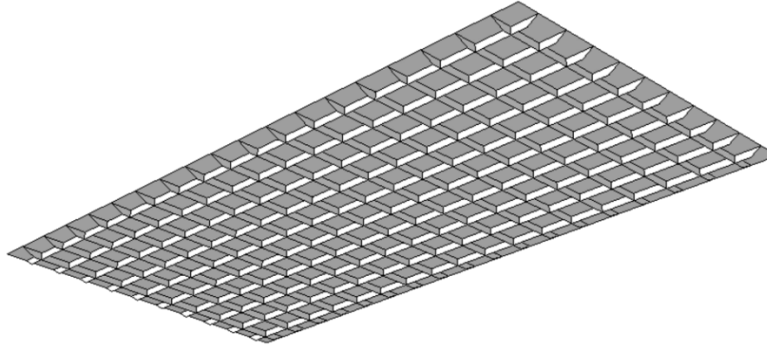


Figure 3.23: Orthogrid Panel Developed by the Boeing Company [2,4]

Table 3-1: Different Classes of Models Used for Fluid-thermal-structural Analysis of an Orthogrid Panel

Name	Pressure	Heat Flux
Uncoupled	RANS over flat panel	Fixed c_h and T_{aw} from RANS over flat panel
Approx.	Classical piston theory	Eckert's reference enthalpy
POD	Kriging interpolant based on POD modes (1200 training points)	
ASD	Flat panel + Kriging interpolant for arbitrary deformations (87 training points)	
RANS	RANS solution over static deformation	

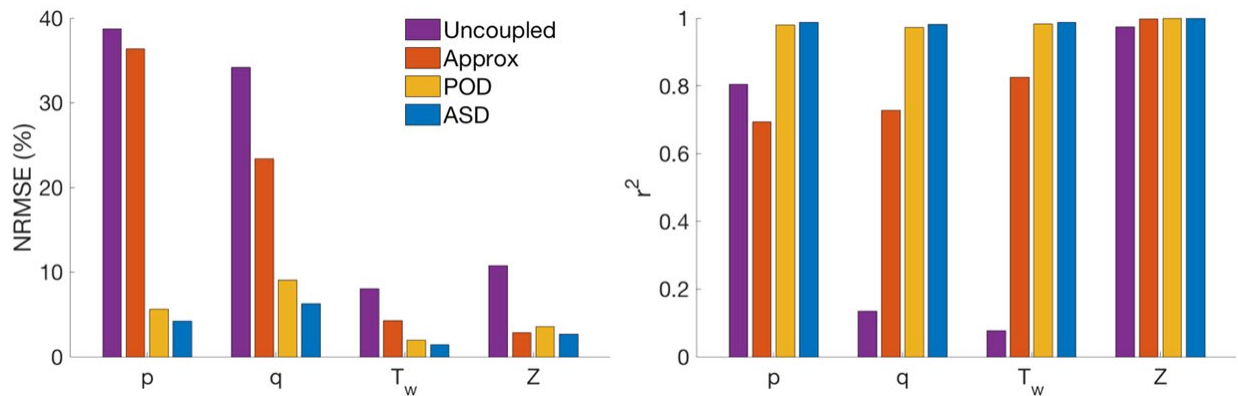


Figure 3.24: Error Metrics in Pressure, Heat Flux, Surface Wall Temperature, and Surface Displacement Using 4 Different Approximations for the Loads

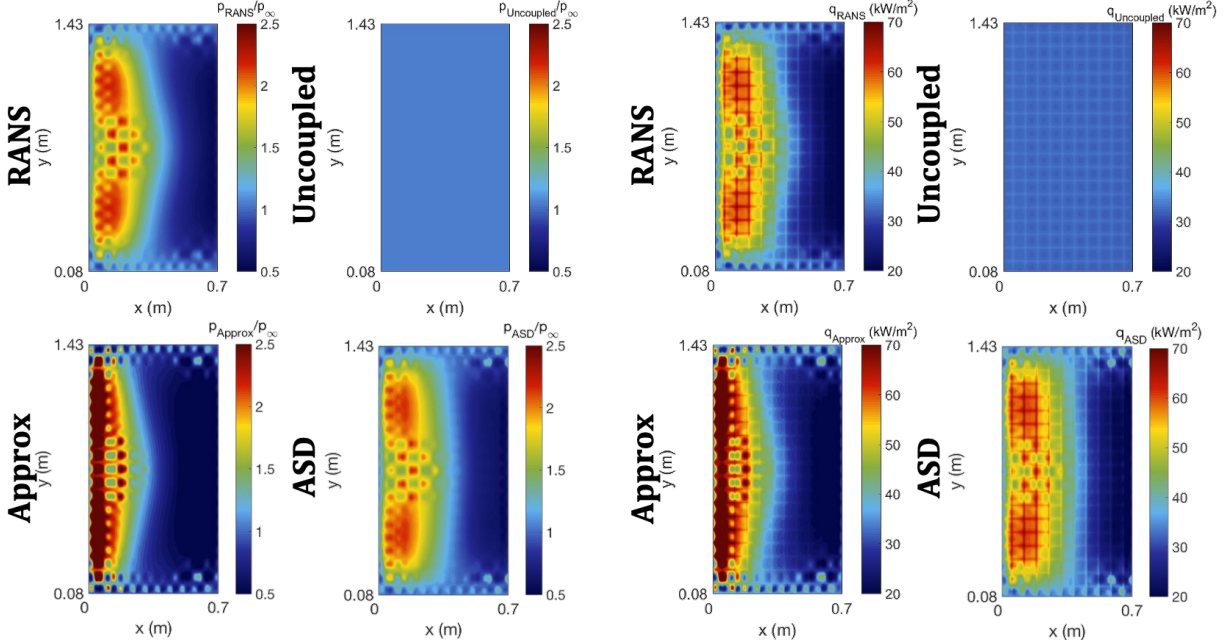


Figure 3.25: Pressure and Heat Flux Surface Contours Comparing 3 Different Simplified Modeling Approaches to the RANS-based Reference Model

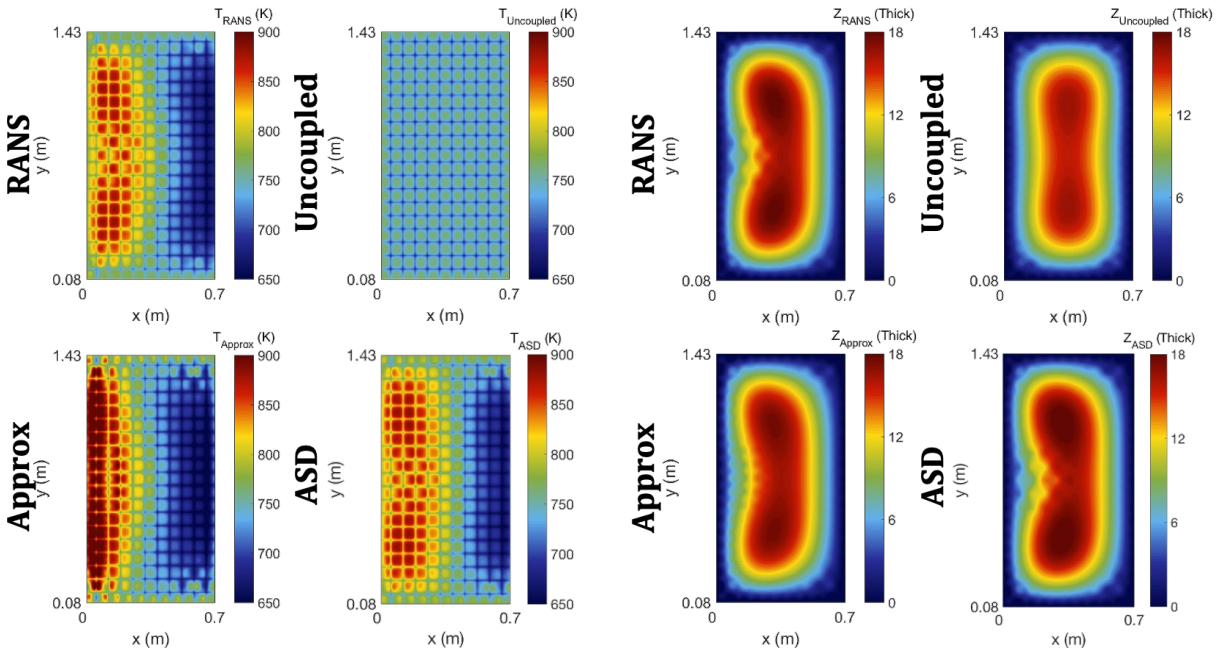


Figure 3.26: Wall Temperature and Displacement Surface Contours Comparing 3 Different Simplified Modeling Approaches to the RANS-based Reference Model

3.1.3. A.3: Nonlinear ROM of a Hat-stiffened Panel

CCSS Personnel: Bret Wainwright (Ph.D. student), Marc Mignolet

Period of Activity: 07/2016-04/2020

Over the last decade, significant progress has been accomplished in ROM modeling with the emphasis switching from methodology development to consideration of more complex structures. Some of the more complicated structures to date are the 9-bay panel [9,10] and the Culler-McNamara one, defined in [16] and analyzed in the context of NLROMs in [13,14], both of which include small stiffeners resulting in some asymmetry of the structure. Other panel considered such as the clamped-clamped curved beam, see project A.1, the piezobeam of [21], and the orthogrid panel [22-23] have more overall asymmetry. The above validations have provided good supporting evidence that the NLROM methodology is applicable to a variety of geometries including stiffeners. In this light, this project focused on providing a validation of the ROM capabilities to a particularly asymmetric panel which would be representative of a built-up structure. A “hat-stiffened” panel was selected as representative of such structures. The careful and detailed assessment of the reduced order predictions carried out in the present effort has first confirmed that this methodology is applicable to even very asymmetrical and complex structures. Moreover, it has also confirmed the findings of project A.4 that highly nonlinear features of the response can be captured within this framework, the present situation being an internal resonance between two modes in the excitation band and a third outside that band. Note finally that the ROM derived above is the starting point of a different investigation on capturing the nonlinearity induced by gaps in built up structures, e.g., due to a broken fastener, within the nonlinear geometric ROM construct.

With these objectives, it was decided to consider a hat-stiffened panel or hat section, such as the one considered using GFEM^{gl} in [24]. Figure 3.27 shows the selected structure.

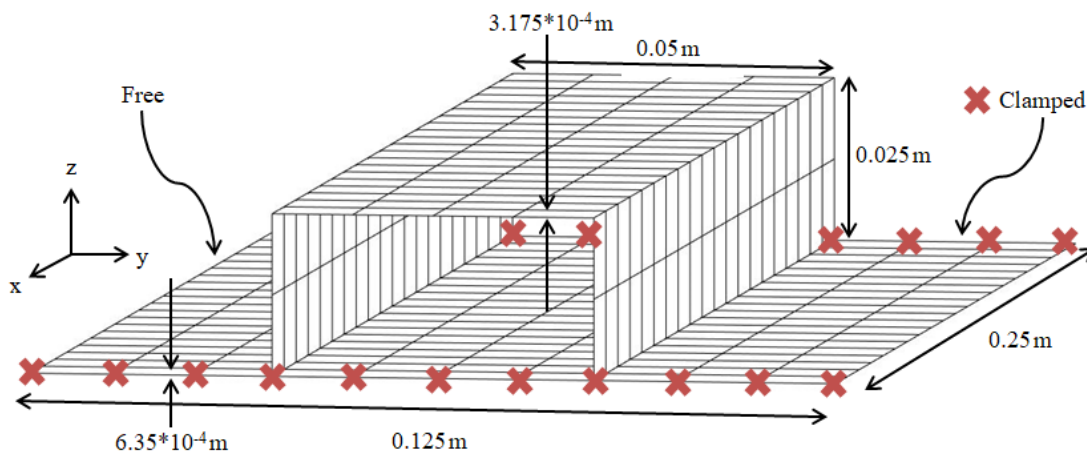


Figure 3.27: Hat-stiffened Panel

It was assumed that the hat stiffener is rigidly attached to the skin so that there is no flange or relief and the structure is monolithic. A FEM of that hat section was built in Nastran and consists of 360 CQUAD4 elements and 378 nodes with a skin thickness of $6.35 \cdot 10^{-4}$ m and a hat thickness of $3.175 \cdot 10^{-4}$ m. The section is 25.4 cm long (along the x directions), 2.54 cm high (in the z direction), and 12.7 cm wide (in the y direction). The material properties of the hat section were selected as

follows: Young's Modulus of $2 \cdot 10^{11}$ Pa, shear modulus of $8 \cdot 10^{10}$ Pa, and density of 7850 kg/m^3 . Clamped boundary conditions were applied along the edges parallel to the y axis, on the skin (but not the hat), preventing motion in all 6 degrees of freedom for these 22 nodes.

Achievements:

The careful and detailed assessment of the ROM predictions carried out in the present effort has first confirmed that the ROM methodology is applicable to even very asymmetrical and complex structures. Moreover, it has also confirmed the findings of project A.4 that highly nonlinear features of the response can be captured within this framework, the present situation being an internal resonance between two modes in the excitation band and a third outside that band. The conditions necessary to achieve such good predictions have been highlighted, i.e., that dual modes associated with the out of band mode participating to the resonance be included in the model and the symptom exhibited by the response when these conditions are not met have been demonstrated. The latter point is particularly important as it is not likely that a ROM user could predict the occurrence of the resonance, especially since its severity depends on the finite element mesh, i.e., on the specific alignment of the natural frequencies. Thus, recognizing the symptoms will trigger a revisit of the ROM basis to include the necessary dual modes.

Finally, it has also been demonstrated that, even though it is excessive, the high frequency content of the ROM response without the necessary dual mode does not affect measurably the fatigue life of the panel and that the ROM without that mode still performs well from that standpoint.

Results and Discussion:

The construction of a ROM for the hat section started with the selection of the linear modes to be considered. Relying on nonlinear static finite element data, 11 linear modes were recognized as significant contributors to the response. Surprisingly, it was observed that some of these modes were high frequency ones, e.g., modes 18 (950 Hz), 30 (1500 Hz), and 34 (1700 Hz). Seeking an explanation, a series of static solutions were devised in which each of the low frequency modes is in turn excited in the nonlinear range and the response is analyzed. These computations demonstrated that the high frequency modes are in fact nonlinearly coupled to the first one. This situation had not been encountered before and it is believed that it is due to the strong asymmetry and more specifically to the absence of nearly transverse and nearly in plane modes. For this structure, every mode involves significant transverse and in plane displacements.

Of the 11 linear modes, it was observed that 5 of those play a dominant role. The selection of the dual modes proceeded first with these 5 modes as dominant and the remaining ones as secondary, but this process led to 66 dual modes. Notwithstanding significant effort towards the identification of the stiffness coefficients, this 77-mode ROM was found to be unstable under dynamic excitations.

In fact, the above situation is an excellent example of the challenges described in project A.4 with regard to dual construction and which led in that project to the optimization of the linear modes, i.e., their rotation, using reference data. This approach was undertaken here and led to 4 POD eigenvectors as being sufficient to represent this static data with the first eigenvector being significantly more dominant than the other 3. As a validation of these observations, a 5-mode ROM was constructed which incorporates the 4 POD eigenvectors and the dual of the first one of these.

Static predictions of this very simple model were found to be very good. However, this model is not appropriate in the dynamic case as it does not correctly predict the in band, [0,500] Hz, natural frequencies.

Retaining the dual mode and adding to the original 11 linear modes led to good static predictions, e.g., see Figure 3.28, and provided a first dynamic ROM, the response of which captured qualitatively the Nastran predicted response. Seeking a quantitative match, duals of the POD eigenvectors and the linear modes were successively added to improve the model. As the predictions of the static response (see Figure 3.28) and the dynamic in band one converged, it was observed that the ROM predictions exhibited a spurious high frequency content centered around two of the high frequency modes included in the model, see Figure 3.29. Moreover, the amplitude of this high frequency content was increasing in comparison to the in-band response as the excitation level increased suggesting a nonlinear behavior.

Improvements of the predictions were obtained first by utilizing the multi-level stiffness coefficients identification approach [25], compare the pink curves in Figure 3.29 with the light green one (obtained with the multi-level identification). Yet, the out of band response was still present, see Figure 3.29(a) in particular.

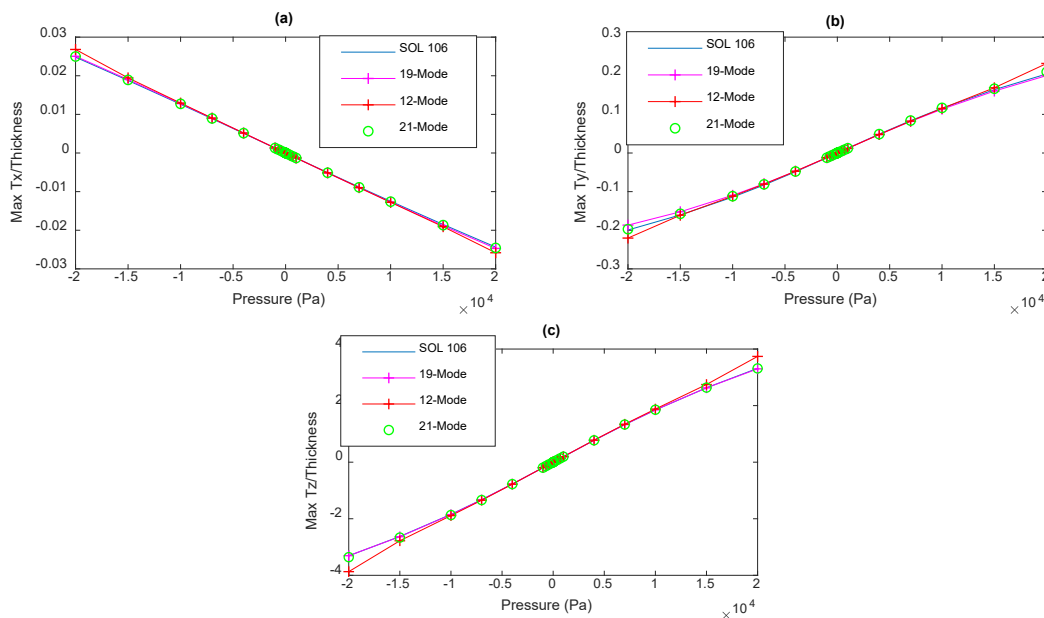


Figure 3.28: Displacements (Normalized by Skin Thickness) vs. Pressure for the Uniform Loading - Maximum Displacements (a) Tx, (b) Ty, and (c) Tz Respectively

Through careful study of the ROM, this high frequency content was eventually determined to be caused by an internal resonance, i.e., an energy transfer between low frequency in-band modes and high frequency out of band modes which had to be included in the basis. Reaching this conclusion was a lengthy process. First, it was observed that adding lumped masses to the structure at specific locations to change the natural frequencies of specific modes would reduce the high frequency content, although not eliminate it.

A second set of structural modifications were made in which the mesh of the hat section was refined first by 4 (by 2 in both directions of the elements), then by 16 (by 4 in both directions of the elements). This remeshing was initially motivated by the desire to compare the Nastran results with those of another finite element code, more specifically of the Air Force code implementing the approach of [19]. Rather surprisingly, it was observed that the ROMs constructed on these meshes, using either Nastran or the Air Force code to identify the coefficients, did not exhibit any significant high frequency content. An investigation of the natural frequencies of the various modes showed significant shifts. This observation, as the lumped mass addition results, suggested that the original FEM exhibited a specific alignment of natural frequencies that created the issue, i.e., an internal resonance.

As a final check, two of the high frequency modes from the ROM basis were removed and a significant reduction of the high frequency content was observed. Note that this removal was not acceptable as it negatively affected the static and in-band dynamic predictions. The latter observation in particular confirms the coupling between the high frequency modes and those in-band.

The source of the high frequency content was eventually identified as an insufficient softening of the motions induced by the high frequency mode in the original model which in turn did not reduce the coupling between the in-band modes and the out-of-band ones as needed. Originally and typically in the dual selection process, no dual modes are selected from the less dominant modes at high frequency even if they are included in the basis. The excessive coupling induced more energy in the out-of-band modes, but it also took the existence of an internal resonance to really amplify the out-of-band response. Specifically, the dominant linear modes 1 and 6 had natural frequencies of 250 Hz and 500 Hz respectively while mode 18 had natural frequency of 1000 Hz which was then excited by the $2 \times \text{mode } 1 + \text{mode } 6$ combination. By including additional dual modes in the basis, specifically those associated with these high frequency linear modes, the interactions could be properly softened, and the high frequency response could be eliminated from the ROM.

Accordingly, a new successful 25-mode ROM was constructed for the hat-stiffened panel, accurately predicting the static and dynamic response of the structure throughout the entire frequency range, even at the higher loadings of 154 dB and 164 dB, see Figure 3.30 and Figure 3.31. Excellent predictions of the static displacements were also obtained. The findings from this investigation provide valuable information for future ROM constructions and demonstrate the importance of including and appropriately capturing high frequency modes.

Interestingly, it was found that the fatigue life of the structure was not significantly affected by the larger than expected out-of-band response. The majority of the damage accumulated by the structure was in fact caused by the in-band response. This is important knowledge because if the internal resonance effects had not been corrected, it would not have had a significant adverse effect on an important by-product of the NLeROM, i.e., the fatigue life prediction.

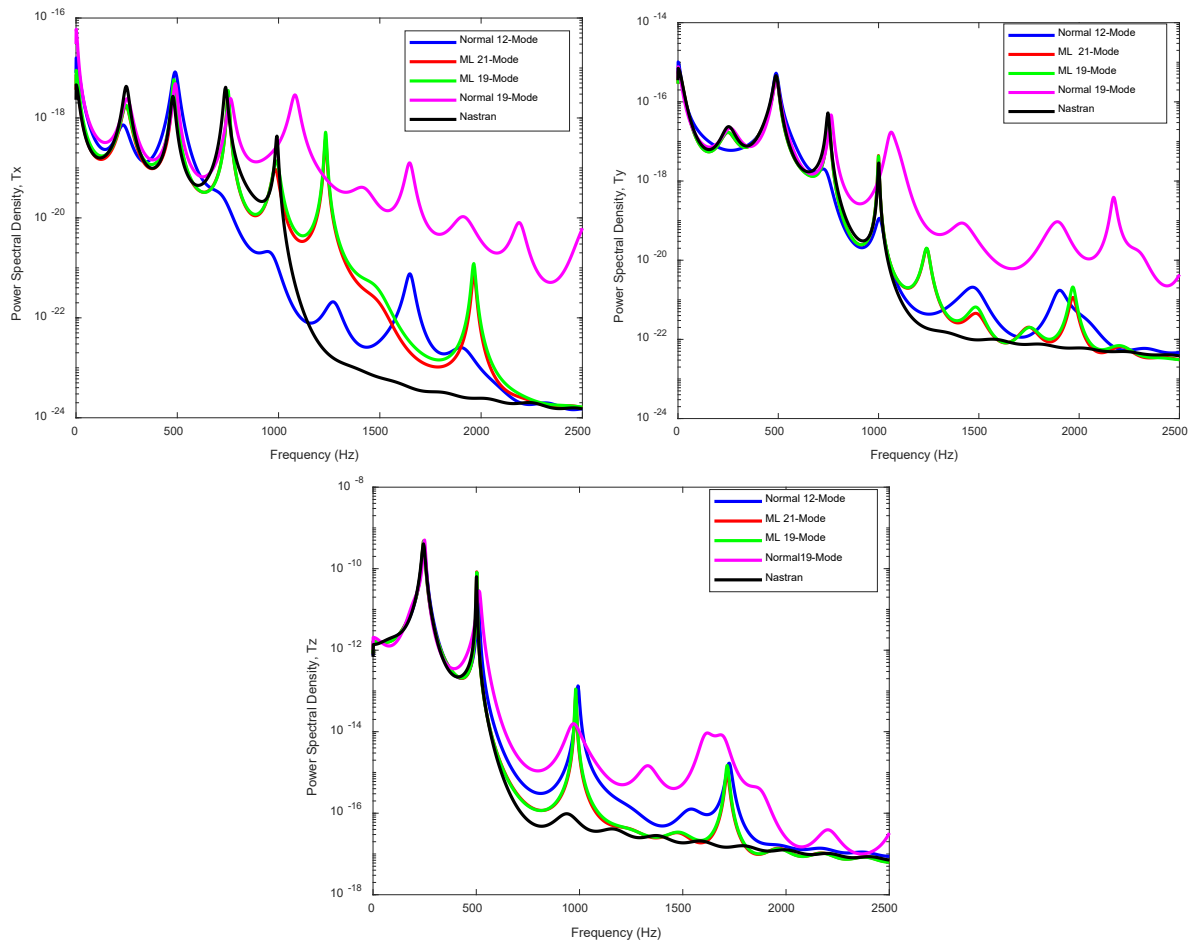


Figure 3.29: Power Spectral Density of the Displacement Along (a) x, (b) y, and (c) z of Node 16 for the OASPL of 143.5 dB, [0,500 Hz] Excitation

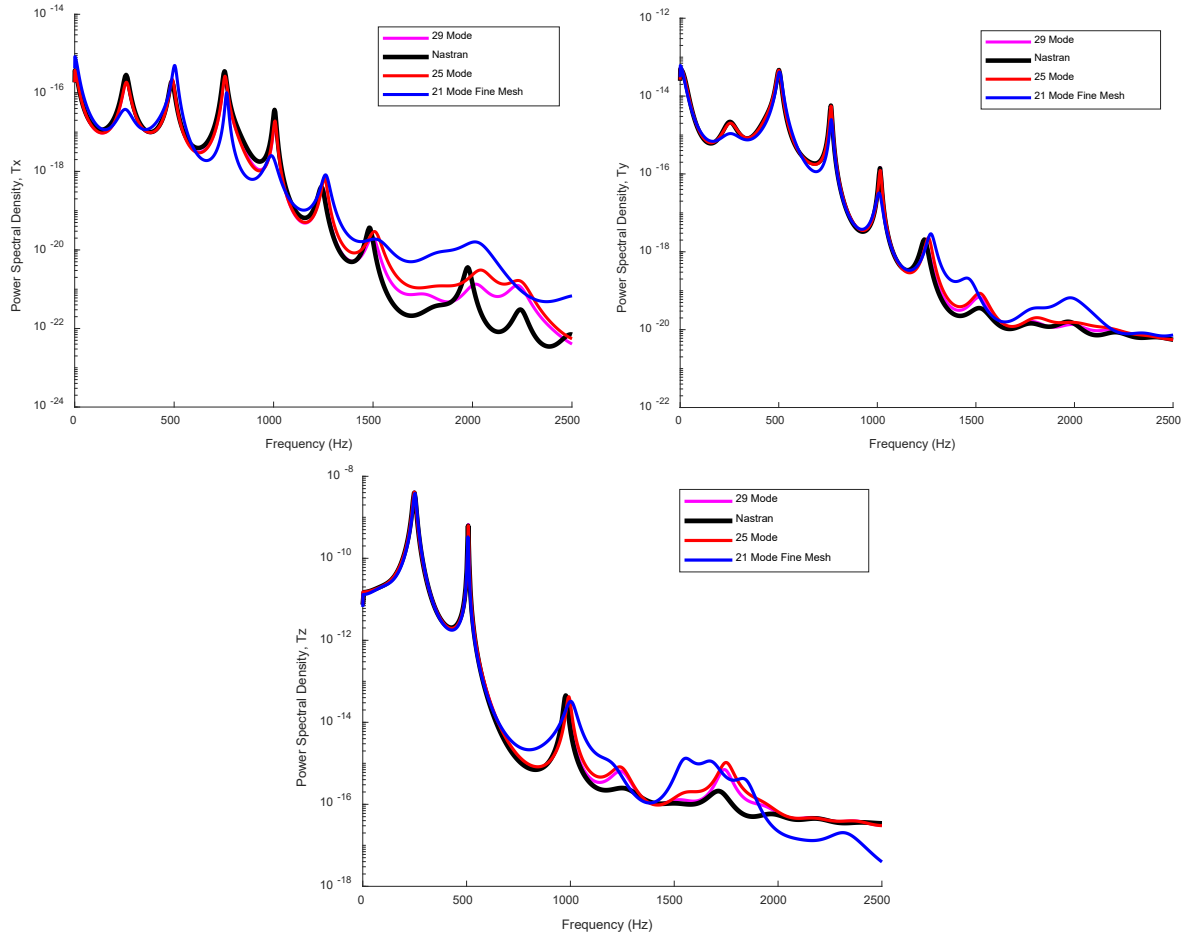


Figure 3.30: Power Spectral Density of the Displacement Along (a) x, (b) y, and (c) z of Node 16 for the Low Nonlinear Loading, OASPL of 154 dB, [0,500 Hz] Excitation

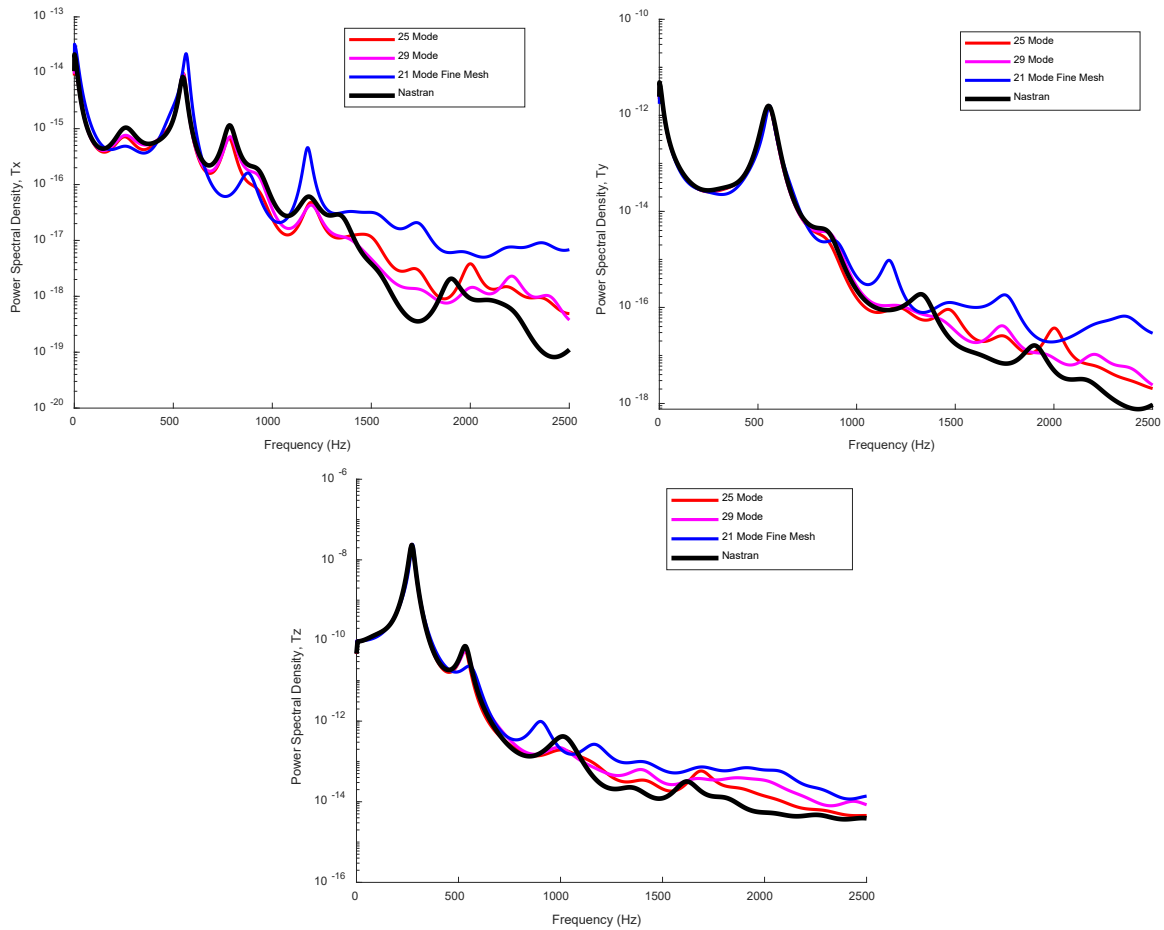


Figure 3.31: Power Spectral Density of the Displacement Along (a) x, (b) y, and (c) z of Node 16 for the High Nonlinear Loading, OASPL of 163.5 dB, [0,500 Hz] Excitation.

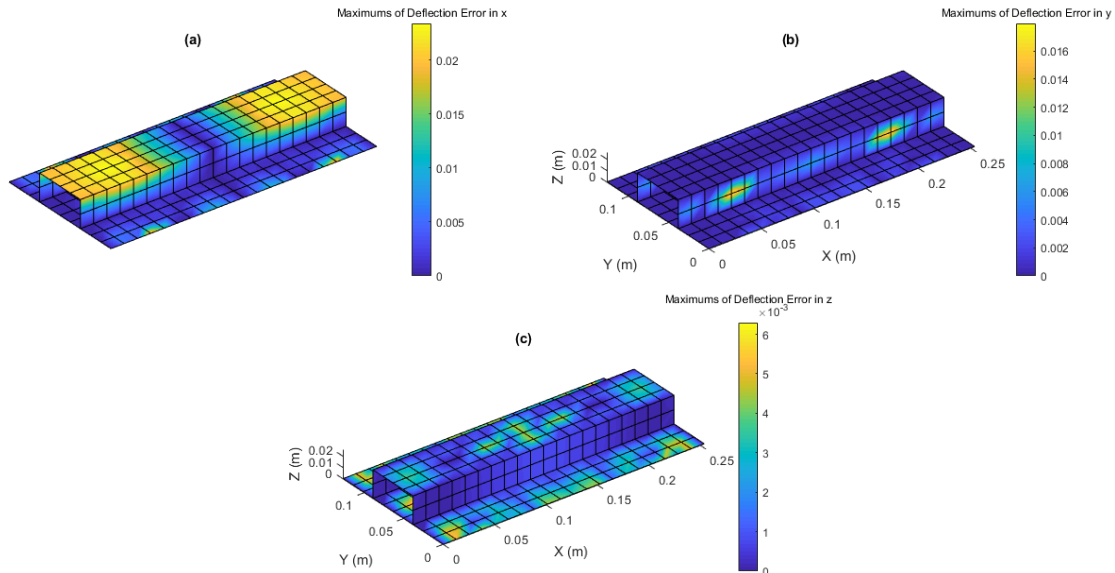


Figure 3.32: Absolute Errors of the 25-mode ROM Static Predictions Normalized by Maximum Deflection in that Direction

3.1.4. A.4: Nonlinear ROM of Structures Exhibiting a Strong Nonlinearity

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Period of Activity: 01/2018-04/2020

Owing to large aerodynamic loads and heating, it is expected that panels of high-speed vehicles will exhibit deformations large enough to induce geometric nonlinearity in the response. For many structures, this nonlinearity leads to notable but not dramatic changes in behavior, e.g., a stiffening as the amplitude of deformations increases. For some structures however, a dramatic change does happen, e.g., a curved panel undergoing snap-through or a flat one experiencing thermal buckling. ROM has been generally straightforward and successful for the former structures, but it has been difficult for those in the latter class. The focus of the present investigation is then on resolving the modeling challenges to obtain stable ROMs providing good predictions of the response of structures exhibiting strongly nonlinearity. This effort demonstrated that the challenges rest mostly with the identification of the ROM coefficients and a novel approach was proposed to improve this identification. The optimization of the basis functions was also proposed and shown to have positive effects on the predictive capabilities and stability. The ROMs thus obtained were shown to provide a good prediction of the onset of the strong nonlinear behavior, snap-through and symmetry breaking specifically, as well as the response thereafter.

Motivation/Background:

The last 15 years have seen a dramatic growth in the capabilities of the nonlinear ROM methodology to efficiently and accurately model a broad range of structures, including some particular complex ones. Of the 35 structures considered by the ASU group, 28 of them have been very accurately modeled by ROMs requiring no further consideration. The ROM modeling of the

other 7 has yielded partial success to different degrees. Among these are only 3 structures that are relevant to panels of high-speed vehicles. Not surprisingly, these structures, described below, are those which exhibit the strongest nonlinearity, most notably snap-through or buckling:

1. The clamped-clamped curved beam considered in [17], see Figure 3.33. The analysis extends to snap-throughs and include the effects of a temperature field as well. While good predictions were eventually obtained, we had to resort to zeroing out of a series of contentious terms and were not able to correctly capture the snap-through at temperatures exceeding those presented.

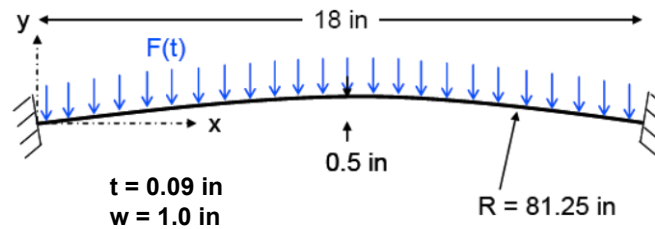


Figure 3.33: Curved Beam Geometry [17]

2. The shallow cylindrical shell introduced in [18]. This shell exhibits, under a uniform pressure, a mode-switching, i.e., mode 1 is the dominant mode for low level responses but is replaced as the prevalent mode at higher levels by mode 2. Good results were obtained in [18] but it is not clear whether, or how much, mode switching occurred in the loading cases considered. The ASU group has encountered difficulties in obtaining a basis, dual modes in particular, providing a good modeling of the response over the entire range of response levels including the mode switching point.

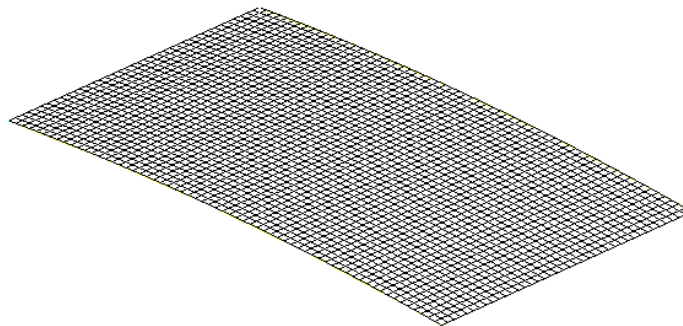


Figure 3.34: FEM of the Shallow Cylindrical Shell [18]

3. The panel of Figure 3.6 which was considered by ROMs without and with temperatures in [13-14]. A structural ROM was obtained that provides a very good modeling of the structural behavior in the response range of the problem. However, just outside that range, the panel exhibits a buckling that involves strongly the stiffener, and which was never successfully captured by the ROM.

The focus of the present investigation is then on resolving the above modeling challenges to obtain stable ROMs providing good predictions of the strongly nonlinear response of these 3 structures.

Achievements:

Significant improvements of the ROM modeling of structures exhibiting a very nonlinear behavior were accomplished. In particular, the clamped-clamped curved beam modeling was very successfully achieved through improvements in both the selection of the basis functions and of the identification of the stiffness coefficients. The work on the identification was prompted by an insightful comparison of the coefficients obtained from a Nastran model and the equivalent one treated with an open source finite element code written by the Air Force Research Lab following [19]. This comparison confirmed the long-held suspicion that a series of coefficients related to the dual modes were not correctly identified when using Nastran, owing to the differences in nonlinear finite element formulations between that code and the ROM. The ROM obtained was able to capture the snap-through statically but also dynamically that is occurs rarely, intermittently, or nearly continuously.

The improvement of the basis selection process developed for the curved beam proved to be very efficient as well for the shell and a ROM and a small size ROM was obtained that provided a very good match of full finite element results, both static and dynamic. Interestingly, the shell undergoes a symmetry breaking that had not been recorded in earlier works and the ROM provided a close prediction of this event. This result and the very good prediction of the snap-through behavior of the curved beam demonstrate that the ROMs not only predict well quantitatively the response but actually capture the physical intricacies of these strongly nonlinear structures.

A detailed investigation of the local buckling of the panel of Figure 3.6 was carried out and it was found that the buckling pattern dramatically changes with small variations of the loading past the buckling point. This behavior precludes a good capturing of the deformations by a small ROM basis but an alternate strategy based on the concepts developed under project B.3 was suggested for further work.

Strategy and Results:

Central to this effort has been the assertion that better predictions by ROMs are obtained when the number of basis functions that have large components is as small as possible. For the linear part of the basis, this assumption was consistent with the state of the art of ROMs at ASU at the beginning of the project, most of the models considered thus far had one dominant linear mode and the predictions had been very good to excellent. When multiple linear modes are dominant, achieving similarly accurate predictions has been more challenging or not achieved.

It is believed that this correlation stems from two challenges of ROM constructions. The first is the basis selection and most notably the determination of the duals which complement the linear modes to form the basis. This process is very straightforward when a single linear mode dominates the response but becomes more challenging when two or more modes play a key role owing to the need to create a set of loadings that induce displacements fields that are representative of the likely variable combination of dominant linear modes. The second challenge relates to the identification of the nonlinear stiffnesses. Specifically, having multiple dominant linear modes also implies that there exists a much larger number of stiffness coefficients that have an important effect on the magnitude of the restoring forces, in particular, coefficients involving indices corresponding to multiple modes.

Based on the above assertion and observations, an optimization of the basis was defined, seeking to concentrate the response on a small subset of modes. For the linear part of the basis, this effort was accomplished using a set of finite element static displacements obtained under relevant loading conditions, referred to as the reference data. These displacements fields are first projected on a series of linear modes and these projections are processed through a POD to determine the most significant combinations of linear modes in the response. Then, the eigenvector(s) with the largest eigenvalue(s) is (are) retained and their full finite element space counterpart determined. This (these) mode(s) then form the core of the linear basis. To this core are finally added the rest of the linear modes which are further orthogonalized.

This process only rotates the linear modes, it does not change the space that they span. Moreover, the space spanned by the dual modes constructed from either the original or the rotated sets of linear modes should also be the same *if all combinations of the linear modes were used to create these duals*. This is however very rarely the case, only a subset of these combinations is used, favoring the modes that are expected to be dominant to minimize the number of retained dual modes, and thus the size of the final basis. Effectively, the rotation of the linear modes has determined which combinations are expected to be the dominant ones, i.e., those that involve the first few eigenvectors. The net effect of the rotation of the linear modes is thus a more compact and relevant set of dual modes for the reference data.

This process was shown to be very efficient in connection with the curved beam and the cylindrical shell leading to linear modes that very well represented the response. Shown in Figure 3.35 and Figure 3.36 are comparisons of the static predictions of the nonlinear response of the shell under uniform pressure, using this information as reference data with 11 rotated linear modes, 6 of which were POD eigenvectors, and 7 duals determined considering the first 2 POD eigenvectors as dominant and the remaining 4 as secondary. Clearly, the ROM predictions are extremely close to the full finite element ones in all directions and in all loading conditions, i.e., in the single well domain, in the two well domain, as well as right at the transition of these two conditions.

A dynamic validation was also carried out under a simulated acoustic excitation that is uniform in space along the mean transverse direction and varying in time as a bandlimited white noise in the frequency range of [0,500] Hz. Shown in Figure 3.37 are the power spectra of the displacement in the three directions at a node located at quarter length of the panel in both x and z directions. An excellent match is again observed.

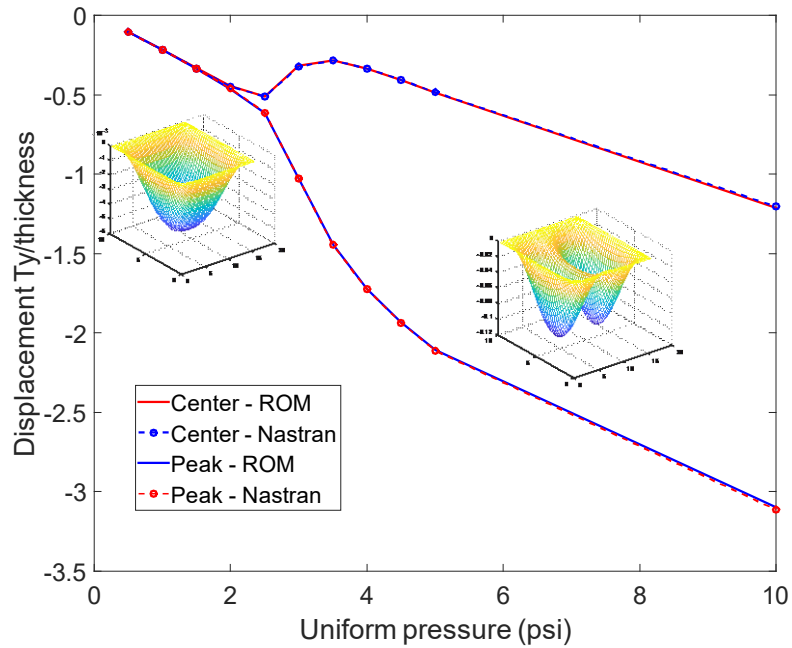


Figure 3.35: Center and Peak Displacements Along the y (Transverse) Direction vs. Applied Uniform Pressure (Nastran and ROM predictions, Shell Model)

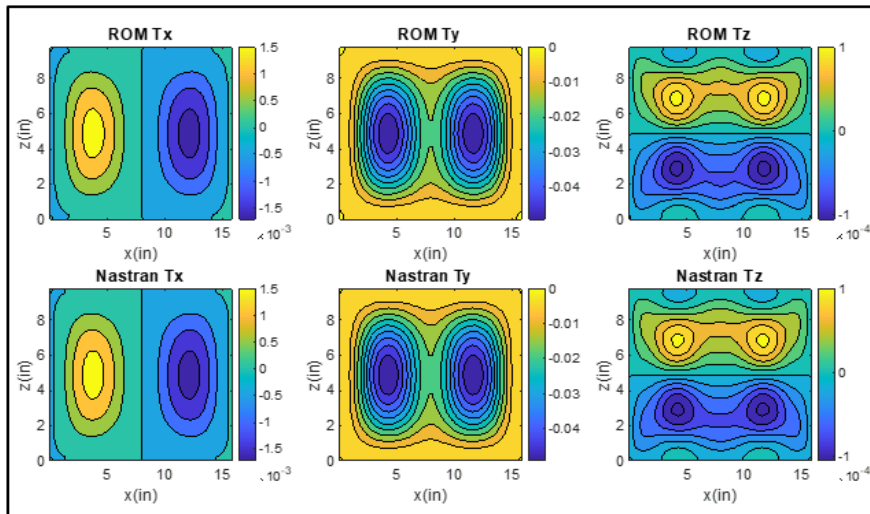
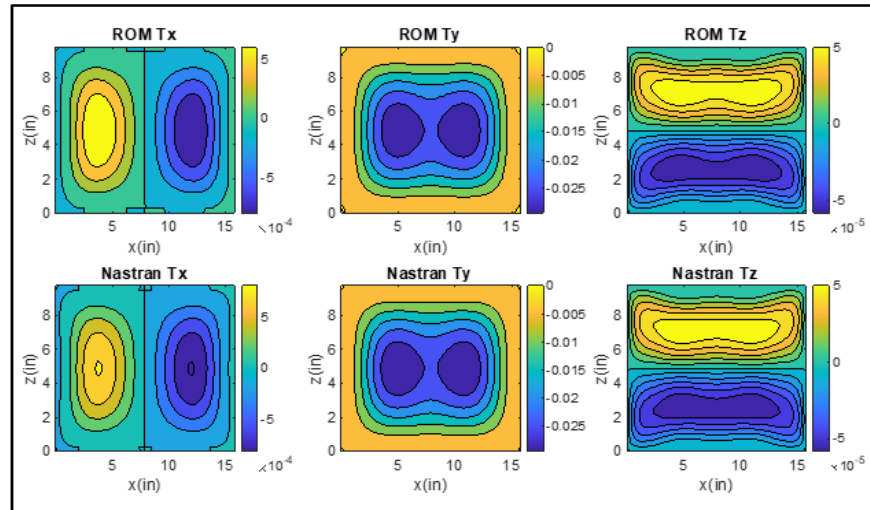
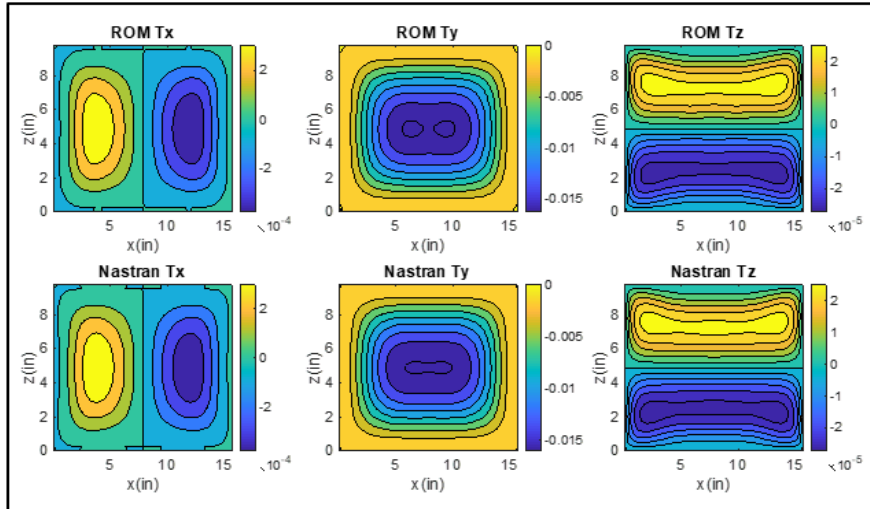


Figure 3.36: Contour Plots of Displacements Along x, y, z as Predicted by Nastran and the ROM for Uniform Pressures of 1.5 psi (top), 2.5 psi (middle), and 3.0 psi (bottom) (Shell Model)

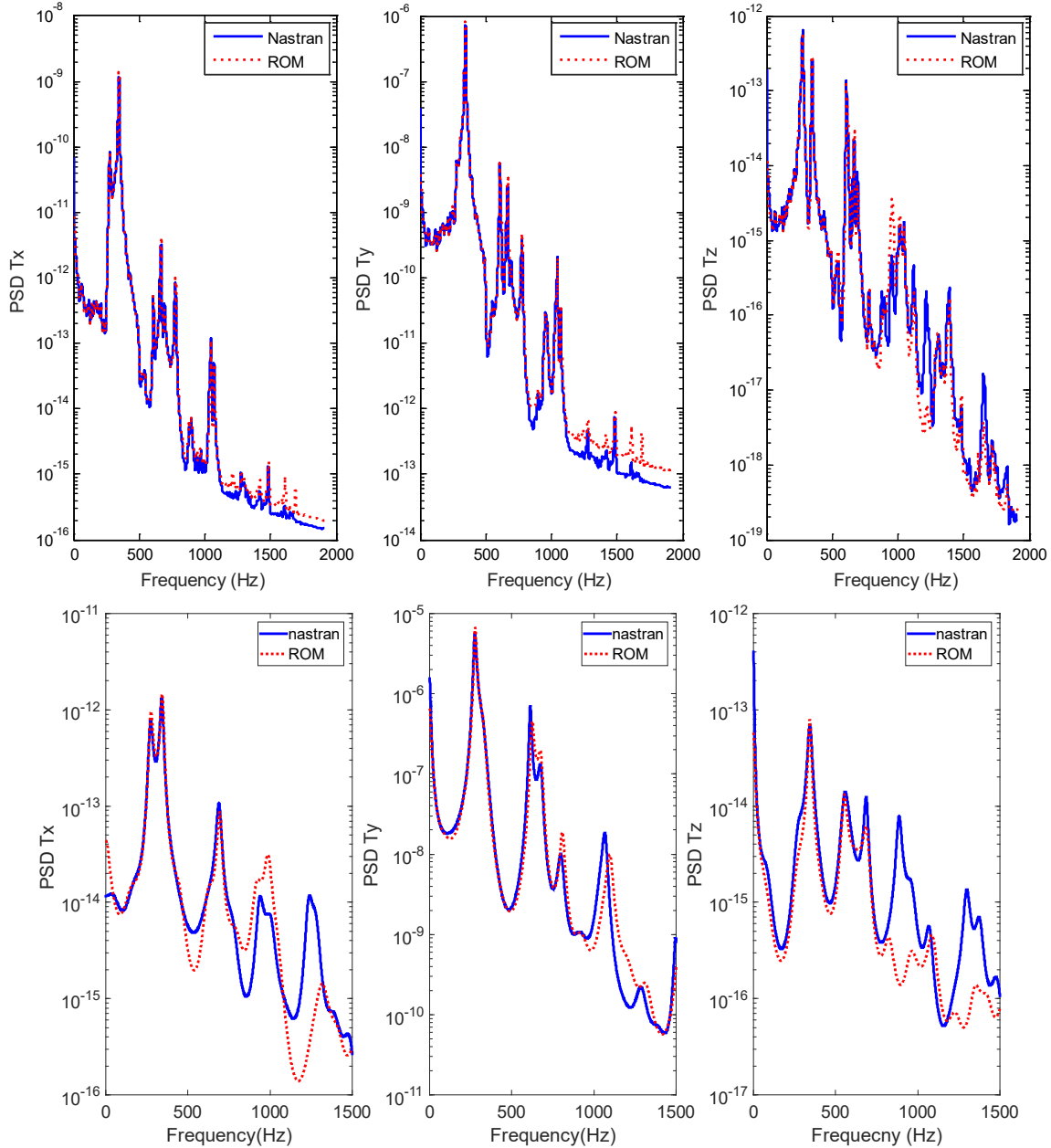


Figure 3.37: Power Spectral Densities of the Displacements in the x, y, and z Directions at a Node Located at Quarter Length of the Panel in Both x and z Directions with OASPL of (top) 150 db & (bottom) 160 db (Shell Model)

An optimization of the dual modes was also proposed motivated by the desire to concentrate the response in a small number of modes to improve the identification/stability of the ROM but also to address situations observed in the past where the number of dual modes necessary was unusually large (e.g., more than twice the number of linear modes). This effort was not carried out on the reference data used for the linear modes to avoid a bias of the model to this data. Rather, it was carried out as a secondary modal reduction, starting from a given basis judged to have too many

dual modes and using its identified stiffness coefficients to determine an optimum linear combination of these duals.

Two separate optimization strategies were considered. The first approach is similar in spirit to the definition of the optimum thermal modes, see project A.1 and more specifically A.1.3. Assuming that there is no direct excitation on the dual modes, or that it has a small effect, the response along the dual modes is induced by its counterpart for the linear modes through the nonlinear stiffness terms, primarily the quadratic ones that couple them. Relying on this observation, it was argued that the combination of dual modes that maximizes the coupling terms with the dominant linear modes would be especially important. This optimization process leads to a classic eigenvalue problem the eigenvectors of which represent the combination of the original duals to form these optimum duals.

The second dual optimization strategy seeks the linear combinations of the original duals that result in the lowest natural frequencies/lowest stiffnesses. It stems from the observation that the duals typically behave quasi-statically and that a larger generalized coordinate will result if the corresponding stiffness is small. Equivalently, motions along the duals that are very stiff should no produce much effect.

An assessment of these optimization efforts was performed on the clamped-clamped curved beam of Figure 3.33. An original set of duals was constructed on the 6 linear modes rotated as discussed above using uniform loading response both below and above snap-through as reference data. This process led to 8 dual modes when considering mode 1 as dominant. These 8 duals provide an excellent representation of the in plane (horizontal) displacements of the beam in all conditions (below and above snap-through), see Figure 3.38.

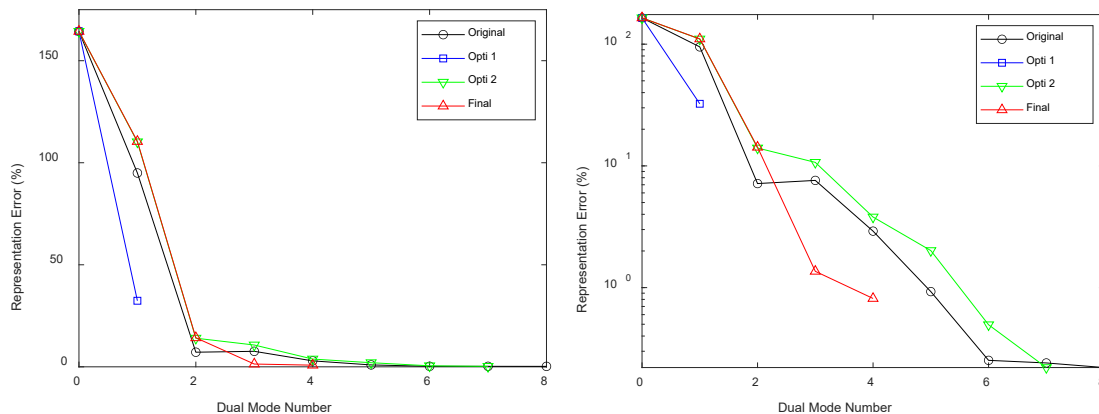


Figure 3.38: Average Representation Error, in %, of the In-plane Displacements Corresponding to Loadings of 2.5, 3, 3.5, 4, and 4.5 lbf/inch (i.e., Post Snap Through) vs. Number of Various Types of Dual Modes - Linear (left), Log Scale (right)

Considering that the first mode of the basis should be dominant, only its coupling with the duals was optimized in the first approach. Accordingly, only one optimized dual can be generated. Nevertheless, this mode seems very efficient in reducing the representation error of the uniform response post snap-through as shown in Figure 3.38 (curve “Opti 1”) for the loadings of 2.5, 3,

3.5, 4, and 4.5 lbf/inch above snap-through. More specifically, this error drops from 164% to 32% with that single dual. For comparison, the first original dual only reduces it to 95%. Enriching further the model would require the consideration of other combinations of the transverse modes beside the 1-1.

It was next desired to assess the benefits of the second dual optimization, i.e., based on the modal analysis of the corresponding blocks of the mass and linear stiffness matrices. An inspection of the resulting eigenvectors demonstrated first that the one associated with the smallest eigenvalue (natural frequency or stiffness) was primarily transverse while all others were primarily in-plane. Moreover, the latter ones were significantly more in plane dominant than the original ones. This finding indicates that this secondary modal reduction actually “concentrates” the in-plane motions in the dual rendering them more efficient to couple with the linear modes. The assessment of these new duals for the representation of the uniform displacement data was carried out as before by evaluating the average in-plane representation error corresponding to the loadings of 2.5, 3, 3.5, 4, and 4.5 lbf/inch, see Figure 3.38. Note in this figure that the new duals were considered in order of increasing eigenvalue and that the transverse dominant one was not included. It is seen that the two in-plane duals with lowest eigenvalues provide a significant drop in the representation error, yet, not quite as large as the original duals. However, the representation error drops consistently with these new duals at the contrary of the original ones. In this regard, note that the increase in representation error for the original duals associated with dual #3 results from this dual being primarily transverse. Thus, it leads to a decrease of the representation error in the transverse error but at the cost of an increase in the in-plane one. In this light, the continuous decrease of the representation error for the new duals is effectively associated with the decoupling induced by the eigenvalue problem. It is concluded from the above discussion that the two dual optimization strategies are both beneficial but in different ways.

To confirm the validity of the above conclusion, the stiffness coefficients of the ROM with optimized linear modes and duals were identified following the tangent stiffness-based approach of [9]. Unfortunately, the predictions from this ROM were either poor or unconverged above snap-through, a situation which had been observed before especially in the context of this structure. This finding motivated a renewed investigation of the stiffness identification problem. To obtain another point of reference, the identification of the stiffness coefficients was also performed with the open source finite element code from the AFRL. Very interestingly, it was observed that this identified ROM was not only stable but provided an excellent match of the Nastran predicted responses. The ensuing comparison of the AFRL code and Nastran identified coefficients, e.g., see Figure 3.39 and Figure 3.40, provided clear support for the long-held perspective that a series of nonlinear coefficients identified from Nastran are not reliable. That is, the stiffness coefficients relevant to transverse or linear modes (K_{tt} , and K_{ttt} in the figures) only are generally well captured – although the cubic ones may not always be, see Figure 3.40. Also, well captured are the quadratic coefficients involving one dual mode and two transverse modes (K_{ttd}/K_{dtt} in the figures). However, all other nonlinear coefficients may/generally exhibit very large errors.

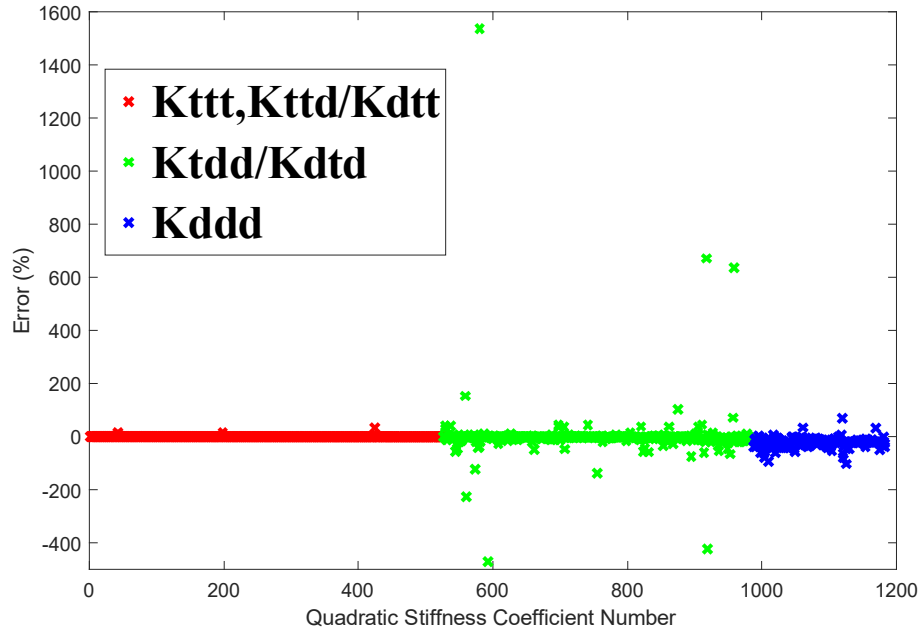


Figure 3.39: Relative Errors of the Nastran Identified Quadratic Stiffness Coefficients in Comparison to Their AFRL Code Counterparts, 6L7D model - Curved Beam

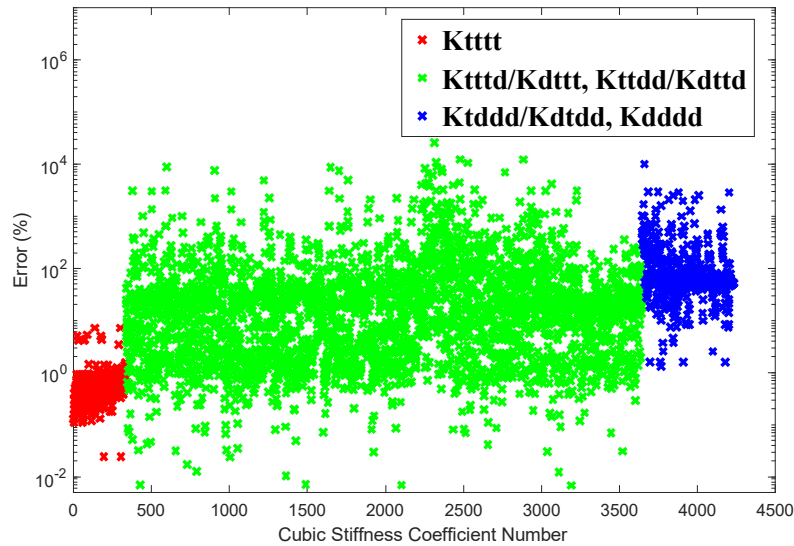


Figure 3.40: Relative Errors of the Nastran Identified Cubic Stiffness Coefficients in Comparison to Their AFRL Code Counterparts, 6L7D Model

Having determined what sets of nonlinear stiffness coefficients are reliably identified, several different remedies can be envisioned. In the absence of data for the structure considered, one approach is to proceed with the coefficients as identified. A second option is to zero out the coefficients which are deemed poorly identified. This is the “cleaning” option that has occasionally been performed in the past. This option traditionally improves the stability of the ROM for

dynamic computations and has often improved predictions because many of the coefficients which are eliminated contribute little to the response. Yet, for structures such as the clamped-clamped curved beam with very large deflections, it is necessary to have a ROM with a more complete set of nonlinear stiffness to obtain an accurate prediction, especially of the post snap-through behavior. In such situations, a third option is developed here to refine the nonlinear stiffness coefficients deemed inaccurate. In fact, two different approaches of “fine tuning” of the ROM stiffness coefficients were also devised and employed in connection with the curved beam. The need to carry this effort stems from the high sensitivity of the ROM response to some of the coefficients.

A first tuning approach based on the matching of modal forces was shown to bring a significant improvement in the validation results, especially under static loading. However, such tuned ROMs may not be stable enough under dynamic loading to give converged results. This is because some stiffness coefficients have been tuned to a value far away from their “correct” values although the error of modal forces calculated from them is small. The second tuning approach was devised to avoid that problem. It is based on the matching of the generalized displacements q_i computed by Nastran and the ROM. This tuning approach was found to be better than the first one yielding stable ROMs. Figure 3.41 shows the loading-unloading curve of the curved beam without and with tuning. Without this operation, the high amplitude branch and the unloading point are poorly predicted. The obtained model also performs well with temperature, see Figure 3.42, and under dynamic conditions, see Figure 3.43.

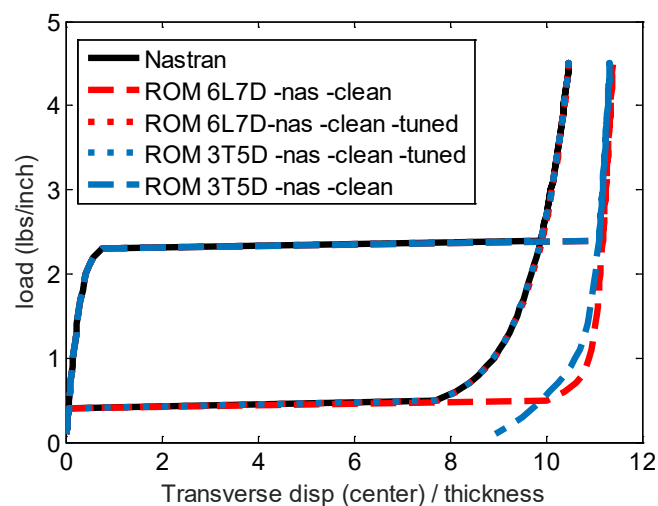


Figure 3.41: Transverse Displacement of Beam Center Under Uniform Load Predicted by Nastran, Cleaned 3T5D and 6L7D ROMs, and Corresponding Extended (“Clean-tuned”) Models with Identified Coefficients

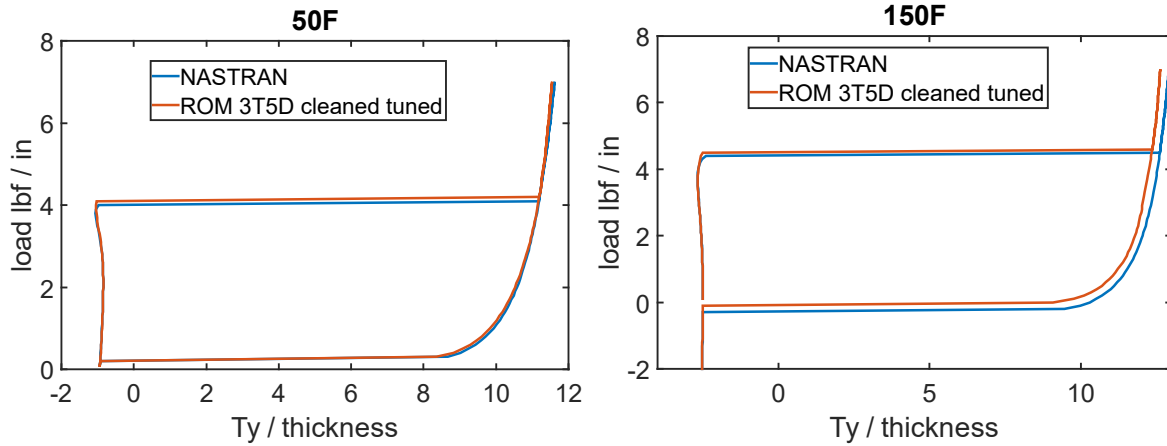


Figure 3.42: Transverse Displacement of Beam Center vs. Uniform Load Including Snap-back at (a) 50F & (b) 150F with Nastran and Extended (“Cleaned-tuned”) 3T5D ROM

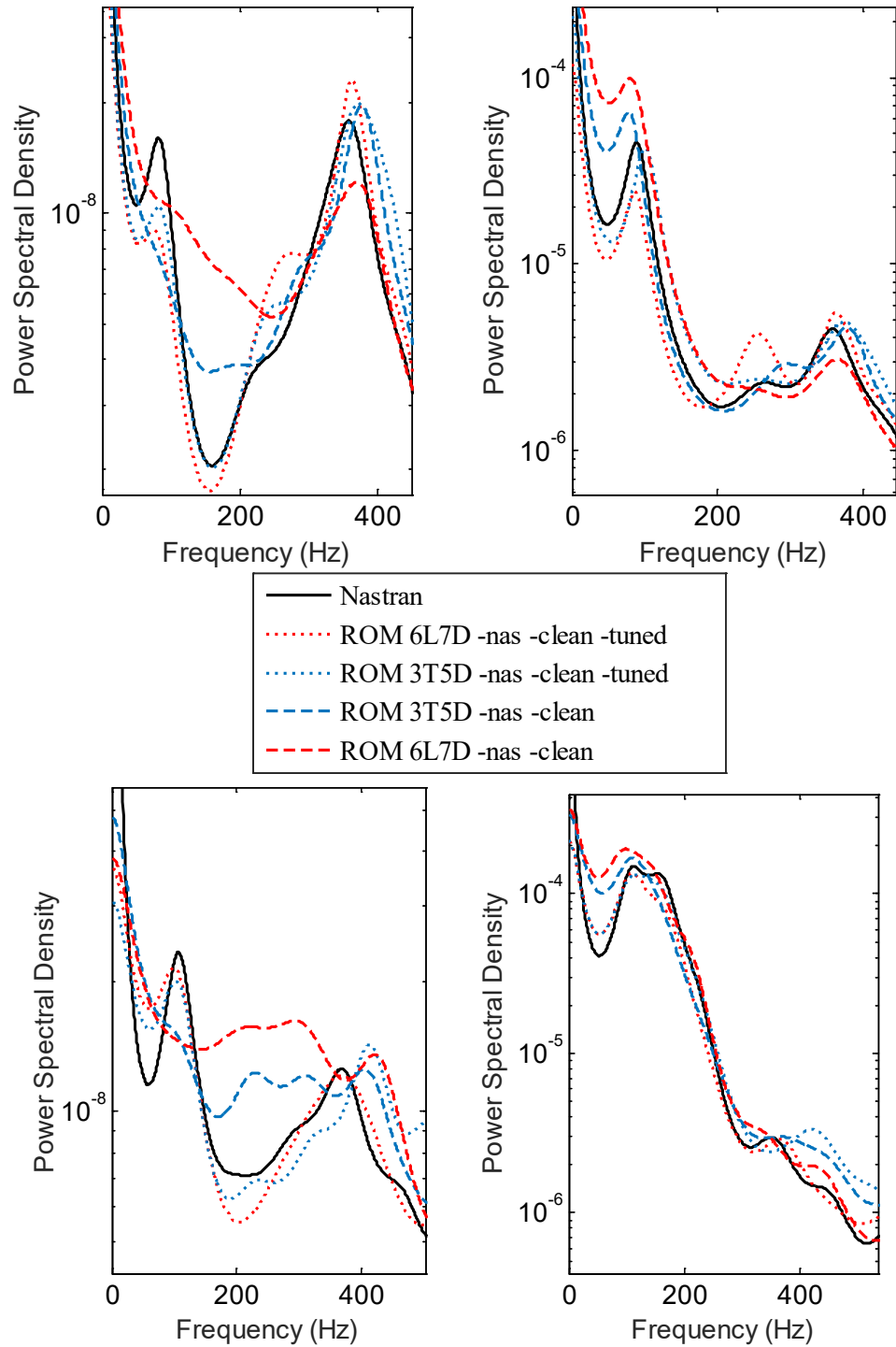


Figure 3.43: Power Spectral Densities of the In-plane (left) and Transverse (right) Displacements at the Quarter Point of Clamped-clamped Beam Under Medium (top) and High (bottom) Acoustic Loading

A final question investigated in this project is the “on-line” assessment of the ROM, i.e., to determine whether it is accurately capturing the response that would be predicted by the underlying FEM/software. A strategy to carry out this effort minimizing the number of calls to the full finite element code was proposed. The results suggest in particular that the monitoring of the eigenvalues of the ROM tangent stiffness matrix and of the occurrence of zeros of the lowest one provide a framework to (i) predict strongly nonlinear events (snap-throughs, buckling, solution changes) and (ii) assess whether they are accurately predicted. With regard to this latter point, the accuracy of the prediction of the load (static or dynamic) at which the event occurs can be ascertained by comparing the eigenvalues of the ROM tangent stiffness matrix and its Nastran equivalent obtained for the same deflection. A good matching is then indicative of an accurate ROM assessment.

3.1.5. A.5: Nonlinear ROM of a Curved Shell under Combined Thermal and Mechanical Loads: Comparison with Experiments

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AFRL Personnel: J.J. Hollkamp, R. Perez, S.M. Spottswood

Period of Activity: 1/2019-4/2020

A recent experiment performed at the Structural Sciences Center focused on the response of a curved panel to a moving heat source. This setup and the associated measured data represents an excellent new test bed for the validation of coupled structural-thermal ROMs as it involves a temperature distribution which evolves over time and space. This investigation has shown that these ROMs can indeed provide an accurate prediction of the structural response but also that they require an appropriate structural basis, especially basis functions capturing well the effects of temperature. The standard structural basis functions, i.e., linear and dual modes were shown not to be sufficient when temperature is acting and enrichments of the basis were thus needed. A series of options to construct these functions have been proposed, classified, and assessed on the experimental data. It is found that the temperature induces three effects that generally interact with each other: a change in stiffness of the structure, an external loading term, and geometric nonlinearity induced by the large deformations. For some temperature distributions, one or two of the above effects dominate but in general all three are present and must be reflected in the choice of enrichments. An approach to bypass the need for enrichments based on their static condensation has been analyzed and shows promise.

Motivation/Background:

This project aims to use recently obtained experimental data of a generic high-speed panel (the Gordon-Hollkamp shell, [18]) to assess and improve the current nonlinear ROM methodology for the coupled structural-thermal analysis of high-speed aircraft structures, in particular for the construction of the basis of the ROM.

For a coupled structural-thermal ROM, a necessary condition is that the structural and thermal bases well represent the displacement and temperature fields. Past efforts have been very fruitful proposing and validating, and the structural-thermal ROM methodology is believed to be in an acceptable state as shown by the ROM predictions in the aero-thermal-structural coupled

simulations. However, this perception may only be a reflection of the very limited validations that have been conducted. The paucity of validation cases for coupled structural-thermal ROM, especially considering unsteady thermal effects, must be addressed to either confirm the appropriateness of the current state of the art or enable its improvement by demonstrating prediction gaps.

The experiment performed at the Structural Sciences Center (SSC) which focuses on the response of a curved panel (the Gordon-Hollkamp shell, [18]) to a moving heat source represents an excellent new test bed for the coupled structural-thermal ROMs as it includes a non-trivial temperature distribution which evolves with time so that unsteady effects are present. The tested curved panel is a part of a cylindrical shell with radius of curvature of 100 inch. A FEM of the curved panel was constructed using 2457 CQUAD4 shell elements (a 64-by-40 mesh) in Nastran, as shown in Figure 3.34. The panel is clamped along all the edges. This FE model is consistent with the FE model [18] constructed in Abaqus so a comparison can be made when necessary.

Two sets of test data of the curved panel were obtained from the SSC.

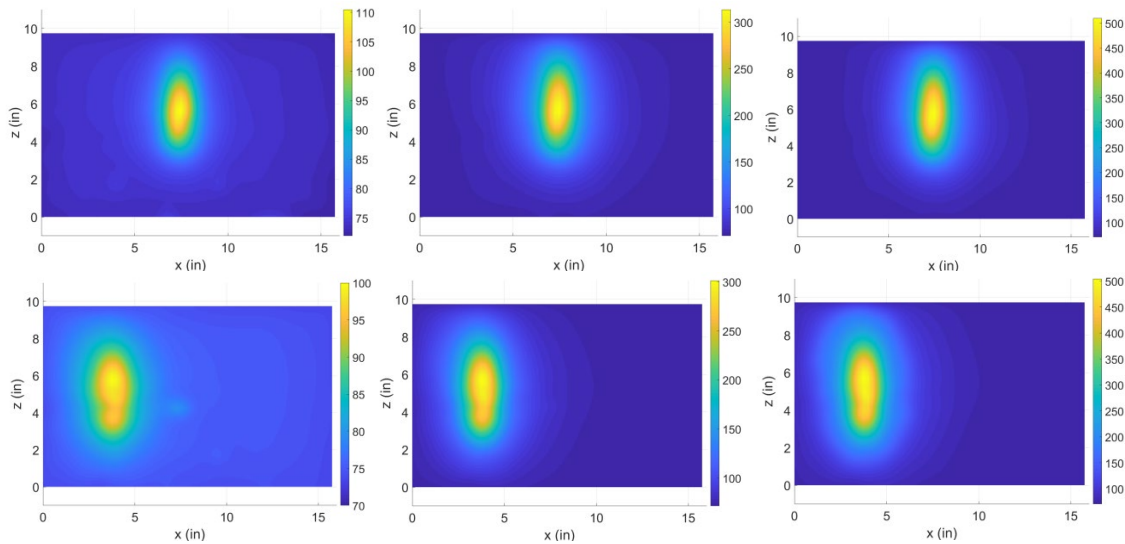


Figure 3.44: Processed Temperature Fields for Usage with the FE Model - Center Heating (top), Quarter Heating (bottom); Left to Right: Low, Medium, and High Peak Temperature

The first set of test data includes a set of six temperature field snapshots and a set of corresponding position coordinate data, both covering the whole panel.

The six temperature field snapshots are divided as two groups: one corresponding to the local heating at the center point (the center heating) and the other at a quarter point (the quarter heating). Each group has three snapshots with different peak temperatures. The six temperature snapshot data were mapped from the measurement grid (2205-by-1555) to the FE mesh (64-by-40), so that they can be used in the ROM construction and validation. In Figure 3.44 are shown the six temperature fields after the processing. This set of six temperature data can be considered as a set of “single-temperature-field” scenarios, in which each data is a single temperature field.

The second set of test data includes a set of 29,848 temperature field snapshots and a set of 99,122 position coordinate data, both covering the whole panel. These snapshots were taken from a heat sweep process in which the heat source moves from the quarter point to the center point. The temperature field data was also processed to obtain the temperature field data on the FE mesh. Six representative temperature snapshots, including the one at the beginning and the one at the end of the heat sweep, are shown in Figure 3.45. This whole set of temperature data can be considered as a “multiple-temperature-field” scenario.

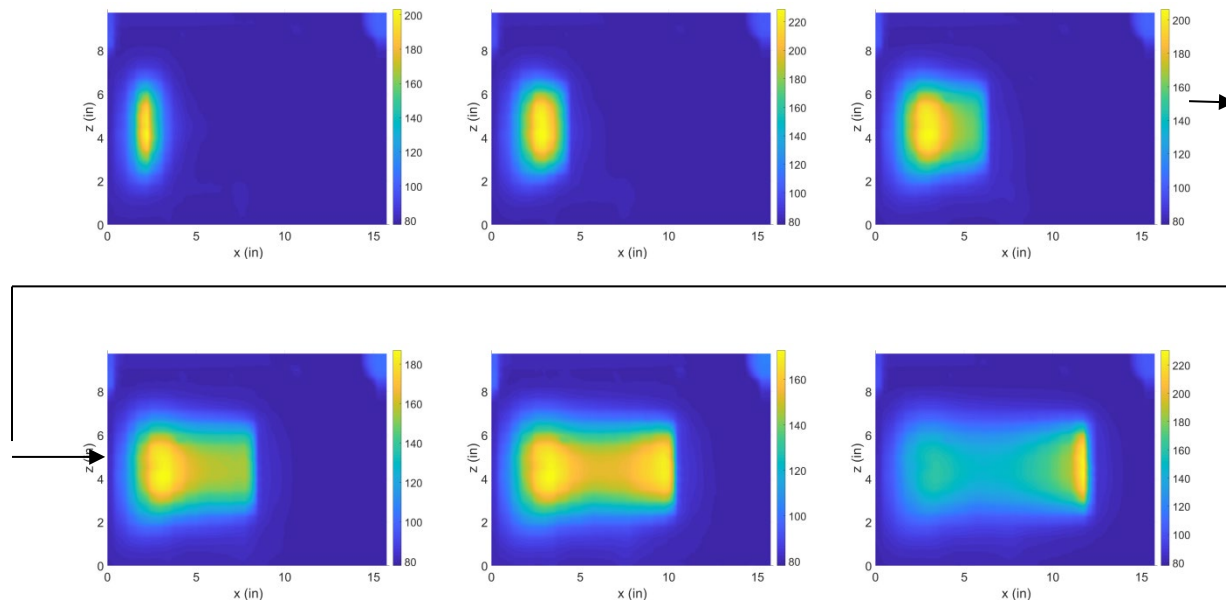


Figure 3.45: Representative Temperature Fields During the Heat Sweep Period

The availability of full field temperature data permits the decoupling of the thermal and structural problems thereby allowing for easier validations of the structural FEM and ROM. Moreover, the availability of full field structural data will permit a close validation of these models.

Achievements:

In the present project, the construction of a coupled structural-thermal NLROM follows the “enrichment” approach, that is, an isothermal (“cold”) NLROM is firstly constructed, then some enrichment modes, which are necessary to account for the thermal effects, are obtained and added to the basis of the isothermal NLROM.

Various structural enrichment options were investigated systematically, from which an optimal enrichment strategy was developed, i.e., using the dominant POD eigenvectors from nonlinear static displacements due to load of temperature fields related to linear combinations of thermal modes. The optimal enrichment strategy was applied to various temperature-field scenarios, and the performance of the constructed ROMs was assessed. It was shown that the strategy performs very well when a small number of thermal modes represents temperature fields well.

When the required number of thermal modes is large, the number of enrichment modes becomes large accordingly, which may bring the instability issue of the NLROM. Methods for the reduction of enrichment modes to improve the NLROM performance were proposed and studied.

Strategy and Results:

Structural Enrichment for Thermal Effects: A Systematic Study of Various Options

The governing equations of the coupled structural-thermal NLROM have been derived based on the thermoelasticity theory. When the structural properties are independent of the temperature and the effects of the latency and the change of geometry are small hence ignored, the governing equations are expressed as [11]

$$M_{ij} \ddot{q}_j + D_{ij} \dot{q}_j + \left[K_{ij}^{(1)} - K_{ijl}^{(th)} \tau_l \right] q_j + K_{ijl}^{(2)} q_j q_l + K_{ijlp}^{(3)} q_j q_l q_p = F_i + F_{il}^{(th)} \tau_l \quad (1)$$

$$B_{ij} \dot{\tau}_j + \tilde{K}_{ij} \tau_j = P_i \quad (2)$$

The thermal effects on the structural deformation are two-folds: on the left hand side (LHS) it alters the linear stiffness of the structure, usually in the softening way which may induce thermal buckling; on the right hand side (RHS) it gives rise to an applied force which induces in plane deformations not well represented by the duals for the membrane stretching effect as shown later.

An isothermal basis of the curved panel is firstly constructed for further enrichment for the thermal effects. The basis is constructed in the regular way. A 19-mode isothermal basis is eventually obtained, which includes the 4 linear modes and 15 dual modes (4L15D). Using the structural responses to the six temperature fields of the single-temperature-field scenario, it was found that the isothermal basis is far from enough to represent the nonlinear static responses well. Moreover, the first 50 linear modes are taken to check the representation error with respect to the linear static responses to the six temperature fields. It turns out that the isothermal basis is not efficient in representing the linear responses either. The structural enrichment for the thermal effects is necessary not only for the nonlinear responses but also for the linear ones. The procedure of constructing the enriched structural basis is as follows:

- 1) An isothermal basis is used as the starting basis for enrichment.
- 2) Linear enrichment: the linear static response to each thermal mode is taken as a linear enrichment mode. The number of linear enrichment modes is thus equal to the number of thermal modes.
- 3) Nonlinear enrichment: temperature fields as linear combinations of the thermal modes are generated and scaled at a set of load levels, and the corresponding nonlinear static responses are found. A POD analysis of these nonlinear static displacements is carried out, and the dominant POD eigenvectors are taken as the nonlinear enrichment modes.

It has been shown in Eqs. (1,2) that the thermal effects are two folds: one left-hand-side (LHS) and one right-hand-side (RHS) effect. When the temperature is high enough, the RHS force is large to induce the nonlinear geometric effect. The nonlinear enrichment is expected to capture such thermal effects.

A set of enrichment options were investigated to see whether a nonlinear enrichment could be successful without the need of the data having all three features. In the following is the list of all the options studied, where the triplet of “1” or “0”, (RHS effect, LHS effect, NL geometric effect),

is used to indicate whether the three features are considered in an option, “1” meaning the feature is considered.

- (1) Hot duals from thermal modes (1,1,1)
- (2) Semi-hot duals from RHS effect of thermal modes (1,0,1)
- (3) Semi-hot linear modes from LHS effect of thermal modes (0,1,0)
- (3a) Buckling modes from LHS effect of thermal modes (0,1,0)
- (4) Hot linear modes from thermal modes (1,1,1)
- (5) Hot Linear-Cold duals (1,0,1)
- (6) Hot linear responses (1,1,0)
- (7) Hot duals from linear responses (1,1,1)

For completeness, it is noted that the linear enrichment corresponds to the triplet (1,0,0) and the cold duals would be cataloged as (0,0,1).

The above enrichment options were implemented with a single-temperature-field scenario, that is, the quarter-heating temperature field at the medium level. For this scenario, the thermal basis has one thermal mode which is the single temperature field. Accordingly, there is only one linear enrichment mode. After adding the linear enrichment mode, the nonlinear enrichment modes derived from each of the above options are added to the 20-mode basis of 4 linear modes, 15 cold duals, and 1 linear enrichment mode (4L15D1EL, common to all options) to obtain the final enriched basis.

Once the basis is obtained, the representation error is computed to study its performance. The representation errors for all the options are shown in Figure 3.46 for the scaled temperature field of quarter heating at the high temperature level with corresponding maximum transverse displacement of 4.01 thicknesses. Note that the first 20 modes (4L15D1EL) are common to all the bases. It can be seen that option 1 is better than the others at all the three displacement levels, and in the transverse and the two in plane directions. Similar behavior is observed for the low temperature (max displacement of 0.24 thicknesses) and the medium (max displacement of 2.55 thicknesses) temperature levels.

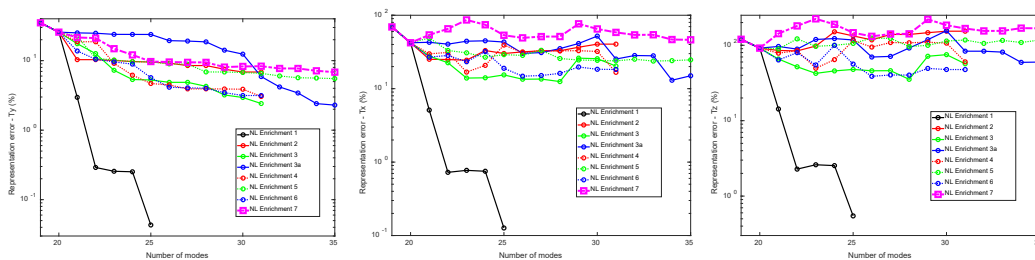


Figure 3.46: Representation Error by Various Enriched Structural Bases of Nonlinear Static Response to Scaled Temperature Field of Quarter Heating - High Displacement Case: 4.01 thicknesses, (a) Transverse, T_y ; (b) In-plane, T_x ; and (c) In-plane, T_z

For the enriched 25-mode basis obtained from the optimal option (option 1), the stiffness coefficients, $K_{ij}^{(1)}$, $K_{ijl}^{(2)}$, and $K_{ijlp}^{(3)}$, and the structural-thermal coupling coefficients, $K_{ijl}^{(th)}$ and

$F_{il}^{(th)}$, were identified. Validations of the NLROM were carried out for the quarter heating at different peak temperatures. Shown in Figure 3.47 are the comparison between the Nastran results and this 25-mode NLROM predictions. An excellent agreement is obtained as well up to the displacement level close to 4 thicknesses.

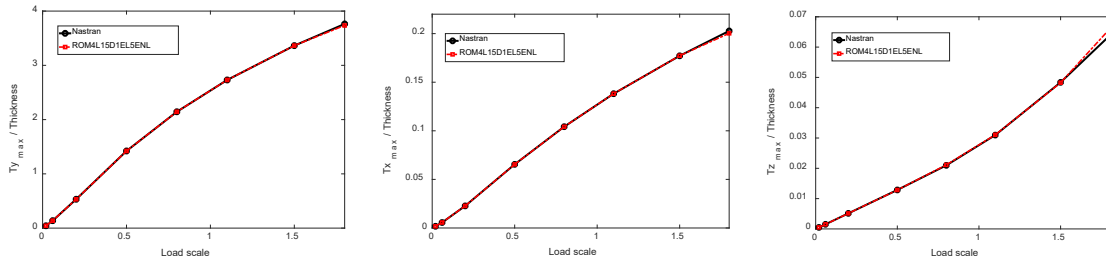


Figure 3.47: Validation of the 26-mode ROM, Quarter Heating. (a) Transverse, T_y ; (b) In plane, T_x ; and (c) In plane, T_z . Maximum Displacement

Structural Enrichment for Thermal Effects: Two-temperature-field Scenario

Before proceeding to the ultimate multiple-temperature-field scenario, the optimal structural enrichment strategy was applied to an intermediate two-temperature-field scenario. This scenario includes two single-temperature-field scenarios, i.e., the ones at the medium temperature level of the quarter and the center heating, plus a linear combination of the two, half-half as shown in Figure 3.48 or a random combination.

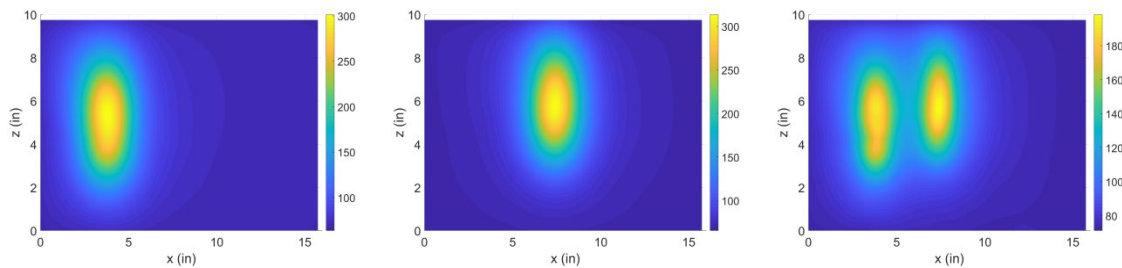


Figure 3.48: Set of 3 Temperature Fields of the Two-temperature-field Scenario (left to right) Quarter Heating, Center Heating, Linear Combination of the Two

The temperature fields corresponding to the quarter and the center heating are taken as two thermal modes, and the optimal enrichment strategy for the single-temperature-field scenario is extended by using the nonlinear static response data (displacement) to the temperatures constructed as a linear combination (half-half) of these two thermal modes. These temperatures are scaled at a set of load levels so that the displacement data cover the range from nearly linear to strongly nonlinear (usually about 4 thicknesses). In total, 16 enrichment modes were selected, leading to a 37-mode (4L15D2EL16ENL) basis.

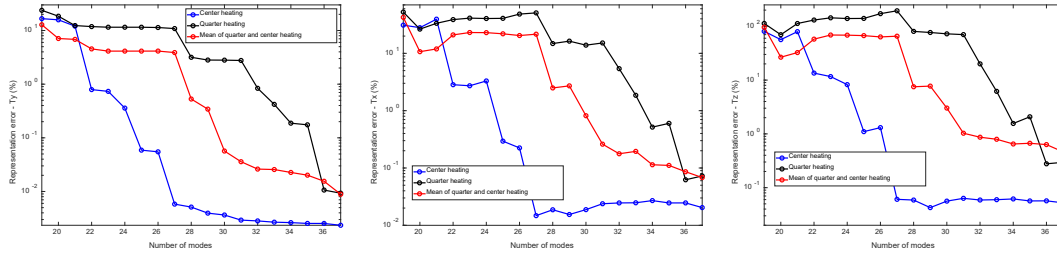


Figure 3.49: Representation Error by the 37-mode and the 38-mode Enriched Structural Bases of Nonlinear Static Responses to Two-temperature-field scenario - (a) Transverse, Ty; (b) In-plane, Tx; (c) In-plane, Tz

The representation error by this basis of the nonlinear displacements due to the three temperature fields are shown and compared in Figure 3.49. It can be seen that the 37-mode enriched basis (with the combination of equal weight) has very small representation errors ($< 1\%$) in the transverse and both in-plane directions, and for all the three temperature fields.

The structural stiffness and the structural-thermal coupling coefficients of the 37-mode enriched basis were identified, and the predictions of structural responses to a random combination the two temperature fields by the ROM were computed and validated against Nastran results. The temperature field is scaled by a load factor up to 2.5, giving rise to the maximum transverse displacement of about 4.5 thicknesses.

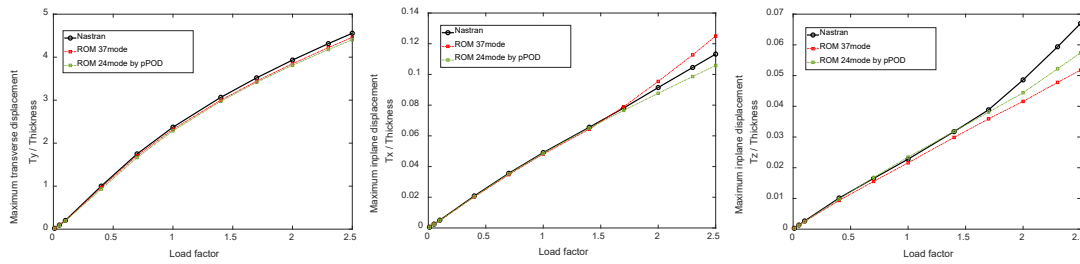


Figure 3.50: Predictions of Nonlinear Static Responses to One-temperature-field of Scenario 4 by the 37-mode Enriched ROM and Their Reduced Counterparts by the pPOD Method - (a) Transverse, Ty; (b) In-plane, Tx; (c) In-plane, Tz

In Figure 3.50 are shown the validation results; the ROM gives very good predictions of transverse displacements and good predictions of in-plane displacements. In the figure are also presented a 24-mode ROM reduced from the 37-mode ROM obtained by the progressive POD (pPOD) method, to be discussed in the sub-section of “reduction of enrichment modes.”

Structural Enrichment for Thermal Effects: Multiple-temperature-field Scenario

In order to apply the optimal enrichment strategy to the multiple-temperature-field scenario, the first task is to construct a thermal basis which represents the multiple temperature fields well. To this end, a thermal basis was constructed by performing the POD analysis of a smaller set of 300 temperature fields, roughly taken every 100 snapshots from the whole set of nearly 30,000

snapshots. The corresponding POD eigenvalues decrease rapidly for the first 50 POD eigenvectors or so, and the decreasing becomes slower afterwards.

By setting the criterion of representation error to be 1%, it was found that the set of 300 temperature fields can be represented very well by taking the uniform temperature as the first thermal mode then adding the first 20 POD eigenvectors to give rise to a 21-mode thermal basis. In fact, the representation error of this thermal basis with respect to the entire set of temperature field data (nearly 30,000 snapshots) is below 0.75%, suggesting that the 21-mode thermal basis might be more than sufficient. As an intermediate step, the first 5 of the 21 thermal modes were taken (for which the representation error is about 6%) and the enrichment process was carried out.

For the linear enrichment, the linear static responses to the temperature loads of these five thermal modes were taken as five linear enrichment modes. The 15 combinations of these five modes with equal scaling on all three modes at 7 different levels were generated and the corresponding nonlinear static responses (displacements) were determined. From the POD analysis of this set of data, 67 nonlinear enrichment modes were selected, giving rise to a 91-mode enriched structural basis which includes the same 4 linear modes and 15 duals as before, plus 5 linear and 67 nonlinear enrichment modes (4L15D5EL67ENL). This basis is quite large and will probably bring some difficulties in the identification of the ROM coefficients. Therefore, the methods of reducing the number of enrichment modes were investigated before proceeding to identify the coefficients of the 91-mode basis.

Reduction of Enrichment Modes by the Progressive POD (pPOD) Method

The progressive POD (pPOD) method [29] was originally developed for the reduction of the CFD data stored in multidimensional arrays. As applied to the reduction of the number of enrichment modes, the basic idea is doing a successive POD operation with the matrix of POD coefficients when projecting the displacement data on the enrichment modes, and using the dominant POD eigenvectors to that is,

This pPOD reduction method was firstly implemented with the 37-mode enriched basis for the two-temperature-field scenario, which has 16 nonlinear enrichment modes. The successive POD leads to 16 secondary POD eigenvectors, and it spears that the first three POD eigenvectors are dominant. Three new enrichment modes can be derived from these three secondary POD eigenvectors to replace the original 16 enrichment modes, and the basis is reduced from 37 modes to 24 modes. The structural stiffness and the structural-thermal coupling coefficients of the reduced 24-mode basis were identified, and the predictions of the ROMs are shown in Fig. AF607, as compared to the original 37-mode ROM and the Nastran results. The pPOD reduced ROM has similar good predictions.

The pPOD reduction method was further applied to the 91-mode enriched basis for the multiple-temperature-field scenario. For this scenario, the displacement data used in the construction of nonlinear enrichment modes is a 3D matrix by its physical nature: the dimensions of structural degrees of freedom, N_{dof} , the load levels, N_{load} , and the combinations, N_{combo} .

There are two arrangements in the implementation of the pPOD method. In the first arrangement (pPOD1), the 2D data blocks, $N_{dof} \times N_{load}$, for each combination out of N_{combo} , were taken

from the displacement data, and the first POD step was carried out one combination by one combination. The dominant POD eigenvectors, selected as the enrichment modes from the first POD step, are stacked together as the final set of enrichment modes. A second POD step is then performed with the matrix of POD coefficients when projecting the displacement data on the final enrichment modes. In the second arrangement (pPOD2), the 2D data blocks, $N_{dof} \times N_{combo}$, for each load level out of N_{load} , were taken from the displacement data, and the first POD step was carried out one load level by one load level. Similarly, the dominant POD eigenvectors, selected as the enrichment modes, are stacked together as the final set of enrichment modes for this arrangement. A second POD step is performed with the matrix of POD coefficients when projecting the displacement data on the enrichment modes.

The six representative temperature fields of the multiple-temperature-field scenario shown in Figure 3.45 were used as temperature loads to compute the nonlinear static displacements. Each temperature field was scaled at 8 load levels, so that the maximum transverse displacements are in the range of 3.2 to 4.0 thicknesses. The displacement data were used to assess the performance of the enriched 91-mode and 69-mode bases obtained from the above two pPOD arrangements, respectively.

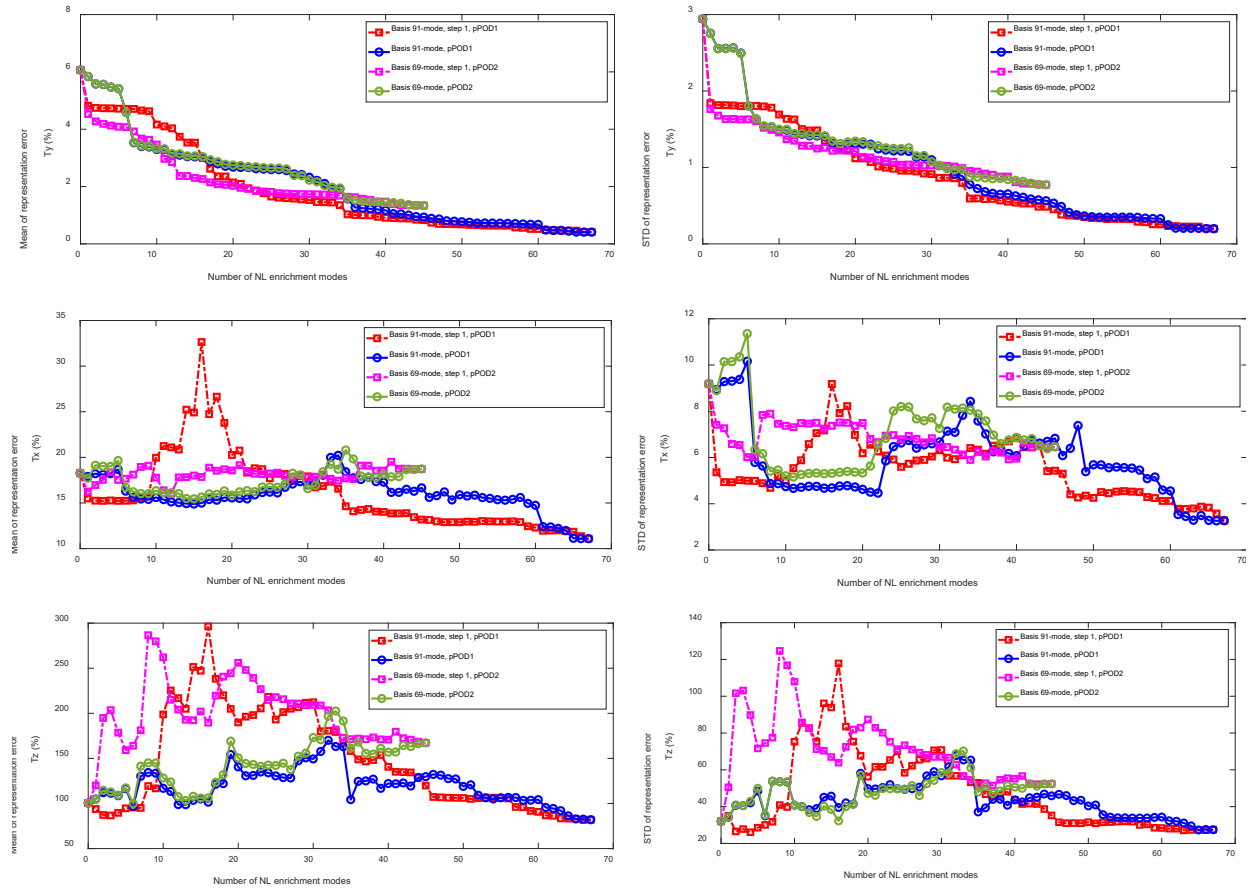


Figure 3.51: Representation Error with Respect to Nonlinear Static Responses to 6 Representative Temperature Fields of the Bases from 2 pPOD Arrangements - (a) Mean; (b) Standard deviation; (from top to bottom) Transverse, T_y ; In-plane, T_x ; In-plane, T_z

In Figure 3.51 are shown the mean (left column) and the standard deviation (right column) of the error for the bases obtained from the two pPOD arrangements. The second pPOD arrangement has almost the same performance as the first one eventually, although the representation error after the first POD step is quite different. In both pPOD arrangements, the first eight pPOD eigenvectors appear to be dominant for the transverse (T_y) and the dominant in-plane (T_x) displacements, and they reduce the representation error quickly. For the other in-plane (T_z) displacement, dominant pPOD eigenvectors cannot be found and the error remain large.

Reduction of Enrichment Modes by the Method of Static Condensation

The reduction of nonlinear enrichment modes is further studied by using the method of the static condensation. For the static condensation to be applicable to a mode, its eigenvalue should be large enough that the response due to the mode can be considered quasi-static and small. To this end, the 37-mode basis for the two-temperature-field scenario is taken as the first example, and the eigenvalues of its 16 nonlinear enrichment modes are computed and compared with those of its 4 linear modes and 15 dual modes. It was found that the range of the eigenvalues of the nonlinear

enrichment modes is between the one of linear modes and the of dual modes, with some overlap. It is thus expected that when the 16 nonlinear enrichment modes are rotated by their eigenvectors, the rotated modes which have larger eigenvalues are not significant and can be statically condensed.

For the structural-thermal coupled ROM, the static condensation is more complicated since the structural-thermal coupling coefficients need to be considered. In addition, the linear coupling stiffness coefficients and the in plane static forces which are usually ignored in the static condensation are considered as well.

The formulation of static condensation is described as follows using a 1T1E ROM as an example, where t and e denote the modes to take (transverse, dual, and dominant enrichment) and the modes to eliminate (non-dominant enrichment), respectively, from the original “full” ROM.

The equations of motion for the static problem are written as

$$K_{tt}^{(1)} q_t - K_{ttl}^{(th)} q_t \tau_l + K_{te}^{(1)} q_e - K_{tel}^{(th)} q_e \tau_l + K_{ttt}^{(2)} q_t^2 + K_{tte}^{(2)} q_t q_e + K_{ttt}^{(3)} q_t^3 = F_t + F_{tl}^{(th)} \tau_l \quad (3)$$

$$K_{ee}^{(1)} q_e - K_{eel}^{(th)} q_e \tau_l + K_{et}^{(1)} q_t - K_{etl}^{(th)} q_t \tau_l + K_{ett}^{(2)} q_t^2 = F_e + F_{el}^{(th)} \tau_l \quad (4)$$

in which the nonlinear terms of the enrichment have already been eliminated consistently with the expectation that the corresponding generalized coordinate is “small”. From Eq. (4), one obtains

$$q_e = \frac{\left[F_e + F_{el}^{(th)} \tau_l \right] - \left[K_{et}^{(1)} q_t - K_{etl}^{(th)} q_t \tau_l + K_{ett}^{(2)} q_t^2 \right]}{K_{ee}^{(1)} - K_{eel}^{(th)} \tau_l} \quad (5)$$

Substituting Equation 5 into Equation 3, and after some manipulations, the reduction equation by static condensation was obtained, written as

$$\begin{aligned} & \left[\hat{K}_{tt}^{(1)} - \hat{K}_{ttl}^{(th)} \tau_l - \hat{K}_{tllm}^{(th)} \tau_l \tau_m \right] q_t + \left[\hat{K}_{ttt}^{(2)} - \hat{K}_{tttl}^{(th)} \tau_l \right] q_t^2 + \hat{K}_{ttt}^{(3)} q_t^3 \\ & = F_t + \hat{F}_{tl}^{(th)} \tau_l + \hat{F}_{tllm}^{(th)} \tau_l \tau_m - K_{te}^{(1)} (F_e / \hat{K}_{ee}^{(1)}) \end{aligned} \quad (6)$$

where the “hat” stiffness coefficients and modal forces are now functions of temperature owing to the dependence of all terms on $\hat{K}_{ee}^{(1)} = K_{ee}^{(1)} - K_{eel}^{(th)} \tau_l$. The linear stiffness matrix and the modal force are quadratic functions, and the quadratic stiffness matrix is a linear function of modal temperature, respectively. That is, the temperature dependence of the condensed model is more complex than of the original model.

This method of static condensation has been carried out with the 37-mode basis for the two-temperature-field scenario. Among the 16 rotated nonlinear enrichment modes, the eigenvalues of the last 10 modes appear to be larger than the rest, thus are currently being considered as the modes to eliminate, i.e., to be condensed. This work is still in progress.

3.2.B: Adaptive Multi-Scaling (Spatial and Temporal)

3.2.1. B.1: Linking Solid and Dimensionally Reduced Models

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Period of Activity: 7/2013 – 02/2020

Long duration simulation of structural components of high-speed aircrafts using 3D solid elements is neither computationally feasible nor necessary, given the geometrical characteristics of these components. Dimensionally reduced models such as plates, shells and beams, can approximate the exact solution with high accuracy, and at a significantly reduced cost, at several regions of such components. Nonetheless, the extreme environment these components are exposed to, leads to complex and fully 3D stress states at several localized regions. Reliable failure and life prediction of these components require computational models able to accurately approximate highly localized three-dimensional stress states. Computational efficiency, however, requires that a combination of shells and fully 3D models be employed. This project aims to formulate and implement a multiscale computational framework capable of efficiently resolve localized effects in large structures. This framework couples structural-scale shell models defined in a commercial software and 3D GFEM discretizations implemented in another code. The coupling is non-intrusive – it requires no modification of the commercial code – and it accounts for two-way interactions between structural and non-linear, time-dependent localized responses around spot welds, fractures, sharp thermomechanical gradients, etc.

A main challenge in combining shells and fully 3D models is that they are governed by different sets of partial differential equations. This challenge has traditionally been dealt with using ad-hoc solutions based on engineering intuition and experience. These methods essentially attempt to enforce displacement continuity between shells and 3D models. This can be formulated at the discrete (finite element) level, or continuum (variational principle) level. In the first case, finite elements for shells are connected with finite elements for 3D elasticity. The connection involves node-to-node equivalence, multi-point algebraic constraints or the use of rigid beams between shells and 3D FEM nodes. This is not only a labor-intensive process but, mostly important, not a robust one. Two analysts will in general get very different solutions depending on how they connected these two classes of elements. Multi-point constraints are not recommended for time-dependent simulations involving, e.g., stress waves since the point-by-point interface between shells and 3D FEMs leads to spurious effects such as reflected waves, artificial stress concentration or singularities. Reliable failure or life assessment is not possible in these models. The second approach to combine shells and 3D models involves, for example, the introduction of a Lagrange multiplier field or one of its variants, such as the so-called mortar element method. A major issue with this approach is the numerical stability of the model.

Methodology Overview

A method [42] has been identified to capture locally large, transient, thermal spatial gradients on relatively course meshes through the so-called GFEM with global-local enrichment functions (GFEM^{gl}). This method can be thought of as a traditional finite element formulation that is augmented with enrichment functions to capture localized events of interest. It combines features

of adaptive mesh refinement with global-local finite element analysis while being computationally efficient and able to capture interactions among multiple spatial scales. In this project, the GFEM^{gl} was combined with the Iterative Global-Local (IGL) [43-46] method with the goal of combining shells with 3D elasticity models. In this framework, the GFEM^{gl} captures localized thermomechanical responses on coarse meshes via enrichment functions provided by parallel simulations of local boundary value problems where local features are accurately modeled and resolved. The IGL, in turn, provides a robust and non-intrusive approach to establish a two-way coupling between structural models defined in a commercial code, with the GFEM^{gl} implemented in another code. The computational framework developed in this project is hereafter denoted as IGL-GFEM^{gl}. Figure 3.52 illustrates the methodology. Technical details on the IGL-GFEM^{gl} are presented in [47, 48]. The main benefits of this computational framework and two application examples are presented in the next sections. Details on the GFEM^{gl} developed as part of this and closely related projects are presented in references [49-53]. Other non-intrusive algorithms of potential interest are described in [54, 55].

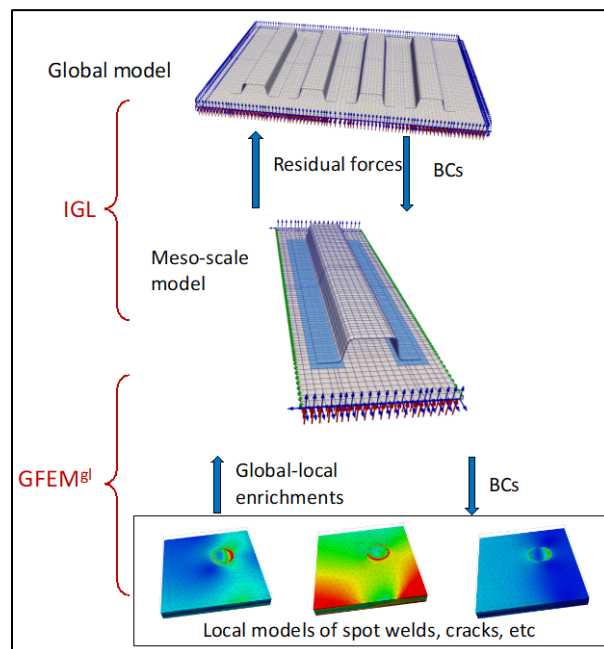


Figure 3.52: Overall Multiscale Framework Combining IGL and GFEM^{gl} [47, 48] - (top) Structural Scale/Global Model, (middle) Meso-scale Model, (bottom) Local Models Defined Around Spot Welds

Features and Benefits of the Multi-scale Framework

In the computational framework developed in this project, the structural model can be solved by legacy FEM codes, thus leveraging the vast library of classical finite elements and algorithms available in these codes. The FEM adopts coarse meshes of defeatures models – small-scale features such as spot welds, cracks, etc., are ignored in this model. The meso-scale model also adopts simple meshes that are compatible with the global one. This makes the transition between global- and meso-scale meshes straightforward. The local model can adopt different element type

from the one adopted in the meso or global model. Automatic mesh refinement based on tetrahedron elements is typically used at this scale. Furthermore, the local mesh need not fit fine-scale features such as cracks or spot welds since local problems are solved using the GFEM as described in [47, 49-53]. It is also noted that the number of degrees of freedom adopted in the local problems has no impact on the meso-scale problems: only three-degrees of freedom are added to meso-scale nodes enriched with local problem solutions, regardless of the local problem size.

Application Examples: Hat-stiffened Panel with One Stiffener

The first example is a hat-stiffened panel with one stiffener. There are 42 spot welds in the domain connecting the skin with the stiffener. The objective of this simulation is to show the effectiveness of the methodology for solving representative structures and handling a large number of local features. Further details can be found in [47, 48].

The geometry of the panel is shown in Figure 3.53. The radius of each spot weld is $r_{\text{weld}} = 0.07$ in. The thickness of the skin panel and stiffeners are $t_{\text{skin}} = 0.0625$ in and $t_{\text{stiff}} = 0.032$ in, respectively. The height of the stiffeners is $h_{\text{stiff}} = 1.0$ in.

As for boundary conditions, a uniformly distributed pressure $p_0 = 1.0$ psi is applied to the surface of the skin panel (i.e., the side where there is no stiffener). The edges at $x = 0$ and $x = 0.5065875$ are assigned symmetry displacement boundary conditions. The edges as $z = 0$ and $z = 15$ are fixed in all directions. The material properties are Young's modulus $E = 1.67 \times 10^7$ psi and Poisson's $\nu = 0.32$.

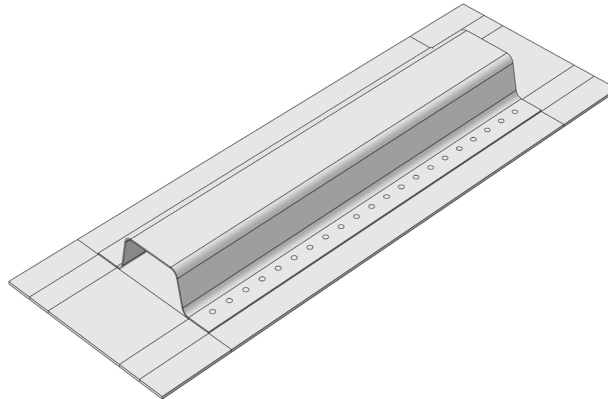


Figure 3.53: Hat-stiffened Panel with One Stiffener

The reference solution of this problem is obtained through a Direct Finite Element Analysis (DFEA) using Abaqus. The reference model is discretized using quadratic tetrahedral elements (Abaqus element C3D10). A zoom in view of the mesh is shown in Figure 3.54. It is noted that this is a high-fidelity model with heavy mesh refinements in the neighborhood of all spot welds in order to capture the localized stress field.

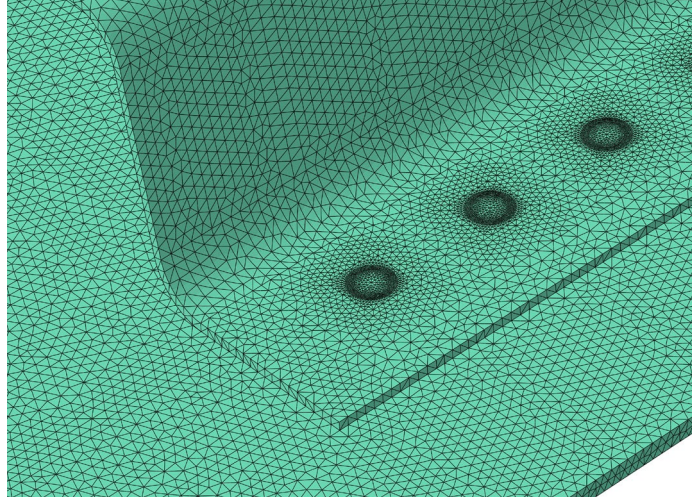


Figure 3.54: Zoomed-in View of Abaqus C3D10 Mesh for the Panel with One Stiffener

The global and mesoscale meshes are shown in Figure 3.55. A typical local problem mesh discretizing a spot weld is also shown. Boundary conditions are shown on the global mesh and the blue region denotes the domain of interest. Mesoscale nodes enriched with a local problem solution are shown as colored glyphs. The global model is solved in Abaqus on a coarse hexahedral mesh. C3D20R elements are adopted. It is noted that the parallel GFEM^{gl} presented in [24] is adopted to bridge the local and mesoscale models and to model the spot welds. The mesoscale and local problems are solved using a GFEM solver. The mesoscale model is discretized using 20-node quadratic hexahedral elements. Along the global-mesoscale interface, the meshes of the two scales match each other. The local models are discretized with linear tetrahedral elements enriched with linear polynomials. Spot welds are represented only at the local scale.

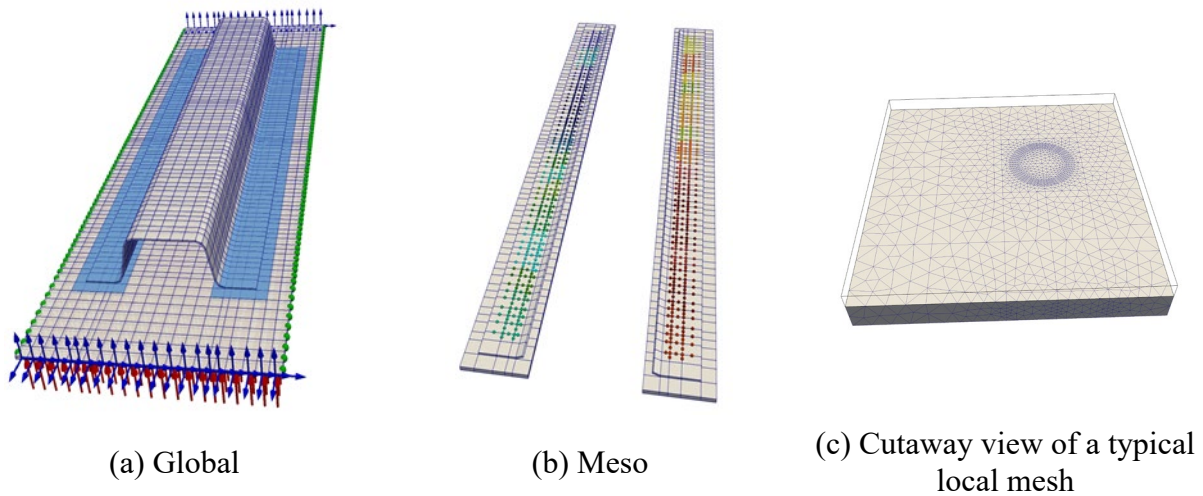


Figure 3.55: Global, Meso, and Local Meshes for Solving Problem of Panel with 1 Stiffener Using IGL-GFEM^{gl}

One advantage of the IGL-GFEM^{gl} is that it avoids the need for representing all local features in the global domain. In this problem, the spot welds are modeled only at the local level while the global and mesoscale models are discretized using coarse and easy-to-generate meshes. Thus, the user time for an IGL-GFEM^{gl} analysis is much less than for a DFEA. In any numerical simulation of representative structures, the model preparation time can be loosely decomposed as mesh generation time and mesh modification time. Mesh generation time is the time spent by the user on discretizing the given structure/model at the beginning of the design and validation process. Mesh modification time is the time spent on modifying the existing mesh in order to account for any changes in the geometry and features during design iterations. Table 3-2 compares the user time of an IGL-GFEM^{gl} simulation to a DFEA based on the stiffened panel problem. Generating the mesh in Abaqus requires carefully partitioning of the domain based on the spot weld locations and geometry. Depending on the partitions the user created and the meshing parameters (e.g., element types and mesh density at different locations), the mesh generator sometimes fails. Multiple trial and error iterations are needed. The Abaqus mesher usually works well when the mesh is not highly refined. However, for the required mesh density in this example, it is not very robust and could fail many times. In contrast, the IGL-GFEM^{gl} does not require densely refined meshes at the global or meso scales. They are coarse and fairly easy to generate. At the local scale, only a representative local mesh needs to be prepared and then the code can automatically handle the repetitive pattern of the spot welds. As for mesh modification, the user time of a DFEA varies depending on the type of design changes made to the target structure. Minor changes in the size, location, and number of spot welds may require relatively small amount of time to modify the existing mesh. However, in many occasions, the change may require the user to regenerate all the partitions and features on the Abaqus model and re-mesh the whole domain, which could be as labor-intensive as the initial mesh generation process. On the other hand, in an IGL-GFEM^{gl} analysis, there is no need to modify the global and meso-scale meshes. The user only needs to regenerate the representative local mesh in order to reflect the changes in local features. To summarize, the multiscale framework developed in this project reduces the user time significantly as compared to a DFEA. Also, many design iterations are often needed when developing realistic products and structural components.

Table 3-2: User Time Comparison - DFEA vs. IGL-GFEM^{gl} Analysis of Stiffened Panel Problem

	Mesh generation	Mesh modification
DFEA	~ 10 hrs	~ 2-10 hrs
IGL-GFEM ^{gl}	~ 2 hrs	~ 1-2 hrs

The problem sizes for the different solution methods are summarized in Table 3-3. It is noted that the IGL-GFEM^{gl} requires significantly less computational resource when dealing with large structural components. The number in parentheses is the number of mesoscale dofs without global-local enrichments.

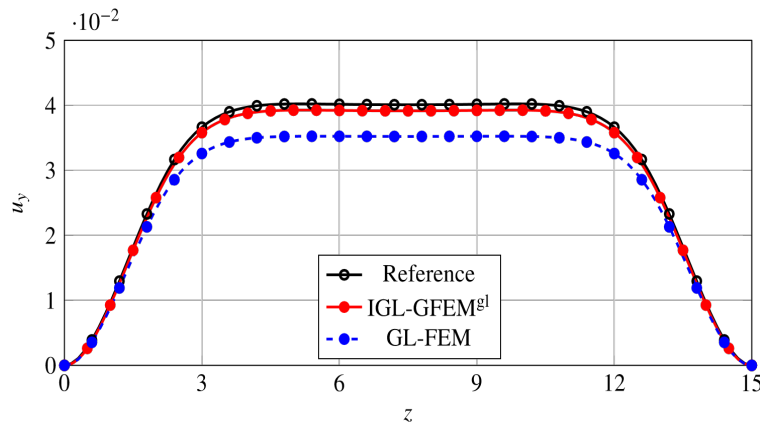
Table 3-3: DFEA and IGL-GFEM^{gl} Problem Sizes in dofs for the Panel with 1 Stiffener

Method	Problem size (dofs)		
	Global	Meso	Local
IGL-GFEM ^{gl}	72,702	97,200 (86,094)	194,964 – 349,512
Reference		18,159,126	

Table 3-4 lists a comparison between the accuracy of the IGL-GFEM^{gl} and GL-FEM for the maximum displacement on the panel. Figure 3.56 plots the out-of-plane displacement u_y along the right edge of the panel. The one-way coupling used in the GL-FEM yields inaccurate solutions and underestimates the deflection of the panel, while the IGL-GFEM^{gl} accurately approximates the global response.

Table 3-4: Maximum Displacement u_y (unit: inch) for Panel with 1 Stiffener Computed with DFEA, GL-FEM, and IGL-GFEM^{gl}

Method	Max u_y	
	Value	Rel. error (%)
IGL-GFEM ^{gl}	0.0393	2.24
GL-FEM	0.0352	12.44
Reference	0.0402	

**Figure 3.56: Displacement u_y Along the Right Edge of Panel from DFEA, IGL-GFEM^{gl}, and GL-FEM Solutions**

The von Mises stress fields obtained from different solution methods are shown in Figure 3.57. It is noted that the global (Abaqus) and mesoscale (GFEM) solutions are patched together in the IGL-GFEM^{gl} and GL-FEM contour plots. It can be observed that the IGL-GFEM^{gl} is able to resolve the localized stress field with high accuracy on a coarse mesh. The GL-FEM, on the other hand, underestimates the stress concentration in the neighborhood of spot welds.

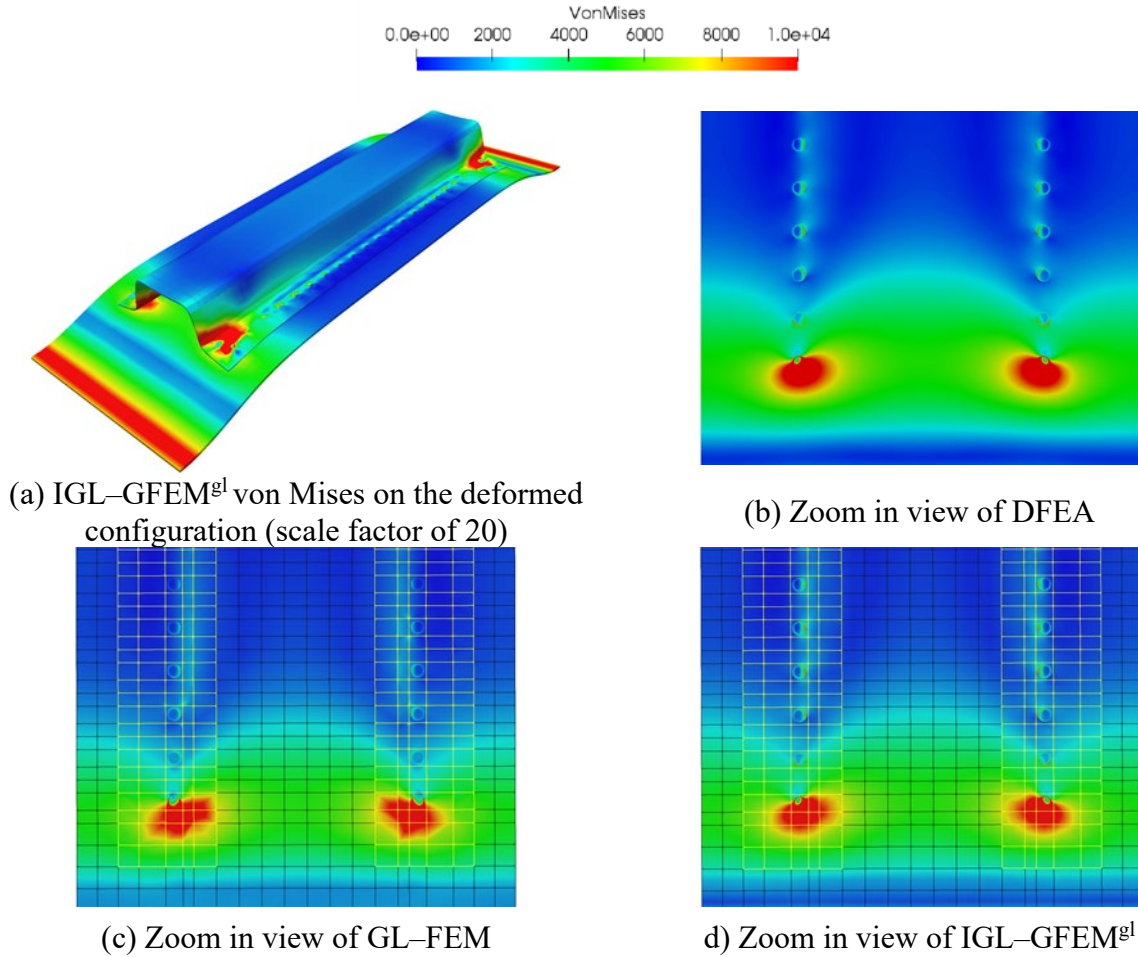


Figure 3.57: Contour Plots of von Mises Stress on Skin of Panel with 1 Stiffener from DFEA, GL-FEM, and IGL- GFEM^{gl} Solutions

Application Examples: Welded T-Joint with a Crack

The welded joint shown in Figure 3.58 is analyzed in this section. The goal of this problem is to demonstrate the ability of the IGL- GFEM^{gl} to adopt shell elements at the structural scale. Further details can be found in [47, 48].

There are two local details that need to be modeled in this problem. The first one is the fillet welds connecting the two plates. Note that the plates are connected only through the welds. There is a zero-thickness seam (denoted by the gray area shown in Figure 3.58) at the interface between the two plates. Those surfaces are traction-free and unconstrained. In other words, the displacement field will be discontinuous across the seam as the structure deforms. The second fine-scale feature is a half-circle crack at the weld-plate interface as shown in Figure 3.58.

The left ($x = 0$) and right ($x = 62$) boundaries of the T-joint are fixed in all directions and the front ($z = 30$) and back ($z = 0$) boundaries are assigned symmetry boundary conditions. The top surface

of the vertical plate ($y = 32$) is assigned uniform tractions $t^-(x, 32, z) = 5$ ksi. Material properties, $E = 2.9 \times 10^4$ ksi and $\nu = 0.3$, are adopted.

The reference solution of this problem is obtained by a Direct GFEM Analysis (DGFEA). The discretization of the reference model adopts linear tetrahedral elements enriched with linear polynomials. Special enrichment functions are used to model the crack.

The global and mesoscale models used in the IGL-GFEM^{gl} analysis are shown in Figure 3.59. The global shell model is defined along the mid-surface of the two plates. It does not contain any local feature. The mesoscale and local models are solved by the GFEM solver. The mesoscale model is discretized using linear hexahedral elements with its nodes not at the interface enriched with quadratic polynomials. The fillet welds are represented at this scale. The local mesh consists of linear tetrahedral elements with linear polynomial enrichments and special enrichments to represent the crack.

The deformed configurations from the DGFEA and IGL-GFEM^{gl} simulations are shown in Figure 3.60. The global and mesoscale solutions are combined to provide the final solution over the whole domain. The maximum vertical displacements obtained from different solution strategies are listed in Table 3-5. The results show that the IGL-GFEM^{gl} with the shell-solid coupling can approximate well the global response. As expected, the GL-FEM significantly overestimates the deformation of the structure.

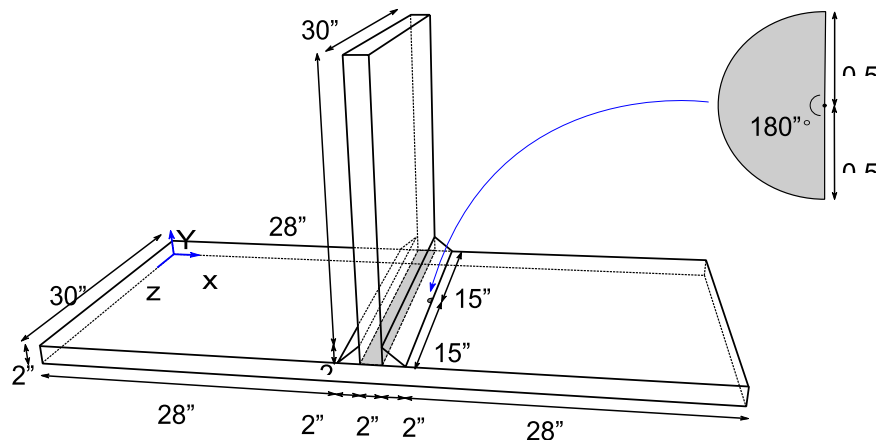


Figure 3.58: Welded T-joint with a Crack

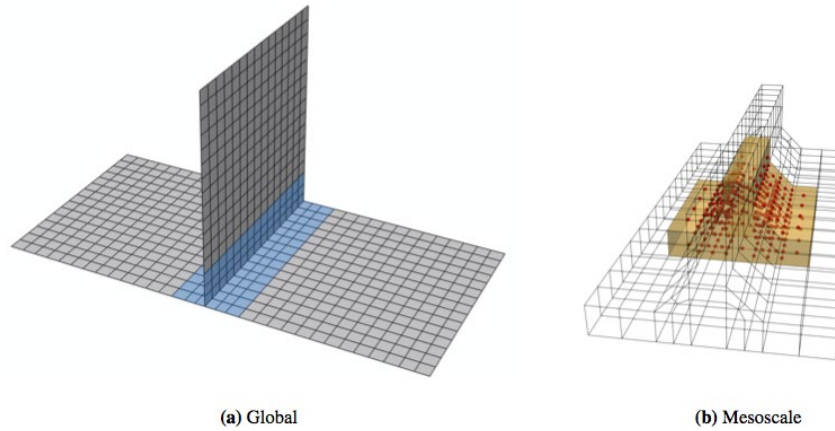


Figure 3.59: Global and Mesoscale Meshes for T-joint with a Crack Solved Using IGL-GFEM^{gl} with sShell-solid Coupling- Blue & Yellow Regions Denote Mesoscale and Local Domains; Red Glyphs Denote Nodes with Global-local Enrichments

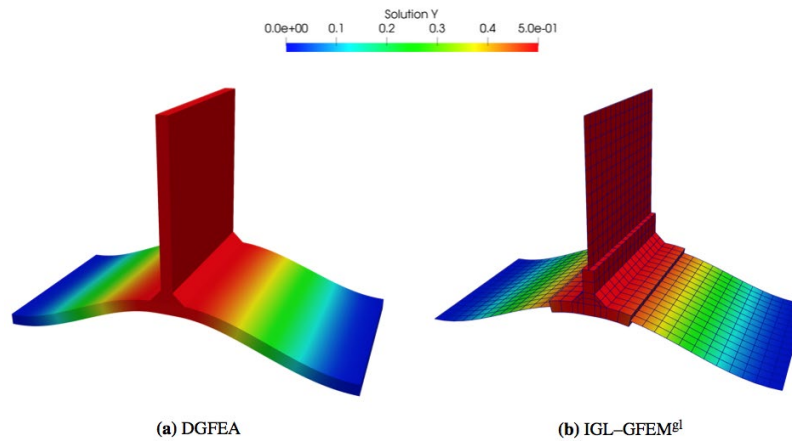


Figure 3.60: Contour Plots of Displacement u_y on Deformed Configuration (Scale Factor of 20) of T-joint from tDGFEA and IGL-GFEM^{gl} Solutions

Table 3-5: Maximum Displacement u_y (unit: inch) for T-joint Problem from DGFEA, GL-FEM, and IGL-GFEM^{gl} Solutions with Shell-solid Coupling

Method	Max u_y	
	Value	Rel. error (%)
IGL-GFEM ^{gl}	0.5092	1.32
GL-FEM	0.6076	17.75
Reference	0.5160	

3.2.2. B.2: Linking Polycrystalline and 3D Solid Models

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Period of Activity: 7/2013 – 4/2020

Structural metals and alloys are generally characterized by heterogeneous polycrystalline microstructures, exhibiting nonuniform dispersions of crystallographic orientations and misorientations, colony structures, multiple phases etc. The mechanical response and failure characteristics of structures of these materials are strongly influenced by the microstructural heterogeneities. To realize microstructural effects in structural simulations, it is important to incorporate material microstructure-integrated multiscale constitutive models in structural analysis models and codes. Yet, structural analysis in engineering practice often ignores microstructural influence. This may be largely attributed to the lack of computationally efficient, microstructure-sensitive constitutive models. Typically, simple material constitutive models like isotropic elasticity or J_2 -plasticity are used, where material properties are either extracted from handbooks. Macro-scale material properties like stiffness, strength and hardening response of metals like Titanium alloys, inherently depend on underlying microstructural features such as crystallographic texture, misorientation and grain size distributions. Simple elasticity or J_2 plasticity models cannot capture the microstructure-dependent mechanical and failure characteristics exhibited by these alloys. To avoid these limitations, this project aims to develop a microstructure-integrated parametrically homogenized constitutive model (PHCM). PHCM bridges length-scales by linking polycrystalline and solid models through explicit representation of microstructural descriptors in macro-scale constitutive models. PHCMs overcome high computational costs of other multiscale methods and enable highly efficient large scale structural simulations.

A systematic development of PHCM that links polycrystalline models with 3D solid models requires a sequence of steps [74] outlined in Figure 3.61. These steps are discussed below.

1. *Generating Statistically Equivalent Virtual Microstructures and SERVEs*: The first step generates 3D statistically equivalent virtual microstructures (SEVMs) with statistical distribution functions that are equivalent to those extracted from electron backscatter diffraction (EBSD) image data sets. These SEVMs capture the statistics of characteristic morphological and crystallographic descriptors, such as (i) grain size, (ii) grain aspect ratio, (iii) grain orientation, (iv) grain crystallographic orientation and (v) crystallographic misorientation with neighboring grains. Sensitivity analysis with respect to these descriptors is used to identify representative aggregated microstructural parameters or RAMPs for constitutive parameters in the PHCM. Subsequently the microstructure-based Statistically Equivalent Representative Volume Element or *M-SERVE* is determined from optimal convergence of morphological and crystallographic statistics of the microstructure [75, 76].
2. *Creating a Micromechanical Image-based CPFE Model of the M-SERVE*: Developing PHCMs requires data from a large number of micromechanical simulations of representative polycrystalline microstructures. A necessary ingredient for this activity is an experimentally validated crystal plasticity FE model of the M-SERVE. In this step, crystal plasticity constitutive parameters are first calibrated from experimental test data, followed by validation of the image based CPFE model with respect to averaged response.

3. *Selecting the Mathematical Forms of PHCM Equations:* A very important aspect in the development of PHCMs is the choice of appropriate mathematical forms of the constitutive relations for a given material. These forms must adequately represent all characteristics of macroscopic response of the material. For example, for the alloy Ti6242S, the chosen forms must reflect microstructure dependent (i) elastic and plastic anisotropy, (ii) tension-compression asymmetry, and (iii) strain-rate and temperature dependencies. Furthermore, the forms must also be consistent with the microscopic crystal plasticity relations.
4. *Identifying Microstructural Descriptors and RAMPS:* In this step, sensitivity analysis is conducted on various constitutive parameters belonging to the PHCM equations, with respect to the identified morphological and crystallographic descriptors and their distributions. Representative aggregated microstructural parameters or RAMPs that represent these descriptors and their distributions in an aggregated sense are proposed. The Sobol analysis [77] is performed to determine dependencies of constitutive coefficients on the RAMPs.
5. *Calibrating PHCM Functional Forms using Machine Learning:* Functional forms of the constitutive coefficients in terms of the RAMPs are derived by a machine learning code Eureqa [78] from an extensive simulation-based database. This database is constructed from CPFE simulations of virtual polycrystalline microstructures for a range of different crystallography and morphology distributions, under various conditions of thermo-mechanical loading. Virtual polycrystalline microstructures are generated in the space of RAMPs for calibrating PHCM constitutive coefficients. Machine learning is subsequently used to obtain calibrated functional forms of constitutive coefficients.
6. *Uncertainty Quantification in PHCM:* Different sources of uncertainties associated with the PHCM development viz. model reduction error, data sparsity error and microstructural uncertainty are quantified using Bayesian inference and the uncertainty in constitutive coefficients is propagated to material response variables such as stresses and plastic strains.
7. *Numerical Implementation of PHCMs in General Purpose FE Codes and Validation with Experiments:* The PHCM thus developed is numerically implemented in the general-purpose code ABAQUS [79] using the UMAT user subroutine. The accuracy and efficiency of the PHCM-based macroscopic FE simulations is demonstrated by comparing with experimental results for different strain-rates and temperatures.

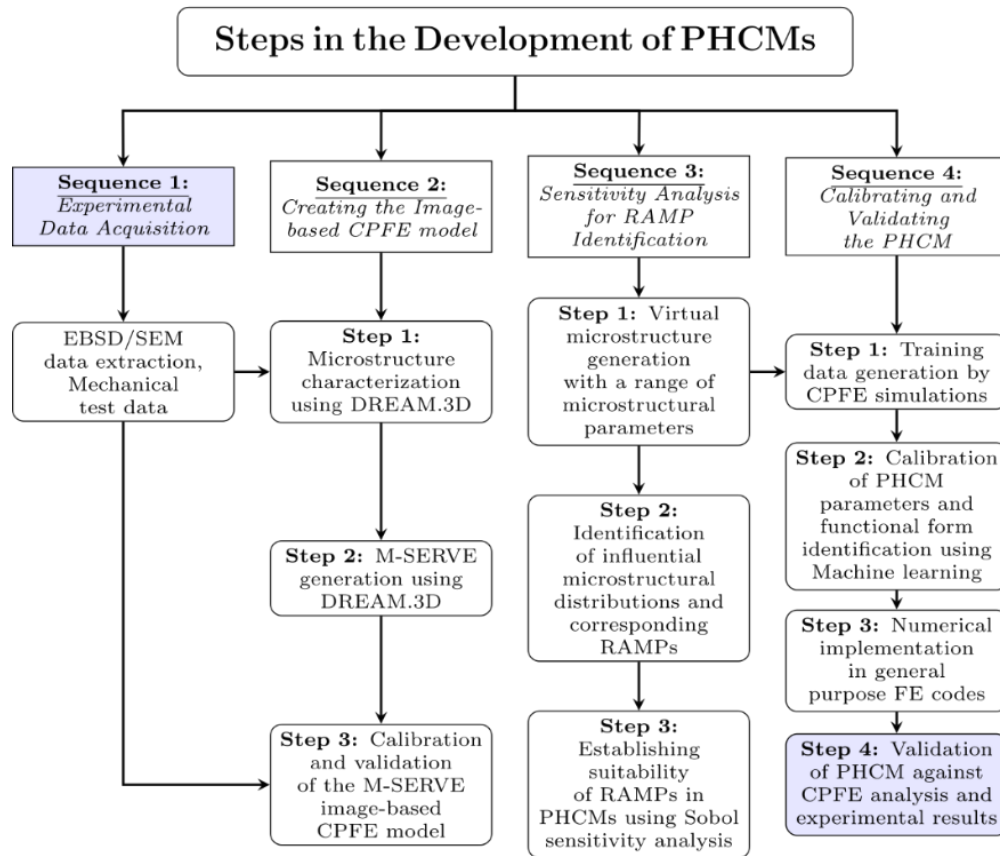


Figure 3.61: Development of PHCM Including Calibration and Validation with Experiments

Each of these steps is discussed in section C.1 and C.2. Further details on PHCM development may be found in [74, 80-82].

3.2.3. B.3: Spatial Multi-Scaling in ROMs

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Period of Activity: 1/2014 – 3/2017

High speed vehicles will invariably experience high loading from aerodynamics and an extreme environment, including high temperature as well as other mechanisms such as corrosion, ablation, etc. It is thus fully expected that damage, including fatigue, crack initiation and propagation, corrosion spots, will take place. To continue to safely operate a vehicle that has such defects will necessitate computational methodologies, ROM in the present context, that take those defects into account because their effects on the stress distribution will be much more important than the geometry and displacement field changes. Moreover, considering that these defects are likely to evolve over time, it is desirable to devise a ROM strategy that starts from the one for the structure

without defect (the “virgin structure”) and enriches it to model the effects of the defect. This goal was achieved in this investigation in three steps. The first of these was the definition of a set of local basis functions that capture the small changes in the displacement field induced by the defect. The ROM coefficients associated with these basis functions were investigated next and it was found that only the linear stiffness ones needed to be accounted for, thus allowing for an expedient updating as the defect changes. Finally, the methodology was implemented in connection with the GFEM^{sl} finite element strategy to achieve maximum accuracy and computational efficiency in capturing the defect effects.

Related research studies [26-28] investigated the applicability and formulation of nonlinear ROMs for structures with stress inducing defects such as notches [26] and cracks [27, 28]. Two key questions considered in these investigations were: (1) whether the displacement-based ROM can accurately capture the stress concentration of the defect when the structure undergoes large deformations, and (2) whether and how the ROM of the virgin structure could be used to predict these stresses.

A positive answer to question (1) was demonstrated in [26] for the case of a beam-like flat panel exhibiting a notch. It was first shown that the ROM directly constructed from the notched panel did lead to a very good prediction of the displacement *and stress* fields even close to the notch. Moreover, with regard to question (2), it was also shown in [26], as a second approach, that the ROM of the virgin panel could be used to predict the stress field of the notched beam through a post-processing of the virgin structure displacements near the notch. More specifically, these displacements would be considered as imposed far field boundary conditions to a local FEM of the notch area the linear static analysis of which would yield the desired stress distribution. A related strategy to this post-processing approach but utilizing the GFEM^{sl} approach was also proposed and successfully demonstrated for a structure with a crack [27]. In fact, this latter approach was naturally extended to study the propagation of the crack [28].

In these post-processing options, the effects of the local defect(s) on the global response of the structure are not included and thus the coupling between the global displacements of the structure and the local behavior due to the defect is only one-way, i.e., from the former to the latter. A full coupling does exist when the nonlinear ROM is constructed directly on the structure with defects, as the first approach of [26], but such a model would have to be completely redone, basis and parameters, when the defects change and/or new defects arise in the structure.

What would be desirable for such situations is to have the ROM of the virgin structure be the foundation of the ROM of the structure with defect and have it enhanced to capture the effects of the defect(s). Then, the change of a defect would only trigger the modification of the enhancements to the virgin ROM. Similarly, the occurrence of a new defect would then only require a further enhancement of the ROM. The formulation and assessment of such a local enhancement approach, addressing both basis and parameters of the ROM, was the focus of the present investigation.

Achievements:

A strategy was proposed in this effort to define a set of local ROM basis functions that capture the behavior of the structure in the neighborhood of the defect. These local basis function *enrich* the virgin basis so that only part of the model must be reconstructed if the defect changes, e.g., the crack propagates. Moreover, the natural coupling of the basis functions with each other implies

that the local behavior, visible through the generalized coordinates of the local basis, will in turn also affect the global response, i.e., the generalized coordinates of the virgin structure.

A particularly important finding of this investigation is that the behavior of the local basis functions and of their coupling with the virgin part of the basis *is effectively linear*, i.e., as long as the defect does not occupy a significant part of the structure, the geometric nonlinear effects are negligible. This finding implies in fact that the change of a small defect can be readily accounted for in the ROM by relying only on linear finite element constructs.

These concepts were first validated on the notched beam of [26]. The connectivity of this approach with the GFEM^{gl} approach was next addressed because this method provides a natural framework for considering and quantifying local effects. More specifically, the combined approach was then utilized on the cracked structure of [27, 28]

Strategy:

Since the coupling of the local basis functions with the virgin ones will be included in the ROM through appropriate coupling stiffness coefficients, it was deemed sufficient that the local enrichments be developed under the expectation that the coupling is only one way, i.e., the response “far” from the defect is governed by the virgin structure basis functions. The response along these modes is then considered as the far field for the determination of the behavior near the crack. As a starting point, validated later on as sufficient, it was then proposed to apply statically a displacement along each mode of the virgin basis separately and determine the difference in displacement in the defect zone between the virgin structure and its counterpart with defect. This ensemble of response differences was then processed through a POD to extract the dominant features which were then considered as the enrichments to the virgin basis to reflect the defect. The static imposition of the displacement appears justifiable because the defect zone is small and thus has a high natural frequency, much higher than the modes of interest of the virgin structure and/or of the excitation.

A first challenge in combining the ROM with local enrichments and the GFEM^{gl} was on determining the local enrichments which are defined within the near field domain. In this zone, there are 2 sets of displacement field data available - the displacement field corresponding to the uncracked shell FE model, and the displacement field computed on the cracked 3D model. One option for the construction of the enrichment basis would be to compute the node-wise differences between these 2 displacement fields, and use these values as the foundation for the enrichment basis functions. This choice, however, overlooks the fact that in addition to the presence of a crack, the local model also utilizes 3D continuum elements, whereas the global FE model uses shell elements. This difference in element types introduces additional differences in the uncracked/cracked displacement fields in the local region, which are not due to the crack itself. In light of this, an uncracked baseline 3D FE model (i.e., the same as the cracked 3D model, just without the crack) was also analyzed to provide a 3D displacement field from which the impact of crack’s presence could be isolated, independently from any difference arising from the use in the defect zone of 3D continuum elements versus shell elements. Therefore, the impact of the crack on the local displacement field is obtained by computing the node-wise displacement differences between the 3D cracked and 3D baseline models. It should be recognized that the enrichment basis

functions constructed as above are identically zero on the far field boundary and in the zone beyond it.

A second challenge was on the determination of the blocks of the linear stiffness matrices corresponding to the enrichments and to their coupling with the global modes. The standard approach used in ROM construction involves the imposition of displacements and the computation of the corresponding forces. Unfortunately, in the GFEM^{gl} methodology, as is the case with hierarchical p -FE methods, many components of the force vector lose the physical meaning that they would otherwise have with the Lagrangian shape functions. Moreover, there is also an increase in the dimension of the force vector for a FE model with a given number of nodes, as compared to an FE approximation built upon Lagrangian shape functions. These aspects of the GFEM^{gl} methodology make the enforced displacement approach more cumbersome. Accordingly, an alternate strategy was adopted which relies on the strain energy.

Consider first the estimation of the diagonal terms K_{ii}^{EE} . They were obtained directly from the GFEM^{gl} model of the defect zone subjected to the displacement field $\underline{u} = q_i^E \underline{\psi}_E^{(i)}$ and the corresponding potential energy U_{ii}^{EE} . Specifically,

$$K_{ii}^{EE} = \frac{2U_{ii}^{EE}}{[q_i^E]^2} \quad (7)$$

Next, the off-diagonal terms $K_{ij}^{EE} = K_{ji}^{EE}$ can then be identified from an imposed displacement field $\underline{u} = q_i^E \underline{\psi}_E^{(i)} + q_j^E \underline{\psi}_E^{(j)}$ and its associated potential energy U_{ij}^{EE} . Specifically,

$$K_{ij}^{EE} = \frac{2U_{ij}^{EE} - K_{ii}^{EE}[q_i^E]^2 - K_{jj}^{EE}[q_j^E]^2}{2q_i^E q_j^E} \quad (8)$$

Finally, the determination of the cross terms K_{ij}^{GE} is achieved similarly from the potential energy U_{ij}^{GE} of the entire structure with defect resulting from the displacement field $\underline{u} = q_i^G \underline{\psi}_G^{(i)} + q_j^E \underline{\psi}_E^{(j)}$, i.e.,

$$K_{ij}^{GE} = \frac{2U_{ij}^{GE} - K_{ii}^{GG}[q_i^G]^2 - K_{jj}^{EE}[q_j^E]^2}{2q_i^G q_j^E} \quad (9)$$

In this regard, note that the FEM of the structure with defect may not be assembled, i.e., it may remain two separate, yet coupled, models – the full model of the virgin structure and the GFEM^{gl} model of the defect zone. In such cases, the potential energy U_{ij}^{GE} can be determined as

$$U_{ij}^{GE} = U'_{ij}{}^{GE} - \hat{U}_{ij}^{GE} + \bar{U}_{ij}^{GE} \quad (10)$$

where $U'_{ij}{}^{GE}$, $\hat{U}_{ij}^{GE}$, and $\bar{U}_{ij}^{GE}$ are the potential energies due to the displacement field $\underline{u}$ of the entire virgin structure, the part of the virgin structure occupied by the defect zone, and the defect zone, respectively.

Results:

The first validation of the proposed concepts was accomplished on the notched beam of Figure 3.62 and Figure 3.63 of which two FEMs were developed. One does reflect the notch while the other does not, it has the same meshing as the first one but the notch is filled with elements. In this manner, the virgin and notched beams exhibit a common set of nodes. The application of the GFEM^{gl} in the second example will remove the need for these two separate models.

The construction of local enrichments for the notch beam were carried out using the 8-mode (4 Linear and 4 Dual modes, 4L4D), ROM of the virgin panel obtained in [26]. Specifically, the zone affected by the notch was selected as the parallelepiped encompassing the entire thickness and width of the panel but extending only 2 thicknesses on either side of the notch center along the panel long side. Next, the displacement field of each of the linear and dual modes (8 total) of the virgin panel ROM was enforced at the boundary of the above zone and the resulting linear static responses were obtained (as Nastran SOL101). Next, the differences between the responses of the notched panel in the affected zone and the modes of the virgin panel in the same region were computed and taken as an enrichment mode. Hence, 8 enrichments were obtained leading to a potential 4L4D8E ('E' for 'Enrichment') ROM basis. It was however found that of the 8 enrichments, only the first two were dominant and thus a 4L4D2E basis was used hereafter. The identification of the linear and nonlinear stiffness coefficients corresponding to this basis was then performed.

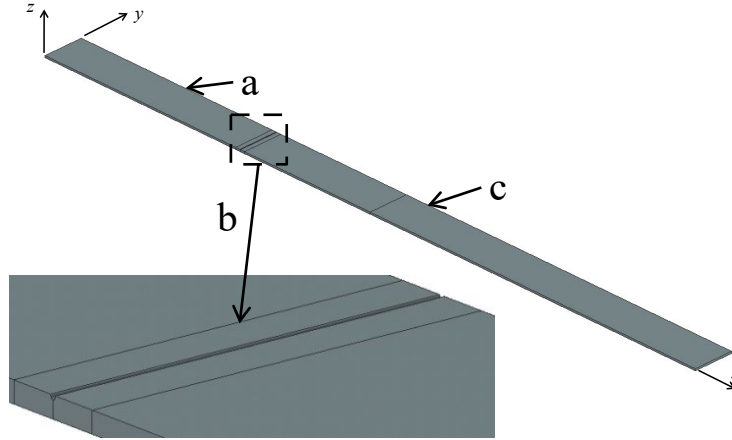


Figure 3.62: Notched Panel Model with (b) Showing Zone Near Notch Modeled with Finer Mesh than (a) and (c) Away from Notch

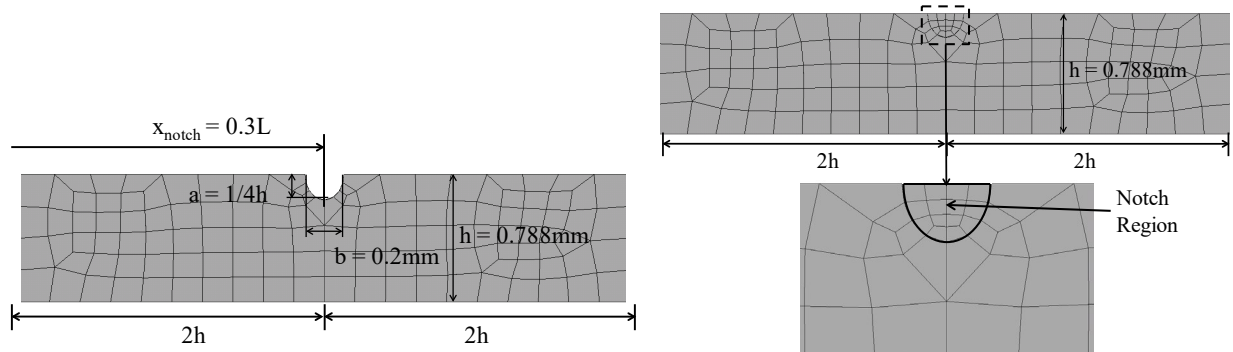


Figure 3.63: Geometry and Finite Element Mesh Near Notch Region: Notched Panel (left) and Virgin Panel (right) Where $L=0.2286$ m and $h=7.88 \times 10^{-4}$ m

In parallel to this ROM (referred hereafter to as the “notched panel ROM”), two “hybrid” ROMs were also constructed and their predictions also assessed in comparison to full Nastran results. The first hybrid ROM was constructed by replacing the linear and nonlinear stiffness coefficients associated with the 4L4D modes in the notched panel ROM by those of the virgin panel ROM. The stress coefficients relevant to the global modes only were also taken as those from the virgin panel. This hybrid ROM is referred to as the full hybrid ROM hereafter and it provides an assessment, when compared to the notched panel ROM, of whether the presence of the notch affects the virgin part of the ROM.

The second hybrid ROM focused on the need or lack thereof to account for the nonlinear stiffness coefficients of the enrichments and those coupling the virgin modes and the enrichments. This hybrid ROM was constructed by zeroing out these nonlinear stiffness coefficients, it is accordingly referred to as the linear hybrid ROM.

An assessment of the 3 different ROMs was carried out on the static response of the panel to a uniform pressure acting on the bottom surface of magnitude equal to 17 kPa. This loading leads to a peak transverse displacement of approximately 4 panel thicknesses, well within the nonlinear

range. Moreover, it would promote the opening of the notch and thus induces larger stress concentrations than a pressure on the top surface.

An excellent matching of the displacements of all three ROMs with Nastran was observed but more significant is the comparison of stresses. Then, shown in Figure 3.64 is the dominant stress S_{xx} along the top edge of the panel ($y=0, z=h$), computed by the three ROMs and the Nastran nonlinear solver (SOL106). The agreement is very good, even in the notch near field, and for all three ROMs. Only a small difference between the predictions of the linear hybrid ROM and the other two ROMs can be seen.

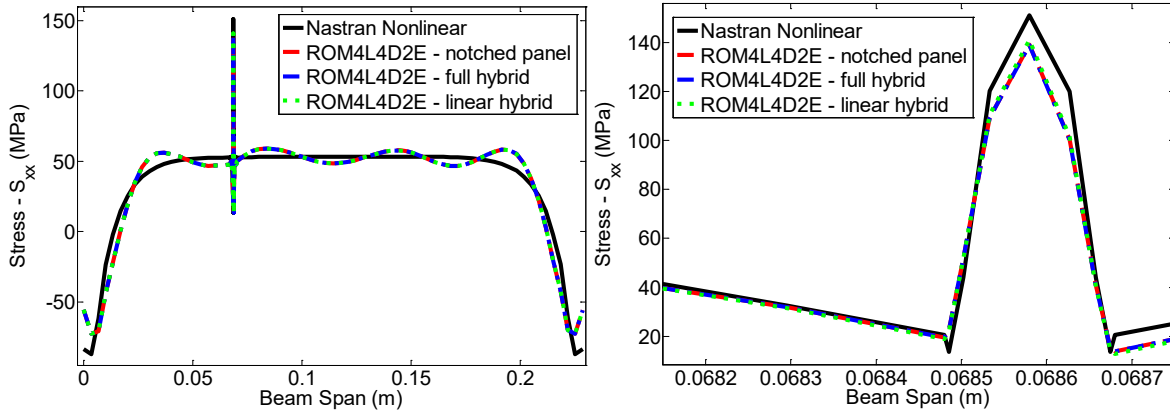


Figure 3.64: Element Stress S_{xx} Near Panel Edge at $y=0, z=h$, Induced by Uniform Pressure of 17 kPa, Comparison of Nastran Nonlinear Static Solution and 3 ROMs (left) Full View; (right) Zoomed View of Notched Region

A similar matching of the ROM and Nastran stress predictions was also obtained in the dynamic case, see Figure 3.65 and Figure 3.66. These power spectra correspond to a simulated acoustic excitation, uniform in space on the panel bottom surface varying randomly in time as a band-limited white noise process in the frequency range $[0, 1042]$ Hz with an overall sound pressure level (*OASPL*) of 147dB.

These comparisons clearly demonstrate that:

- (i) the enriched ROM basis provides the desired modeling of the displacements and stresses both away from and in the neighborhood of the defect,
- (ii) that the ROM parameters relevant to the virgin ROM basis may remain those from the virgin ROM, and
- (iii) that the necessary ROM parameters involving the enrichments are only the linear stiffness coefficients, both the self-terms of these modes and their coupling with the virgin ROM basis.
- (iv) A direct result of these findings is that no nonlinear finite element analysis of the structure with defect needs to be carried out, neither for the construction of the enrichments nor for the identification of the related ROM parameters.

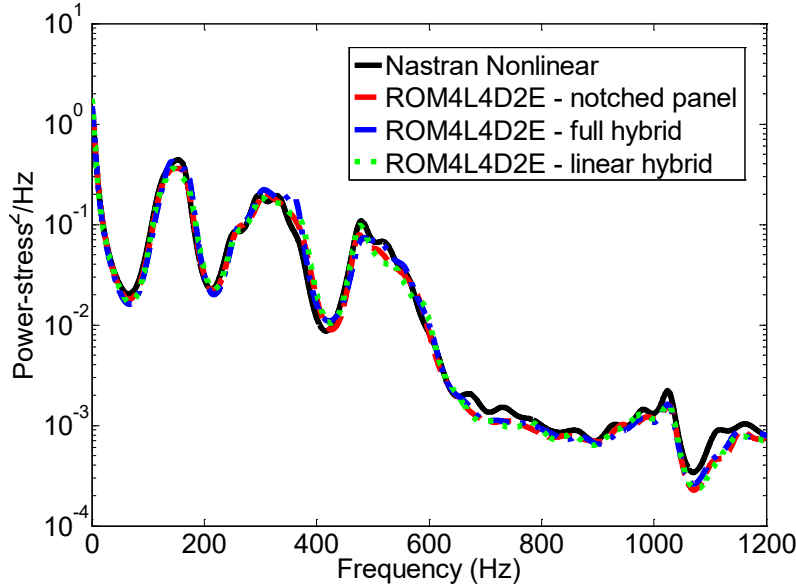


Figure 3.65: Power Spectral Density of Sxx Element Stress Near Notch Tip at $y=0$, $z=h$ (OASPL = 147 dB)

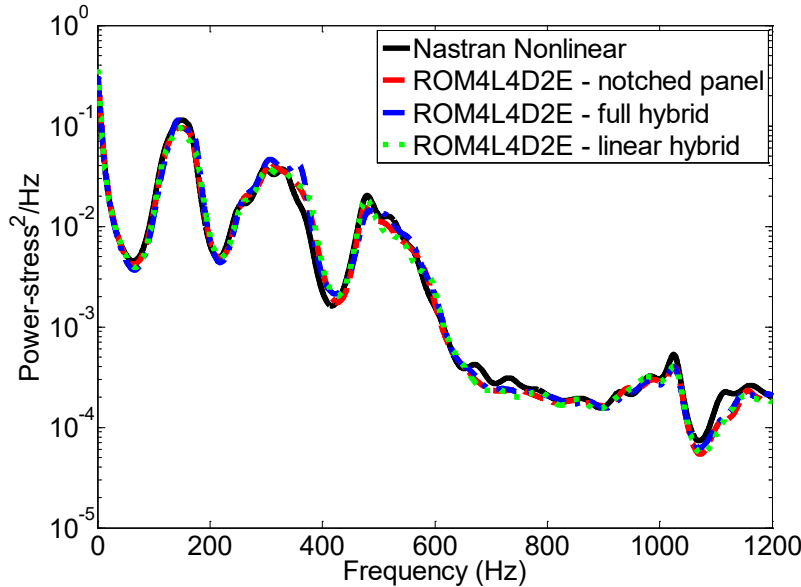


Figure 3.66: Power Spectral Density of Sxx Element Stress at 2 panel thicknesses from Notch Tip; $y=0$, $z=h$ (OASPL = 147 dB)

A direct result of these findings is that no nonlinear finite element analysis of the structure with defect needs to be carried out, neither for the construction of the enrichments nor for the identification of the related ROM parameters.

Based on these findings, the investigation moved to the next phase, i.e., the coupling of the above ROM methodology with the GFEM^{gl} approach. In this approach, two discretizations of the

structure are utilized: (1) a fixed, coarse global discretization and (2) a highly adapted, potentially evolving local discretization defined in a region of localized interest. Each discretization constitutes a separate, but linked boundary value problem (BVP) to be analyzed. The second discretization yields a specially tailored enrichment function through the solution of a highly adapted local BVP in the localized region of interest. Its boundary conditions are derived from the solution of the problem computed on the coarse global discretization. The solution of this local BVP then has knowledge of the localized physics embedded in it and it is used as the local approximation space to enrich the global solution space for the global BVP.

Consider more specifically the cracked blade model shown in Figure 3.67. It has been loosely divided in the vicinity of the crack into a far field region, a near field region, and defect zone. The far-field and near-field regions are modeled using the Nastran shell elements (CQUAD4). Following the GFEM^{gl} approach, both the near-field region and the defect zone are modeled using 27-node, quadratic hexahedron 3D brick elements and there is one layer of such elements through the plate thickness. The interaction between these two models occurs at the far field/near field boundary where the displacements from the Nastran (shell) model are imposed as Dirichlet BCs to the solid 3D model.

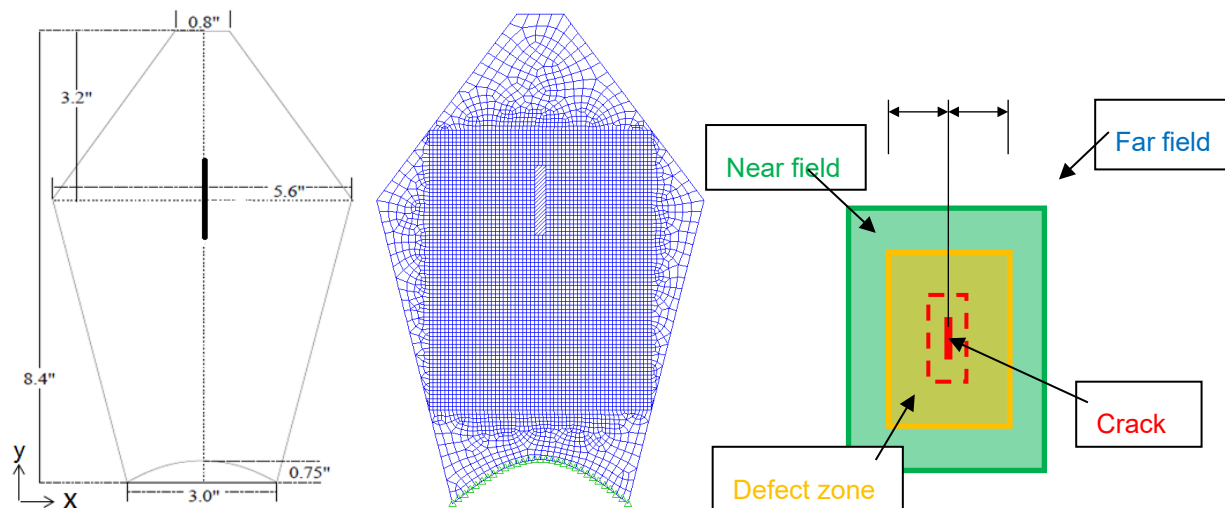


Figure 3.67: Test Structure: (a) Geometry and Dimension (b) Global Finite Element Meshing (c) Sketch of Global Finite Element in Neighborhood of Crack

The ROM modeling of the virgin blade was first undertaken and a basis with 8 linear modes and 9 duals (8L9D) was selected and identified. The corresponding ROM was then found to provide an excellent agreement of Nastran predictions. The displacements of each of these 17 modes were next imposed as boundary conditions at the 50 nodes separating the near and far field zones (see Figure 3.67(c)). For each of these 17 cases, the static responses at the 42 nodes located at the periphery of the defect and near-field zones were determined using the GFEM^{gl} approach. The differences between these responses and the corresponding computations carried out without the crack in the GFEM models (each cracked blade length having its own GFEM model) were then evaluated and a POD analysis of the 17 42-component vectors was carried out. Shown in Figure 3.68 are the eigenvalues of these POD analyses showing that 4 to 6 modes are typically sufficient

to represent the effects of the crack at the near field – defect zone boundary. Nevertheless, all eigenvectors were retained as enrichments in the ensuing analysis leading to 4 separate (one for each crack length) 8L9D17E nonlinear ROMs. The linear stiffness coefficients corresponding to the enrichments alone or with the global modes were identified as discussed in Eqs. (7)-(10) thereby completing the construction of the cracked blade ROM.

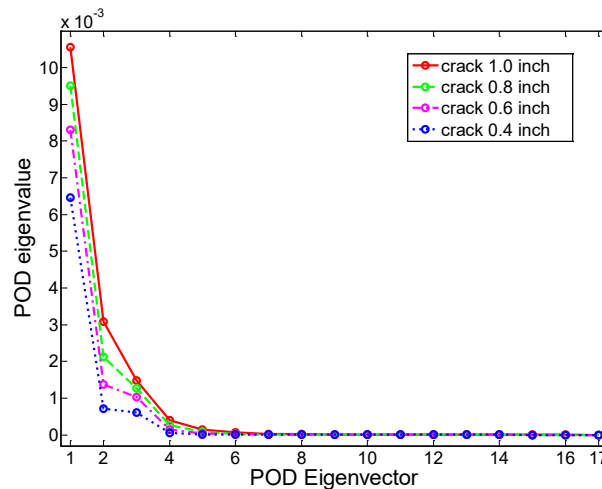


Figure 3.68: Eigenvalues of the Enrichment POD Analyses

A series of computations were carried out to validate the constructed ROM and assess the effects of the crack on the blade response. First, as expected, it was found that the displacements far away from the crack, e.g., at point *A*, see Figure 3.67(a), are essentially unaffected by the crack, statically or dynamically. However, significant effects of the cracks are observed, predominantly in the *x* direction (perpendicular to the crack), along the near field – defect zone boundary and shown in Figure 3.69 are the norm of the three displacements of these 42 nodes obtained in steady state response under a 20 g harmonic motion of the blade support. As expected the deviations from the virgin blade model increase with increasing blade crack and the effects are negligible in the transverse direction.

The coupling of the Nastran and GFEM^{gl} FEMs allowed not only displacements to be predicted but also crack related quantities, e.g., strain energy and stress intensity factor (SIF), as shown in Figure 3.70 and Figure 3.71, which clearly demonstrate the effects of the cracks.

The combination of the ROM and GFEM^{gl} methodologies has thus been showed to provide a computationally efficient strategy to predict the nonlinear geometric response of structures with defects that requires only minimal changes as the size of the defect changes. While not discussed here, the presence of multiple defects does not alter the formulation, it will only be necessary to add local enrichments for each of the defects and identify the corresponding linear stiffness matrices.

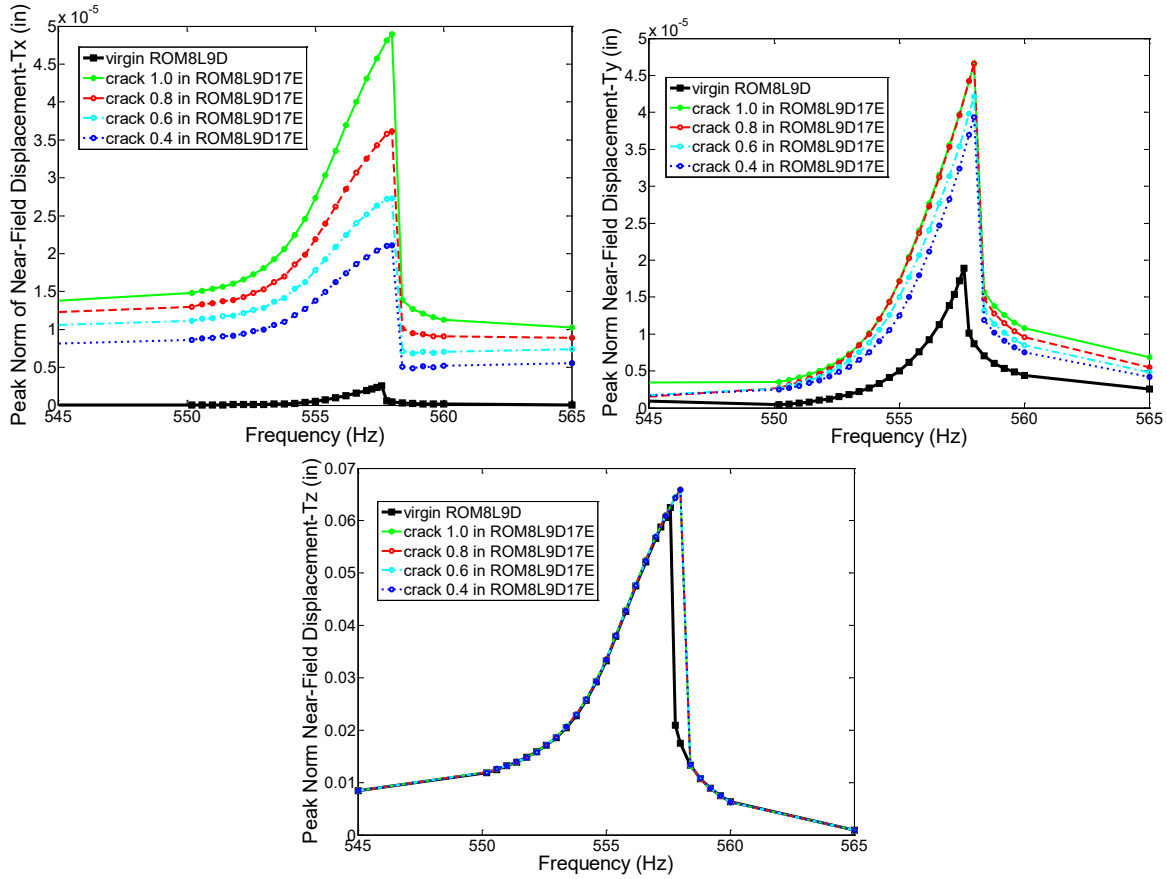


Figure 3.69: Peak Value of Euclidean Norm of Vector of Steady State Deflections at Nodes Along Near-field/Defect-zone Boundary as a Function of Frequency of Clamp Motions (20 g peak)

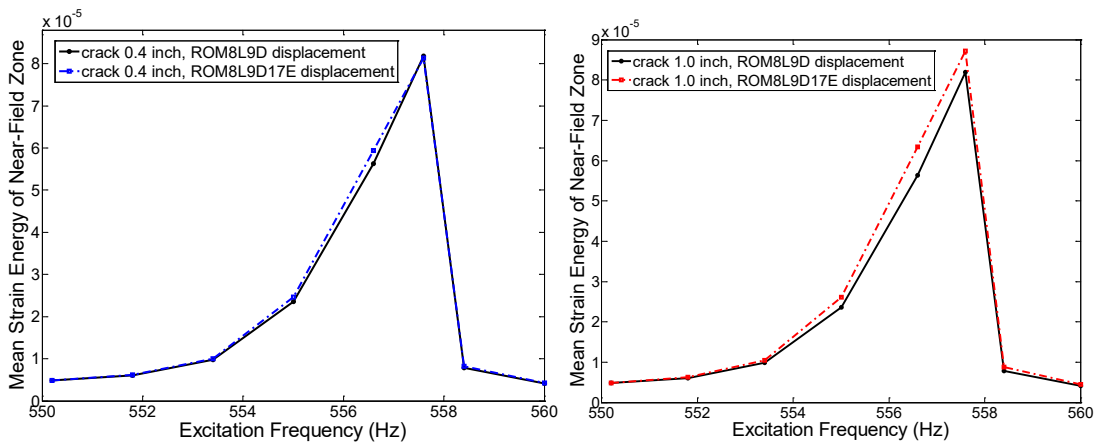


Figure 3.70: Mean Strain Energies over a Cycle in the Defect Zone for Crack Lengths (a) 0.4 in and (b) 1.0 in as Functions of the Frequency of Excitation (20g peak), ROMs With and Without Enrichments

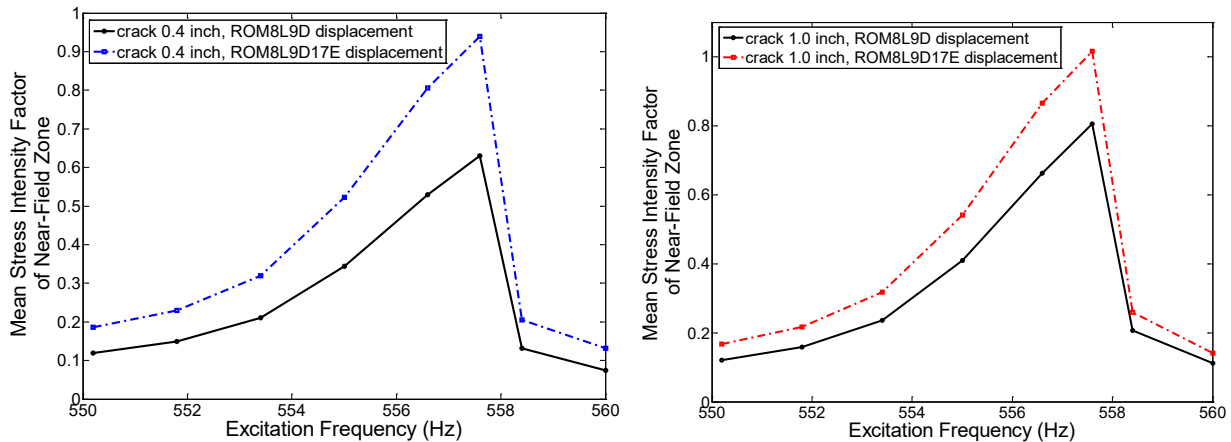


Figure 3.71: Mean SIF in Defect Zone for Crack Lengths (a) 0.4 in and (b) 1.0 in as Functions of the Frequency of Excitation (20g peak), ROMs With and Without Enrichments

3.2.4. B.4: Temporal Multi-Scaling

CCSS Personnel: Brent Miller (PhD Student), Marshall LeVett (MS Student), Chris McClurg (MS Student), Jack McNamara

AFRL Personnel: B. Smarslok, T. Eason, S.M. Spottswood

Period of Activity: 07/2013 – 08/2016

This project focuses on efficient managing of the disparate characteristic time scales associated with fluid-thermal-structural interactions. Two different strategies are developed and assessed. The first approach is based on loose coupling of partitioned fluid, thermal, and structural solvers. Here the goal is maintaining stability and the order of accuracy of the fluid, thermal, and structural solvers for the coupled response without the need to impose sub-iterations between each. Both a predictor implicit and predictor-corrector approach is considered, where the former is most appropriate for quasi-steady and CFD surrogate class of aerodynamic models and the latter is best when using time-accurate CFD. Significant speedups in computational efficiency are obtained without degradation in the numerical accuracy. In order to further reduce computational cost of long-time record simulation, parallel time marching strategies are investigated. Here the goal is to leverage the coarse and fine scales of the problem to develop a parallel processing algorithm for the time response. The literature is reviewed and preliminary results are provided.

Motivation and Background

A challenge with strongly coupled fluid-thermal-structural interactions is the disparity in time scales between the different fields, which leads to conflicting requirements for long time record simulation due to slowly evolving responses using relatively small-time steps to capture rapidly evolving responses. This motivates the design of time-marching algorithms capable of leveraging characteristic time scale differences of the different fields. Partitioning the solution process is a common and logical approach to the problem. Here, separate, tailored solvers are used to compute the fluid, thermal and structural responses and coupling is achieved through careful exchange of

boundary conditions at the interfaces. The partitioned approach may be used with loose or strong coupling. Loose coupling is achieved by exchanging information between solvers only once per update, where an update may be a single time step or multiple time steps. Conversely, strong coupling requires subiterations to converge the coupled solutions to a desired tolerance at each update. Because loosely coupled schemes do not require subiterations and thus are less expensive per time step than strongly coupled schemes, their development is desirable in order to maximize computational efficiency. However, the challenge with loose coupling is maintaining time accuracy and numerical stability of the multiphysics solution [56-58].

Beyond seeking to maximize computational efficiency, which motivates loosely coupled solvers that only exchange information at relevant time intervals, the time to a solution can remain impractical because of the large amount of time steps needed for a long-time record solution. In other words, it is important to note that the total time required to generate a solution is given by:

$$\left(\frac{\text{wall time}}{\text{iteration}} \right) \times (\# \text{ of iterations}) = \text{total time required for solution}$$

Thus, while loosely coupled time marching schemes (as well as ROMs) address the cost per iteration, total time to solution can remain impractical if the number of iterations required is significant. In the context of fluid-thermal-structural interactions, the fine scale response of the fluid result in a high number of iterations needed to cover the global solution response time driven by the thermal response of the system. Thus, time marching schemes are desired that can mitigate the inherent bottleneck that develops when a fine time scale time integration is needed for one field, compared to coarser time integration for other fields. Parallel, or parareal, time marching strategies are one such approach that offers promise in this regard and was also a focus of research [59-61].

This project was broken into two parts. The focus of the first part was on loosely coupled time integration approaches. The focus of the second part was on parareal time integrators.

Loosely Coupled Time Integration of Fluid-Thermal-Structural Integration

A generalized framework for partitioned coupling of fluid-thermal-structural interactions using quasi-steady fluid models is shown in Figure 3.72 below. Note that this scheme will also work with CFD surrogate models that incorporate a correction for unsteady effects as shown in Figure 3.15. Before the first step, the solvers are assumed to be synchronized at the same point in time. The sequence is as follows [56]:

1. Displacement, velocity and temperature are passed from the thermal solver to heat flux solver;
2. Heat flux is computed and passed to the thermal solver;
3. The thermal solution is updated one thermal time iteration;
4. The updated thermal solution is passed to the structural solver;
5. Displacement, velocity, and temperature are passed from the structural solver to the pressure solver;
6. Pressure is computed and passed to the structural solver;
7. The structural solution is updated one structural time iteration;

8. Steps 5-7 are repeated until the structural solution is advanced to the same point in time as the thermal solver;
9. Updated displacements and velocities are passed to the thermal solver for the cycle to repeat.

A loosely coupled scheme previously developed in Ref. [56] was transitioned to the CCSS that was designed to preserve 2nd order time accuracy when using basic engineering models and CFD surrogates. This scheme is denoted as a predictor implicit integrator and was designed with 2nd order accurate predictors of pressure and heat flux to cover the thermal step. Furthermore, sub-cycling of the structure is carried out using 2nd order interpolation of the temperature field.

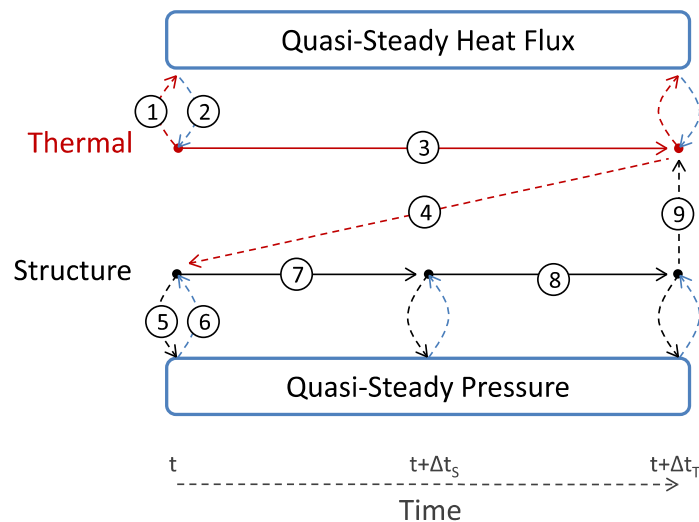


Figure 3.72: Sequence of Coupling Scheme Using Quasi-steady and CFD Surrogate Solvers for Pressure and Heat Flux

As part of this project, the above loosely coupled scheme was extended to enable incorporation of time-accurate solvers for the fluid domain, e.g., unsteady CFD predicted loads. A schematic of this extended scheme is shown in Figure 3.73. As before, the solvers are assumed to be synchronized at the same point in time. The sequence is as follows [57]:

1. Heat flux is passed from the fluid solver to the thermal solver;
2. The thermal solution is updated one thermal time step;
3. Updated temperature is passed to both the fluid and structural solvers;
4. Pressure is passed from the fluid solver to the structural solver;
5. The structural solution is updated one structural time step;
6. Structural displacements and velocities are passed from the structural solver to the fluid solver;
7. The fluid solution is updated one fluid time step;
8. Step 7 is repeated until the fluid solver is updated to the same point in time as the structural solver;
9. Steps 4-8 are repeated until the structural and fluid solvers are updated to the same point in time as the thermal solver.

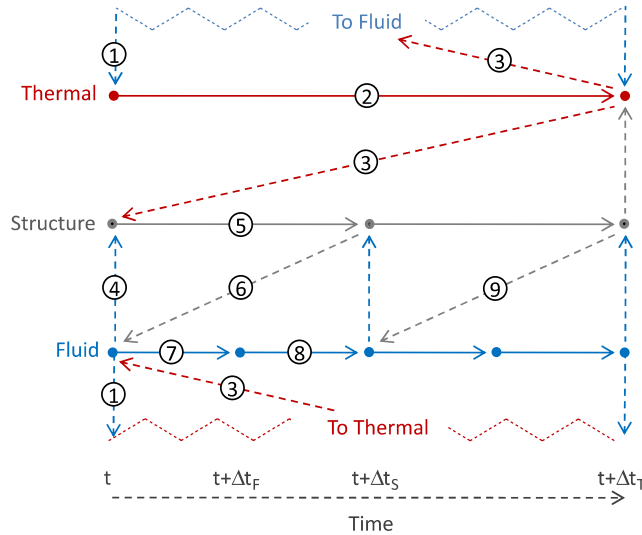


Figure 3.73: Sequence of Coupling Scheme Using Unsteady CFD Solvers

In order to preserve the 2nd order accuracy of the solvers used the predictor implicit scheme described above was extended as follows:

1. Fluid load (pressure and heat flux) predictors were developed using 2nd order extrapolation;
2. 2nd order linear temperature interpolation was used during sub-cycling of the fluid and structural solvers;
3. Cubic displacement interpolation used for sub-cycling of fluid solver;

Corrections of the structural and thermal solutions made with the updated fluid load to match fluid loads between each solver.

Main Results Using Loosely Coupled Time Integrators

A key take-away from this research is that loosely-coupled time integrators represent a significant speed-up in computational simulation of fluid-thermal-structural interactions. Specifically, cases studied indicated a 2-10X speed up in computational time compared to strongly-coupled schemes that use sub-iterations during transfer of boundary conditions between solvers. However, it is also important to carefully design these schemes in order to avoid inaccurate response predictions. An example of this is shown in Figure 3.74 for the aerothermoelastic flutter response of a skin panel computed using URANS CFD. Here the basic implicit scheme, which is a loosely coupled scheme that does naïve transfer of information between solvers, is characteristically different in both magnitude and spatial variance compared to the predictor-implicit scheme which matches the reference solution of a strongly coupled simulation. Even worse, in this case the magnitude response of the flutter is under-predicted compared to the truth solution.

Complete details on the development and implementation of these time integrators is available in Refs. [56-58].

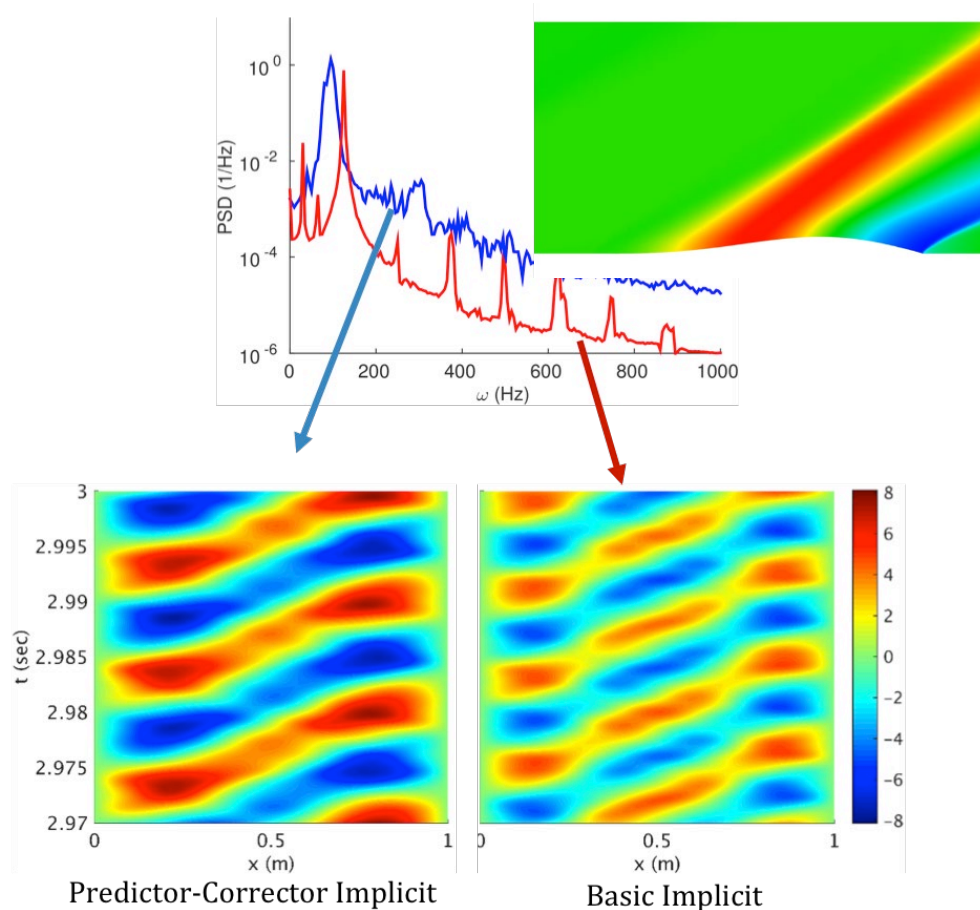


Figure 3.74: Comparison in Aerothermoelastic Response of a Skin Panel Using URANS CFD with Predictor-Implicit and Basic Implicit Time Marching Schemes for Fluid-thermal-structural Interactions

Parallel Time Integration of Fluid-Thermal-Structural Integration

As discussed above, the use of loosely coupled time integrators addresses inefficiencies introduced by passing information between solvers. However, it does not fully address the bottleneck introduced by small time scale physics over long time records. As such, a preliminary investigation was carried out on the ability of parallel in time, or parareal, integrators to address this issue. The parareal algorithm is explained in Figure 3.75 and Figure 3.76. A basic example is shown in Figure 3.77.

While not inherently a multi-scale approach, the breaking of the problem into coarse and fine scale solutions aligns with multi-physics problems, such as fluid-thermal-structural interactions, that have disparate time scales. Here, the thermal time scale represents a coarse scale, while the structural and fluid problems are at a finer scale.

A basic implementation of this was examined for the aerothermoelastic response problem as shown in Figure 3.78. Here a coarse scale aerothermoelastic response was carried out at the thermal response scales of the problem. This was then used to initialize a set of fine scale aerothermoelastic

responses computed using the loosely-coupled scheme above, where the time interval of each response was the thermal time step size. These fine scale steps were carried out in parallel and the process shown in Figure 3.77 was repeated until the solution converged.

1. On the entire time domain, discretize time with the use of coarse time steps.
 - Designate the coarse time values as $T(0) = T_0, T_1, \dots, T_N = T(\text{end})$.
 - Designate the coarse time slices created as $S_N = [T_{N-1}, T_N]$.
2. On each of the coarse slices, discretize time with the use of fine time steps.
 - Designate the fine time values as $T_{N-1} = t_0, t_1, \dots, t_J = T_N$.
3. On the entire time domain, initialize a solution by time-marching on the coarse scale.
 - Designate the coarse solution as $Y_N = Y(T_N)$.
4. On each of the coarse slices, use the coarse solution values as ICs to find a fine scale solution.
 - Designate the final value obtained on S_N as $y_N = y(t_J)$.
5. On the entire time domain, find the coarse jumps.
 - Designate the coarse jumps as $\Delta_N = y_N - Y_N$.
6. Propagate the coarse jumps to correct the coarse solution, obtaining new values for Y_N .
7. Repeat to step 4, if necessary (until the solution converges.)

Figure 3.75: Description of the Parareal Time Marching Algorithm [62]

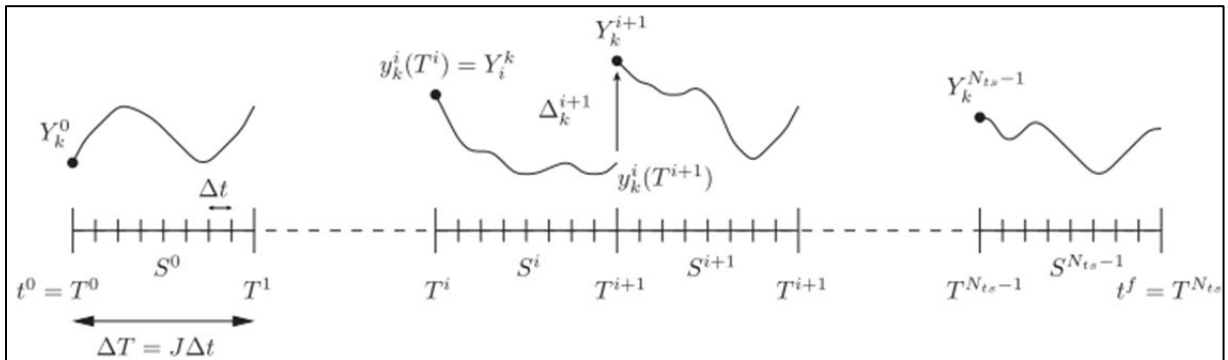


Figure 3.76: Illustration of Predictor-corrector Parareal Method [62]

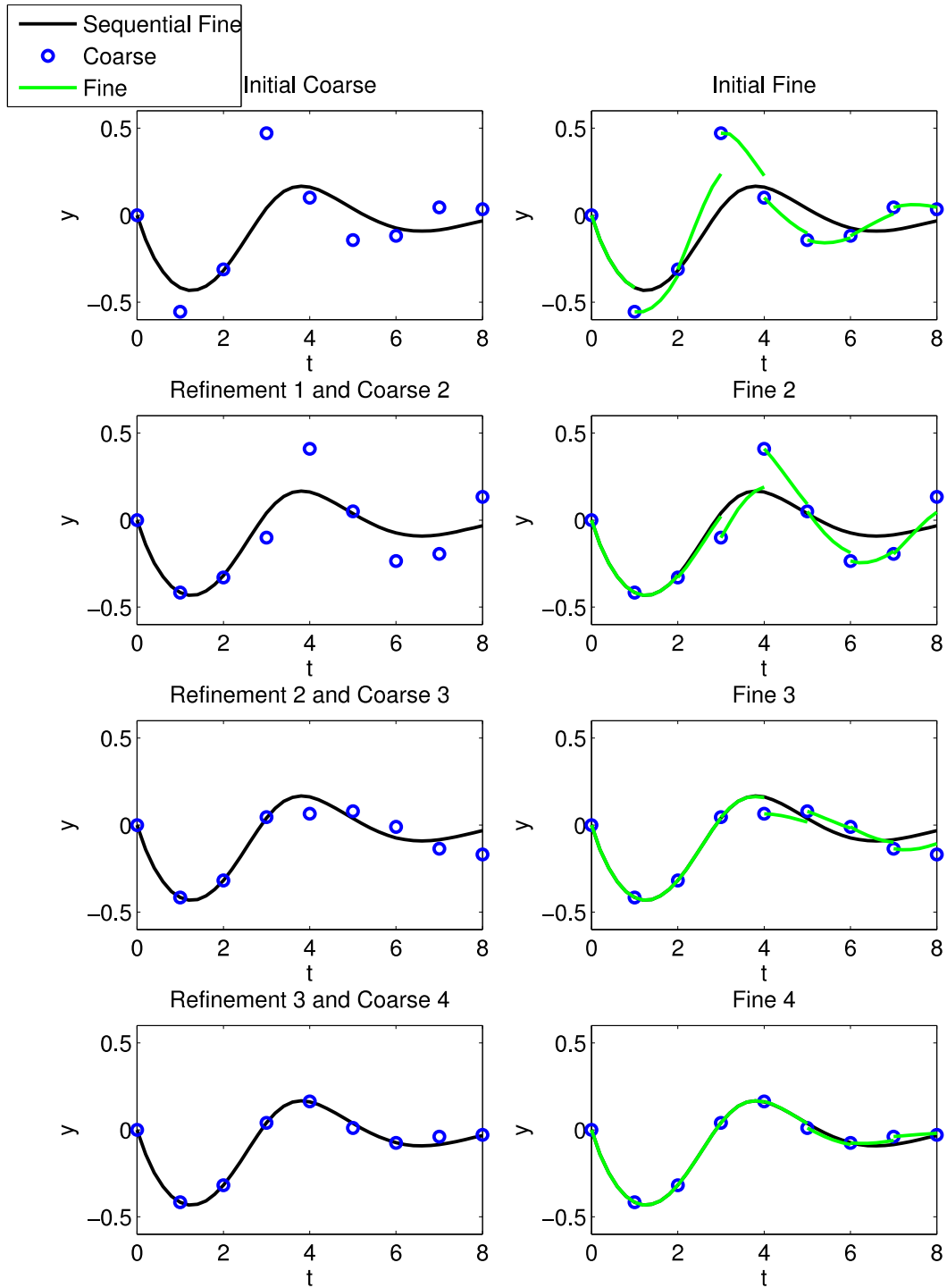


Figure 3.77: Example of a Parareal Time Integration Progression

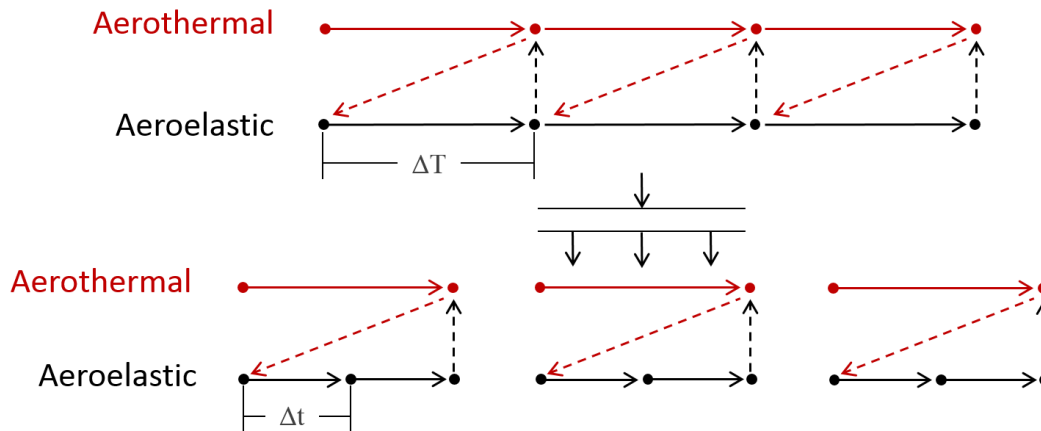


Figure 3.78: Coarse (top) and Fine (bottom) Time Discretization Using a Parareal Time Marching Approach with a Loosely Coupled Partitioned Aerothermoelastic Solver

A typical result is shown in Figure 3.79. This represents the mid-panel displacement for the aerothermoelastic response of a skin panel. Initially the panel buckles into the flow field due to the increased temperature from the flow field. The panel then has a quasi-static, post-buckled response until roughly 25 seconds, at which point the panel snaps through and initiates a dynamic limit cycle response. Here the parareal integration does an excellent job at capturing the quasi-static response. However, the scheme becomes unstable when transitioning to the dynamic limit cycle response. Separate investigations demonstrated that the parareal approach was capable of predicting dynamically unstable response. Thus, the failure of the scheme in this case seems to stem from the transition of a quasi-static response to a strong dynamic response.

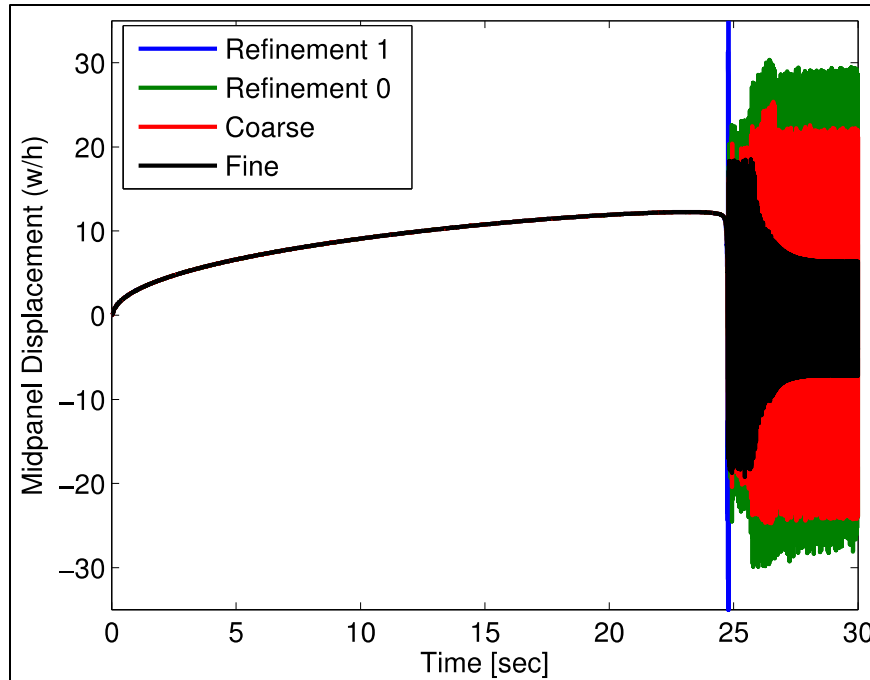


Figure 3.79: Mid-panel Displacement Using a Parareal Time Integration for Aerothermoelastic Response

Subsequent to these findings a deep literature review was carried out in order to better understand the rapidly evolving parareal research landscape. Shown in Figure 3.80 is a list of all publications between 2001 and 2016 when this research project was paused. This demonstrates a high degree of activity on the approach and a lack of maturity. Thus, it was concluded at this stage to halt the revisit this research at a later date.

Complete details and research results generated for this project are detailed in Refs. [59-61].

Date	Algorithm	Author(s)	Institution	Notes on name	Application
2001	Parareal	Lions et al.	Pierre-and-Marie-Curie University	--	linear, nonlinear PDE
2002	Parareal	Baffico et al.	Pierre-and-Marie-Curie University	--	molecular dynamics (ab initio)
2003	Parareal	Fischer et al.	Pierre-and-Marie-Curie University	--	Naiver-Stokes
2003	PITA1	Farhat et al.	University of Colorado	Parareal Implicit Time-integrator	unsteady Piston flow (1D); 2nd-order structural dynamics; fluid-structure interaction
2004	Parareal	Trinidade et al.	Escola Superior Náutica	--	unsteady, incompressible Naiver-Stokes
2005	NLMG		Ferien-Akademie	FAS and NMG	diffusion (2D)
2006	PAVI	Kale et al.	Stanford University	Parallel Asynchronous Variational In	nonlinear elastodynamics
2006	PITA2	Farhat et al.	Stanford University	modified PITA	plate free vibration; FE assembly dynamic response
2006	SIPC Parareal	Bal et al.	Columbia University	symplectic interpolated predictor-co	Hamiltonian system (1D)
2007	Parareal	Gander et al.	University of Geneva	--	heat; advection
2007	PITA2	Gander et al.	University of Geneva	modified PITA	2nd-order ODE
2008	KSE Parareal	Gander et al.	University of Geneva	Krylov subspace-enhanced	2nd-order ODE; heat
2008	Parareal	Gander	University of Geneva	--	wave, advection
2008	Parareal	Harden	Florida State University	--	nonlinear PDEs (with FEM and ROM)
2008	SDC Parareal	Minion et al.	University of North Carolina	Spectral Deferred Correction	Lorenz
2009	PITA3	Cortial et al.	Stanford University	nonlinear PITA	spherical cap (nonlinear); clamped plate (nonlinear)
2009	PPHC Parareal	Chouly et al.	Inria Research Center	partitioned parabolic-hyperbolic cou	Fluid-structure interaction
2009	SMTS Parareal	Audouze et al.	Ecole Centrale Paris	symplectic multi-time step	molecular dynamics (1D, 3D)
2009	TDG Parareal	Mercerat et al.	Institut de Physique du Globe de Paris	time-discontinuous Galerkin	acoustic wave (1D)
2010	RIDC	Christlieb et al.	Michigan State University	Revision Integral Deferred Correction	advection- diffusion, Brusselator
2010	SI Parareal	Dai et al.	Pierre-and-Marie-Curie University	first version of symmetric Parareal	harmonic oscillator; Kepler (2D); solar system
2010	SDC Parareal	Minion	University of North Carolina	Spectral Deferred Correction	Lorenz, Burgers'
2011	KSE Parareal	Ruprecht et al.	University of Italian Switzerland	Krylov subspace-enhanced	linear, hyperbolic acoustic- advection system (2D)
2011	MGIT	Friedhoff et al.	Lawrence Livermore National Laboratory	Multi-Grid In Time	diffusion (1D)
2011	PE	Gander et al.	University of Geneva	ParaExp	diffusion with oscillating source, wave, advection
2011	PITA4	Cortial	Stanford University	staggered PITA	nonlinear spherical cap
2011	S2 Parareal	Dai et al.	Pierre-and-Marie-Curie University	second version of symmetric Parareal	wave; Burgers'
2011	SWR Parareal	Gander et al.	University of Geneva	Schwarz Waveform Relaxation Parareal	heat
2012	Parareal	Nielsen	Technical University of Denmark	--	test; Bernoulli; linear ODE system, Van der Pol ; diffusion (2D); free surface water wave
2012	PFASST	Emmett et al.	University of North Carolina	Parallel Full Approximation Scheme	Burgers', Kuramoto-Silvashinsky
2012	RB Parareal	Chen et al.	Brown University	reduced basis	nonlinear PDEs
2013	KDC Parareal	Bu et al.	Ewha Womans University	Krylov Deferred Correction	linear DAE, nonlinear DAE, Van der Pol
2013	MGRIT	Falgout et al.	Lawrence Livermore National Laboratory	Multi-Grid Reduction In Time	diffusion (2D, 3D)
2014	A Parareal	Haut et al.	Los Alamos National Laboratory	asymptotic Parareal	highly oscillatory PDE
2014	MGRIT	Dobrev et al.	Lawrence Livermore National Laboratory	Multi-Grid Reduction In Time	heat
2014	MGRIT	Falgout et al.	Lawrence Livermore National Laboratory	Multi-Grid Reduction In Time	unsteady flow over cylinder (Strand2d, RANS)
2014	NLMG		University of Leeds	FAS and NMG	nonlinear 2nd-order diffusion
2015	MGRIT*	Dobrev et al.	Lawrence Livermore National Laboratory	Multi-Grid Reduction In Time	ODE system
2015	MS Parareal	Ariel et al.	ICES, UT-Austin	Multi-Scale	HiOsc, Volterra-Lotka
2015	Parareal	Steiner et al.	Università della Svizzera italiana	--	nonlinear Naiver-Stokes
2015	PEBK	Kooij et al.	University of Twente	ParaExp with Block Krylov	advection- diffusion, Burgers'
2016	MGRIT*	Falgout et al.	Lawrence Livermore National Laboratory	Multi-Grid Reduction In Time	moving mesh PDE

Figure 3.80: List of Research Studies Carried Out on Parareal Algorithms Between 2001 – 2016

3.2.5. B.5: Extraction of SIFs of 3D Fractures in Anisotropic Materials

CCSS Personnel: Bryce Mazurowski (M.S. Student), Armando Duarte

AFRL Personnel: B. Gockel and P. O'Hara

Period of Activity: 08/2017 – 4/2020

Anisotropic materials are extensively used in many practical engineering applications of interest to the US Air Force. Single crystal and directionally solidified materials used in turbine blades and titanium alloys such as Ti-6242 used in structural components exposed to extreme environments are known to exhibit orthotropic behavior. Predictive simulations of crack growth in this class of materials must take into account their directional properties. Simplified calculations resulting from assumptions of isotropy are not acceptable for most applications of interest to the US Air Force where safety margins must be kept at a minimum.

This project focuses on the development and implementation of an accurate and computationally efficient method for the extraction of SIFs of 3D fractures in anisotropic materials. These parameters can be used to drive 3D fracture growth and to provide fatigue life estimates of representative high-speed structural components.

Methodology Overview

Analytical or handbook solutions for 3D fracture problems in anisotropic materials are significantly limited due to the complexity of the problem and the large number of parameters characterizing the stiffness of anisotropic materials. As a result, the FEM is often used for solving 3D fracture problems in anisotropic materials. However, the creation of FEMs for complex 3D crack geometries or mixed-mode crack propagation simulations often requires user intervention and high computational times [64]. Enriched FEMs have shown the ability to generate accurate solutions for 3D fracture problems while avoiding the aforementioned issues encountered by standard FEM.

Most techniques currently used to compute quantities of interest for crack propagation simulations, SIFs in particular, do not directly extend to anisotropic material systems. As such, this an open area of research, required to accurately address crack propagation in structural components composed of anisotropic materials.

The CCSS co-PI's research group has recently developed [65] an accurate and computationally efficient method for the extraction of SIFs of 3D fractures in *isotropic* materials. The method is based on the displacement correlation method (DCM) and a GFEM enriched with singular functions from the asymptotic expansion of the elasticity solution in the neighborhood of a crack. It is shown in [65] that the DCM, with proper enrichment of the GFEM mesh, has an accuracy and robustness comparable to domain integral methods at a fraction of the computational cost. In this project, the DCM presented in [65] was reformulated such that it can be applied to general anisotropic materials and, in particular, to orthotropic materials such as Ti-6242.

This required the derivation of the elasticity solution in the neighborhood of fractures in anisotropic materials. This derivation was based on the works of [66], [67], and [68]. Figure 3.81 shows the three coordinate systems inherent to the DCM for anisotropic materials. This extraction method uses the expansion of the elasticity solution to relate SIFs to jumps of the displacement

field across the crack surface. This relation leads to a coupled system of equations for the SIFs, in contrast with the case of isotropic materials in which the SIFs are uncoupled. Details on the DCM for anisotropic materials can be found in [69, 70].

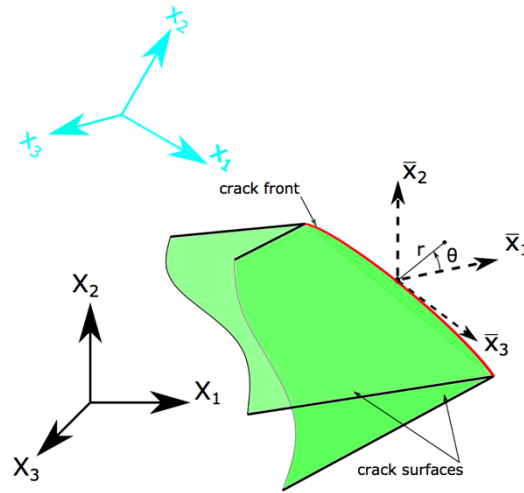


Figure 3.81: Crack Front, Global, and Material Coordinate Systems Used in DCM for Anisotropic Materials [69, 70]

Transition to AFRL and CCSS Personnel

The DCM for anisotropic materials developed in this project was implemented in the GFEM platform ISET. This platform integrates research projects from Thrusts A, B and C. This integration effort was part of the project I1: GFEM Integration w/ CFD Surrogates and Continuum Damage Modeling. An example presented in Section 4.1 showcases the integration of this and projects B1: Linking Solid and Dimensionally Reduced Models and C2: Continuum Level Homogenized Models for Deformation and Creep.

Results from this project have been made available for all personnel, from both academia and AFRL, involved in these projects. They will also feed directly into other AFRL research thrusts (Spradlin and O'Hara) on the modeling and simulation of mixed-mode crack growth in granularly-driven orthotropic material systems of direct interest to the USAF.

Verification Problem: Inclined Elliptical Crack

The problem of an elliptical crack in a cuboid domain is solved in this section. The geometry of the problem is shown in Figure 3.82. The dimensions of the cube and the fracture are chosen such that $c/L = 3/40$ and $a/c = 9/15$. The problem is solved with both the Orthotropic I and Orthotropic II materials listed in Table 3-6. The varied alignment of the crack front changes the material properties at each point the SIFs are calculated.

The global GFEM mesh used to solve the problem using the GFEM developed in Project B1 [71, 72] is shown in Figure 3.82. This GFEM allows the adoption of a fairly coarse mesh as shown in the figure, and it need not fit the crack geometry.

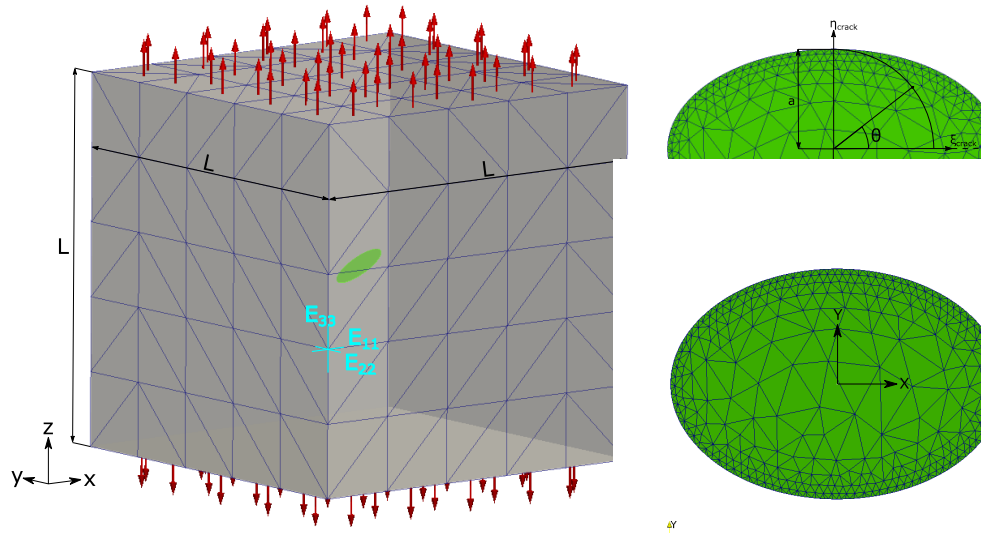


Figure 3.82: Geometry and Mesh Used for Inclined Elliptical Crack in a Cube of Orthotropic Material

Table 3-6: Material Properties for Orthotropic I and Orthotropic II Materials

	Orthotropic I	Orthotropic II
E_{11}	8.000×10^6	2.475×10^6
E_{22}	2.475×10^6	8.000×10^6
E_{33}	8.000×10^6	2.475×10^6
ν_{12}	0.0360	0.1114
ν_{13}	0.0360	0.1114
ν_{23}	0.1114	0.0360
G_{12}	7.000×10^5	7.000×10^5
G_{13}	3.861×10^6	1.114×10^7
G_{23}	7.000×10^5	7.000×10^5

The SIFs reported in [68] are taken as a reference. The normalized SIFs extracted with the DCM developed in this project and reference values computed with the 3DFAS code [68] are presented in Figure 3.83. The agreement between the method developed in this project and the reference values from [68] is excellent for all three SIFs and both materials, attesting the accuracy of the developed DCM.

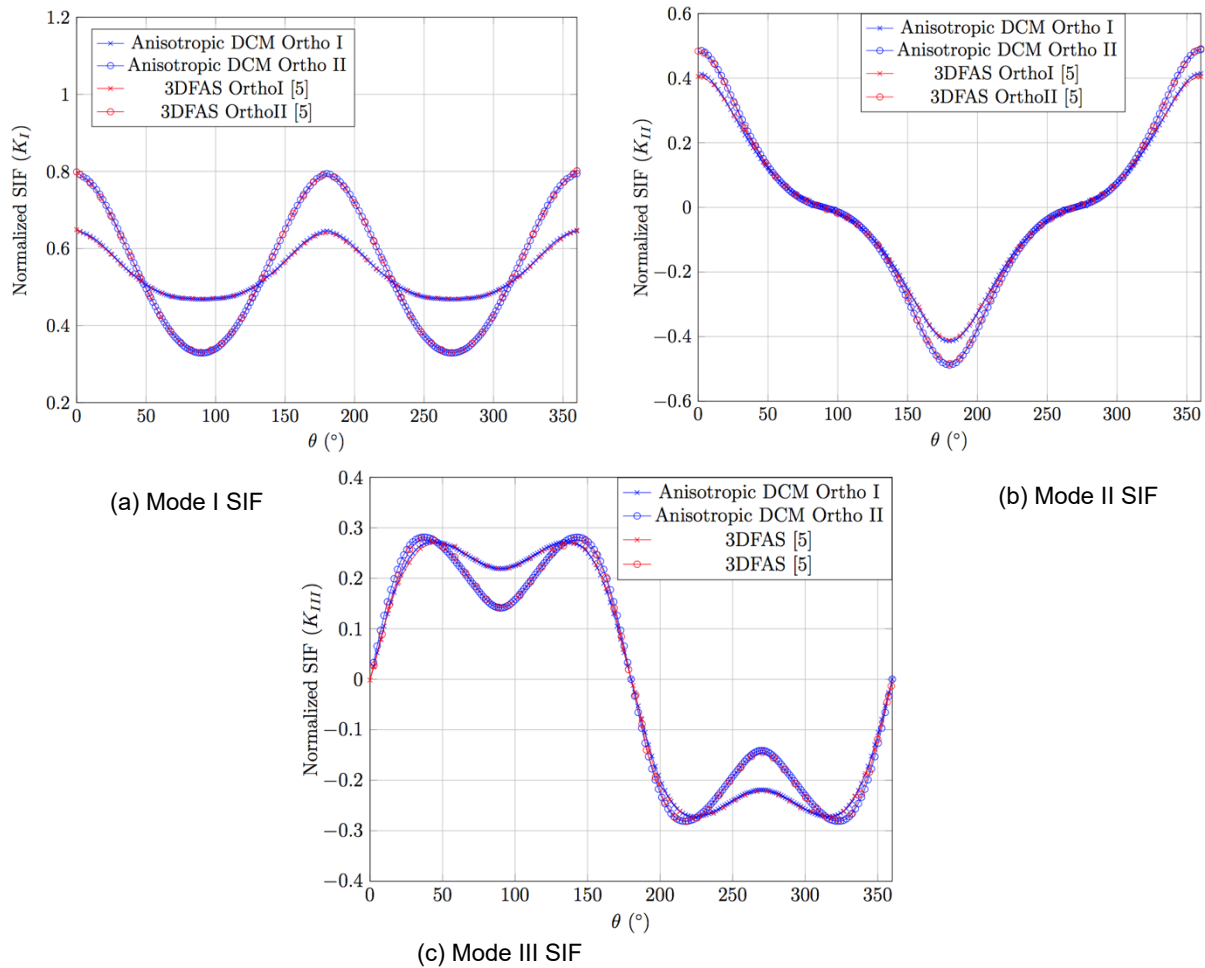


Figure 3.83: Normalized SIFs Extracted with DCM developed in this Project and Reference Values Computed with 3DFAS Code [68]

Application Problem: SIFs at Lap Joint with Three Spot Welds

A lap joint with three spot welds is chosen to showcase performance of the anisotropic DCM when linked with the multiscale structural analysis framework developed in project B1: Linking Solid and Dimensionally Reduced Models, as well as the state of the art Ti-6242 material model developed in project C2: Continuum Level Homogenized Models for Deformation and Creep.

The geometry of the problem is shown in Figure 3.84. Dirichlet boundary conditions are applied on the left side, $u_x(0, y, z) = 0.0$ and the right side, $u_x(7, y, z) = 0.01$. A coarse mesh is used to discretize the global domain, while each spot weld has a fine-scale local problem. The local problems utilize classical GFEM enrichments for fracture mechanics problems to represent the spot weld connection without the need to explicitly mesh the geometry. The global problem is used to provide the boundary conditions for the local problem, the solution from the local problems are then used as enrichment functions on the global mesh to add in the fine-scale structural details to the domain. This analysis procedure is depicted in Figure 3.85.

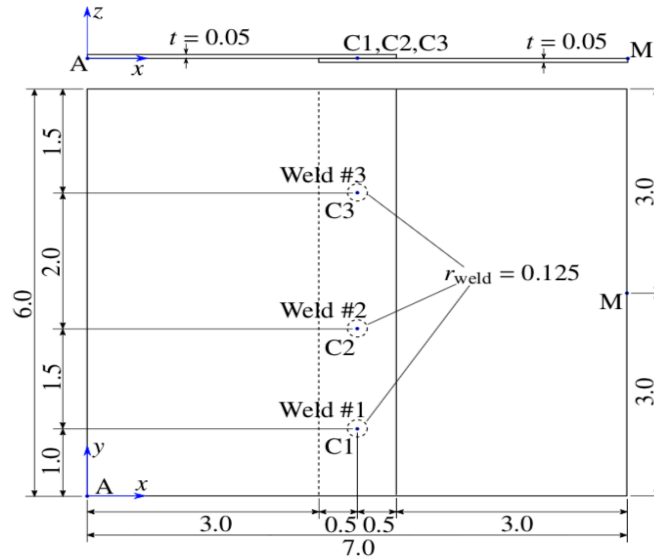


Figure 3.84: Geometry of Lap Joint with 3 Spot Welds, Dimensions in Inches

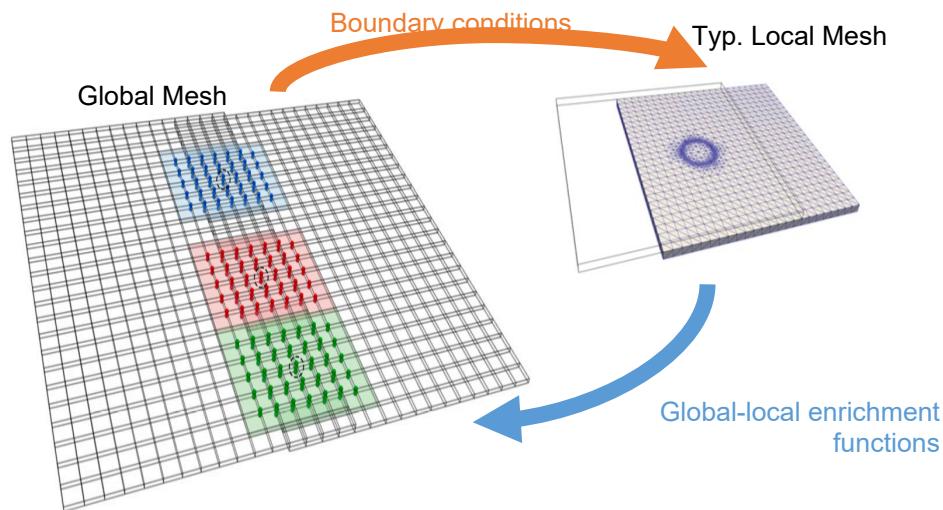


Figure 3.85: GFEM^{gl} Analysis Procedure Developed in Project B1 Applied to Three-weld Lap Joint Problem

This problem is solved with four different material models. Two of these are anisotropic and are generated from the Abaqus UMAT implementation of the Ti-6242 material model developed in project C2. The GFEM solver ISET can utilize an Abaqus UMAT to set the material properties. This had to be slightly modified to accommodate the new features of the Ti-6242 UMAT. Kearns texture parameters [73], g_i , and the material symmetry axis are the main inputs to the UMAT, which determine the relative stiffness of the material and its global orientation, respectively. The two anisotropic material models generated from the UMAT are taken to be the cases resulting in maximum anisotropy. This is done by setting a single Kearns parameter to one and the other to

zero. The other two materials are isotropic and based on the largest and smallest moduli from the anisotropic cases. All four materials are fully described in Table 3-7.

Table 3-7: Material Properties for Four Materials Used in Three-weld Lap Joint Problem

	Isotropic 1	Isotropic 2	JHU UMAT, $g_1 = 1.0$	JHU UMAT, $g_2 = 1.0$
E_1	2.172×10^7	1.554×10^7	2.172×10^7	1.554×10^7
E_2	2.172×10^7	1.554×10^7	1.554×10^7	2.172×10^7
E_3	2.172×10^7	1.554×10^7	1.554×10^7	1.554×10^7
ν_{12}	0.325	0.325	0.320	0.229
ν_{13}	0.325	0.325	0.456	0.320
ν_{23}	0.325	0.325	0.320	0.456
μ_{12}	8.198×10^6	5.865×10^6	7.496×10^6	7.496×10^6
μ_{13}	8.198×10^6	5.865×10^6	5.327×10^6	7.496×10^6
μ_{23}	8.198×10^6	5.865×10^6	7.496×10^6	5.327×10^6

The two anisotropic materials provide a way to assess the effect of rotating the rolling direction of the plates by ninety degrees. The global alignment of both Kearns parameters is shown on a typical spot weld in Figure 3.86 along with the parametric angle, β , that is used to plot SIFs.

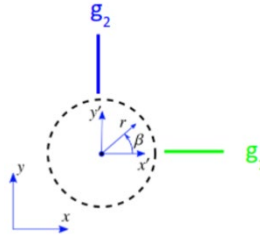


Figure 3.86: Material Alignment with Respect to Global Coordinates in Terms of Kearns Texture Parameters with Parametric Angle β Shown for Typical Spot Weld

Mode I SIFs for each spot weld are shown in Figure 3.87 with respect to parametric angle β . Material anisotropy provides clear differences in SIFs from the two isotropic materials even at the relatively low level of anisotropy exhibited by Ti-6242. The two cases of material isotropy do not put an upper and lower bound on the SIFs obtained from the anisotropic material models. The overall form of the SIF curves from each of the four materials are the same, but they differ in the magnitude of the peaks.

On top of the ability to extract smooth and accurate SIFs from fractures in anisotropic materials, this anisotropic DCM developed in this project can be seamlessly incorporated into the multiscale analysis framework developed in project B1 and can rely on the UMAT developed in project C2 to define the material.

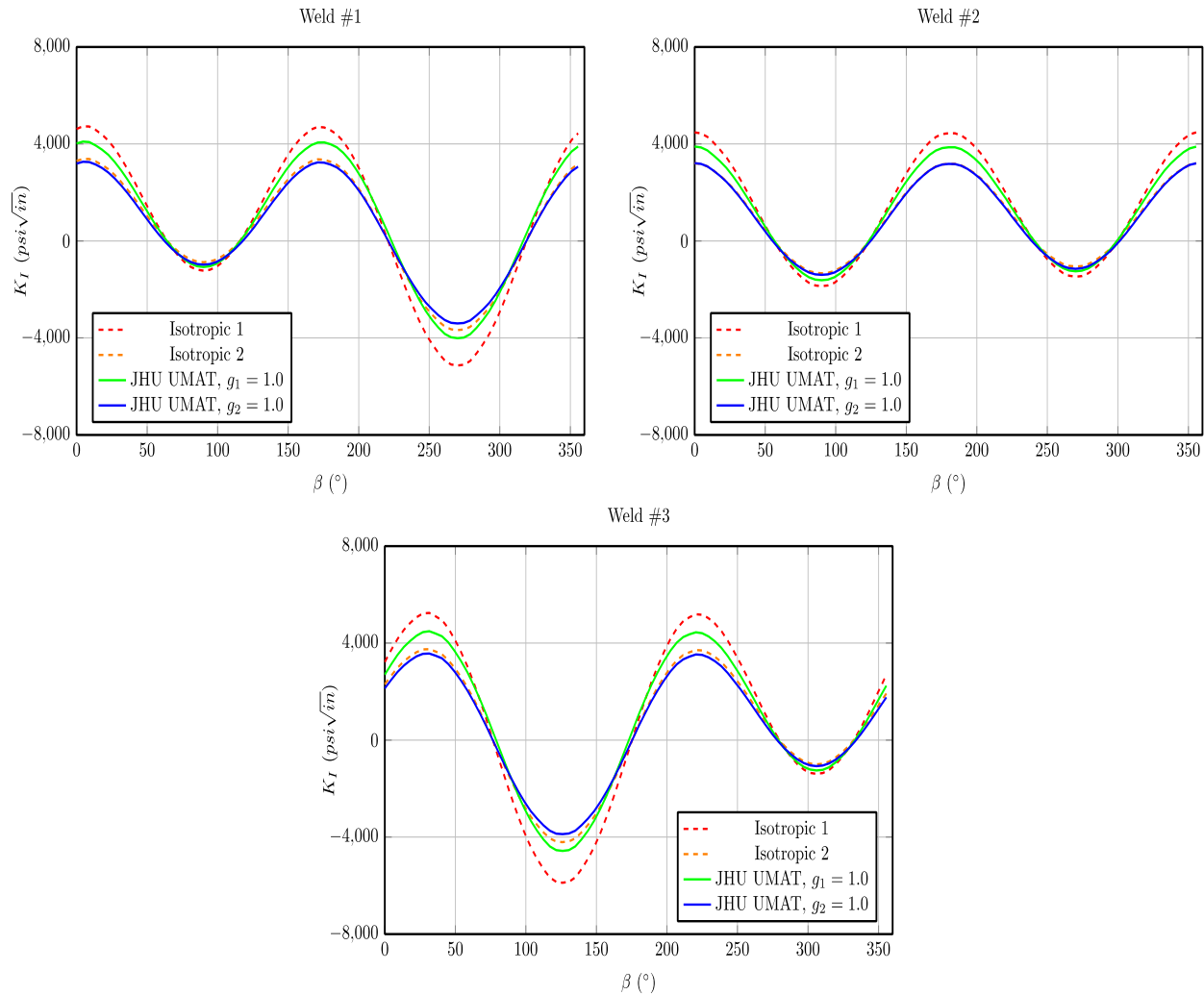


Figure 3.87: Mode I SIFs Each of the Three Spot Welds with Respect to Parametric Angle β

3.3.C: Adaptive Material Constitutive/Damage Modeling

3.3.1. C.1: Micromechanical Deformation, Creep and Crack Nucleation Model Development

CCSS Personnel: Deniz Ozturk (Ph.D Student), Shravan Kotha (Ph.D Student), Somnath Ghosh

AFRL Personnel: B. Gockel

Period of Activity: 7/2013 – 12/2019

Robust micromechanical models that account for deformation, creep and crack nucleation are necessary to predict mechanical behavior and eventual crack initiation in Titanium alloys. This project aims to develop and calibrate micromechanical models that account for detailed mechanisms of deformation and crack nucleation. Specific tasks in this project include the enhancement of crystal plasticity FEM to account for temperature dependency of material

properties of Titanium alloys along with its calibration and validation from experiments provided by AFRL at different temperatures and strain rates. This project also develops a probabilistic crack nucleation model that is calibration and validated based on experiments provided by Adam Pilchak at AFRL.

Introduction

A dual-phase Titanium alloy Ti6242S is considered in this modeling. Samples of this alloy have been experimentally characterized in earlier work [83, 84] and exhibit a bimodal (duplex) microstructure as shown in Figure 3.88. The bimodal microstructure is characterized by equiaxed primary α grains consisting of *hcp* crystals and transformed β grains consisting of alternating laths of α (*hcp*) and β (*bcc*) phases. Size and rate-dependent image-based crystal plasticity FE (CPFE) models of deformation in polycrystalline Titanium alloys have been developed and calibrated in [83-87]. However, in light of the new experimental data available at different strain rates and temperatures in [88], the crystal plasticity parameters for the primary- α phase are recalibrated in this work. The CPFE model is summarized in this section along with its calibration. The grain level crack nucleation model for Titanium alloys is discussed at the end of the section.

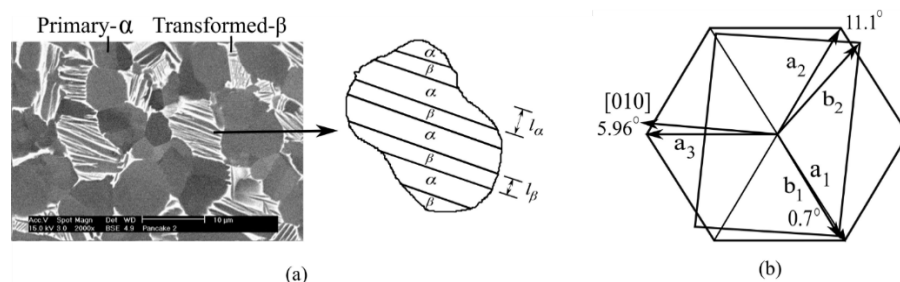


Figure 3.88: (a) Scanning Electron Microscopy Image of a Primary α -transformed β Microstructure [84] where Primary α Grains are Shown in Gray and Transformed β Colonies are Shown in Alternating Gray and White; (b) Burgers Orientation Relationship Between *hcp* and *bcc* Crystals Within Colonies Showing Misorientation Between Different Slip Systems

Generation of Microstructure-based Statistically Equivalent RVEs

3D statistically equivalent virtual microstructures (SEVMs) for polycrystalline Ti alloys are generated from EBSD surface scan data using DREAM.3D software [89]. Following developments in [90, 91], this software segments grains by grouping neighboring voxels with nearly congruent crystallographic orientations and subsequently extracts parent grains statistics from 2D EBSD surface data on crystallographic orientation and misorientation distributions, as well as on morphological distributions of grain size, near neighbors, aspect ratio etc. 3D size and aspect ratio distributions are estimated from the surface data by applying stereological projections while 2D surface crystallographic orientation and misorientation distribution functions are directly used in 3D crystallographic distributions. The DREAM.3D software matches the morphological distribution functions of the generated virtual and experimental microstructures by packing complex shaped grains with assumed morphological distributions and near-neighbor constraints.

3D statistically equivalent representative volume elements (SERVEs) are obtained from the SEVMs from convergence of statistical distributions of morphological, crystallographic and material response functions [75, 76, 92]. The microstructure-based SERVE or M-SERVE is classified as one that is based on convergence of morphological and crystallographic distributions of the microstructure, while property-based SERVE or P-SERVE is determined from the convergence of material response functions. Convergence tests are done to seek the minimum M-SERVE size at which characteristic feature statistics converge, following steps outlined in [75, 76]. An M-SERVE consisting of 529 grains is generated from the EBSD scan of a Ti6242S duplex annealed sheet given [88]. The M-SERVE, along with the comparisons of pole figures, grain size and misorientation distributions is shown in Figure 3.89. For micromechanical analysis, the M-SERVE is meshed into 450272, 4-noded constant strain tetrahedral (CST:TET4) elements using the meshing software [93]. An F-bar patch method developed in [94] is implemented for relieving volumetric locking in the TET4 elements.

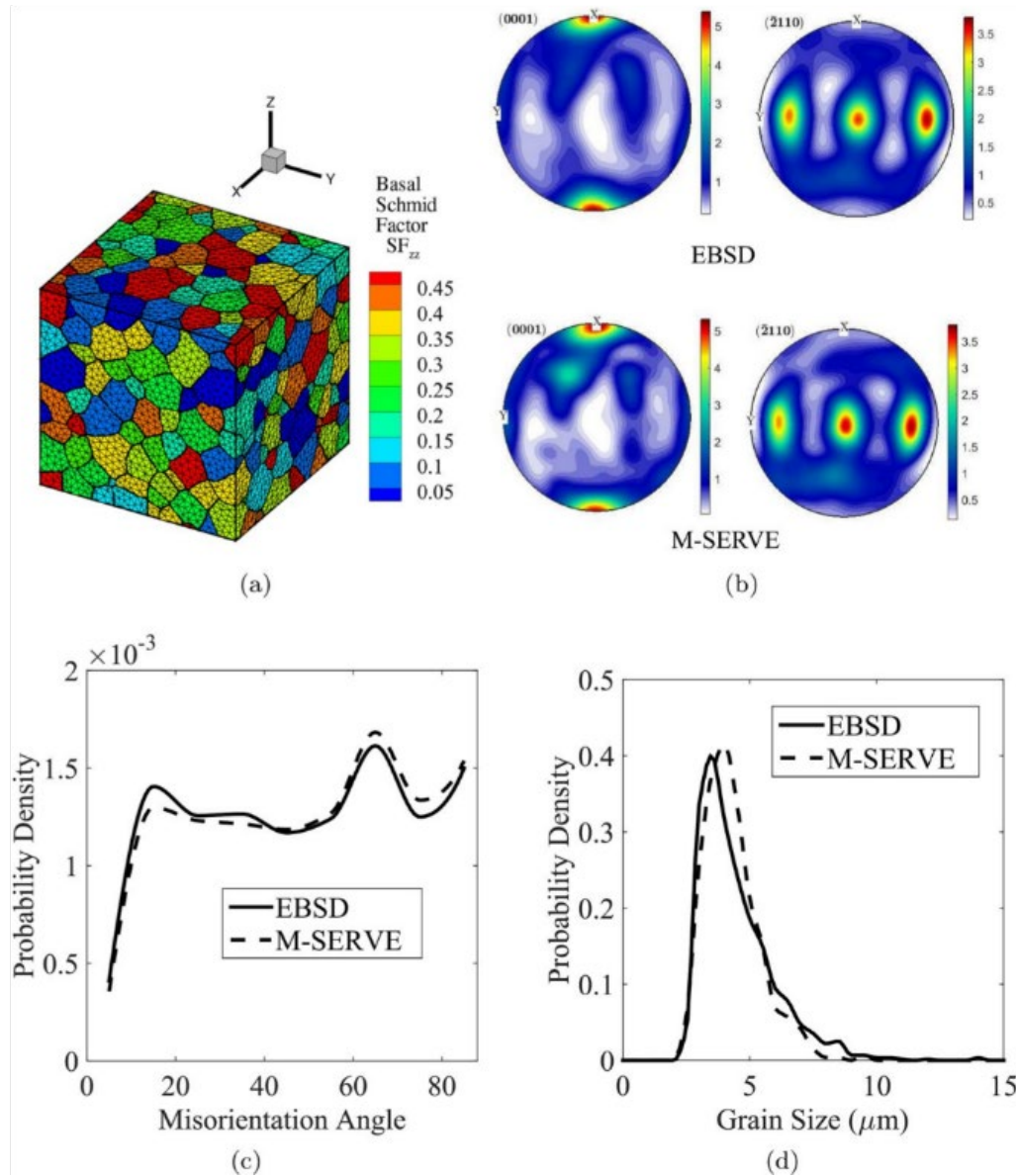


Figure 3.89: (a) Simulated 529 Grain M-SERVE of a Ti6242S Polycrystalline Microstructure Created by DREAM.3D Software Discretized into 450272 TET4 Elements; Comparison of: (b) M-SERVE and EBSD Data-based Pole Figures, (c) Probability Density of Misorientation Distribution and (d) Probability Density of Grain Size Distribution of M-SERVE and EBSD data

Image-based Crystal Plasticity FEM for Micromechanical Simulations of M-SERVE

The bimodal microstructure of Ti6242S is characterized by equiaxed primary α grains consisting of *hcp* crystals and transformed β grains consisting of alternating laths of α (*hcp*) and β (*bcc*) phases. The volume fraction of the α and β lamellae in the transformed β colonies are assumed to be 88% and 12% respectively, from experimental observations discussed in [83, 95]. The *hcp*

crystal lattice consists of a total of 30 different slip systems divided into 5 different slip families, viz. basal $\langle \mathbf{a} \rangle$ ($\{0001\}\{11\bar{2}0\}$), prism $\langle \mathbf{a} \rangle$ ($\{10\bar{1}0\}\{11\bar{2}0\}$), pyramidal $\langle \mathbf{a} \rangle$ ($\{10\bar{1}1\}\{11\bar{2}0\}$), 1st order pyramidal $\langle \mathbf{c} + \mathbf{a} \rangle$ ($\{10\bar{1}1\}\{11\bar{2}3\}$) and 2nd order pyramidal $\langle \mathbf{c} + \mathbf{a} \rangle$ ($\{11\bar{2}2\}\{11\bar{2}3\}$). Similarly, the *bcc* crystal system consists of a total of 48 different slip systems divided into 3 different slip families - $\mathbf{b}_1$ ($\{110\}\{111\}$), $\mathbf{b}_2$ ($\{112\}\{111\}$), $\mathbf{b}_3$ ($\{123\}\{111\}$). During processing, the nucleation and growth of the α laths within the transformed β matrix follows one of 12 possible crystallographic orientations, given by Burgers orientation relationship (BOR) expressed [96] as $(101)_\beta \parallel (0001)_\alpha$, $[\bar{1}\bar{1}\bar{1}]_\beta \parallel [2\bar{1}\bar{1}0]_\alpha$. An example of this relationship is shown in Figure 3.88b, which aligns $\mathbf{a}_1$ ($[2\bar{1}\bar{1}0]$) slip direction of *hcp* crystal with the *bcc* $\mathbf{b}_1$ ($[\bar{1}\bar{1}\bar{1}]$) slip direction. This constitutes a *soft* slip mode since plastic slip is easily transmitted at the lath boundary [84]. On the other hand, significant misalignment exists between α phase $\mathbf{a}_2$ ($[\bar{1}2\bar{1}0]$) and β phase $\mathbf{b}_2$ slip directions, and also between the $\mathbf{a}_3$ ($[\bar{1}\bar{1}20]$) and all $\langle 111 \rangle_\beta$ directions in the β phase. These slip systems constitute *hard* slip modes as plastic slip is arrested at the lath boundary. As a result of the soft and hard slip modes, the ease of slip transmission for $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ basal and prism slips varies significantly [83].

In the crystal plasticity model, the primary α phase is explicitly modeled using 30 slip systems. A computationally efficient equivalent homogenized model has been developed for transformed β grains [83] based on the Taylor model assumption of uniform deformation gradient for all phases with known volume fractions. The equivalent homogenized model has 78 aggregated slip systems corresponding to 30 secondary slip systems and 48 β slip systems in the transformed β grain. The general crystal plasticity formulation is the same for both *hcp* and *bcc* phases with the only difference introduced in the hardening laws.

Crystal Plasticity Constitutive Relations for *hcp* and *bcc* Phases

The crystal plasticity model introduces a multiplicative decomposition of the total deformation gradient ($\mathbf{F}$) into elastic ($\mathbf{F}^e$), thermal ($\mathbf{F}^\theta$) and plastic deformation gradients ($\mathbf{F}^p$) as:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^\theta \mathbf{F}^p \quad (11)$$

The second Piola-Kirchhoff (PK) stress ($\mathbf{S}$) in the thermally expanded configuration is related to elastic Green-Lagrange strain $\mathbf{E}^e = \frac{1}{2}(\mathbf{F}^{eT} \mathbf{F}^e - \mathbf{I})$, by,

$$\mathbf{S} = \mathbf{C}(\theta) : \mathbf{E}^e \text{ where } \mathbf{C}(\theta) = \mathbf{C}|_{\theta=296K} - \hat{\mathbf{C}}\theta \quad (12)$$

Here $\mathbf{C}(\theta)$ is the temperature (θ) dependent elastic stiffness tensor and $\mathbf{C}|_{\theta=296K}$ is the stiffness tensor at a reference temperature of 296K. $\hat{\mathbf{C}}$ represents the change in elastic stiffness tensor per unit increase in temperature. The evolution equations for thermal and plastic deformation gradient are assumed to be given by,

$$\dot{\mathbf{F}}^\theta = \dot{\theta} \boldsymbol{\alpha} \mathbf{F}^\theta \text{ and } \mathbf{L}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1} = \sum_{\alpha=1}^{nslip} \dot{\gamma}^\alpha \mathbf{s}_0^\alpha \quad (13)$$

Where, α represents the second order thermal expansion tensor and $\mathbf{s}_0^\alpha = \mathbf{m}_0^\alpha \otimes \mathbf{n}_0^\alpha$ is the Schmid tensor for a slip system (α) obtained using slip system normal ($\mathbf{m}_0^\alpha$) and slip direction ($\mathbf{n}_0^\alpha$). n_{slip} is the total number of slip systems which correspond to 30 and 48 for *hcp* and *bcc* phases, respectively. The flow rule governing the plastic slip rate ($\dot{\gamma}^\alpha$) on each slip system is given by

$$\dot{\gamma}^\alpha = \dot{\gamma}^\alpha \left\langle \frac{|\tau^\alpha - \chi^\alpha| - \tau_{GP}^\alpha}{g^\alpha + \tau_p^\alpha + \tau_{GF}^\alpha} \right\rangle^{\frac{1}{m}} \text{sign}(\tau^\alpha - \chi^\alpha) \quad (14)$$

Here, $\dot{\gamma}^\alpha$ is the reference slip rate, m is the strain rate sensitivity exponent, τ^α is the resolved shear stress and χ^α is the slip system back-stress. Evolution of χ^α is given by Armstrong-Frederick type non-linear kinematic hardening law [97] as

$$\dot{\chi}^\alpha = c\dot{\gamma}^\alpha - d\chi^\alpha|\dot{\gamma}^\alpha| \quad (15)$$

with c and d representing direct hardening and dynamic recovery coefficients, respectively. τ_{GP}^α and τ_{GF}^α are the hardening contribution from geometrically necessary dislocations (GND) due to short and long-range stresses, given by,

$$\tau_{GP}^\alpha = c_1^\alpha G^\alpha b^\alpha \sqrt{\rho_{GP}^\alpha}, \tau_{GF}^\alpha = \frac{Q^\alpha}{c_2^\alpha b^{\alpha^2}} \sqrt{\rho_{GF}^\alpha} \quad (16)$$

c_1^α and c_2^α are the material constants. G^α , Q^α and b^α correspond to shear modulus, activation energy and Burgers vector respectively. ρ_{GP}^α and ρ_{GF}^α represent GND densities parallel and normal to slip plane and are obtained from curl of plastic deformation gradient [87]. The slip system hardening resistance g^α due to statically stored dislocations is represented using the following hardening law with stress saturation:

$$\dot{g}^\alpha(\theta, t) = \sum_{\beta=1}^{n_{slip}} q^{\alpha\beta} h^\beta |\dot{\gamma}^\beta|, g^\alpha(\theta, 0) = g_0^\alpha(\theta) + g_{HP}^\alpha \quad (17)$$

Where, $g_0^\alpha(\theta) = \bar{g}_0^\alpha - \hat{g}^\alpha \left[1 - \exp\left(-\frac{\theta - \theta_{ref}^\alpha}{\hat{\theta}^\alpha}\right) \right]$ captures the temperature dependency of g^α with calibrated constants $\bar{g}_0^\alpha$, $\hat{g}^\alpha$ and $\hat{\theta}^\alpha$ for each slip system in primary alpha phase [74]. $g_{HP}^\alpha = \frac{K^\alpha}{\sqrt{D}^\alpha}$ is the slip system resistance due to Hall-Petch effect and D^α is the characteristic length-scale governing size-effect [84]. D^α for different slip systems of *hcp* and *bcc* phases are based on the soft or hard slip for a given slip system and are given in [81]. The hardening-rate on individual slip systems of *hcp* components evolves as

$$h^\beta = h_0^\beta \left| 1 - \frac{g^\beta}{g_s^\beta} \right|^r \text{sign}\left(1 - \frac{g^\beta}{g_s^\beta}\right) \text{ and } g_s^\beta = \bar{g}_s^\beta \left(\frac{\dot{\gamma}^\beta}{\dot{\gamma}} \right)^n, \quad (18)$$

h_0^β and g_s^β correspond to the initial hardening rate and saturation stress, respectively. r and n are the hardening and saturation exponents, respectively. For the *bcc* phase, the evolution of self-hardening rate is given by,

$$h^\beta = h_s^\beta + \text{sech}^2 \left[\left(\frac{h_0^\beta - h_s^\beta}{\tau_s^\beta - \tau_0^\beta} \right) \gamma_a \right] (h_0^\beta - h_s^\beta) \quad (19)$$

Here, $\gamma_a = \int_0^t \sum_{\beta=1}^{nslip} |\dot{\gamma}^\beta| dt$ is the accumulated slip on all *bcc* slip systems at a given point. The parameters h_0^β and h_s^β are the initial and asymptotic hardening rates, while τ_0^β and τ_s^β correspond to initial and asymptotic saturation stress. Finally, a yield point phenomenon attributed to precipitate shearing on the basal and prismatic slip systems in *hcp* systems is represented using [74],

$$\tau_p^\alpha = \tilde{\tau}_p^\alpha \exp \left(-\frac{\bar{\varepsilon}_p}{\bar{\varepsilon}_p^*} \right) \quad (20)$$

Here, $\tilde{\tau}_p^\alpha$ and $\bar{\varepsilon}_p^*$ are the yield point phenomenon stress and plastic strain magnitudes respectively and $\bar{\varepsilon}_p = \int_0^t \|D^p\| dt$ is the effective plastic strain. The temperature dependency of $\tilde{\tau}_p^\alpha$ is introduced using the following relationship.

$$\tilde{\tau}_p^\alpha = \bar{\tau}_p^\alpha + \hat{\tau}_p^\alpha \exp \left(-\frac{\theta - \theta_{ref}}{\bar{\theta}^\alpha} \right) \quad (21)$$

Where, $\bar{\tau}_p^\alpha$, $\hat{\tau}_p^\alpha$ and $\bar{\theta}^\alpha$ are the calibrated constants [74]. For *bcc* phase, the yield point phenomenon is not seen in experimental observations and is not considered in the present study.

It has been observed in experiments that Ti alloys exhibit tension-compression asymmetry in their overall response. This has been attributed to mechanisms such as residual stresses in colonies during the growth processes and differential slip transmission mechanisms, depending on the loading direction [84]. The crystal plasticity parameters are separately calibrated in tension and compression and a stress-state dependent, weighted averaging scheme is employed to determine different slip system parameters. The weight W_t for tensile parameters is determined based on the lode angle θ , corresponding to the local stress state in the π -plane. The lode angle is measured clockwise from the third positive principal axis [98]. The π -plane is divided into 6 regions by pure tensile and compressive stress axes. The weighting parameter W_t for tensile parameters changes smoothly from 0 to 1 corresponding to pure compressive and tensile stress axes respectively. The weighted averaging ensures that the hardening parameters change smoothly for all the stress states. The weight for tension is given as:

$$W_t = \frac{1}{2} (1 + \cos 3\theta) \quad (22)$$

$$\text{with } \cos \theta = \frac{S_3^{dev}}{2\sqrt{J_2}}, \sin \theta = \frac{\sqrt{3}(S_2^{dev} - S_1^{dev})}{2\sqrt{J_2}} \quad (23)$$

Where S_1^{dev} , S_2^{dev} and S_3^{dev} are the principal values of the deviatoric part of the second P-K stress tensor and J_2 is its second invariant [81].

Equivalent Homogenized Model for Transformed β Colonies

In CPFE simulations, each grain in the M-SERVE is assumed to consist of either primary α or transformed β phase. In transformed β grains consisting of alternating laths of secondary α (*hcp*) and β (*bcc*) phases, an equivalent homogenized model has been developed in [83] using assumptions of a uniform deformation gradient in the Taylor model for both *hcp* and *bcc* phases. The resulting model for colonies consists of an equivalent single crystal with 78 slip systems. The Cauchy stresses σ in each individual phase is:

$$\sigma_{ij}^{hcp} = \frac{1}{|F_e^{hcp}|} F_{ik}^{e^{hcp}} S_{kl}^{hcp} F_{jl}^{e^{hcp}}, \sigma_{ij}^{bcc} = \frac{1}{|F_e^{bcc}|} F_{ik}^{e^{bcc}} S_{kl}^{bcc} F_{jl}^{e^{bcc}} \quad (24)$$

Using a volume-fraction based weighted-averaging rule, the homogenized stress in transformed beta colonies σ^{TB} is obtained from the stresses in individual phases and their volume fractions as,

$$\sigma_{ij}^{TB} = v_f^{hcp} \sigma_{ij}^{hcp} + v_f^{bcc} \sigma_{ij}^{bcc} \quad (25)$$

where, v_f^{hcp} and v_f^{bcc} are the volume fractions of the α and β laths in the colonies that are weights. In [83], these are taken to be 88% and 12% respectively.

Calibration and Validation of Crystal Plasticity Model

The parameters of the crystal plasticity model summarized in previous sections have been calibrated using different single crystal and polycrystalline experiments in [83- 86, 99]. With the new experimental data [88] available at different strain rates and temperatures for primary- α Ti6242S, some parameters of the crystal plasticity model are recalibrated in [74]. The calibrated parameters along with their temperature dependencies are given in [74, 81]. The temperature dependencies of parameters are calibrated using experimental data at $\theta = 296K, 373K$ and $589K$ and the calibrated crystal plasticity model is validated at $\theta = 473K$. The calibrated and validated stress-strain response at different temperatures and strain rates is given in Figure 3.90. This crystal plasticity model is used in all subsequent simulations in the current work.

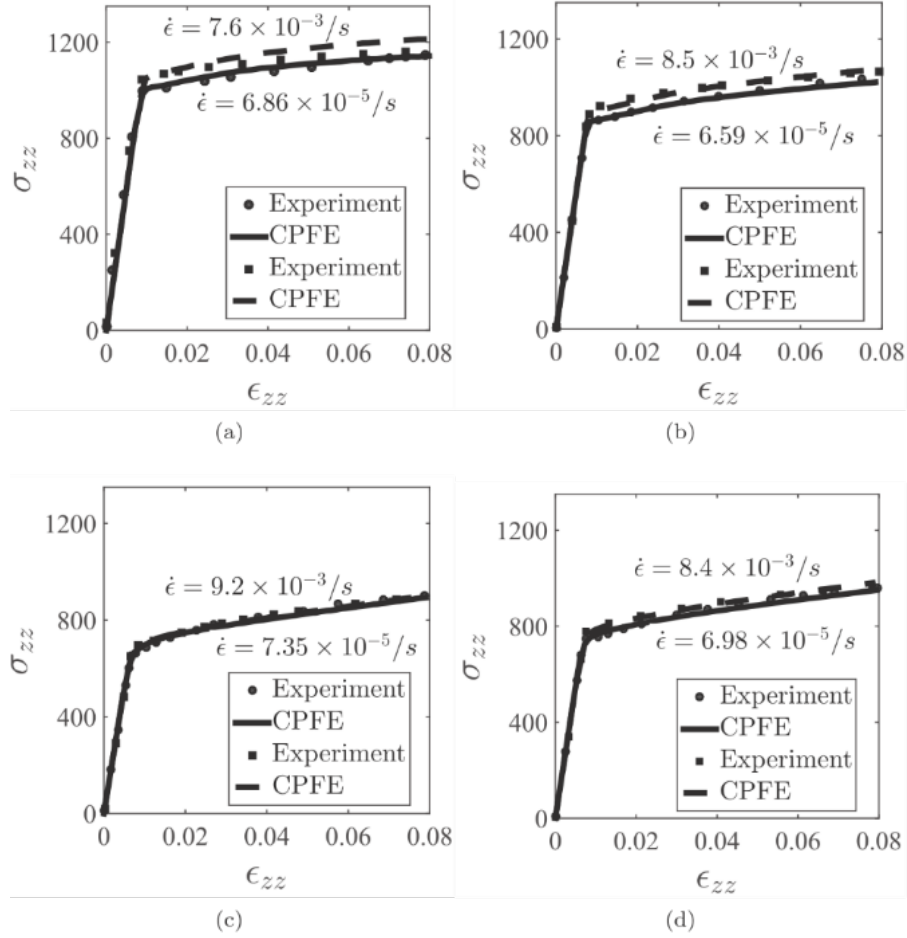


Figure 3.90: Comparison of CPFE Simulated, Volume-averaged True Stress-logarithmic Strain Response with Experimental Data in [88] at Different Temperatures: (a) 296 K, (b) 373 K, (c) 589 K for Calibration, and (d) 473 K for Validation

Grain-level Crack Nucleation Model

The CPFE crack nucleation model has been developed and validated in [100 – 102]. The models are rooted in load-shedding phenomenon, which has been observed to result in near-basal, quasi-brittle dwell fatigue crack nucleation. The inter-granular crack nucleation model in [100, 101] is based on the premise that a wedge crack nucleates in the hard grain with dislocation pile-up in the contiguous soft-grain boundary due to closure failure along a Burgers circuit surrounding the piled-up dislocations. In this non-local model, the hard grain crack nucleation criterion ahead of dislocation pile ups is stated in terms of a nucleation variable R as:

$$R = T_{eff}\sqrt{c} \geq R_c = \frac{K_c}{\sqrt{\pi}} \quad (26)$$

where K_c is a material dependent fracture toughness. $T_{eff} = \sqrt{\langle T_n \rangle_+^2 + \beta T_t^2}$ is the effective traction on a crack facet with a normal $\hat{n}^{cra}$. T_n and T_t are respectively the normal and shear components

of the traction vector and β is the ratio of the critical normal and shear fracture toughness. The length c of the wedge-shaped crack due to lattice incompatibility can be expressed in terms of the crack opening displacement B , which is calculated by integrating Nye's dislocation tensor $\mathbf{A} = \nabla \times \mathbf{F}^p$ [87, 100]. It should be emphasized that the model does not assume the crack surface $\hat{\mathbf{n}}^{cra}$ to lie on a particular crystallographic plane. Rather, among the potential set of wedge cracks with different orientations, that with the largest value of R governs the nucleation process from that point. Therefore, the orientation of a nucleated crack is solely governed by micromechanics. This model has been extended in [102] to account for the large number of slip bands and the uncertainty in local crystal strength R_c due to the crystallographic defects at the tip of each impingement. The probability of nucleation for the domain is calculated using extreme value theory as:

$$P_{nucl} = 1 - \exp \left[- \sum_{i=1}^{n_{GB}} \left(\frac{R_i}{R_{c,0}} \right)^k \rho_d A_i \right] \quad (27)$$

where n_{GB} is the number of CPFE nodes at grain boundaries, k is the Weibull modulus and $R_{c,0}$ is a characteristic nucleation strength parameter. ρ_d is the defect or slip band density evolving with cycles and A_i is the effective surface area around each grain boundary node i that is obtained by Voronoi partitioning. Nucleation probability in the polycrystalline domain P_{nucl} is calculated in every time increment using Eq. (27). The model is able to predict the time, location and orientation of nucleating cracks in polycrystalline microstructures [100, 102].

3.3.2. C.2: Continuum Level Homogenized Models for Deformation and Creep

CCSS Personnel: Shravan Kotha (Ph.D Student), Deniz Ozturk (Ph.D Student), Somnath Ghosh

AFRL Personnel: B. Smarslok, B. Gockel

Period of Activity: 7/2013 – 4/2020

This project develops a computationally efficient, microstructure sensitive parametrically homogenized constitutive model (PHCM) for Titanium alloys like Ti6242 for integration in structural simulations. PHCMs play an important role in material microstructure-informed structural response prediction. These models account for fundamental deformation characteristics exhibited by Titanium alloys such as, anisotropy, tension-compression asymmetry, history/path-dependence, Bauschinger effect, etc. PHCMs are thermodynamically consistent, ROMs, in which microstructural morphology and crystallographic distributions are explicitly represented using *Representative Aggregated Microstructural Parameters* or (RAMPs). Machine learning tools are employed to obtain these functional forms using micromechanical time-dependent plastic deformation and fatigue crack nucleation data-sets that are generated from image-based crystal plasticity finite element simulations. The PHCMs are coupled with Bayesian calibration to quantify different uncertainties, which are then propagated to predict uncertainty in material response (UQ-PHCM). Analogous to PHCM, the micromechanical grain level crack nucleation simulations are used to obtain a Parametrically Homogenized Crack Nucleation Model (PHCNM). The UQ-PHCMs are readily incorporated in commercial FE software like ABAQUS through user-defined material modeling interfaces such as UMAT, for microstructure-sensitive structural

response predictions. Versions of the UQ-PHCMs have been distributed to CCSS for integration in the UIUC ISET framework.

Introduction

PHCMs have been developed for both primary- α (for e.g., Ti7) and dual phase α/β Titanium alloys (for e.g. Ti6242S) in [81, 103]. A generic PHCM framework for dual phase α/β Titanium alloys is presented in this section however PHCM calibration for a primary- α Titanium alloy Ti6242S is only given. More details on PHCM may be found in [74, 80, 81, 103].

Representative Aggregate Microstructural Parameters (RAMPs) in PHCM

Parameters of PHCM equations manifest explicit dependence on microstructural descriptors. Specifically, the constitutive parameters are expressed as functions of Representative Aggregate Microstructural Parameters (RAMPs). These RAMPs characterize different crystallographic and morphological distributions of a microstructure and enable the connection between macroscopic mechanical properties and underlying microstructure. From systematic sensitivity analysis in [74], only the crystallographic texture, misorientation, grain size distribution and lath size have been found to influence the homogenized mechanical response of primary α alloys. The corresponding RAMPs that are used to characterize these microstructural distributions are delineated below.

Texture Intensity Parameter and Material-Symmetry Axes: The texture tensor ($\mathbf{I}^{\text{tex}}$) characterizes the crystallographic c-axis orientation of hcp crystals within a SERVE of the poly-crystalline microstructure. It is defined as:

$$\mathbf{I}^{\text{tex}} = \frac{1}{V} \sum_{i=1}^{n_G} \hat{\mathbf{c}}^{(i)} \otimes \hat{\mathbf{c}}^{(i)} V^{(i)} \quad (28)$$

where, $\hat{\mathbf{c}}^{(i)}$ and $V^{(i)}$ are the unit vector along the c-axis and the volume of i^{th} grain in the microstructural SERVE of total volume of V with n_G number of grains. In [74, 80] the texture tensor has been shown to completely characterize the crystallographic texture of polycrystalline Ti alloys. The eigen-values (g_α) and eigen-vectors ($\mathbf{v}_\alpha$) of $\mathbf{I}^{\text{tex}}$ represent the corresponding RAMPs, termed as the “texture intensity parameters” and “material-symmetry axes”, respectively.

Lattice Orientation with respect to Material-Symmetry Axes: The volume-averaged slip system orientations of a polycrystalline SERVE determine its disposition to plastic slip. In PHCMs, this propensity is accounted for by a RAMP called “Orientation with respect to Material-Symmetry Axes” or ($\overline{OMA}_{\alpha\beta}$). It is defined in terms of the basal and prism Schmid tensors for each grain with respect to the material symmetry axes and is expressed as:

$$\overline{OMA}_{\alpha\beta} = \frac{1}{V} \sum_{i=1}^{n_G} \text{Max} \left\{ \left| \mathbf{v}_\alpha \cdot \mathbf{S}_{0,basal}^{(i)} \cdot \mathbf{v}_\beta \right|, \left| \mathbf{v}_\alpha \cdot \mathbf{S}_{0,prism}^{(i)} \cdot \mathbf{v}_\beta \right| \right\} V^{(i)} \quad (29)$$

$\mathbf{S}_{0,basal}^{(i)}$ and $\mathbf{S}_{0,prism}^{(i)}$ correspond to the Schmid tensors for basal and prism a-slip in i^{th} grain of the SERVE. Plastic anisotropy in polycrystalline Ti alloys is expressed as a function of $\overline{OMA}_{\alpha\beta}$.

Grain-Pair Misorientation Parameter: The misorientation distribution is quantified using a RAMP called the “Grain-Pair Misorientation Parameter” ($\bar{A}_{\theta_{mis}}$). It represents the fraction of grain-pairs with less than 15° misorientation angle θ_{mis} between their $\hat{c}$ axes. It measures the ease of slip transfer across grain boundaries and is defined as:

$$\bar{A}_{\theta_{mis}} = \frac{\text{Grain boundary surface area with } \theta_{mis} < 15^\circ}{\text{Total grain boundary surface area in the polycrystalline SERVE}} \quad (30)$$

Mean and Standard Deviation of Grain Size Distribution: The grain size plays an important role in determining the effective slip-system resistance in crystal plasticity relations [84]. Accordingly, RAMPs are identified to represent the aggregate grain size distribution in the SERVE. For Ti alloys, the grain size distribution in the SERVE has been identified to be represented adequately by a log-normal distribution function [90, 92]. The corresponding RAMPs are represented as the mean ($\bar{D}_g^\mu$) and standard deviation ($\bar{D}_{ln}^\sigma$) of the log-normal distribution defined as:

$$\bar{D}_g^\mu = \frac{1}{n_G} \sum_{i=1}^{n_G} D_i, \bar{D}_{ln}^\sigma = \sqrt{\frac{1}{n_G} \sum_{i=1}^{n_G} [\ln(D_i) - \bar{D}_{ln}^\mu]^2} \text{ where, } \bar{D}_{ln}^\mu = \frac{1}{n_G} \sum_{i=1}^{n_G} \ln(D_i) \quad (31)$$

Here D_i is the diameter of i^{th} grain in the polycrystalline SERVE and $\bar{D}_g^\mu$ is the average grain size. $\bar{D}_{ln}^\mu$ and $\bar{D}_{ln}^\sigma$ are the mean and standard deviation of the log-normal fit to the grain size distribution from the DREAM.3D code [89].

Alpha and Beta lath thickness (l_α and l_β): The response of the transformed β phase in the polycrystalline ensemble depends on the distributions of α and β lath thicknesses, in addition to grain size. This is because, the characteristic length in the Hall-Petch relationship of crystal plasticity model in Equation 17 depends on the orientation of α and β laths with respect to loading direction. Different characteristic lengths are employed for loading along different directions [84]. Therefore, the thicknesses l_α and l_β of the α and β laths are considered as RAMPs in the PHCMs for the transformed β phase. However, as the volume fraction of secondary α in colonies is assumed to be constant (88% in the current work), only l_β is considered as an independent RAMP. A value of $l_\alpha \sim 3l_\beta$ has been determined for 88% volume fraction of secondary α in colonies in [84].

A summary of sensitivity analysis along with the corresponding RAMPs for each microstructural distribution are given in Table 3-8.

Table 3-8: Sensitivity of Elastic and Plastic Response to Various Microstructural Descriptors and Corresponding RAMPs of Polycrystalline Primary α and Transformed β Phases

Microstructural Descriptors	Primary α				Transformed β			
	Elastic Model		Plastic Model		Elastic Model		Plastic Model	
	Sensitivity	RAMP	Sensitivity	RAMPs	Sensitivity	RAMPs	Sensitivity	RAMPs
Crystallographic texture	Strong	$\mathbf{I}^{tex}$	Strong	$\text{OMA}_{\alpha\beta}$	Strong	$\mathbf{I}^{tex}$	Strong	$\text{OMA}_{\alpha\beta}$
Crystallographic misorientation	Weak	-	Moderate	$\bar{A}_{\theta_{mis}}$	Weak	-	Moderate	$\bar{A}_{\theta_{mis}}$
Grain size	Weak	-	Strong	$\bar{D}_{ln}^{\mu}, \bar{D}_{ln}^{\sigma}$	Weak	-	Strong	$\bar{D}_{ln}^{\mu}, \bar{D}_{ln}^{\sigma}$
Lath thickness	-	-	-	-	Weak	-	Strong	l_{α}, l_{β}
Grain aspect ratio	Weak	-	Weak	-	Weak	-	Weak	-
Grain orientation	Weak	-	Weak	-	Weak	-	Weak	-

Constitutive Equations with Microstructural Dependencies and Representation in PHCM

The Ti alloy Ti6242S exhibits a variety of fundamental deformation characteristics such as anisotropy, tension-compression asymmetry, Bauschinger effect, strain rate and temperature dependency in its homogenized mechanical response. These response characteristics are attributed to different grain-scale mechanisms. Constitutive equations of plasticity that form the PHCMs are meticulously chosen to represent the aforementioned mechanical response characteristics. Analogous to the equivalent homogenized model for transformed β colonies in CPFE, an equivalent model that considers the volume fraction of primary α and transformed β phases within a polycrystalline aggregate is formulated in [81] using Taylor assumption. The validity of this formulation is demonstrated in [81]. In the present section, the constitutive equations of PHCM for dual phase α/β Titanium alloy Ti6242S are summarized however, the calibration results are only given for primary α phase. Furthermore, consistent with the crystal plasticity formulations, the PHCM-based macroscopic constitutive relations are assumed to admit a multiplicative decomposition of the total deformation gradient $\bar{\mathbf{F}}$ into elastic, thermal and plastic components as $\bar{\mathbf{F}} = \bar{\mathbf{F}}^e \bar{\mathbf{F}}^{\theta} \bar{\mathbf{F}}^p$, where the overbar symbol corresponds to a macroscopic variable used in PHCM. Here $\bar{\mathbf{F}}^e$ is the macroscopic elastic deformation gradient, $\bar{\mathbf{F}}^{\theta}$ is the macroscopic thermal deformation gradient and $\bar{\mathbf{F}}^p$ is the macroscopic plastic deformation gradient. $\bar{\mathbf{F}}^{\theta} \bar{\mathbf{F}}^p$ defines an intermediate, thermally expanded configuration, corresponding to the overall deformation in every increment. Functional dependencies and representation of the constitutive parameters in terms of RAMPs are discussed below (see [80] for more details).

Anisotropic elasticity in PHCM

The RAMP-dependent macroscopic elastic stiffness tensor $\bar{\mathbb{C}}$ in PHCM relates the macroscopic second Piola-Kirchhoff stress tensor ($\bar{\mathbf{S}} = |\bar{\mathbf{F}}^e| \bar{\mathbf{F}}^{e^{-1}} \cdot \bar{\boldsymbol{\sigma}} \cdot \bar{\mathbf{F}}^{e^{-T}}$) in the thermally expanded intermediate configuration, to the elastic Green-Lagrange strain $\bar{\mathbf{E}}^e = \frac{1}{2} (\bar{\mathbf{F}}^{eT} \bar{\mathbf{F}}^e - \mathbf{I})$. It is expressed using the relation:

$$\bar{\mathbf{S}} = \bar{\mathbb{C}}(\mathbf{I}^{tex}, \bar{\boldsymbol{\theta}}) : \bar{\mathbf{E}}^e \quad (32)$$

Where the RAMP $\mathbf{I}^{tex}$ is defined in Eq. (28). $\tilde{\theta} = \frac{\theta - \theta_{ref}}{\theta_{ref}}$ is the normalized temperature and θ_{ref} is the reference temperature. $\bar{\mathbb{C}}$ is assumed to be orthotropic and θ_{ref} is chosen to be 296K. The explicit parametrized form of $\bar{\mathbb{C}}(\mathbf{I}^{tex}, \tilde{\theta})$ in material symmetry coordinate system is given in Table 3-9. The material symmetry coordinate system is represented in terms of the eigenvectors $\mathbf{v}_\alpha$ of $\mathbf{I}^{tex}$. With deformation, this system is assumed to undergo a rotation expressed as:

$$\mathbf{R}^{mat}(t) = \bar{\mathbf{R}}^e(t) \mathbf{R}^{mat}(0) \text{ where } \bar{\mathbf{R}}^e(t) = \bar{\mathbf{F}}^e(t) \bar{\mathbf{U}}^{e^{-1}}(t) \quad (33)$$

$\mathbf{R}^{mat}(0)$ corresponds to the initial material symmetry orientation. It is expressed in a Cartesian coordinate system with unit vectors $\mathbf{e}_\alpha$ as:

$$\mathbf{R}^{mat}(0) = R_{\alpha\beta}^{mat} \mathbf{e}_\alpha \otimes \mathbf{e}_\beta = \mathbf{v}_\beta \cdot \mathbf{e}_\alpha (\mathbf{e}_\alpha \otimes \mathbf{e}_\beta) \quad (34)$$

Plastic Flow Rule and Anisotropic Yield Function in PHCM

The PHCM plastic flow rule accounts for anisotropy and strain-rate dependency of plastic flow. It is formulated as a power-law equation as:

$$\bar{\mathbf{L}}^p \approx \bar{\mathbf{D}}^p = \dot{\bar{\mathbf{F}}}^p \dot{\bar{\mathbf{F}}}^{p-1} = D_0^p \left(\frac{Y}{Y_0} \right)^{\frac{1}{m}} \bar{\mathbf{N}} \quad (35)$$

where $\bar{\mathbf{L}}^p$ and $\bar{\mathbf{D}}^p$ are the macroscopic plastic velocity gradient and rate of plastic deformation tensor, respectively. D_0^p and m are the reference strain-rate and the rate-sensitivity exponent, respectively. Time integration of $\bar{\mathbf{L}}^p$ yields the plastic deformation gradient $\bar{\mathbf{F}}^p$ in PHCM. Plastic anisotropy in PHCM is expressed by an effective transformed stress (Y), defined as [104],

$$Y = [(|\lambda_1| - \lambda_1)^a + (|\lambda_2| - \lambda_2)^a + (|\lambda_3| - \lambda_3)^a]^{\frac{1}{a}} \quad (36)$$

where k and a are respectively the tension-compression asymmetry parameter and the yield surface exponent that control its shape. λ_1 , λ_2 and λ_3 are the principal values of a transformed effective stress $\bar{\Sigma}$, defined as,

$$\bar{\Sigma} = \mathbb{L}(\overline{OMA}_{\alpha\beta}, \theta): (\bar{\mathbf{S}} - \bar{\mathbf{X}}) \quad (37)$$

where $\mathbb{L}$ is a temperature and microstructure-dependent fourth order anisotropy tensor. This tensor is expressed in the material symmetry coordinate system and its matrix form [105] is given by:

$$\mathbb{L} = \begin{bmatrix} \alpha_{11} & \beta_{12} & \beta_{12} & 0 & 0 & 0 \\ \beta_{12} & \alpha_{11} & \beta_{12} & 0 & 0 & 0 \\ \beta_{12} & \beta_{12} & \alpha_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma_{12} & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma_{13} & 0 \\ 0 & 0 & 0 & 0 & 0 & \gamma_{23} \end{bmatrix}$$

Plastic incompressibility constraint leads to the following relationship among the coefficients of the anisotropy tensor.

$$\beta_{12} = \frac{1}{2}(\alpha_{33} - \alpha_{22} - \alpha_{11}), \beta_{13} = \frac{1}{2}(\alpha_{22} - \alpha_{33} - \alpha_{11}), \beta_{23} = \frac{1}{2}(\alpha_{11} - \alpha_{22} - \alpha_{33})$$

Bauschinger effect in PHCM is represented using a modified Armstrong-Frederick type non-linear kinematic hardening law, in which back-stress $\bar{\chi}$ evolution is given by,

$$\dot{\bar{\chi}} = C\bar{D}^p - \left(D - E \left[\exp \left(\left\langle \frac{-\bar{\chi} : \bar{N}}{G} \right\rangle \right) \right] \right) \|\bar{D}^p\| \bar{\chi} \quad (38)$$

where C, D, E, G are the direct hardening and dynamic recovery coefficients, respectively. The plastic flow is along the normal to the flow surface, defined as,

$$\bar{N} = \frac{\partial Y}{\partial \bar{S}} / \left\| \frac{\partial Y}{\partial \bar{S}} \right\| \quad (39)$$

where $\|\cdot\|$ is the norm defined in Eq. (41). A large number of micromechanical CPFE simulations are performed at different temperatures ranging from 296K to 589K, for polycrystalline microstructures with different crystallographic orientations [80]. A machine learning code Eureka [78] is used to extract the functional forms of the anisotropy tensor $\mathbb{L}$ coefficients in terms of the RAMP $\bar{O}MA_{\alpha\beta}$ and temperature θ . The functional forms of α_{ii} and γ_{ij} are given in Table 3-9. The yield surface parameters are calibrated to be $a = 3$ and $k = -0.058$.

Anisotropic Hardening Model in PHCM

Hardening laws for primary α phase: Anisotropic hardening in the PHCM for primary α phase is formulated as a microstructure-dependent strain hardening Voce-type law [106], in which the flow stress Y_0 is expressed as:

$$Y_0 = \tilde{Y}_0 + \hat{\alpha} \exp \left(- \left(\frac{\bar{\varepsilon}_p}{\hat{\beta}} \right)^{0.75} \right) + \bar{H} \left(1 - \exp(-b\bar{\varepsilon}_p) \right) \quad (40)$$

Where, Y_0 is the initial flow stress. $\hat{\alpha}$ and $\hat{\beta}$ are microstructure and loading direction-dependent parameters that capture the yield point phenomenon observed in Ti alloys, and $\bar{H}$ represents the hardening slope. The parameter b controls the cyclic hardening-rate [107], and $\bar{\varepsilon}_p$ is the effective plastic strain defined as:

$$\bar{\varepsilon}_p = \int_0^t \|\bar{D}^p\| dt = \int_0^t \sqrt{\frac{2}{3} \bar{D}^{p'} : \bar{D}^{p'}} dt \quad (41)$$

Where $\bar{D}^{p'} = \bar{D}^p$ is the deviatoric part of $\bar{D}^p$. The hardening parameters in PHCM depend on crystallographic orientation, misorientation and grain size distributions, as well as temperature. The crystallographic orientation and load-direction dependency of the hardening parameters is

expressed in terms of a dimensionless parameter, defined as:

$$R_Y = \frac{Y(\mathbb{L}; (\bar{\mathbf{S}} - \bar{\chi}))}{Y(\mathbb{I}^{dev}; (\bar{\mathbf{S}} - \bar{\chi}))} \quad (42)$$

R_Y accounts for the amount of $\langle \mathbf{a} \rangle$ type basal and prismatic slip in the polycrystalline aggregate for a given loading, and hence the anisotropy in hardening response. Its microstructure-dependency comes from the orientation dependency of $\mathbb{L}$, and loading direction dependency is accounted for through second P-K stress $\bar{\mathbf{S}}$.

Hardening laws for transformed β phase: The macroscopic hardening response of the transformed β phase depends on the strain-rate and the tension-compression stress-state, in addition to anisotropy of the single crystal hardening parameters. To capture the rate-dependent hardening response, a saturation stress-based hardening law (as in the CPFEM model) is assumed for the transformed β phase. The microstructure-dependent flow stress is given as:

$$Y_0 = \bar{Y}_0(t) + \hat{\alpha} \exp \left(- \left(\frac{\bar{\epsilon}_p}{\bar{\beta}} \right)^{0.75} \right) \quad (43)$$

and the evolution of $\bar{Y}_0$ is given as:

$$\dot{\bar{Y}}_0(t) = \bar{H} \|\bar{\mathbf{D}}^p\| \text{ and } \bar{Y}_0(0) = \tilde{Y}_0 \quad (44)$$

where $\bar{H}$ is the microstructure-dependent hardening-rate expressed as:

$$\bar{H} = \bar{H}_0 \left| 1 - \frac{Y_0}{Y_{sat}} \right|^{\bar{r}} \text{sign} \left(1 - \frac{Y_0}{Y_{sat}} \right) \quad (45)$$

$\bar{H}_0$ represents the initial hardening rate and $\bar{r}$ is an exponent controlling the rate of hardening. Y_{sat} is the saturation stress given as:

$$Y_{sat} = Y_{sat}^{Ref} \left(\frac{\|\bar{\mathbf{D}}^p\|}{D_0^p} \right)^{\bar{n}} \quad (46)$$

Where Y_{sat}^{Ref} is a reference saturation stress and $\bar{n}$ is a saturation exponent, which controls the strain-rate dependency of hardening. The PHCM hardening parameters for the transformed β phase are calibrated from CPFEM simulations under uniaxial tension and compression loads. The calibration accounts for tension-compression asymmetry of single crystal hardening parameters for the secondary α phase in the CPFEM model. Weighted averaging of the calibrated parameters is used for the PHCM hardening parameters subjected to arbitrary loading. The weighting function W_t for tensile hardening parameters is determined from the PHCM-based macroscopic stress tensor using Eq. (12), for consistency with tension-compression states in CPFEM.

Micromechanical CPFEM simulations performed at temperatures ranging from 296K to 589K on

polycrystalline SERVEs with different crystallographic orientation, misorientation and grain size distributions, are used to obtain the functional forms of hardening parameters, given in Table 3-9 for polycrystals with primary- α phase. The functional forms for polycrystals with transformed- β phase are given in [81].

Uncertainty Quantification and Propagation in PHCM

The deterministic PHCMs summarized in the above sections inherently has different sources of uncertainties. These are listed below:

- Model reduction error associated with the functional forms employed in PHCM for constitutive parameters,
- Data sparsity error due to the finite size of microstructural and micromechanical CPFE simulation data-sets used in the PHCM calibration,
- Uncertainty in microstructure or RAMPs due to the natural variability in microstructure associated with thermo-mechanical processing.

An uncertainty-quantified PHCM (UQ-PHCM) framework has been developed in [81, 82] that is only summarized here.

Bayesian Inference of the Functional Forms of PHCM Coefficients

In the stochastic PHCM, the constitutive parameters are considered to be probabilistic and their generalized expression is given as:

$$\theta_i(\mathbf{x}_R) = \sum_k^{n_b} C_{ik} \phi_k(\mathbf{x}_R) + \varepsilon_{m,i} \quad (47)$$

where θ_i represents the set of PHCM constitutive parameters in Table 3-9. $\phi_k(\mathbf{x}_R)$ is the set of n_b basis functions, used for representing the functional form of the constitutive parameters in terms of the RAMP-set $\mathbf{x}_R$. $\mathbf{C} = [C_{ik}]$ is the set of random coefficients in the functional form, to be inferred from the CPFE-based calibration dataset using Bayesian inference. $\varepsilon_{m,i}$ represents the model reduction error. It is assumed to be an independent Gaussian random variable with zero mean and variance $\sigma_{m,i}^2$, where the parameters $\sigma_{m,i}$ are identified using maximum likelihood estimation. Using the micromechanical CPFE dataset $\mathcal{D}$, the posterior distribution of coefficients $\mathbf{C}$ is expressed using the Bayes rule as:

$$p(\mathbf{C}|\mathcal{D}) \propto p(\mathcal{D}|\mathbf{C})p(\mathbf{C}) \quad (48)$$

where $p(\mathbf{C})$ and $p(\mathbf{C}|\mathcal{D})$ are the prior and posterior distributions of the coefficients in the functional form. The posterior distribution contains the uncertainty due to calibration data sparsity. $p(\mathcal{D}|\mathbf{C})$ is the probability density of producing the data $\mathcal{D}$ with a given set of coefficients $\mathbf{C}$, also referred to as the model likelihood. In this work, non-informative, flat priors $p(\mathbf{C}) \propto 1$ are used to avoid subjective bias of the posterior distribution. Using Hamiltonian Monte Carlo technique [108] with No-U-Turn sampler [109] the posterior distributions of constitutive parameters are sampled and their statistical moments are embedded in UQ-PHCM.

Table 3-9: Calibrated Functional Forms for Different Constitutive Parameters in PHCM in Terms of RAMPs

Functional forms for constitutive parameters in PHCM for primary alpha alloy Ti6242S						
<u>Elastic stiffness coefficients:</u>						
$\bar{C}_{mat,ijkl}(\mathbf{I}^{tex}, \tilde{\theta}) = \sum_{\alpha=1}^3 g_{\alpha} \left[C_{ijkl}^{hcp}(\mathbf{v}_{\alpha}, \theta = \theta_{ref}) - C_{ijkl}^{\theta}(\mathbf{v}_{\alpha}) \tilde{\theta} \right]$						
Stiffness Coefficient/index ($ijkl$)	1111	1122, 1133	2222, 3333	2233	1212, 1313	2323
$C_{ijkl}^{hcp}(\mathbf{v}_1, \theta = \theta_{ref})$ (GPa)	204.0	86.0	170.0	98.0	51.0	36.0
$C_{ijkl}^{\theta}(\mathbf{v}_1)$ (GPa)	9.12	4.07	13.52	2.12	4.97	5.27
<u>Anisotropic yield coefficients:</u>						
Without using summation convention and for cyclic permutations of $\{i, j, k\} = \{1, 2, 3\}, \{2, 3, 1\}, \{3, 1, 2\}$,						
$\begin{aligned} \alpha_{ii} &= 0.002312 + 0.000644\tilde{\theta} + 0.017956\overline{MA}_{jk}\overline{MA}_{ii}^2 - 0.000120\overline{MA}_{ik} \\ &\quad - 0.002520\overline{MA}_{jk} - 0.004097\overline{MA}_{ii} \\ &\quad - 0.003048\overline{MA}_{jk}\overline{MA}_{ii}^2\tilde{\theta} \\ \gamma_{jk} &= 0.003986 + 0.000966\tilde{\theta} + 0.000402\overline{MA}_{ik}\tilde{\theta} + 0.018495\overline{MA}_{jk}^2 \\ &\quad - 0.013892\overline{MA}_{jk} - 0.007760\overline{MA}_{ij}\overline{MA}_{ik} \\ &\quad - 0.001315\overline{MA}_{jk}\tilde{\theta} + 0.017787\overline{MA}_{ij}\overline{MA}_{ik}\overline{MA}_{jk} \end{aligned}$						
<u>Hardening Parameters:</u>						
$\begin{aligned} \tilde{Y}_0 &= 0.465 + \frac{\bar{K}_D}{\sqrt{\bar{D}_g^{\mu}}} - 0.288\bar{D}_{ln}^{\sigma} + 0.506(1 - \bar{A}_{\theta_{mis}}) - 0.264(1 - \bar{A}_{\theta_{mis}})^2 \\ \hat{\alpha} &= -37R_Y(1 - 0.089\tilde{\theta}) + 0.183(1 - 0.0135\tilde{\theta}) \\ \hat{\beta} &= 1.3R_Y(1 - 0.92\tilde{\theta}) + 0.001345(1.49 + 0.136e^{0.5\tilde{\theta}}) \\ \bar{H} &= 769R_Y(0.80 + 0.44e^{-6.6\tilde{\theta}}) + 2.07(0.85 + 0.08e^{2.88\tilde{\theta}}) - \frac{\bar{H}_D}{\sqrt{\bar{D}_g^{\mu}}} \\ m &= 0.0651 - 0.0526e^{0.182\tilde{\theta}}, D_0^p = 0.0023 s^{-1}, C = 23795 \text{ MPa}, D = 214, b = 0.5 \\ \bar{K}_D &= 0.348 \text{ MPa}\sqrt{\mu\text{m}}, \bar{H}_D = 0.60 \text{ MPa}\sqrt{\mu\text{m}} \end{aligned}$						

Uncertainty Propagation in PHCM

The uncertainty in constitutive parameters, inferred using Bayesian calibration, is next propagated to material response variables such as stresses and plastic strains using an uncertainty propagation method. This process uses a Taylor series expansion-based uncertainty propagation (UP) method, introduced in [82]. Considering $\xi = \{\xi^i\}$ to represent the evolving state vector containing all constitutive parameters $\theta = \{\theta_i\}$ and the state variables like $\bar{\mathbf{F}}^p, \bar{\chi}, \bar{\epsilon}_p$, the PHCM incremental time-integration scheme is expressed as:

$$\xi_{(n+1)} = \mathfrak{T}[\xi_{(n)}; t_{(n)}; t_{(n+1)}] \quad (49)$$

where the RHS is the time-integration operator over a time-step $[t_{(n)}, t_{(n+1)}]$ in the incremental solution process. The random variables in state vector $\xi_{(n)}$ have a joint probability distribution with mean $\mu_{(n)} = \{\mu^i\}_{(n)}$ and covariance $\Sigma_{(n)} = [\Sigma^{ij}]_{(n)}$. Using Taylor expansion, the time-integrator $\mathfrak{T}[\xi_{(n)}]$ is expanded about $\mu_{(n)}$, which allows expressing the mean $\mu_{(n+1)}$ and covariance $\Sigma_{(n+1)}$ of the state vector $\xi_{(n+1)}$ at time $t_{(n+1)}$ as:

$$\mu_{(n+1)}^i = \bar{\mathfrak{T}}^i + \frac{1}{2} \bar{\mathfrak{T}}_{km}^i \Sigma_{(n)}^{km} \quad (50)$$

$$\Sigma_{(n+1)}^{ij} = \bar{\mathfrak{T}}_k^i \bar{\mathfrak{T}}_m^j \Sigma_{(n)}^{km} + \frac{1}{4} \bar{\mathfrak{T}}_{km}^i \bar{\mathfrak{T}}_{rs}^j (\Sigma_{(n)}^{kmrs} - \Sigma_{(n)}^{km} \Sigma_{(n)}^{rs}) \quad (51)$$

Where $\bar{\mathfrak{T}}^i = \mathfrak{T}[\mu_{(n)}]$ is the time integrator evaluated at the mean state $\mu_{(n)}$. $\bar{\mathfrak{T}}_k^i$ and $\bar{\mathfrak{T}}_{km}^i$ are the partial derivatives of the time-integrator evaluated at $\xi_{(n)} = \mu_{(n)}$, expressed as:

$$\bar{\mathfrak{T}}_k^i = \left. \frac{\partial \xi_{(n+1)}^i}{\partial \xi_{(n)}^k} \right|_{\mu_{(n)}} \quad \text{and} \quad \bar{\mathfrak{T}}_{km}^i = \left. \frac{\partial^2 \xi_{(n+1)}^i}{\partial \xi_{(n)}^k \partial \xi_{(n)}^m} \right|_{\mu_{(n)}} \quad (52)$$

The fourth-order central moment $\Sigma_{(n)}^{kmrs}$ in Eq. (51) is approximated using the Isserlis' theorem [110], based on the covariance matrices $\Sigma_{(n)}^{km}$. The series expansion-based expressions are used to propagate the uncertainty to output variables such as Cauchy stress at every time step. The expansion-based UP method has been found to be computationally efficient and its accuracy is verified by comparing the calculated stochastic response with Monte Carlo simulations in [82].

Parametrically Homogenized Crack Nucleation Model (PHCNM)

Analogous to the PHCM, a parametrically homogenized crack nucleation model (PHCNM) is developed next, as a means of identifying macroscopic hotspots with probable crack nucleation in the underlying microstructure. The PHCNM is a probabilistic surrogate model formulated from micromechanical CPFE model and simulation data. Consistent with the grain-scale crack nucleation model in Eq. (27), the nucleation probability in a macroscopic volume element is given as:

$$\bar{P}_{nuc} = 1 - \exp \left[- \left(\frac{\bar{R}}{R_{c,0}} \right)^k V \right] \quad (53)$$

$\bar{R}$ corresponds to a macroscopic nucleation variable, $R_{c,0}$ and k are Weibull parameters and V is the volume of the macroscopic element. A larger volume has a higher likelihood of containing a defect, which can nucleate a crack under the given loading conditions.

PHCNM is calibrated based on microscopic analyses performed on a large set of M-SERVEs under a range of relevant loading histories. A two-way multi-scaling is employed in which macroscopic FE model of a test specimen with location-specific RAMPs, is simulated for dwell loading

consistent with experiments (see [103] for more details). 500 macroscopic elements are randomly picked from the gage section of the model to conduct top-down CPFE analysis of the local M-SERVE and estimate the microscopic crack nucleation probability P_{nucl} using Eq. (27). The boundary conditions of the microscopic analyses are obtained from the macroscopic solution in the gage section, which deviates from the uniaxial stress state externally applied to the specimen due to material heterogeneity in the gage section. Details of building the specimen model and the top-down multi-scaling are given in [103]. The inverse of Eq. (53) is used to calculate $\bar{R}$ in terms of the microscopic probability P_{nucl} , as $\bar{R} = R_{c,0}[-\ln(1 - P_{nucl}) / V]^{1/k}$ for the entire deformation history of each M-SERVE. The calibration dataset is finally analyzed by the machine learning software Eureqa [78] to express the macroscopic nucleation variable $\bar{R}$ in terms of evolving macroscopic state variables and RAMPs identified by sensitivity analysis. The established functional form $\bar{R} = \bar{R}(\bar{\sigma}_{max,pr}, \bar{\epsilon}_p, N, \bar{D}_g^\mu, \bar{A}_{\theta_{mis}}, g_L)$ is given in [103], in terms of (i) maximum principal macroscopic stress $\bar{\sigma}_{max,pr}$ (ii) total effective plastic strain $\bar{\epsilon}_p$, (iii) number of load cycles N , (iv) mean grain size $\bar{D}_g^\mu$, (v) misorientation measure $\bar{A}_{\theta_{mis}}$ and (vi) texture intensity parameter along the maximum principal tensile stress axis (n_σ), i.e. $g_L = \sqrt{n_\sigma \cdot I^{tex} \cdot n_\sigma}$. In a macroscopic analysis, $\bar{\sigma}_{max,pr}$ and $\bar{\epsilon}_p$ are obtained using PHCM. For each element in a macroscopic FE simulation, nucleation probability $\bar{P}_{nucl}$ is calculated using Eq. (53) by substituting the functional form for $\bar{R}$ in terms of the evolving state variables and RAMPs.

Integration of UQ-PHCM into the Commercial FE Code ABAQUS and its Calibration

The solution process for the finite deformation PHCM equations in previous sections is detailed in [80]. The UQ-PHCM based model is incorporated in the commercial FE software ABAQUS [79] using the user-material subroutine (UMAT). The general work-flow with the sequence of steps in the UQ-PHCM-based structural analysis is shown in Figure 3.91.

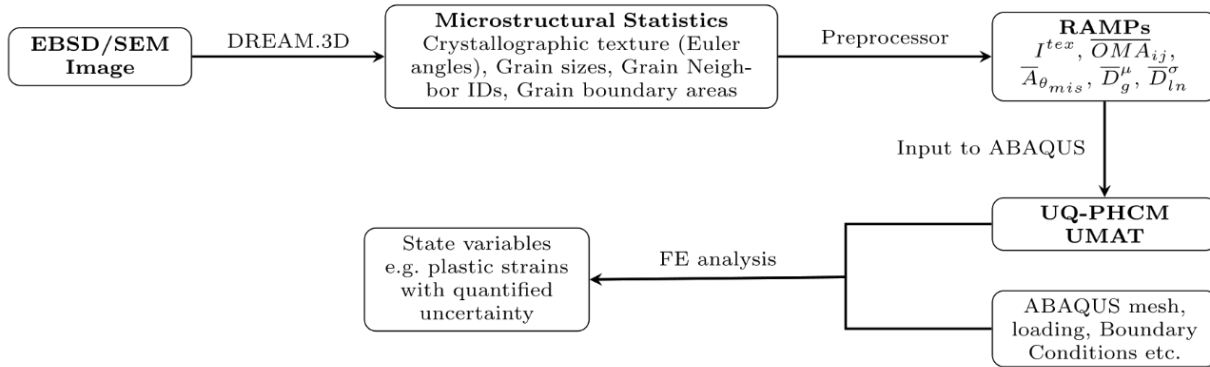


Figure 3.91: Sequence of Steps in the Structural Analysis Workflow with UQ-PHCM

The first step in the analysis requires extracting different morphological and crystallographic descriptors of a polycrystalline microstructure, viz. Euler angles of individual grains, grain sizes, grain boundary areas and grain-neighbor information. These descriptors are extracted from electron back-scattered diffraction (EBSD) images of the microstructures using the DREAM.3D code [89]. An “in-house” pre-processing code takes these microstructural descriptors as input and

calculates RAMPs using Equations 28-31. These RAMPs are inputs to the UQ-PHCM UMAT, which is called at every integration point in the structural analysis model. The mean and standard deviation of various response quantities such as Cauchy stress and effective plastic strain are evaluated using Equations 50 and 51 at every time step and stored as state variables. Similarly, the crack nucleation probability is obtained at every integration point using Equation 53 and stored as a state variable.

Following the sequence of steps described above, PHCM-based predictions are validated with tensile tests, conducted at different strain-rates and temperatures for the alloy Ti6242S [88]. The (0001) and (1120) pole figures corresponding to EBSD scan in [88] are given in Figure 3.92a. The RAMPs corresponding to this EBSD microstructure are obtained and given in Table 3-10. These RAMPs are input as material parameters into ABAQUS UMAT, and functional forms delineated in Table 3-9 are used to obtain different anisotropy and hardening parameters.

Table 3-10: RAMPs Evaluated from EBSD Scan in Test Specimen and Used as Inputs for the PHCM

RAMP	Value
$[g_1, g_2, g_3]$	[0.1784, 0.2731, 0.5484]
ν_1, ν_2, ν_3	[0.89 -0.04 0.46], [-0.45 0.07 0.89], [-0.07 -0.99 0.04]
$\overline{OMA}_{11}, \overline{OMA}_{22}$	0.4384, 0.4319
$\overline{OMA}_{33}, \overline{OMA}_{12}$	0.3525, 0.3975
$\overline{OMA}_{13}, \overline{OMA}_{23}$	0.3830, 0.3830
$\bar{A}_{\phi_{mis}}$	0.1213
$\bar{D}_g^\mu, \bar{D}_{ln}^\sigma$	4.0660 μm , 0.2560

For the PHCM validation, the tensile test specimen used in [88] is modeled using ABAQUS. The model consists of a converged mesh of 20989, 10-noded tetrahedral C3D10 elements, as shown in Figure 3.92b. Minimum boundary conditions are used at one end of the specimen to restrain the rigid body motions and the other end of the specimen is pulled with a time-dependent displacement field corresponding to constant strain-rate experimental loading given in Figure 3.93. The stress strain response obtained at different strain rates and temperatures is shown in Figure 3.93 (see [80] for more details).

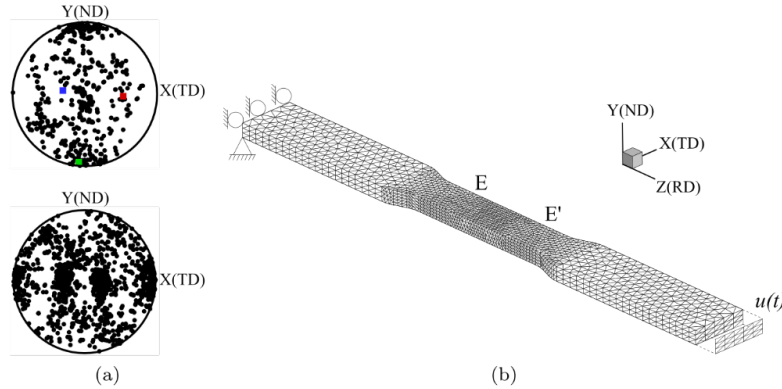


Figure 3.92: (a) (0001) and (1120) Pole Figures of Virtual Microstructure Generated from Statistics of EBSD Scan Given in [88], and (b) Geometry of Tensile Test Specimen Shown with Boundary Conditions, Mesh and Applied Loading

The elastic response is accurately predicted by the PHCM simulations at all the temperatures with a reduction in stiffness at higher temperatures. The PHCM simulations also correctly predict the experimentally observed strain-rate sensitivity and its dependence on temperature. While the initial yield stress is accurately predicted at room temperature, the hardening is slightly over-predicted by the PHCM for the higher strain-rate. For a total strain of 8%, each simulation takes about 20 min on 2 cores of the HHPC cluster at JHU. This set of comparisons between experiments and PHCM predictions demonstrates the accuracy and the computational efficiency of PHCM.

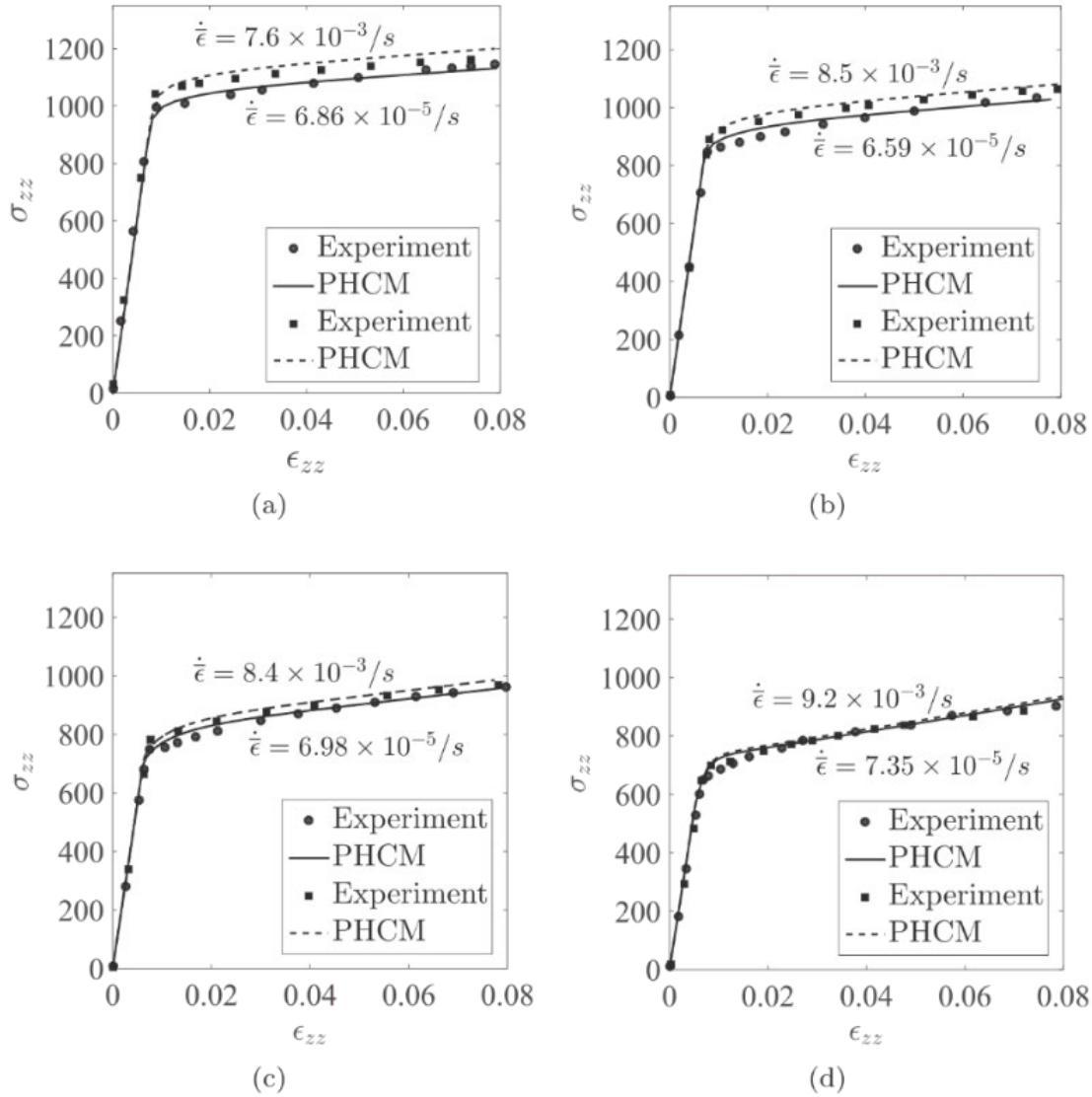


Figure 3.93: Comparison of PHCM Predicted Stress-strain Response with Experiments at Different Temperatures: (a) 296 K, (b) 373 K, (c) 473 K, and (d) 589 K

Parametric Studies on Structural Response Using PHCM

The influence of microstructure on structural response is assessed using the UQ-PHCM-based ABAQUS simulations. Structural analysis is performed on a built-up, ortho-grid panel shown in Figure 3.94a.

FEM of the Built-up Ortho-grid Panel

A built-up panel, made of the Ti alloy Ti6242S, is analyzed under realistic loading conditions to evaluate the influence of microstructure on a structural component. This panel is a part of a high-speed aerospace structure [4]. It consists of a thin sheet of skin supported by evenly-spaced stiffeners along the length and width of the skin, forming an ortho-grid, as shown in Figure 3.94a.

Following [41], the skin is assumed to be clamped on all sides. Its top surface is subjected to a non-uniform, time-dependent pressure loading plotted in Figure 3.94b. This surface pressure profile is obtained from fluid-structure interaction analysis performed in [41]. The pressure is scaled in this work to match the maximum panel deflection obtained in [41]. The time-history of the maximum pressure on the panel is plotted in Figure 3.95a. The panel is meshed with 27712, 20-noded brick elements in ABAQUS that use reduced integration. Capabilities of the UQ-PHCM-based simulations are demonstrated by comparing its predictions with other models for different microstructural and thermal loading conditions.

Effect of Microstructure on Structural Response

The influence of microstructure on structural response is studied by considering three different microstructures viz. MS1, MS2 and MS3 that have varying crystallographic textures. The MS2 in Figure 3.95b is from EBSD scans of the Ti alloy Ti6242S in [88]. MS1 and MS3 are however synthetically generated microstructures, such that there is an increasing volume fraction of c-axis poles aligned along v_3 axis from MS1 to MS3. This is shown in the crystallographic pole figures given in Figure 3.96. All three microstructures have identical average grain-size. The corresponding RAMPs are delineated in Table 3-11, showing values input to the UQ-PHCM-based analysis. The increasing microstructural texture strength is reflected in the

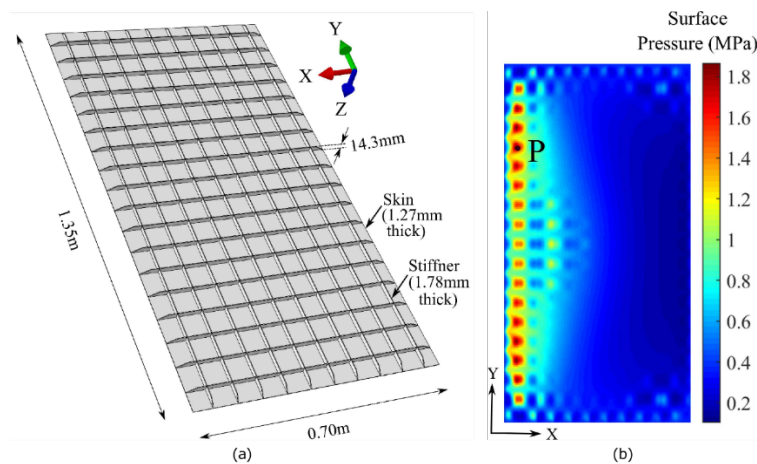


Figure 3.94: (a) Geometry of Ortho-grid Panel with Skin Being Clamped on all Sides, (b) Contour Plot of Aerodynamic Pressure on Skin Obtained by Fluid-structure Interaction (FSI) Analysis in [110]

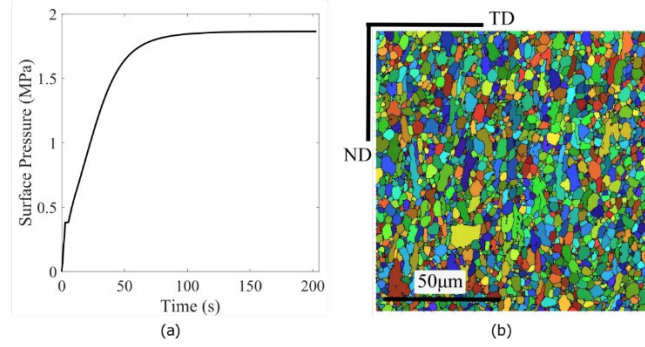


Figure 3.95: (a) Pressure History Plotted at the Point ‘P’ Corresponding to Maximum Pressure in Figure 3.94b, and (b) EBSD Scan of MS2 Microstructure for Alloy Ti6242S

respective RAMPs. The texture intensity parameter g_3 corresponding to material symmetry axis v_3 increases from MS1 to MS3, which indicates that a larger volume fraction of c-axis poles is aligned with v_3 for MS3. A fourth microstructure MS4, identical to microstructure MS3 but with a larger grain size, is studied for grain-size effects. The microstructures studied are appropriate for representing crystallographic textures in rolled sheets with decreasing thicknesses from MS1 to MS3. For such rolled sheets, the direction normal to the rolling direction would align with the v_3 direction. Assuming that the panel is built from rolled sheets of skin and the stiffeners, the RAMPs are assigned to elements in the mesh, such that the normal to the skin and stiffeners align along the v_3 direction of the crystallographic texture.

Table 3-11: RAMPs, Evaluated from Characteristics of 4 Microstructures, Used as Input to PHCM-based Structural Analysis

RAMPs	MS1	MS2	MS3	MS4
$[g_1, g_2, g_3]$	[0.130, 0.406, 0.464]	[0.178, 0.273, 0.548]	[0.097, 0.263, 0.64]	[0.097, 0.263, 0.64]
v_1	[-0.98, -0.18, -0.045]	[0.88, 0.46, 0.04]	[0.13, 0.99, -0.013]	[0.13, 0.99, -0.013]
v_2	[-0.17, 0.96, -0.21]	[-0.45, 0.89, -0.066]	[0.99, -0.13, 0.06]	[0.99, -0.13, 0.06]
v_3	[0.081, -0.20, -0.97]	[-0.06, 0.04, 0.99]	[0.06, -0.021, -0.99]	[0.06, -0.021, -0.99]
$\overline{OMA}_{11}, \overline{OMA}_{22}$	0.4543, 0.4030	0.4383, 0.4319	0.4613, 0.4379	0.4613, 0.4379
$\overline{OMA}_{33}, \overline{OMA}_{12}$	0.3900, 0.3937	0.3525, 0.3974	0.3136, 0.4152	0.3136, 0.4152
$\overline{OMA}_{13}, \overline{OMA}_{23}$	0.4008, 0.3534	0.3830, 0.3830	0.4078, 0.3784	0.4078, 0.3784
$\overline{A}_{\theta_{mis}}$	0.1003	0.1213	0.1847	0.1847
$\overline{D}_g^\mu, \overline{D}_{ln}$	4.0660 μm , 0.2560	4.0660 μm , 0.2560	4.0660 μm , 0.2560	25.000 μm , 0.2560

FE analysis of the panel is performed at room temperature with loading conditions discussed as before. Each simulation takes a wall-clock time of approximately 1.7hrs on 12 CPUs using ABAQUS standard, with only a fraction of this time actually spent on the PHCM execution. Contour plots of the Von Mises stress and the effective plastic strain at the end of the loading are shown in Figure 3.97 for the MS2 microstructure. The corresponding temporal evolution at a critical location ‘A’ in Figure 3.97a, is plotted in Figure 3.98 for all three microstructures. The structural response gradually changes with the variation of MS1 $\rightarrow$ MS3 crystallographic textures. Since the panel undergoes asymmetric bending about its Y-axis, the X-direction stiffeners are subjected to maximum bending. For this deformation, the microstructure MS3 is expected to have softer response i.e. it accumulates more plastic strain compared to MS1 and MS2. This is because, larger volume fraction of (1120) poles of MS3 are aligned with the X-axis of the X-stiffener,

compared to MS1 and MS2. This results in activation of a larger volume fraction of prismatic and basal slip systems in this microstructure, leading to higher accumulated plastic strain and consequently smaller Von Mises stress. Figure 3.98 demonstrates that PHCM-based simulations correctly predict this behavior and thus provide a connection between the structural response and the underlying microstructural crystallography.

The influence of the grain size (a PHCM RAMP) is also studied through the microstructure MS4 that has a larger average grain size of 25 μm . Due to the dependency of the initial yield stress on the average grain-size, MS4 with the higher grain size yields at a smaller stress and accumulates more plastic strain as compared to MS3 under identical loading conditions. This is seen in Figure 3.98, where the Von Mises stress and the effective plastic strain at the location 'A' in the panel are plotted. The predicted Von Mises stress and the effective plastic strain at the end of loading are given in Table 3-12 for all microstructures. The relative difference in a response variable (X) is defined as: $(X - X_{\text{Ref}})/X_{\text{Ref}}$ where X_{Ref} corresponds to MS4. The Von Mises stress and effective plastic strain change by +16% and -20% respectively across the range of microstructures considered. The effect of each RAMP on structural response is discerned through this analysis. It provides a basis for designing optimal set of RAMPs (material design) for robust structural performance.

Table 3-12: Predicted Von Mises Stress and Effective Plastic Strain at Location 'A' in Figure 3.97a and their Relative Differences at End of Loading for Different Microstructures

Model	Von Mises Stress		Effective Plastic Strain	
	Prediction (MPa)	Relative Difference %	Prediction	Relative Difference %
MS1-PHCM	982	15.5	0.0069	-19.8
MS2-PHCM	975	14.8	0.0073	-15.9
MS3-PHCM	949	11.7	0.0077	-10.6
MS4-PHCM	850	Ref	0.0086	Ref

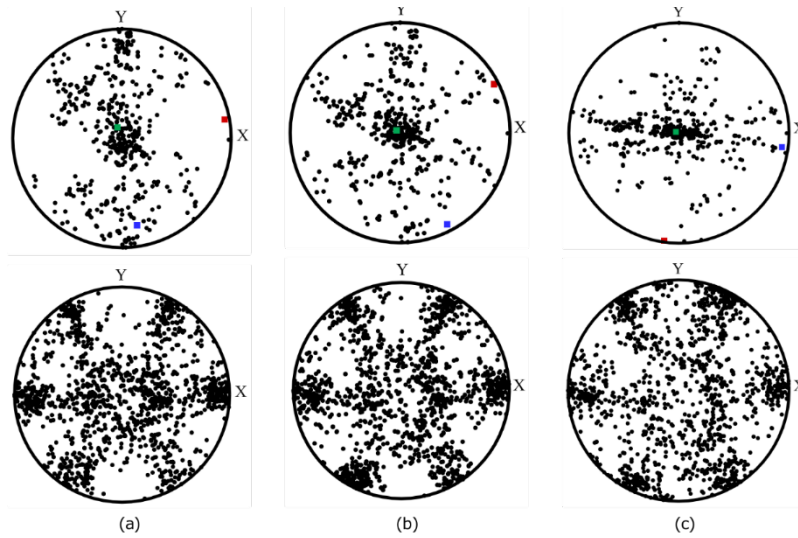


Figure 3.96: (a) (0001)-top and (1120)-bottom, Pole Figures for (a) MS1 (b) MS2 (c) MS3 and MS4, Material Symmetry Axes Marked in (0001) Pole Figures with v_1:Red, v_2:Blue and v_3:Green

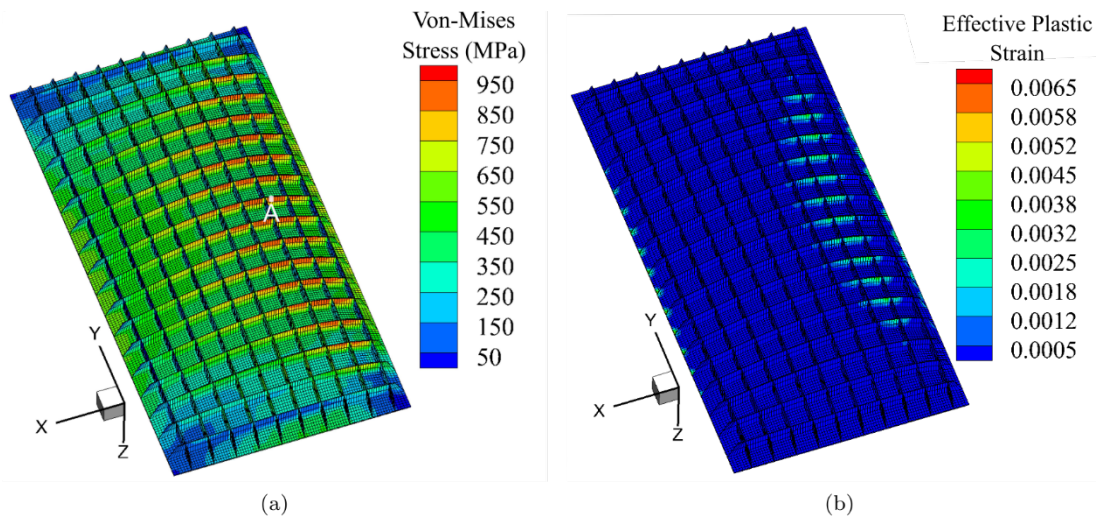


Figure 3.97: Contour Plots of (a) Von Mises Stress and (b) Effective Plastic Strain in Panel at End of Loading Obtained Using PHCM-based ABAQUS Simulations for Microstructure MS2

Comparing PHCM-based Predictions with Isotropic Elasticity and J_2 -Plasticity Predictions

The predictions of PHCM-based simulations are compared with those by isotropic elasticity and J_2 -plasticity in this study. These models do not capture microstructural dependencies in the structural response. For a consistent comparison, these models are derived as special cases of the PHCM. For example, the isotropic elasticity model is obtained by making the texture intensity

parameters $g_1 = g_2 = g_3 = \frac{1}{3}$ corresponding to a uniform texture and increasing Y_0 in Eq. (40) to a large value. The resulting homogenized elastic stiffness corresponds to a uniformly textured polycrystalline microstructure exhibiting isotropic symmetry. Similarly, J_2 -plasticity is derived by setting parameters in Eq. (36) to:

$$a = 2, k = 0, \mathbb{L}_{ijkl} = \mathbb{L}_{ijkl}^{dev} = \frac{1}{2}(\delta_{il}\delta_{jk} + \delta_{ik}\delta_{jl}) - \frac{1}{3}\delta_{ij}\delta_{kl}$$

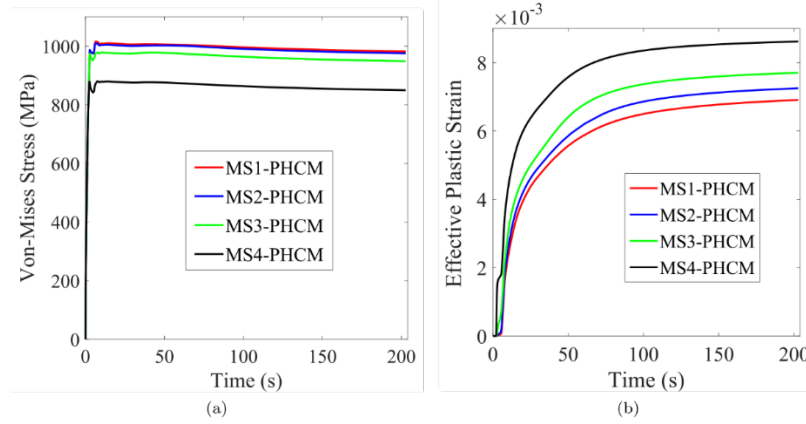


Figure 3.98: Comparison of Temporal Evolution of: (a) Von Mises Stress and (b) Effective Plastic Strain at a Location ‘A’ in Figure 3.97a, Obtained from PHCM-based ABAQUS Simulations for Microstructures Shown in Figure 3.96

The hardening parameters are calibrated from homogenized results of CPFE simulations of a uniaxially loaded microstructure with a uniformly textured polycrystalline aggregate. These hardening parameters are calibrated to be:

$$\tilde{Y}_0 = 1340 \text{ MPa}, \hat{\alpha} = 64 \text{ MPa}, \hat{\beta} = 0.0053, \bar{H} = 3274 \text{ MPa}$$

The panel is further analyzed using these constitutive models under the same set of loading and boundary conditions as discussed before. Figure 3.99 compares the temporal evolution of the Von Mises stress and the effective plastic strain at location ‘A’ with that of the PHCM-based response for microstructure MS4. The response predicted by isotropic elasticity model differs significantly from that by PHCM. Due to the absence of plasticity, the elasticity model cannot predict stress relaxation in the panel. The relative errors in the Von Mises stress and effective plastic strain predictions by the elasticity and J_2 -plasticity models, in comparison with the MS4-based PHCM predictions, are tabulated in Table 3-13. The relative error in a response variable (X) is defined as: $(X - X_{Ref})/X_{Ref}$ where X_{Ref} corresponds to MS4. The elastic model overestimates the Von Mises stress by 82% and underestimates effective plastic strain by 100%. J_2 plasticity model on the other hand, overestimates the Von Mises stress by 20% and underestimates the effective plastic strain by 21%. These errors will increase with the other microstructure based PHCM predictions. For structural analysis, a combination of these errors in various response quantities may lead to a large error in the prediction of extreme properties, such as time to crack nucleation. This study demonstrates the advantages of the PHCMs for microstructure-sensitive structural predictions that surpass other constitutive models.

Table 3-13: The Von Mises Stress and Effective Plastic Atrain at ‘A’ in Figure 3.97a Predicted by Isotropic Elasticity and J2-plasticity Models and Their Relative Errors with MS4-based PHCM Predictions

Model	Von Mises Stress		Effective Plastic Strain	
	Prediction (MPa)	Relative Error %	Prediction	Relative Error %
MS4-PHCM	850	Ref	0.0086	Ref
J ₂ -Plasticity	1018	19.8	0.0069	-20.4
Isotropic Elasticity	1545	81.8	0.0000	-100.0

Effect of Temperature on Structural Response

Ti alloys like Ti6242S exhibit temperature-dependent mechanical behavior, as discussed in [88]. This includes temperature-dependent elasticity, plastic anisotropy, initial yield stress, hardening and strain-rate sensitivity. With increasing temperature, Ti6242S yields at smaller stresses due to thermal activation, while exhibiting higher material hardening. Studies in [88] have shown that strain-rate sensitivity decreases with an increasing temperature, eventually vanishing at 589 K. To comprehend the influence of temperature-dependent material properties on structural response, parametric studies of the panel are conducted using PHCM-based ABAQUS simulations at a range of temperatures from 296 K to 589 K. The RAMPs for the microstructure MS2 are assigned to all the elements. The panel is subjected to appropriately scaled surface pressure loading given in previous sections at four different temperatures viz. 296 K, 373 K, 473 K and 589 K. The Von Mises stress and effective plastic strain at location ‘A’ in the panel, from the FE analyses are plotted in Figure 3.100. Due to thermal softening, the material requires smaller stresses to yield as the temperature increases, and thus accumulates higher plastic strain. Diminishing strain-rate sensitivity and increased material hardening with temperature, leads to smaller stress relaxation at higher temperatures as seen in Figure 3.100. This demonstrates the capability of PHCM to account for both microstructure and temperature-dependent mechanical response.

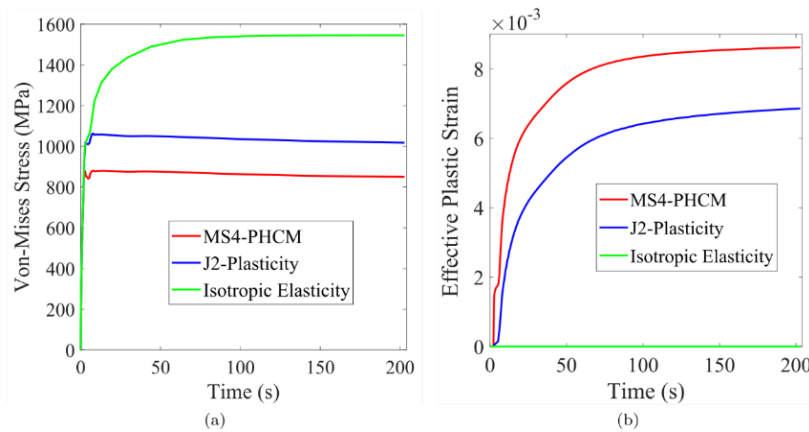


Figure 3.99: Comparison of Temporal Evolution of: (a) Von Mises Stress and (b) Effective Plastic Strain, at a Location ‘A’ in Figure 3.97a Obtained Using Isotropic Elasticity, J2-plasticity and PHCM-based ABAQUS Simulations for MS4

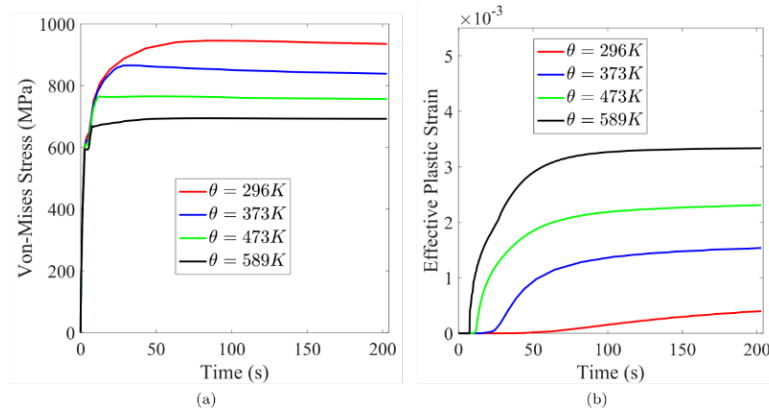


Figure 3.100: Temporal Evolution of: (a) Von Mises Stress and (b) Effective Plastic Strain for Different Temperatures at Panel Location ‘A’ in Figure 3.97a with MS2-based PHCM Simulations

Influence of Microstructural Uncertainty on Structural Response

The model reduction and data sparsity errors represent uncertainties accrued during the calibration stage of the PHCM. They account for the deviation of the PHCM model prediction from the target homogenized CPFE response. These two aspects of the UQ-PHCM for dual-phase Ti6242S have been studied in a recent paper by the authors [81]. The present section focuses on the effect of microstructural uncertainty in structure-scale material response to demonstrate the capabilities of UQ-PHCM in a practical setting. Microstructural uncertainty is incorporated in UQ-PHCM using stochastic RAMPs, which are obtained from the EBSD scans of the material. To obtain the stochastic RAMPs, the EBSD scan in Figure 3.95b is repeatedly sampled with 35 μm x 35 μm boxes, following a method described in [103]. This spatial sampling generates a distribution of RAMPs, which represents the natural variability of the microstructure as captured by the EBSD scan. The statistical moments of the RAMPs are calculated from the samples and incorporated into UQ-PHCM. The mean and standard deviation of RAMPs are given in Table 3-11 and Table 3-14, respectively. In the present study, the microstructural uncertainty is only propagated to plastic response, while the elastic response is assumed to be deterministic. Correspondingly, the RAMPs that determine the elastic response in PHCM viz. g_1 , g_2 and g_3 are kept at their mean values.

Table 3-14: Standard Deviation of RAMPs Estimated from EBSD Scan of MS2 Microstructure in Figure 3.95b

RAMP	$\overline{OMA}_{11}$	$\overline{OMA}_{22}$	$\overline{OMA}_{33}$	$\overline{OMA}_{12}$	$\overline{OMA}_{13}$	$\overline{OMA}_{23}$	$\overline{D}_g^\mu$	$\overline{A}_{\theta_{mis}}$
Standard Deviation	0.01065	0.01560	0.05013	0.02211	0.02589	0.029311	0.16788	0.03646

The RAMPs are assigned to all the elements of the FE model of the panel in Figure 3.94a, and is subjected to loading conditions discussed before. Using the Taylor expansion-based uncertainty propagation method, uncertainty in the RAMPs is propagated to stresses and plastic strains. The Cauchy stress σ_{xx} and the effective plastic strain at location ‘A’ of the panel are plotted in Figure 3.101, along with 1- σ intervals that indicate their standard deviation. It should be noted that the mean response in this figure is same as the deterministic results of MS2 in Figure 3.98. The standard deviation in σ_{xx} and effective plastic strain at the end of loading are 23.36 MPa and

0.000272 respectively. These variations in the Cauchy stress and the effective plastic strain at ‘A’ are due to the uncertainty in material microstructure. The present implementation of UQ-PHCM only gives the mean and standard deviation of material response quantities. The Taylor expansion-based uncertainty propagation can be extended to obtain higher order moments, albeit at a higher computational cost.

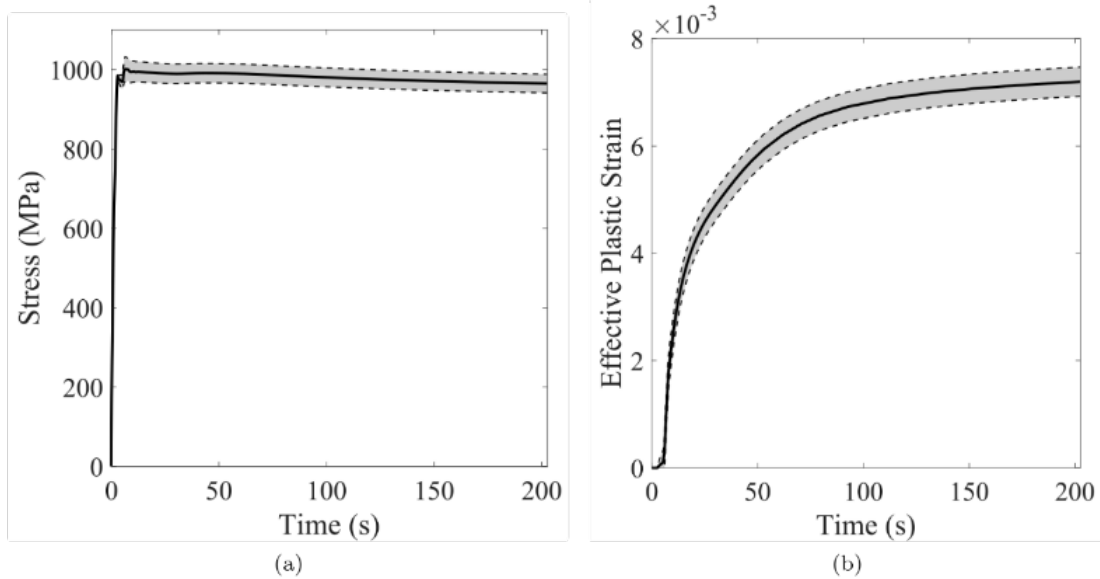


Figure 3.101: Propagated Uncertainty in: (a) Cauchy Stress σ_{xx} and (b) Effective Plastic Strain at Location ‘A’ in Figure 3.97a Due to Microstructural Uncertainty with Solid Line Representing Mean Response and Dotted Lines Corresponding to $1-\sigma$ Intervals Representing Standard Deviation of Response

4. COLLABORATION CENTER INTEGRATION PROJECTS OVERVIEW AND RESULTS

As depicted in Figure 4.1, two capstone integration efforts were carried out in order to aggregate advancements into a combined multi-scale, multi-physics simulation framework capable of handling the complexities shown in Figure 1.1. The core of the framework is the UIUC ISET multi-scale simulation code. The first integration effort, led by UIUC, focused on expanding the capabilities of this code to couple with relevant fidelity fluid models developed at OSU and incorporate advanced continuum level material evolution and damage models developed at JHU. The second integration effort, led jointly by OSU and the AFRL/RQ Structural Sciences Center, refined the fluid-thermal-structural interactions capability of this framework in order to incorporate localized loadings.

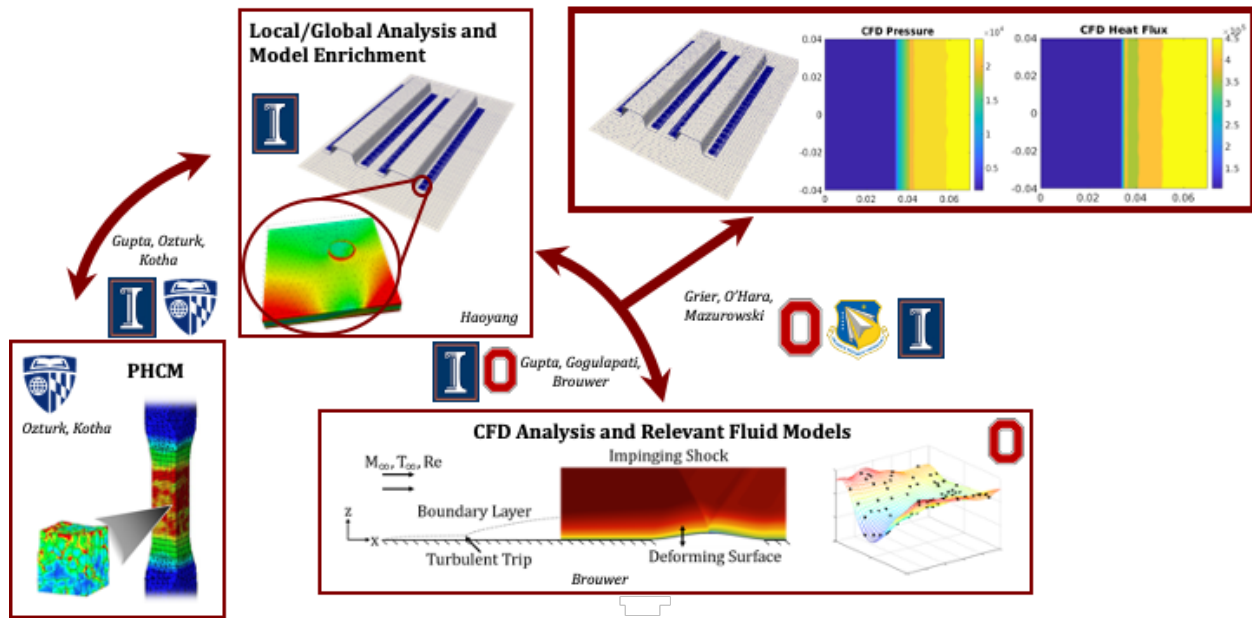


Figure 4.1: Overview of Integration Tasks to Enable Multi-scale, Multi-physics Analysis of High-speed Structural Systems

4.1. I.1: GFEM Integration w/ CFD Surrogates and Continuum Damage Modeling

CCSS Personnel: Piyush Gupta (UIUC), Deniz Ozturk (JHU), Shravan Kotha (JHU), Abhijit Gogulapati (OSU), Kirk Brouwer (OSU), Armando Duarte, Somnath Ghosh, Jack McNamara

AFRL Personnel: T. Eason, P. O'hara, B. Smarslok, S.M. Spottswood

Period of Activity: 8/2016 – 7/2017

Motivation and Objectives

It is now well established that the successful design and development of reusable high-speed aircraft necessitates revolution in structural analysis capabilities. This is rooted by the need to simultaneously address: 1) the unavoidable requirement for optimal weight structural systems so

as to enable a flight system responsive to the demanding performance goals of the USAF, and 2) the resulting extreme environment that such a structural system must repeatedly survive. In other words, the viability of a high-speed aircraft is dependent on accommodating conflicting constraints that seek to minimize weight (inherently increasing compliance) while surviving an extreme (thermal-mechanical) operating environment. Achievement of this requires consideration of multi-scale (in time and space) and multi-physics (fluid-thermal-structural-material) aspects in the structural analysis, where there are strong two-way linkages between the loading environment, the structural response, and the material evolution/damage. This project aims at addressing this need through the integration of three key research thrusts that independently addresses different aspects of this problem. In particular, this integration project combined analysis methods developed as part of the following CCSS projects and thrust areas:

- A2: Enhancement and Refinement of CFD Surrogates
- B1: Linking Solid and Dimensionally Reduced Models
- C2: Continuum Level Homogenized Models for Deformation

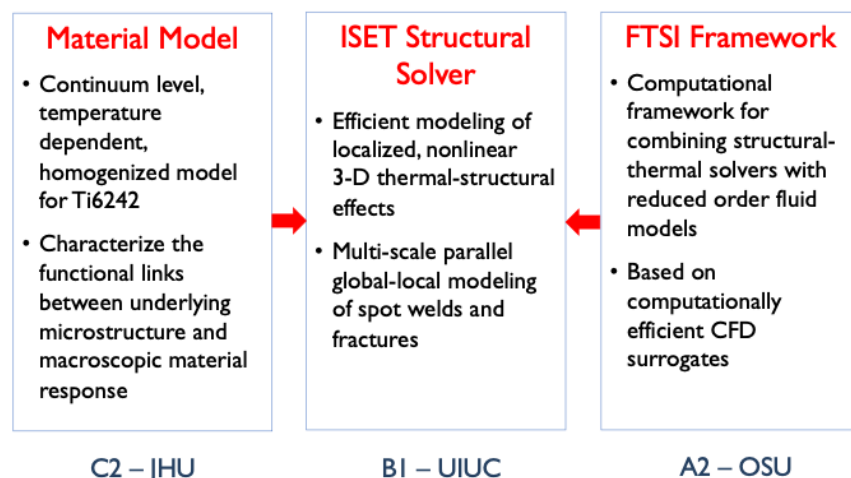


Figure 4.2: Overview of Integrated CCSS Projects

Figure 4.2 presents an overview of CCSS projects that were integrated in this effort. The project was staffed by a post-doctoral fellow which was co-advised by the co-PIs of the projects listed earlier. The next sections report on the efforts of each phase of this project and present the solution of representative multi-physics problems.

Phase I: Integration of Thrusts B and C

This project phase focused on the integration of continuum level homogenized material models for deformation (Project C2), with the multiscale GFEMs (Project B1). The integrated computational framework was built around ISET – a GFEM research software developed at the University of Illinois at Urbana-Champaign (UIUC).

Main Tasks Completed in Phase I of the Project:

1. Transition of JHU linear elastic material model for Ti6242 to UIUC research group. The model was provided as an Abaqus UMAT subroutine. The model uses two material parameters. The user must also provide the material coordinate system.
2. Selection of verification and target application problems.
3. Design and implementation of material models in ISET. This implementation was later on replaced by one based on a generic Abaqus UMAT interface, as described below.
4. Verification of computational framework. Several problems involving orthotropic materials were solved using ISET and Abaqus for verification purposes. These included a cantilever beam and a three-bay panel.
5. Implementation of a generic Abaqus UMAT framework for linear material models. This implementation allows straightforward transition to ISET of material models originally developed for Abaqus – no changes in user code is required. The UMAT material was implemented as an external module to ISET with the following features
 - The material library with UMAT is compiled as a shared object (.so);
 - It is dynamically loaded at run time;
 - There is no need to re-compile ISET: A user can create and update the material library;
 - It is noted that the implemented setup is not limited to a JHU UMAT: It can use any elastic (isotropic or orthotropic) UMAT subroutine.
6. Abaqus UMAT: Extension to non-linear material models. The implementation followed the same strategy as for the linear case. It was verified with a J2 plasticity model. The implementation can potentially be used with other plasticity models, but it was tested only for J2 plasticity.

Details on the user interface implemented in ISET are available in the ISET Reference Manual [118]. All tasks listed above were reported at TIM 06 and 07.

Phase II: Integration of Thrusts A and B

The goal of this phase was the integration of OSU Relevant Fluid Models (RFMs), based on theoretical and CFD-surrogate methods, with the multiscale GFEMs developed in Thrusts areas A and B, respectively. The integrated computational framework was built around ISET, like in Phase I. The integrated framework is able to model and simulate a representative high-speed panel subjected to time-dependent thermo-mechanical loads. The loads are provided by RFMs (from Project A2) and the transient thermo-mechanical response is computed with the multiscale GFEM implemented in ISET (as part of Project B1). The thermo-mechanical loads are coupled to the thermo-mechanical response.

The target representative high-speed structural component analyzed in this project phase was a built-up panel with hat stiffeners and a large number of spot welds. Further details in this application problem are presented below.

Main Tasks Completed in Phase II of the Project:

1. Transition of OSU RFMs to UIUC research group. FORTRAN and MATLAB source code were shared with the UIUC team. The post-doc working on the project visited OSU

to get acquainted with OSU code usage, its Application Programming Interface (API), verification problems solved by the code, etc.

2. Selection of verification and target application problems was performed in consultation with OSU and AFRL collaborators.
3. Design and implementation of GFEM-RFM coupling. The coupled FTSI algorithm implemented in ISET is illustrated in Figure 4.3. The algorithm can adopt either Abaqus or ISET without changes since the functionality implemented in ISET mimics the behavior of corresponding functions available in Abaqus. Some highlights of the implementation are
 - The design of the coupling between the OSU FTSI solver and ISET adopts the same strategy as for the implementation of Abaqus user material models in ISET: It is implemented against the Abaqus API for (FORTRAN) user subroutines, instead of coding directly into ISET.
 - It allows the integration of ISET with OSU FTSI solver non-intrusively – no modifications of OSU code are necessary to support its integration with ISET.
 - The FTSI code base can be changed/improved without requiring modifications to ISET.
 - It adopts a dynamic library, similar to one used for UMATs.
 - No need to recompile ISET or to have its source code;
 - Facilitate transition of integrated code to OSU, JHU, ASU, and AFRL.
4. Verification of computational framework. One of the verification examples solved during this phase of the project is presented below.
5. Solution of target multi-physics problems with the GFEM-RFM computational framework, as reported below.

All project tasks were reported at TIM 07 and at the Advances in Structural Sciences Meeting (TIM 08) on March 2018.

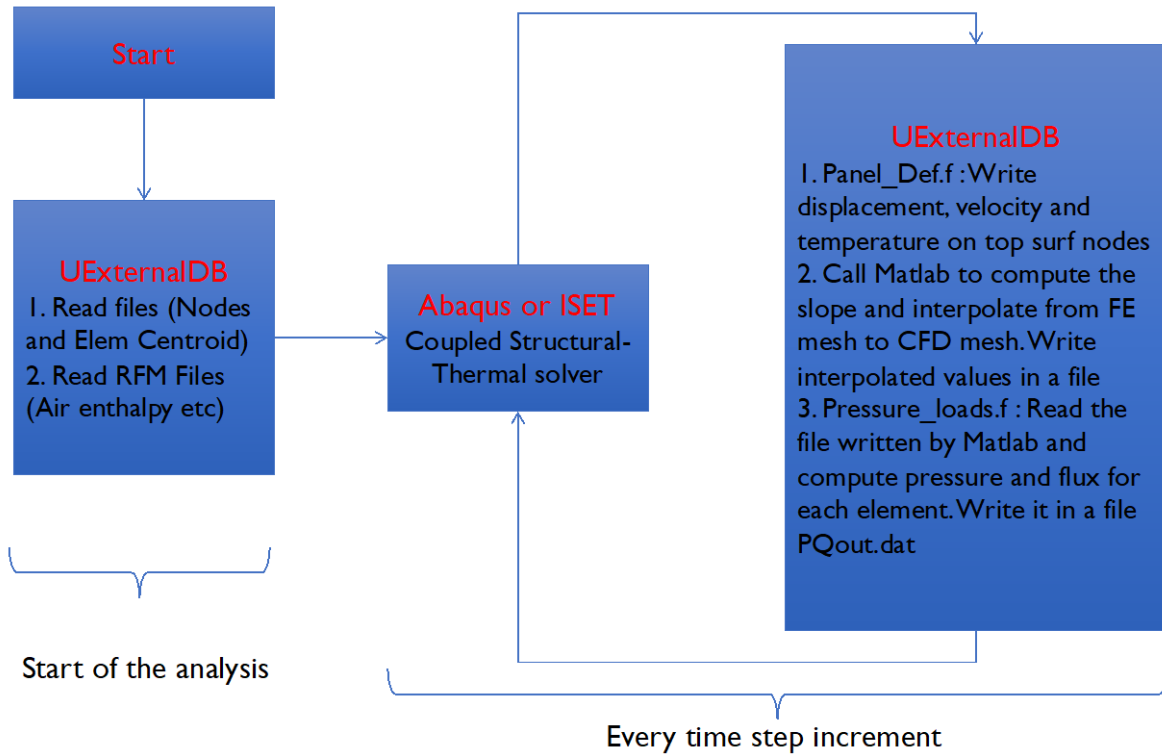


Figure 4.3: Coupled FTSI Algorithm Implemented in ISET

Verification of Coupled FTSI Implementation

The verification example reported in this section is taken from the paper “Measurement and simulation of high-speed fluid-structural interaction on a cantilevered plate in a Mach 6 Flow” by Currao et al. [111]. This is a fully coupled problem with a cantilevered plate subjected to fluid pressure and thermal loading. The problem is illustrated in Figure 4.4.

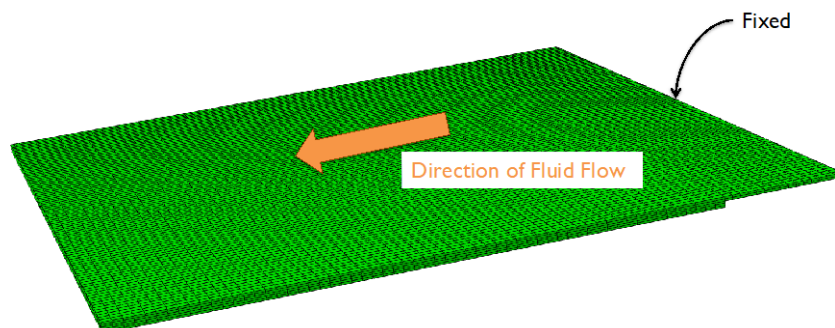


Figure 4.4: Cantilevered plate subjected to Mach 6 air flow.

Figure 4.5 and Figure 4.6 compare results from Abaqus and ISET. The agreement is excellent in all cases. Further details on this problem, step-by-step instructions to solve it using ISET and OSU FTSI code, and post-process its solution are presented in the ISET Tutorial [119].

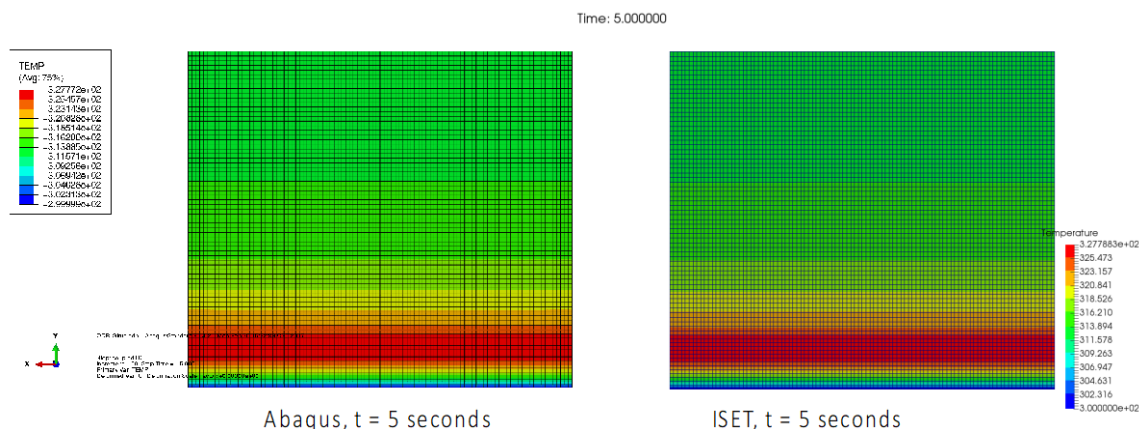


Figure 4.5: Cantilevered Plate Subjected to Mach 6 Air Flow: Temperature Field Computed by Abaqus and ISET at $t = 5$ sec

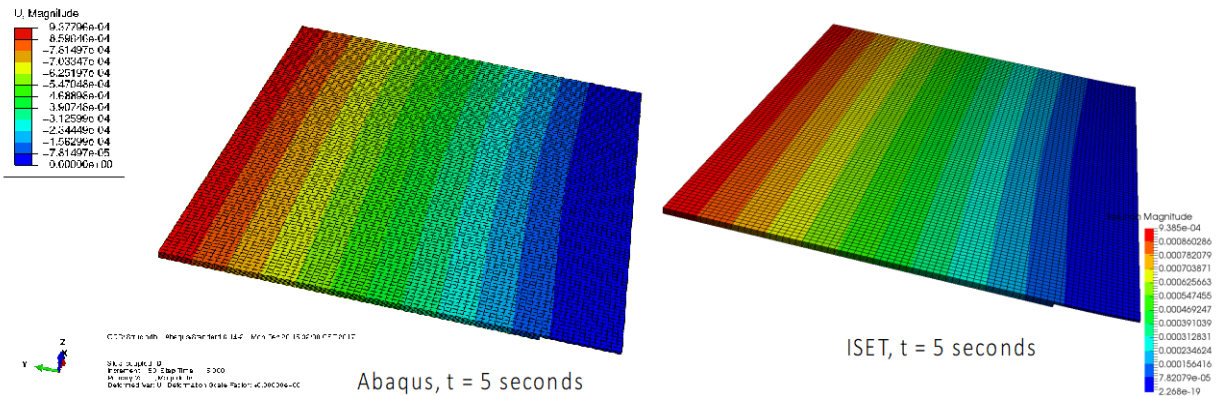


Figure 4.6: Cantilevered Plate Subjected to Mach 6 Air Flow: Contour Plot of Displacement Magnitude Computed by Abaqus and ISET at t = 5 sec

Multi-Physics Simulation of a Hat-stiffened Panel with Spot Welds

The hat-stiffened panel showed in Figure 4.7 is solved in this section using ISET and the OSU FTSI framework. Spot welds are used to connect the panel skin to hat stiffeners. Figure 4.8 shows the prescribed boundary conditions and the GFEM^{sl} mesh. The time-dependent aerodynamic pressure and heat flux on the top surface are provided by the OSU FTSI framework coupled to ISET. The panel is simulated for 5 seconds.

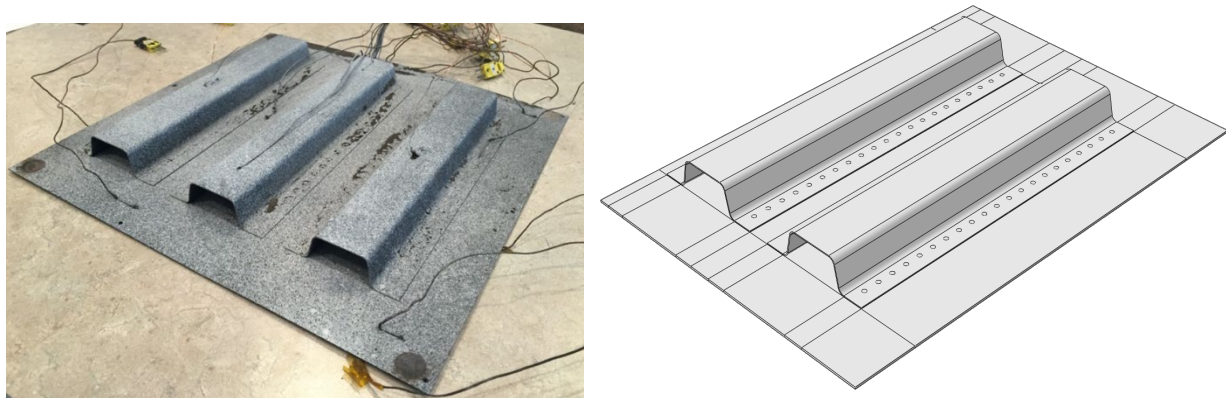


Figure 4.7: Hat-stiffened Panel with Spot Welds (With One Hat-stiffener Missing) and Half-panel Geometry

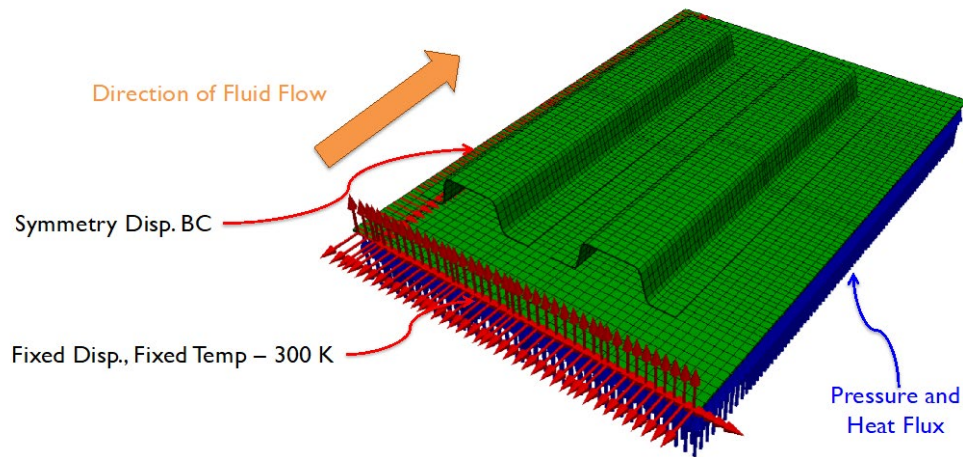


Figure 4.8: Boundary Conditions and GFEM^{gl} for Hat-stiffened Panel with Spot Welds that Need not be Meshed in the GFEM^{gl}

The GFEM^{gl} model shown in Figure 4.8 has 417,876 degrees of freedom. A DFEA model able to provide similar accuracy to the GFEM^{gl} requires 36,350,529 degrees of freedom – about 87 times more degrees of freedom. In addition, the generation of such model requires significantly more user time than in the case of the GFEM^{gl}.

Figure 4.9 shows the von Mises stress on the panel skin (on the skin side connected to the hat stiffeners). The stress is computed at time = 0.2 s, which is the critical time, and using two models – a GFEM^{gl} model and one that represents the welds using point constraints. The later underestimate the stress by a factor of 1.88. This shows the importance of accounting for the true geometry of the welds.

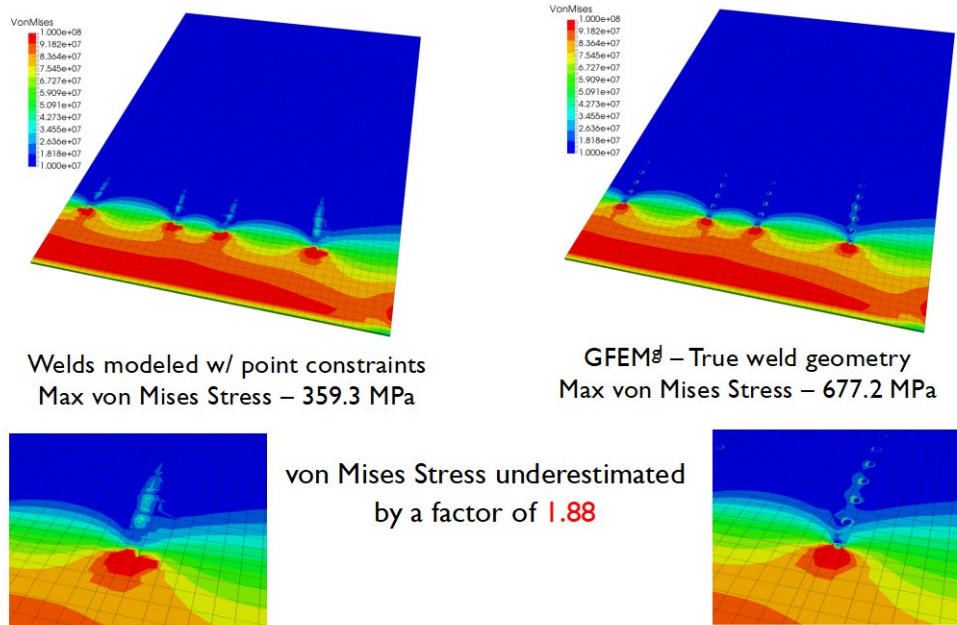


Figure 4.9: Comparison of von Mises Stress Computed by GFEM^g and by Model that Represents Welds Using Point Constraints; Latter Underestimates Stress by a Factor of 1.88

Further details on this problem, step-by-step instructions to solve it using ISET and OSU FTSI code, and post-process its solution are presented in the ISET Tutorial [119].

Transition to AFRL and CCSS Personnel

The integrated computational framework was built around ISET – a GFEM research software developed at the University of Illinois at Urbana-Champaign (UIUC). The ISET source code was made available to AFRL personnel involved in this project. In addition, efforts were made to facilitate new ISET users to get familiar with the code as quickly as possible. A detailed ISET References Manual [118] and a tutorial covering problems solved in this and other CCSS projects was prepared [119] and provided to the Structural Sciences Center. The tutorial provides step-by-step instructions to create GFEM models, solve it using ISET and the OSU FTSI code, and post-process results in a user-friendly graphical interface. YouTube videos covering the compilation of ISET and post-processing its results using Paraview were also created. In addition, hundreds of quality assurance tests covering all aspects of the methods implemented in ISET were shared with AFRL personnel.

4.2.I.2: Response of a Built-up Structure to Localized Loadings

CCSS Personnel: Ben Grier (OSU), Haoyang (UIUC), Bryce Mazurowski (UIUC), Jack McNamara, Armando Duarte

AFRL Personnel: P. O'hara, B. Smarslok, K. Brouwer, T. Eason

Period of Activity: 1/2019 – 2/2020

Introduction

This project seeks to provide a computationally feasible framework capable of capturing multi-scale linkages between coupled structural response and aerothermal loads. The multi-scale, multi-physics ISET capability developed in the previous integration effort was used as the computational infrastructure for the integration effort. Thus, this work follows directly from the integration effort discussed above, which linked relevant fidelity models (RFMs) for environment loadings and homogenized material models (HMMs) into the UIUC ISET code. This integration project builds upon the previous effort by incorporating matured versions of RFMs to carry out thermo-structural analysis of a built-up structural panel. It also advances the fluid-thermal-structural interaction framework in ISET to enable the passing of localized fluid loads to the thermal and structural solvers. As such, it represents the integration of the following CCSS projects and thrust areas:

1. A2: Enhancement and Refinement of CFD Surrogates
2. B.1: Linking Solid and Dimensionally Reduced Models
3. I.1: GFEM Integration w/ CFD Surrogates and Continuum Damage Modeling

The carrying out of these efforts was divided amongst OSU, AFRL/RQ, and UIUC as denoted in Figure 4.10.

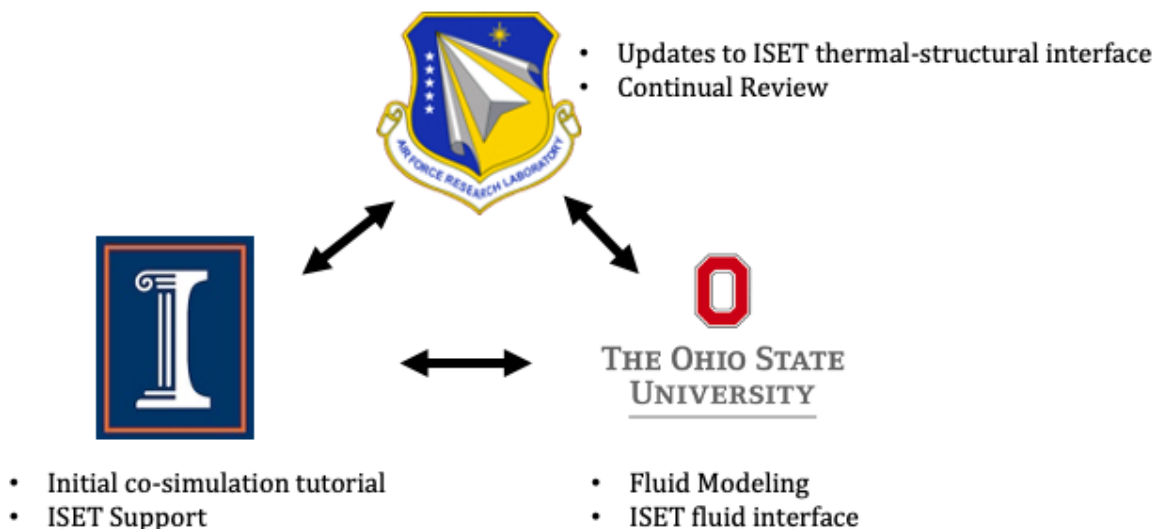


Figure 4.10: Tasks for Second Integration Project Taken on by Each Group

Code Development

As noted, the major extension of the ISET framework was to incorporate more advanced relevant fidelity models for the fluid loadings and to extend the fluid-thermal-structural interactions framework to allow transfer of localized loads to the thermal-structural solver capabilities in ISET. Figure 4.11 represents a high-level overview of the interface. ISET is controlled through TCL file, which subsequently manages the coupling to user defined functions (UDF) containing the various loads solvers (basic engineering, CFD surrogates, or CFD). The UDFs manage bash scripting calls for starting and pausing the different solvers, MATLAB for interpolating between grids, and the different fluid solvers.

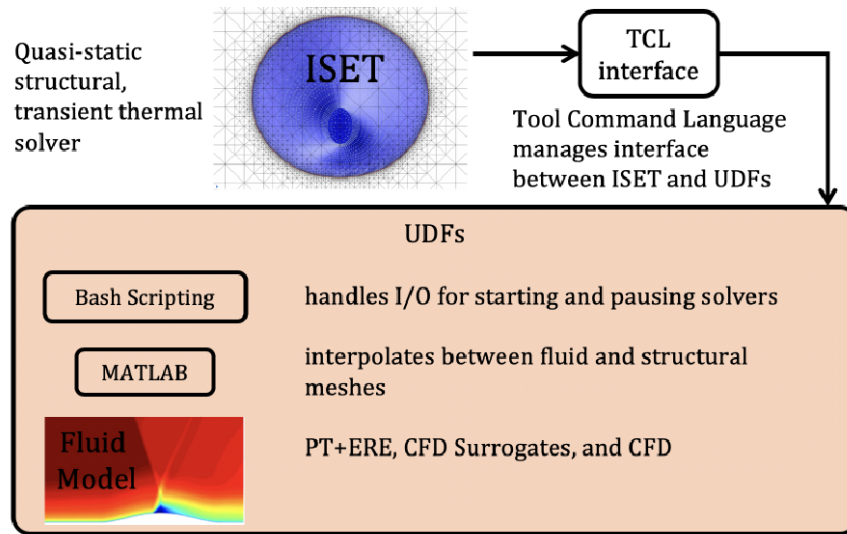


Figure 4.11: Overview of the Fluid-Thermal-Structural Interaction Framework Using ISET

In the first integration effort localized structural features were examined using the coupled framework: spot-welds were modeled through local enrichments and sub-surface features. However, all fluid loads were smoothly varying. Furthermore, the loads were transferred to the ISET solver at the coarse mesh. As shown in Figure 4.12, application of localized fluid loads on the coarse mesh for GFEM results in smearing of the loads rather than application on the refined, localized mesh in the global-local formulation.

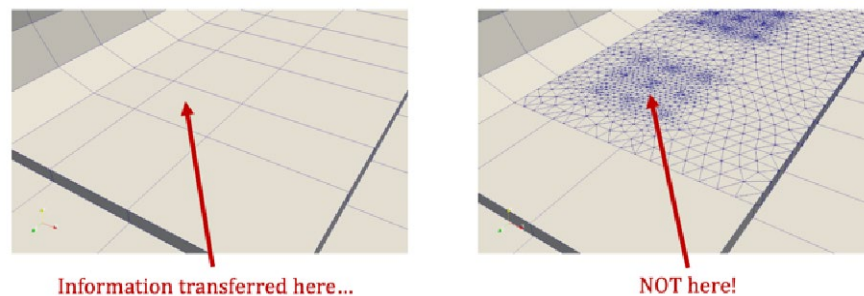


Figure 4.12: Global Mesh (left) Where Fluid Loads Were Previously Implemented and Local Mesh (right) Where Loads are Needed

Dr. Patrick O'Hara of the AFRL/RQ Structural Sciences Center led the effort to modify the ISET code such that the fluid and finite element information is passed at the GFEM integration points rather than the global mesh. Integration points are not confined to the same locations or number of points between time steps, which allows for moving shock and geometry capabilities. This is illustrated in Figure 4.13, where an increase of integration points occurs due to a geometric localization such as a surface crack. Local refinement can also be manually added to the simulation as needed to account for localized fluid loading that is unknown a priori to the GFEM solver.

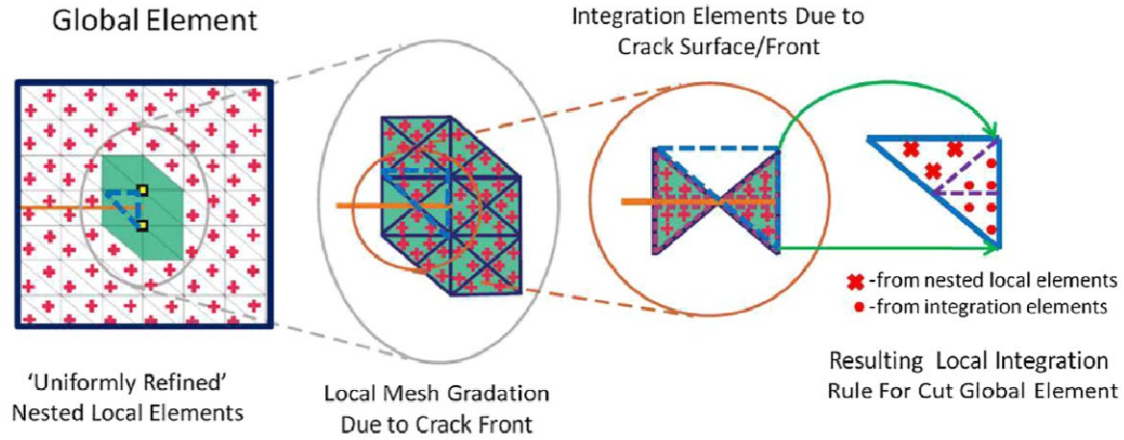


Figure 4.13: Integration Points on a Global Element Due to a Crack Surface

UDFs are used to transfer fluid loads (heat flux and pressure) from the fluid solvers to the GFEM integration points. Currently this interface has been tested with basic engineering models (piston theory and Eckert's reference enthalpy) and CFD loads. Extension to accommodate CFD surrogates is relatively straight forward.

Verification Cases

A simple, 72 element bar with varying heat flux boundary conditions was used for verification of the multi-scale, multi-physics framework. In all 3 cases detailed below, the boundary conditions were implemented both using built-in ISET functions and the coupled framework.

CASE A: Spatially Constant Heat Flux

The heat flux on the top surface is defined by:

$$q(t) = \begin{cases} -50000 (5 - |5 - t|) & t \leq 10 \\ 0 & t > 10 \end{cases}$$

CASE B: Linearly Varying Heat Flux

The heat flux on the top surface is defined by:

$$q(x, t) = \begin{cases} -50000x (5 - |5 - t|) & t \leq 10 \\ -50000x & t > 10 \end{cases}$$

CASE C: Gaussian Distribution of Heat Flux

$$q(x, t) = \frac{-750 (1 - e^{-15t})}{0.025} e^{\frac{-0.5(x-5.3)^2}{0.25^2}}$$

The solutions for each case are extracted at 10 seconds and compared in Figure 4.14 - Figure 4.16. The three verification cases clearly exhibit an increase in maximum difference with the increase in surface heat flux complexity. For a spatially constant heat flux the error is near precision of all written files required by the coupled framework's I/O. There is a significant increase in the difference when using the spatially linear and Gaussian heat flux distributions. However, each of these differences are 5 orders of magnitude less than the heat flux at the given locations, indicating errors are fractions of a percent. Thus, while the exact source of these discrepancies have not been tracking down, all cases are deemed to be within an acceptable threshold for use of the framework.

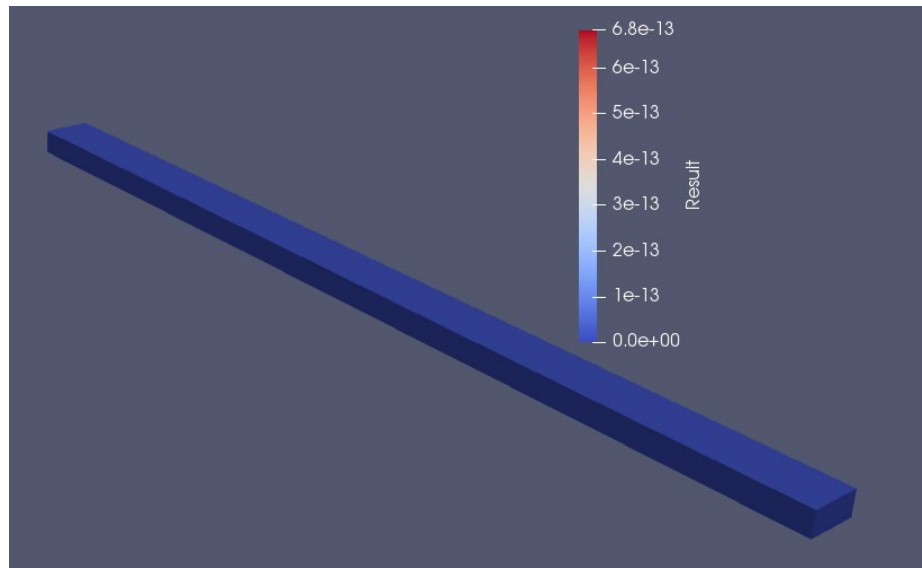


Figure 4.14: Absolute Differences in Heat Flux When Using ISET With and Without Coupled Framework for Case A (Spatially Constant Heat Flux)

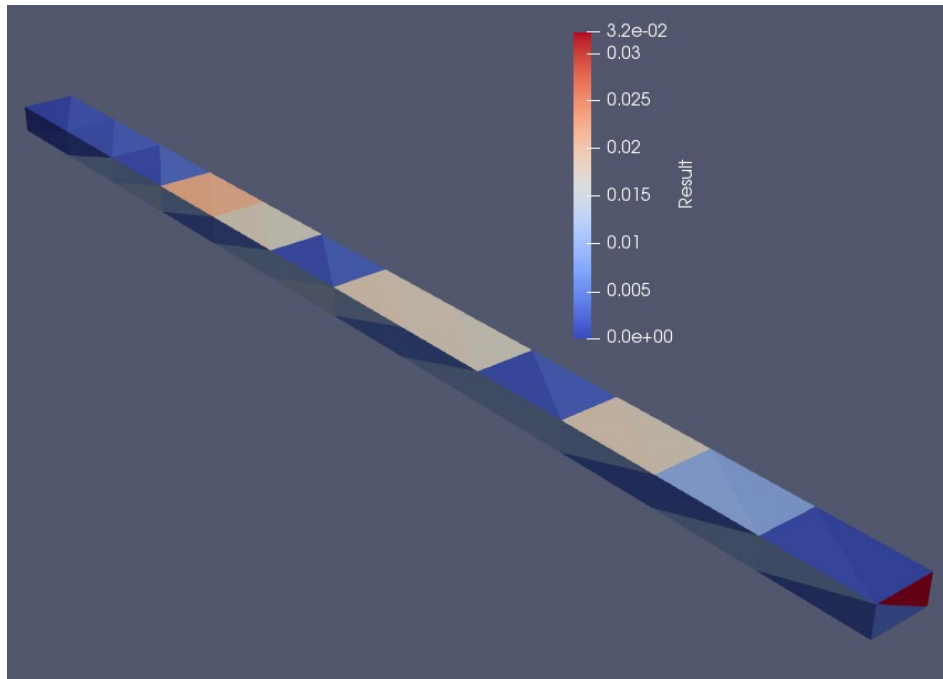


Figure 4.15: Absolute Difference in Heat Flux When Using ISET With and Without Coupled Framework for CASE B (Linearly Varying Heat Flux)

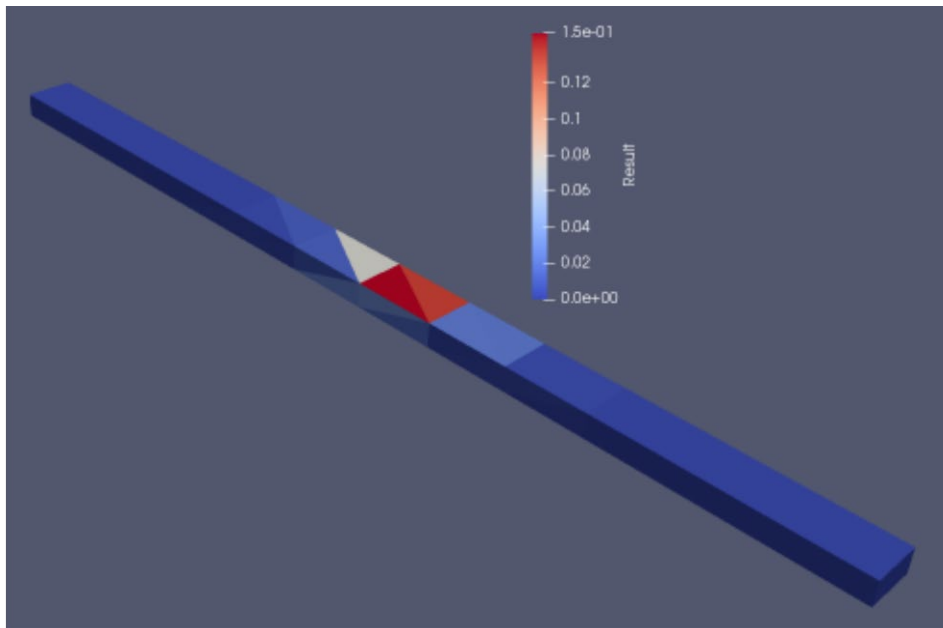


Figure 4.16: Absolute Difference in Heat Flux When Using ISET With and Without Coupled Framework for CASE C (Gaussian Distribution of Heat Flux)

Further details on this problem, step-by-step instructions to solve it using ISET and OSU FTSI code, and post-process its solution were added to the ISET tutorial document [119]. An accompanying video demonstration was also developed.

Transition to AFRL and CCSS Personnel

The enhanced ISET multi-physics framework was made available to AFRL personnel involved in this project. The documentation of Integration Project II provides step-by-step instructions to expand upon the tutorial from Integration Project I [119] to include compiling the expanded code, and running a case with both piston theory/Eckert's Reference Enthalpy and CFD. A video recording covering the example walk through was also created.

5. RELATED / LEVERAGED RESEARCH PROJECTS

Throughout the CCSS duration, several additional research projects were developed with external support based on the work carried out through the center. A short summary and associated references for each are provided.

5.1.OSU/ASU Collaboration

As depicted in Figure 5.1, OSU and ASU carried out an effort to couple the OSU relevant fluid models (basic engineering models, CFD surrogates, and CFD) to the ASU thermo-structural ROMs. The first phase of this collaboration focused on simulating experiments conducted by the AFRL/RQ Structural Sciences Center to simulate the response of a thin-gauge panel to shock-boundary layer interactions. The second phase of this effort, funded by the Boeing Company, focused on application of this capability to the orthogrid panel shown in Figure 5.1. in addition to developing a complete reduced order aerothermoelastic modeling framework, a co-simulation framework was developed based on the commercial Abaqus finite element code for thermo-structural analysis. This framework served as the basis for the multi-physics capability discussed in Section 4 for the two integration projects. These capabilities were transitioned to both Boeing and the AFRL/RQ Structural Sciences Center.

This effort led to the following publications documenting the work: Refs. [22, 23, 112].

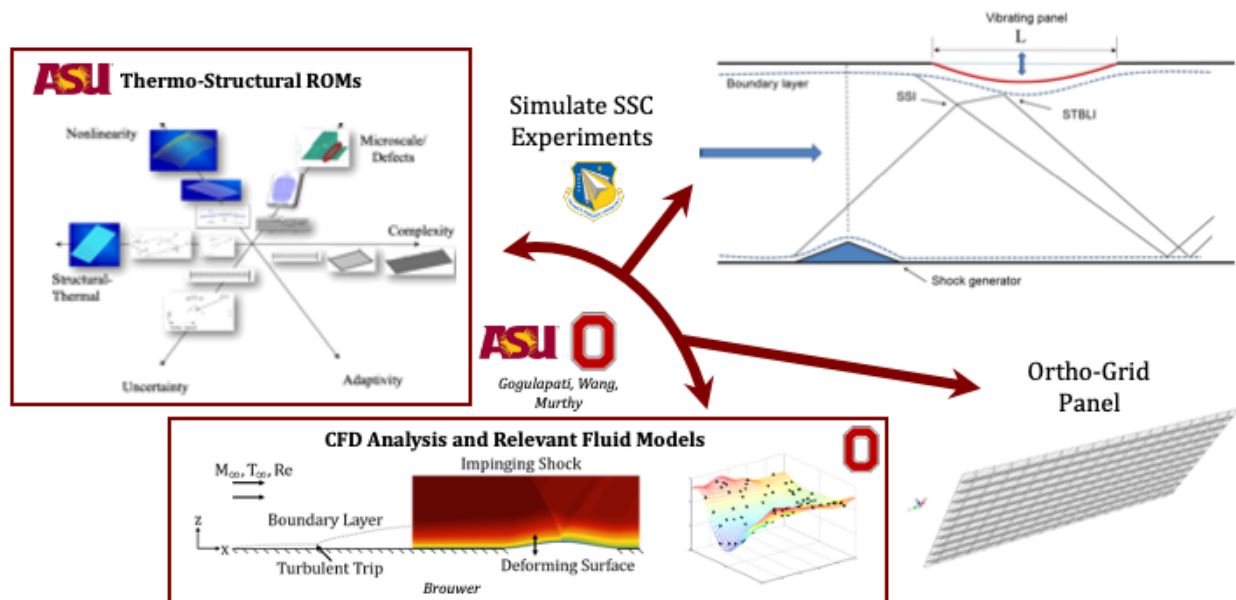


Figure 5.1: Integration of OSU Relevant Fidelity Models With ASU Thermo-structural ROMs

5.2. OSU DAGSI Project I: Incorporation of Damage Accumulation Models into Fluid-Thermal-Structural Analysis Frameworks

In building towards a multi-physics capability, we recognized a lack of understanding on the impacts of material damage in a coupled fluid-thermal-structural interaction framework. A

research project, funded by the AFRL/Defense Associated Graduate Student Innovators (DAGSI) student-faculty fellowship, was undertaken to incorporate and study the impacts of, plastic deformation on multiple loading cycles of skin panels. The developed framework is shown in Figure 5.2, and extends from the original co-simulation framework discussed in Section 5.1 by incorporating UMATs for advanced constitutive models. Capabilities gained here were leveraged for the first integration project discussed in Section 4.

This effort led to the following publication documenting the work: Ref. [113]

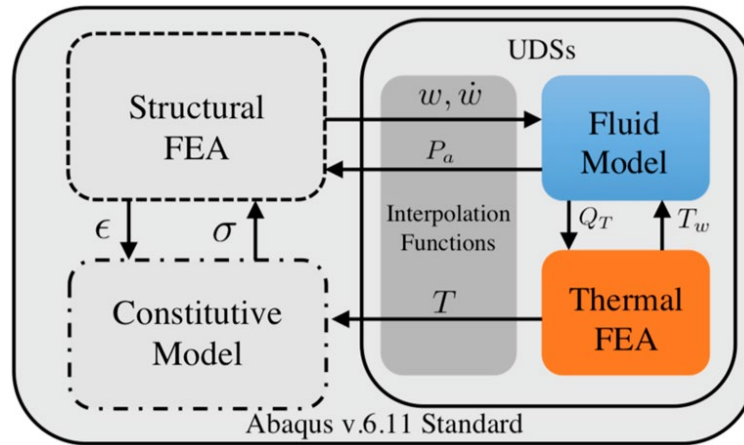


Figure 5.2: Fluid-thermal-structural-material Interaction Framework Built Around Abaqus

5.3. OSU DAGSI Project II: Discrete Solution of the Navier-Stokes Equations Using a Generalized Finite Element Formulation

Recognizing the multi-scale capabilities of the generalized finite element formulation, a second AFRL/DAGSI student-faculty fellowship project was proposed and awarded to study the application on multi-scale fluid flows. This project is currently being co-advised by Dr. Patrick O'Hara of the AFRL/RQ Structural Sciences Center, and came about because of technical interchanges between the academic and government teams in the CCSS.

The following publications document progress of this work: Refs. [114, 115]

5.4. OSU/CalTech AFOSR Project: Dynamics of Interactions Between Turbulent Boundary Layers and Compliant Surfaces

The highest fidelity flow models considered in the CCSS are URANS CFD, which grossly approximates the fine scale features of turbulence. While it is widely recognized that resolving turbulence may be important for accurate structural loads predictions, doing so is not computationally tractable in a general sense. Thus, research efforts are needed to identify the fundamental mechanisms of energy transfer between a turbulent boundary layer and a compliant surface. Using identified knowledge gaps from the CCSS, an AFOSR project was proposed and awarded to carry out such a study. The work is a joint computational and experimental campaign

by OSU and CalTech. OSU is carrying out LES of flows over compliant boundaries, while CalTech is carrying out experiments.

The following publications document progress of this work: [116, 117]

6. KEY ACCOMPLISHMENTS

6.1. Technical Training of Future Research Engineers

The most significant accomplishment of the CCSS was the technical training and vectoring of 17 graduate students and 5 post-doctoral scientists on DOD relevant problems.

6.2. Advancements to the State-of-the-Art Since 2013

Capabilities and understanding in high-speed structural sciences have advanced considerably since the initiation of the CCSS with a primary focus was on simulation methods and tools, as well as combined environment experimentation.

Efforts on simulation capabilities has yielded powerful multi-fidelity, multi-physics frameworks. For environment modeling, this involves RANS to LES level flow modeling coupled to either high fidelity or reduced order thermo-structural solvers. This includes *direct coupling* of RANS and LES solvers to both high fidelity finite element and reduced order thermo-structural solvers for quasi-static analysis or short time record dynamic analysis. *Indirect coupling*, using CFD surrogates, enables long time record dynamic response prediction at a RANS level of flow modeling. Multi-scale thermo-structural solvers, such as the UIUC ISET code, enables the resolution of localized thermal and structural loads/features (e.g., shock impingements, cracks, spot welds, rivets, bolts, etc.). Nominally this analysis is for quasi-static, geometrically linear structural analysis using 3D finite elements. However, the demonstrated capability for non-intrusively coupling to commercial finite element solvers unlocks the ability to capture geometrically nonlinear responses on dimensionally reduced elements such as shells and beams. Further, the use of finite element solvers enables the incorporation of advanced, micro-structurally informed, material evolution and damage models, such as JHUs Parametrically Homogenized Constitutive Models (PHCMs). Nonlinear reduced order thermo-structural models have broadly matured to enable the prediction of the response and temperature of medium complexity structures, with demonstrations on stiffeners, cracks, and notches. Strongly nonlinear behaviors (snap-throughs, buckling) are also accommodated provided that they are expected.

A major development in high-speed structural sciences is the emergence of combined environment (mechanical-thermal-acoustic, fluid-thermal-structural) testing of representative, built-up structural panels in conjunction with the development of advanced techniques for detailed measurements of fluid, thermal, and structural field responses. This includes the building of expertise for carrying out multi-physics experiments, along with stretching and creatively using existing ground based experimental facilities. Efforts here have enabled several discovery experiments, as well as the capability and understanding to acquire validation quality datasets.

In this context, the following are specific advancements due to the CCSS activities:

- Formalized loosely coupled time marching schemes for co-simulation of fluid-thermal-structural interactions
- Established of a foundation for multi-fidelity co-simulation frameworks with fluid models ranging from basic engineering models up to implicit Large Eddy Simulation
- Formalized workflow and assessment metrics for CFD surrogates

- Identified coupling parameters between structural deformation and fluid response for improved understanding in the presence of shock-boundary layer interactions and generalization of structural deformation in CFD surrogate construction
- Developed a user friendly and computationally efficient, multiscale and multi-physics GFEM:
 - Ability to bridge panel- and connection-scale mathematical models and discretizations: It allows the selection of most appropriate model (shell or 3D elasticity) and discretization at each scale of the problem
 - Accommodates multi-physics, time-dependent, nonlinear responses
 - What-if scenarios can be easily run by the analyst:
 - Number and location of spot welds
 - Defective welds: Are they “good enough”?
- Non-intrusive coupling of commercial and research codes.
 - The simulation framework has the ability to incorporate features into a component model which are initially absent from an initial de-featured model defined in a commercial code.
 - The methodology can be applied to fasteners such as spot welds and rivets, as well as cracks.
 - It provides higher fidelity than sub-modelling / break-out modeling: An accuracy comparable to a direct analysis with all scales captured by a single (large) model.
- Parametrically Homogenized Constitutive Model (PHCM) is developed for Titanium alloy Ti6242 that accounts for microstructure influence in structural response prediction
- Parametrically Homogenized Crack Nucleation Model (PHCNM) is developed from grain-level crack nucleation simulations to predict microstructure-dependent probability of nucleation in a macroscopic structural analysis
- PHCM is enhanced with uncertainty quantification (UQ) to quantify and propagate uncertainties in microstructure and multi-scale model development
- Developed component centric ROMs which are as small-size ROMs providing an accurate prediction of the response of part of a stiffened structure without focusing on the rest of it. Running in parallel the different component centric ROMs of the different parts of the structure yields the response of all of it much faster than using a single large-size ROM for the entire structure.
- Developed a multiscale approach to incorporate into the ROM of a virgin structure a local basis that models the effects of one or multiple defects such as notches, cracks, etc. Connected this methodology with the GFEMgl approach for an efficient and accurate capture of the local changes in displacements and stresses due to these defects.
- Clarified and improved the construction, basis selection and coefficients identification, of ROMs for strongly nonlinear structures exhibiting snap-throughs, symmetry breaking, internal resonance, etc. Demonstrated the capability of the ROMs to correctly predict (i) the onset of these events and (ii) the response when they occur.
- Improved the structural basis selection to capture the displacement induced by a time varying temperature field.

- Extended the thermal ROM in introducing basis functions that (i) affect most strongly the structural response to capture accurately the thermal-structural coupling as well as (2) complement these functions to capture the entire temperature field. Moreover, an efficient approach was formulated and validated for the computationally efficient evaluation of the ROM capacitance and conductance matrices for time varying temperature fields when the thermal conductivity and/or specific heat is temperature dependent.

6.3. Transition of Technology

- Incorporation of UIUC developed GFEM technologies in other places:
 - Implementation of GFEM^{gl} approach in large-scale parallel solver at Sandia (Plews)
 - Damage modelling at Army Corps of Engineers (Fillmore)
 - Modelling of multiple, interacting hydraulic fractures (ExxonMobil)
 - Implementation into commercial FE solver PUMA (Birner & Schweitzer)
 - Methodology adopted by other university research groups
 - Ohio State University – modelling of fluid flows (McNamara)
 - Duke – phase fields used to model damage in local problems (Dolbow)
 - University of Bonn, Germany - peridynamics used to model fractures in local problems (Schweitzer)
 - Polytechnic University of Catalunya, Spain – combined GFEM with PGD (Huerta)
- UQ-PHCM and PHCNM are successfully incorporated in commercial FE codes and representative structural panel problems were simulated
- Delivered the UMATs for integration with AFRL/RQ and SSC simulation platforms, as well as to OEMs like Pratt & Whitney and GE.
- CFD surrogates and co-simulation capabilities transitioned to the AFRL and industry

6.4. Publications

A full list of publications through support of the CCSS are provided in Appendix A. Furthermore, a listing of publications directly tied to each project are provided in each description. Final publication counts are as follows:

- Journal: 29 in print, 10 in revision/review/preparation
- Conference: 35
- Dissertations/Theses: 12
- Presentations by students/post-docs at external meetings: 40

6.5. Supplemental Funding Sources

Considerable additional funding resources were brought to the CCSS through academic cost share from each academic institution, fellowships awards to students (university, NDSEG, DAGSI), and summer internships funded through CRDInAL.

7. FUTURE RECOMMENDATIONS

Informed high-speed vehicle design with transformative performance gains and lifecycle cost estimates require improved understanding and capabilities in the following broad, and interrelated, areas of structural sciences:

- a) Coupled response prediction and validation in the presence of complex flow conditions (transitional/turbulent/shock impingements), nonlinear thermal-structural interactions, and material evolution/damage;
- b) Multi-scale thermo-structural analysis.

Recommendations for the next decade of research in these areas are provided here following three high-level themes:

1. Cooperative exercising of established simulation and experimental capabilities in parallel with focused efforts for technology transfer from academia to DOD laboratories and industry;
2. Continued discovery and basic research on the coupled physics;
3. Continued investment in both reduced-order and high-fidelity multi-scale methods;

While predictive methods and tools have advanced considerably, relatively little work has focused on the integration and use of these tools for representative structures subject to extreme, combined environments. The need for this comes at a logical mesh point with new experimental capabilities discussed above. Thus, demonstration cases should be collaboratively developed between simulation and experimental experts for both the acquisition of validation cases and identification of needed refinements. Here, the goal is to address the question: “How well can we do what we can do?”. Further, we also need to address the related question: “How well do we need to do it?”. Comparison (e.g., on stresses) of computational predictions to experimental measurements on carefully calibrated experiments provides a first answer to this question. A more complete one, however, should consider the variability of the geometry and structural property that will exist on different vehicles and the same vehicles as a function of flight time. Once again, experimental efforts will be key in generating data that will permit the assessment of the computational methods with and without uncertainty as well as the calibration of this uncertainty.

In parallel to directed efforts on answering the above questions is the need to transfer the mature aspects of capabilities to the DOD and industry. Conveniently, an excellent pathway for technology transition are integration type efforts that would be required to satisfactorily carry out the work recommended above.

While there are many notable advances in the area, there remains a continued need for discovery through basic research on the coupled physics. A deep understanding is needed on conditions that enable energy transfer between fine scale fluid dynamics in transitional/turbulent/SBLI conditions and the thermo-structural response. Similarly, lack of general understanding on the nature of energy transfer during nonlinear thermal-structural interactions on built-up structures regularly confounds the generation of reduced-order models. Targeted and cooperative research is required using both experiments and high-fidelity simulation tools. Here it is important to recognize that success is **not** achieved by simply carrying out expensive studies on coupled field problems; but

rather the identification, and expanded understanding, of those conditions where current understanding cannot explain or predict the thermo-structural response without detailed analysis.

Finally, continued investments should be made towards response prediction of increasingly complex, multi-scale problems. While not an exhaustive list, capabilities we prioritize at this time are the ability to:

1. carry out high-fidelity analysis of localized features with nonlinear structural dynamics (including damping);
2. incorporate coupled loads that require resolution of fine scale fluid dynamics over relevant thermo-structural response scales;
3. detect if and when during a particular mission the multi-physics computational model becomes inaccurate with the ensuing focus to adapt it to continue the simulation with fidelity.
4. Incorporation of microstructural damage and failure into homogenized constitutive models; and use of such models for materials by design, structural location-specific material design, and design of additive manufacturing-based materials and components.

Continued attention, with specific focus on these problems, should be given to (spatio-temporal) multi-scale computational mechanics and methods, as well as ROM strategies derivative from them.

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APPENDIX: List of Publications Generated With CCSS Support

7.1. Journal Papers

1. J. A. Plews and C. A. Duarte. "Bridging multiple structural scales with a generalized finite element method." *International Journal for Numerical Methods in Engineering*, 102(3–4):180–201, 2015.
2. J. A. Plews and C. A. Duarte. "Generalized finite element approaches for analysis of localized thermo-structural effects." *International Journal for Numerical Methods in Engineering*, 104(6):408-438, 2015.
3. J.A. Plews and C.A. Duarte. "A two-scale generalized finite element approach for modeling localized thermoplasticity." *International Journal for Numerical Methods in Engineering*, 108(10):1123-1158, 2016.
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7.2. Conference Papers

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7.4.Ph.D. Dissertations

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