



**AFRL-RQ-WP-TR-2017-0086**

**STRUCTURAL-SCALE LIFE PREDICTION OF  
AERO-STRUCTURES EXPERIENCING COMBINED  
EXTREME ENVIRONMENTS**

**Thomas G. Eason, III  
Air Force Research Laboratory  
Hypersonic Sciences Branch**

**Ravinder C. Chona  
Aerospace Systems Directorate**

**JUNE 2017  
Final Report**

**DISTRIBUTION STATEMENT A: Approved for public release.  
Distribution is unlimited.**

*See additional restrictions described on inside pages*

**AIR FORCE RESEARCH LABORATORY  
AEROSPACE SYSTEMS DIRECTORATE  
WRIGHT-PATTERSON AIR FORCE BASE, OH 45433-7542  
AIR FORCE MATERIEL COMMAND**

## NOTICE AND SIGNATURE PAGE

Using Government drawings, specifications, or other data included in this document for any purpose other than Government procurement does not in any way obligate the U.S. Government. The fact that the Government formulated or supplied the drawings, specifications, or other data does not license the holder or any other person or corporation; or convey any rights or permission to manufacture, use, or sell any patented invention that may relate to them.

This report was cleared for public release by the USAF 88th Air Base Wing (88 ABW) Public Affairs Office (PAO) and is available to the general public, including foreign nationals.

Copies may be obtained from the Defense Technical Information Center (DTIC)  
(<http://www.dtic.mil>).

AFRL-RQ-WP-TR-2017-0086 has been reviewed and is approved for publication in accordance with assigned distribution statement.

X



---

Thomas Eason  
Work Unit Manager  
Hypersonic Sciences Branch  
High Speed Systems Division

X



---

Michael Brown, Chief  
Hypersonic Sciences Branch  
High Speed Systems Division

X



---

James H. Miller  
Principal Advisor  
High Speed Systems Division  
Aerospace Systems Directorate

This report is published in the interest of scientific and technical information exchange, and its publication does not constitute the Government's approval or disapproval of its ideas or findings.

\*Disseminated copies will show “//Signature//” stamped or typed above the signature blocks.

<b>REPORT DOCUMENTATION PAGE</b>				<i>Form Approved</i> OMB No. 0704-0188	
<p>The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. <b>PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.</b></p>					
<b>1. REPORT DATE (DD-MM-YY)</b> June 2017		<b>2. REPORT TYPE</b> Final		<b>3. DATES COVERED (From - To)</b> 30 September 2014 – 30 September 2016	
<b>4. TITLE AND SUBTITLE</b> STRUCTURAL-SCALE LIFE PREDICTION OF AERO-STRUCTURES EXPERIENCING COMBINED EXTREME ENVIRONMENTS				<b>5a. CONTRACT NUMBER</b> In-house	
				<b>5b. GRANT NUMBER</b>	
				<b>5c. PROGRAM ELEMENT NUMBER</b> 61102F	
<b>6. AUTHOR(S)</b> Thomas G. Eason, III (AFRL/RQHF) Ravinder C. Chona (AFRL/RQ)				<b>5d. PROJECT NUMBER</b> 3002	
				<b>5e. TASK NUMBER</b>	
				<b>5f. WORK UNIT NUMBER</b> Q195	
<b>7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)</b> Hypersonic Sciences Branch (AFRL/RQHF) High Speed Systems Division Air Force Research Laboratory, Aerospace Systems Directorate (AFRL/RQ) Wright-Patterson Air Force Base, OH 45433-7542 Air Force Materiel Command, United States Air Force				<b>8. PERFORMING ORGANIZATION REPORT NUMBER</b> AFRL-RQ-WP-TR-2017-0086	
<b>9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)</b> Air Force Research Laboratory Aerospace Systems Directorate Wright-Patterson Air Force Base, OH 45433-7542 Air Force Materiel Command United States Air Force				<b>10. SPONSORING/MONITORING AGENCY ACRONYM(S)</b> AFRL/RQHF	
				<b>11. SPONSORING/MONITORING AGENCY REPORT NUMBER(S)</b> AFRL-RQ-WP-TR-2017-0086	
<b>12. DISTRIBUTION/AVAILABILITY STATEMENT</b> DISTRIBUTION STATEMENT A: Approved for public release. Distribution is unlimited.					
<b>13. SUPPLEMENTARY NOTES</b> PAO Case Number: 88ABW-2017-2314; Clearance Date 15 May 2017. This is a work of the U.S. Government and is not subject to copyright protection in the United States.					
<b>14. ABSTRACT</b> Reusable high-speed air platforms are critical to the global reach and superiority of tomorrow's USAF. These platforms experience long-duration, combined and intense, thermo-mechanical-acoustic loads over significant portions of their structure. Designing and fielding these platforms requires the capability to probabilistically assess the structural life under complex loading environments. Today's state of the art methods cannot address structural reliability under combined environment conditions due to inadequate understanding of the interactions between the various applicable material failure mechanisms and the continuously-evolving material/structural states. Lack of the necessary knowledge has resulted in significant repair and replacement costs for existing USAF platforms like the B-2 where zones of the aircraft are required to operate under combined, thermo-acoustic-mechanical loads. Current practices for margin prediction are rooted in analysts' past experience, a heavy reliance on testing, and limited choices to tailor material attributes.					
<b>15. SUBJECT TERMS</b> lifing, combined environment, uncertainty, probabilistic, interacting damage modes					
<b>16. SECURITY CLASSIFICATION OF:</b>			<b>17. LIMITATION OF ABSTRACT:</b> SAR	<b>18. NUMBER OF PAGES</b> 28	<b>19a. NAME OF RESPONSIBLE PERSON (Monitor)</b> Thomas G. Eason <b>19b. TELEPHONE NUMBER (Include Area Code)</b> NA
<b>a. REPORT</b> Unclassified	<b>b. ABSTRACT</b> Unclassified	<b>c. THIS PAGE</b> Unclassified			

## TABLE OF CONTENTS

<b>Section</b>	<b>Page</b>
List of Figures .....	ii
List of Tables .....	iii
Forward .....	v
1 Summary .....	1
2 Introduction .....	2
3 Probing Interacting Damage Modes .....	4
4 Capturing Uncertainty in Fatigue Life Data .....	6
5 Fatigue and Creep Life Prediction .....	8
6 Simulating Short Crack Growth in Grain Scale Models.....	11
6.1 Task 1: Machine learning.....	11
6.2 Task 2: Computational Crack Growth in a Polycrystal .....	11
6.3 Task 3: Representative Volume Element size for crack growth.....	14
References.....	18
Appendix A Personnel .....	19
Appendix B List of Publications.....	20

## List of Figures

Figure 1. Damage Mode Interaction as a function of Temperature and Stress.....	5
Figure 2. Fatigue life of Ti-64 at three temperatures.....	6
Figure 3. Correlation Between Mean Life and Deviation of Mean life with the Addition of New Metallic Systems of Ti-6242 and AL7075.....	7
Figure 4. An example of Stationary Kriging vs. LOC-Kriging with the Gray Indicating Regions of Uncertainty.....	9
Figure 5. Analytical Life Model Used as the Truth Model.....	9
Figure 6. Example of LOC-Kriging with the Analytical Model in Red using a Four LOC-Kriging.....	10
Figure 7. Example of Physics Informed LOC-Kriging Predictions.....	10
Figure 8. Algorithm of Proposed Image-Based Method for Predicting Arbitrary Crack Growth.....	12
Figure 9. Initial Crack Surface.....	13
Figure 10. Crack Surface Following First Crack-Growth Increment.....	13
Figure 11. Crack Surface Following Second Crack-Growth Increment.....	13
Figure 12. Predicted Crack Fronts within a Synthetic Polycrystal.....	13
Figure 13. Limitations of Method Include Large Dependencies on Voxel Spacing.....	14
Figure 14. Left: algorithm for generating a single value of RVE* using FE analysis.....	16
Figure 15. Idealized Polycrystal with semi-circular surface crack, shown with exaggerated deformation. Colors correspond to different grains. J-integral calculated along the crack front (N/μm).....	17

## **List of Tables**

Table 1. IN617 Experimental Test Matrix to Fill in Gaps in Existing Data. ....	5
Table 2. Life Model Performance Comparison for Root-Mean-Square Error, Maximum 1 Sigma Standard Deviation, and Integral of the Mean-Square-Error.....	10

## Foreward

This final report documents the work accomplished under the in-house work unit Q195, Structural-Scale Life Prediction of Aero-Structures Experiencing Combined Extreme Environments, performed Oct 1, 2013 –Sept 31, 2016. The work was conducted by the Air Force Research Laboratory, Aerospace Systems Directorate, AFRL/RQ in collaboration with thirteen visiting scientists, graduate students, and in-house researchers. Ravi Penmesta was the Principal Investigator from Oct 1, 2013 to February 14, 2016 and Ravi Chona was the Principal Investigator for February 15, 2016-September 30, 2016. This work was sponsored by AFOSR under LRIR 14RQ09COR. The purpose of this report is to document progress in each of the research thrusts and assess promising approaches that should be carried over for use in high speed platform lifing. Contributions to science were disseminated through conference papers and journal articles and documented in the publications section of this report. As such, the bulk of this report is contained in section 5 covering collaborations from the summer of 2016 where at the close of this casefile, minimal dissemination has occurred and ideas are maturing into an actionable execution plan.

# 1 Summary

Reusable high-speed air platforms are critical to the global reach and superiority of tomorrow's USAF. These platforms experience long-duration, combined and intense, thermo-mechanical-acoustic loads over significant portions of their structure. Designing and fielding these platforms requires the capability to probabilistically assess the structural life under complex loading environments. Today's state of the art methods cannot address structural reliability under combined environment conditions due to inadequate understanding of the interactions between the various applicable material failure mechanisms and the continuously-evolving material/structural states. Lack of the necessary knowledge has resulted in significant repair and replacement costs for existing USAF platforms like the B-2 where zones of the aircraft are required to operate under combined, thermo-acoustic-mechanical loads. Current practices for margin prediction are rooted in analysts' past experience, a heavy reliance on testing, and limited choices to tailor material attributes. A unique aspect of this research effort was that it addressed both (i) the combined environment interactions between the material damage mechanisms and (ii) the confidence that can be placed in the methods used to predict the structural life. While progress was made, additional research effort should be devoted to understanding material level deformation mechanisms and damage initiation under combined-environment complex loading. At the structural level, further effort is required in upscaling the material scale information to the structural scale simulation in a manner which preserves the quantities of interest.

## 2 Introduction

In reviewing current practice for predicting the life of extreme environment structures, the accepted process is to predict the damage for the anticipated failure modes and select the most damaging mode to set the life margin. This process ignores interaction between life limiting failure modes. For the discussion herein, failure mode will refer to life limiting failure modes where either time or cycles are used to express the exposure. For structures where one failure mode dominates, this method can provide a satisfactory engineering answer. However, there are situations where a single failure mode does not dominate so the damage from each failure mode is added together using superposition to account for the total degradation similar to a Miner's rule in fatigue.[1] These two approaches are shown in equation 1.

$$D_{total} = \begin{cases} \max(D_{fat}, D_{cr}, D_{env}) \\ D_{fat} + D_{cr} + D_{env} \end{cases} \quad (1)$$

Where  $D_{total}$  represents the ratio of the total damage done towards crack initiation and the damage modes considered are fatigue ( $D_{fat}$ ), creep ( $D_{cr}$ ), and environmental ( $D_{env}$ ). When  $D_{total}$  is one, crack initiation is declared to have occurred. While this approach is an extremely crude approximation to reality, it is one of the simplest to employ to account for interacting damage. Regardless of the approach taken to model damage or interaction, what is the best way to quantify the confidence in predictive capability of crude to sophisticated models? Secondly, what must be done to increase the accuracy and confidence in the methods, and how far down into the material scale must the structural community go to evaluate interacting failure modes? As a first attempt in answering these questions the following research objectives were pursued:

- Develop methods to (i) accurately capture the interactions between structural damage drivers and material failure mechanisms and (ii) probabilistically predict the life of aero-structures subjected to combined extreme environments.
- Develop methods to quantify confidence in the predicted margins of safety on the life of aero- structures experiencing combined extreme environments.

While not all failure modes will interact, the present research focused on fatigue, creep, and environmental crack initiation in Inconel 617 and Titanium 6242S. These metallic material systems were chosen due to their proposed use in hypersonic platform concepts as well as the fact that they are relatively well characterized material systems.

Equally important are the metrics used to quantify the confidence in structural life predictions for combined environments. These metrics become critical when integrating models of different fidelity into a coherent analysis framework. Under such circumstances, both the capability to assess the confidence in the entire simulation as well as each of the individual models that drive the simulation need to be understood. Having a rational means of determining when a higher fidelity model should be selected becomes of critical importance when attempting to increase the confidence in the simulation prediction. While the complete simulation framework with confidence intervals is beyond the scope, the present research was focused on models and metrics that could be used to quantify confidence for structural life prediction operating in combined environments. These environments from a structural life prediction viewpoint require evaluating

creep, fatigue and environmental effects at a minimum. These failure modes are tied to material scale deformation where mechanisms can interact.

### 3 Probing Interacting Damage Modes

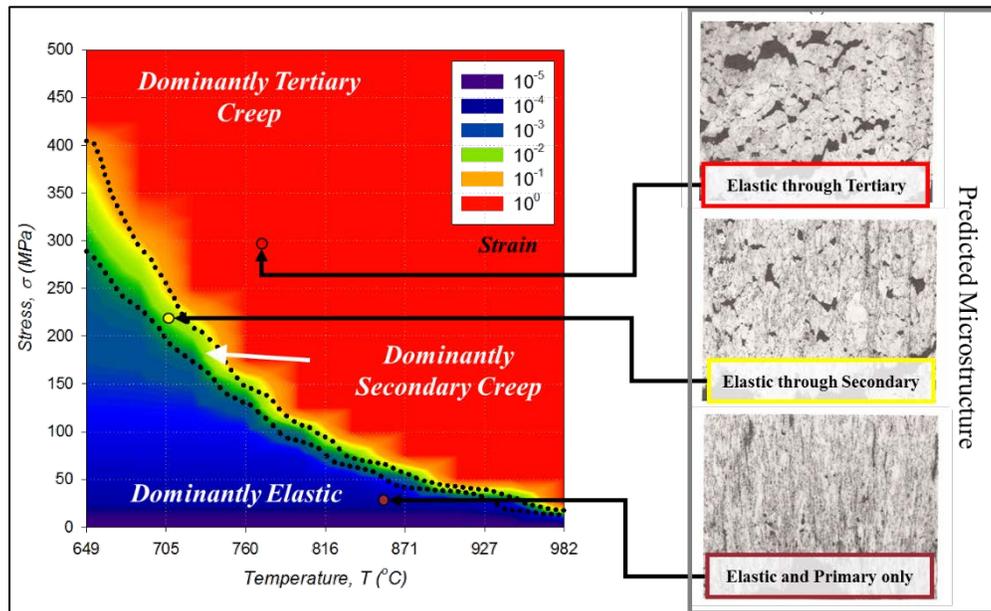
One of the first activities undertaken was to examine the existing data for these material systems and what tests needed to be performed if damage interactions were of interest. Data was found addressing tensile, isothermal-fatigue, creep, and corrosion behavior while data was lacking in the areas of multiaxial fatigue, creep, and compression behavior. The existing data were used to build models for the individual damage modes and implemented using standard structural lifing practices for combined environments by the PI (Dr. Penmetsa). For the individual damage modes, an automated process was used to rapidly calibrate all the parameters and then the life was assessed given a strain-temperature history. This exercise was used to identify gaps in current prediction methods and provide a baseline. The primary gap observed by the PI at the time was a lack of models that accounted for elastic-plastic-creep behavior. Accurate models describing these deformation mechanisms are important as they allow the strain life approach to be implemented to identify regions where crack nucleation is likely to occur. In concert with the modeling efforts, a series of experiments were performed to probe the damage interaction models as shown in Table 1. The goals of the experiments were to:

- Identify the deformation response and mechanisms for candidate alloys under expected service conditions
- Determine crack initiation life trends and compare with published data
- Draw out microstructural-level mechanisms associated with crack initiation.

The results of the tests were used to generate failure mode maps identifying where combined mechanisms interact and relate to material scale deformation. An example of this is Figure 1 where elastic to creep dominated response is shown along with the microstructure in the different regimes. The blue region indicates the stress and temperature where elastic response dominates and the red region is where tertiary creep dominates. The region between the dotted lines, green to yellow shows a transition in behavior. This work was accomplished by the PI (Ravi Penmetsa) in collaboration with Prof. Gordon at UCF during his sabbatical at Wright-Patterson.

**Table 1. IN617 Experimental Test Matrix to Fill in Gaps in Existing Data.**

Specimen	Fatigue Loading	Phasing	Strain Ratio	Strain Range	Minimum Temperature	Maximum Temperature	Temperature Rate	Mechanical Strain Rate	Dwell	Dwell Type	Estimated Number of Cycles to Failure	Estimated Wall Clock Time
			$R\epsilon$	$\Delta\epsilon$ (in/in or )	$T$ (°F)	$T$ (°F)	$\dot{T}$ (°F/s)	$\dot{\epsilon}$ (1/s)	$td$ (sec)	$N$ (cycles)	$t$ (hrs)	
IN-1	Thermal Step	-	-	-	68	1600	-	-	-	-	175	0.32
IN-2	LCF	-	-1	0.0077	1400	1400	0	1.00E-03	0	-	1429	6
IN-3	LCF	-	-1	0.0077	1200	1200	0	1.00E-03	0	-	2065	9
IN-4	Creep-Fatigue	-	-1	0.0077	1400	1400	0	1.00E-03	120	Comp	476	18
IN-5	Creep-Fatigue	-	-1	0.0077	1200	1200	0	1.00E-03	120	Comp	688	26
IN-6	Creep-Fatigue	-	$-\infty$	0.0077	1400	1400	0	1.00E-03	120	Comp	476	18
IN-7	TMF	OP	$-\infty$	0.0077	400	1400	18	1.39E-04	0	-	143	4
IN-8	Creep-TMF	OP	$-\infty$	0.0077	400	1200	18	1.73E-04	120	Comp	207	12
IN-9	Creep-TMF	OP	$-\infty$	0.0077	400	1400	18	1.39E-04	120	Comp	143	9



**Figure 1. Damage Mode Interaction as a Function of Temperature and Stress.**

## 4 Capturing Uncertainty in Fatigue Life Data

This work was performed in collaboration with Professor Hill of Air Force Institute of Technology and worked towards a model to capture dispersion in fatigue life data separately from a mean life model. The model used a robust measure for calculating deviation at individual design points, allowing for the incorporation of censored data, and builds a regression model for capturing trends across the design space. Nonparametric testing addresses the adequacy of the dispersion model by comparing results with residuals of a predictive life model. Diagnostics, both quantitative and qualitative, are utilized for the dispersion model and predictive life model. A Bayesian extension of the model allowed for predictive life and deviation estimations through sampling predictive distributions.[2] The novel result of the model shows potential for a reduction in fatigue testing costs by incorporating characteristics in dispersion. As an example of this approach, fatigue data at three different temperatures and minimum over maximum stress intensity ratio's , R ratio's, were used as shown in Figure 2 to develop a correlation between standard deviation in life and mean life in Figure 3. To investigate the correlation, additional data was added from Ti-64 and AL7075. It is interesting to note that the relationship does not fit well at the ends for Al7075 tested at an R of 0 as well as Ti6246 at the low end of mean life. Nevertheless, the result may allow for empirical insight into the fatigue process; the relationship between the predictive variables. In addition, the log deviation estimations parallel the relationship between predictive variables and log life estimations. This result may allow structural engineers to draw inferences about material behavior and may be extended to provide dispersion estimations in sparse or poorly-behaved test data sets. Although further investigation is needed, the number of runs in subsequent fatigue experiments, and their associated costs, may be reduced. This work was done in collaboration with the PI (Ravi Penmetsa), Raymond R. Hill, Darryl K. Ahner, and Brent D. Russell of Department of Operational Sciences, Air Force Institute of Technology.

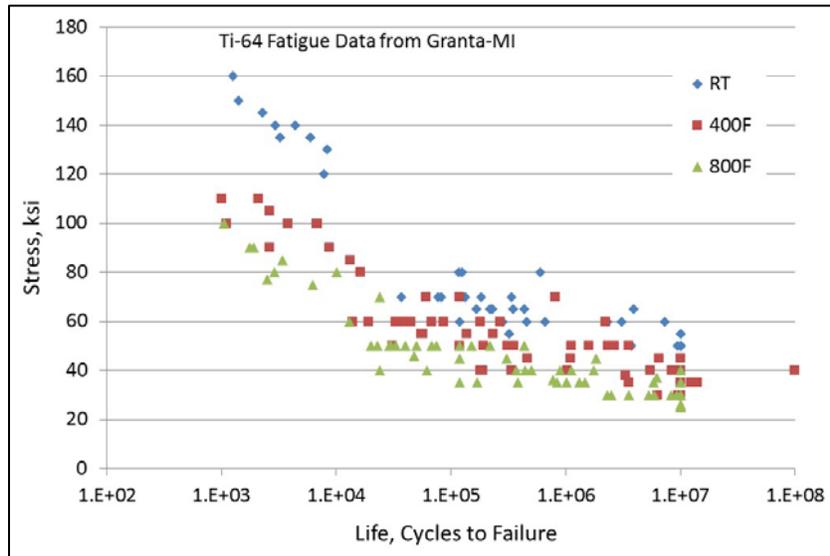
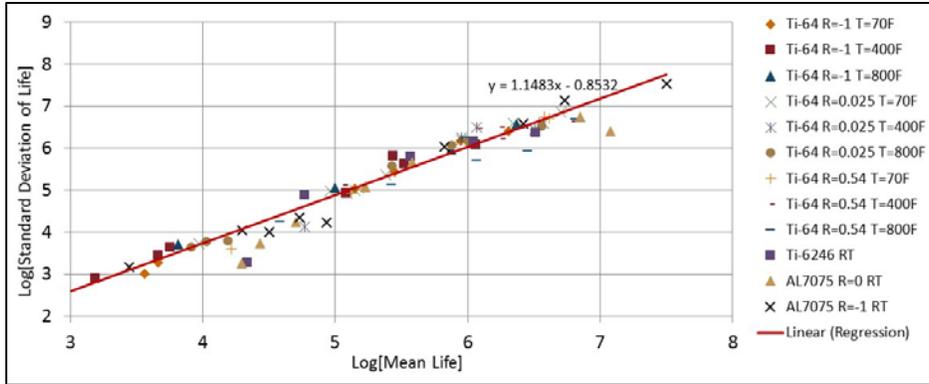


Figure 2. Fatigue Life of Ti-64 at Three Temperatures.



**Figure 3. Correlation Between Mean Life and Deviation of Mean Life with the Addition of New Metallic Systems of Ti-6242 and AL7075.**

## 5 Fatigue and Creep Life Prediction

The use of a Locally Optimized Covariance Kriging method to span the gaps between test data was explored.[3] From a structural technology perspective, fatigue and creep predictions under the transient thermo-mechanical acoustic loadings are essential to assess flight critical damage states with high confidence. Therefore, collecting high-quality material data from physical experiments are of the utmost importance to achieve high confidence. However, the amount of material information necessary for a single composite component can become enormous when considering a large variety of loading conditions at varying temperature conditions. The thought was to leverage surrogate models to help fill in missing test conditions and assess the confidence in those predictions. Surrogate models are not new and are utilized in many engineering applications where actual function evaluations are computationally expensive. Kriging is a flexible surrogate model method best suited for interpolating nonlinear system responses with a limited number of training points. It is commonly used to alleviate the high computational cost associated with common design exploration techniques, e.g., uncertainty quantification and multidisciplinary design optimization. However, when the underlying function shows varying degrees of nonlinear behavior within a design domain of interest, Kriging, with a stationary covariance structure, can result in low quality prediction and overly conservative expected mean squared error. This effect is often amplified by data collected adaptively and unevenly such as in the case of most lifing data. In this research, the locally optimized covariance Kriging (LOC-Kriging) Method is proposed to capture the non-stationarity of the underlying function behavior where the gray around the mean response is shown in Figure 4. In LOC-Kriging, nonstationary behavior of an underlying function is identified with a statistical test process and approximated by aggregating a finite number of locally optimized stationary covariance structures. Compared to a traditional stationary Kriging, the method provides an efficient and flexible computational framework not only to capture transitional system behaviors, but provides the opportunity to impose our physical understanding in building a surrogate model. Practical significance of the method was demonstrated using a fatigue and creep life model for a hypersonic aircraft with *Figure 5* showing the truth model used to perform LOC-Kriging. The variable  $X_1$  is the temperature and  $X_2$  is the stress amplitude which results in a mean life in cycles under the various loading conditions. To capture the fatigue life behavior, four LOC windows are identified and optimized by the proposed process with the results shown in *Figure 6*. It is immediately evident the LOC methodology produces an adequate prediction. However, the contour still shows the discrepancy from the expected monotonic behavior. To address this issue, the weighting function,  $\delta$  is used to relax the stochastic process. The relaxation is used to generate a Physics-Informed (PI) LOC-Kriging model shown in *Figure 7*. The performance comparisons of Physics-Informed LOC-Kriging and stationary Kriging are shown in *Table 2*. The relaxed LOC-Kriging method improves all three performance measures. In this example, the underlying physics of the fatigue-creep interaction is imposed on the surrogate utilizing an additional weighting function. The proposed function is kept general so that it can be implemented in many different aerospace applications where the physical trend is well understood and a regression model would be inadequate. This work was a collaboration between the PI (Ravi Penmetsa), Daniel L. Clark, Jr., Ha-Rok Bae, and Koorosh Gopal of Wright State University.

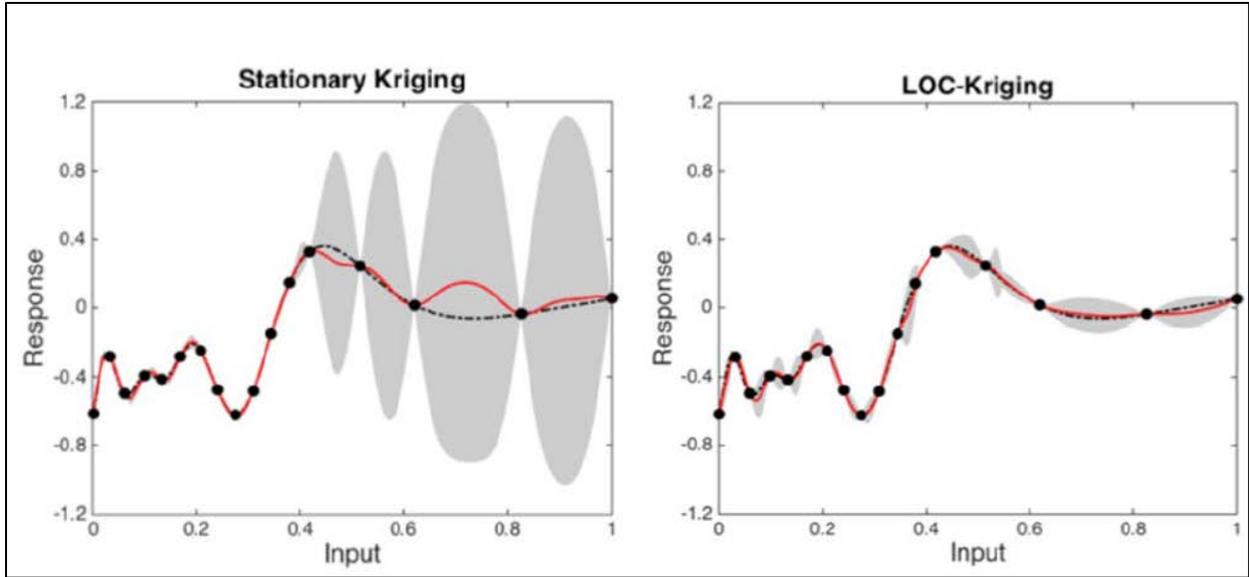


Figure 4. An example of Stationary Kriging vs. LOC-Kriging with the Gray Indicating Regions of Uncertainty.

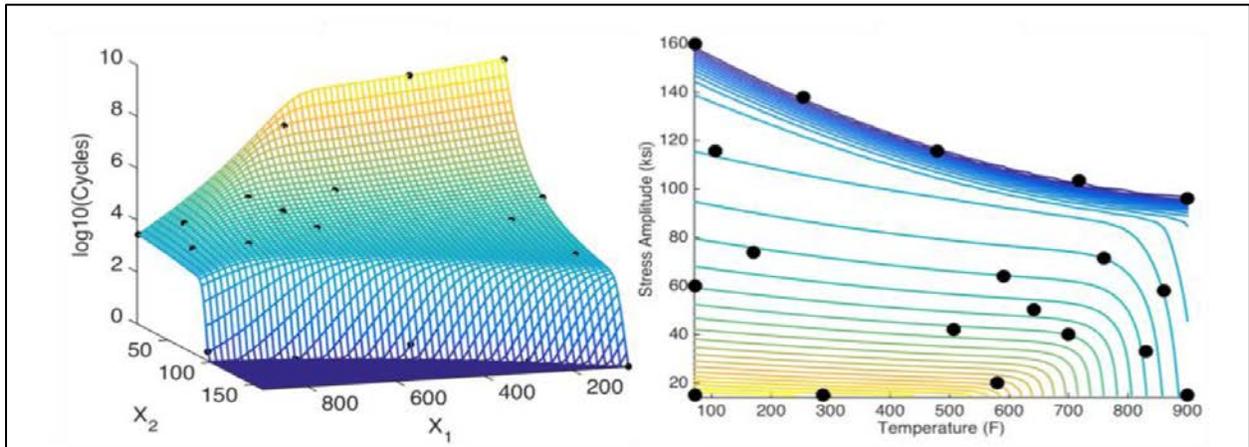


Figure 5. Analytical Life Model used as the Truth Model.

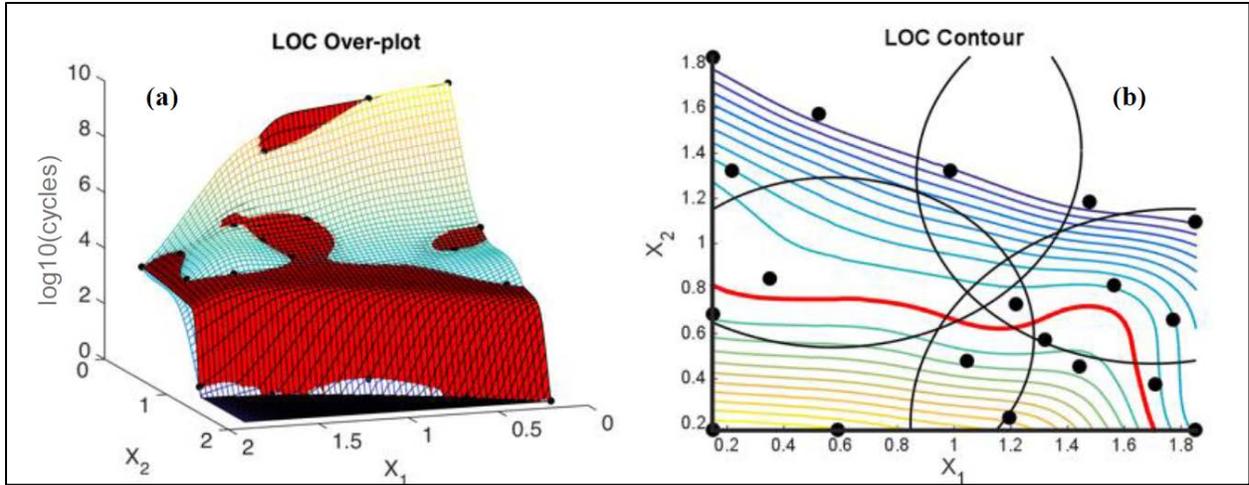


Figure 6. Example of LOC-Kriging with the Analytical Model in Red using a Four LOC-Kriging.

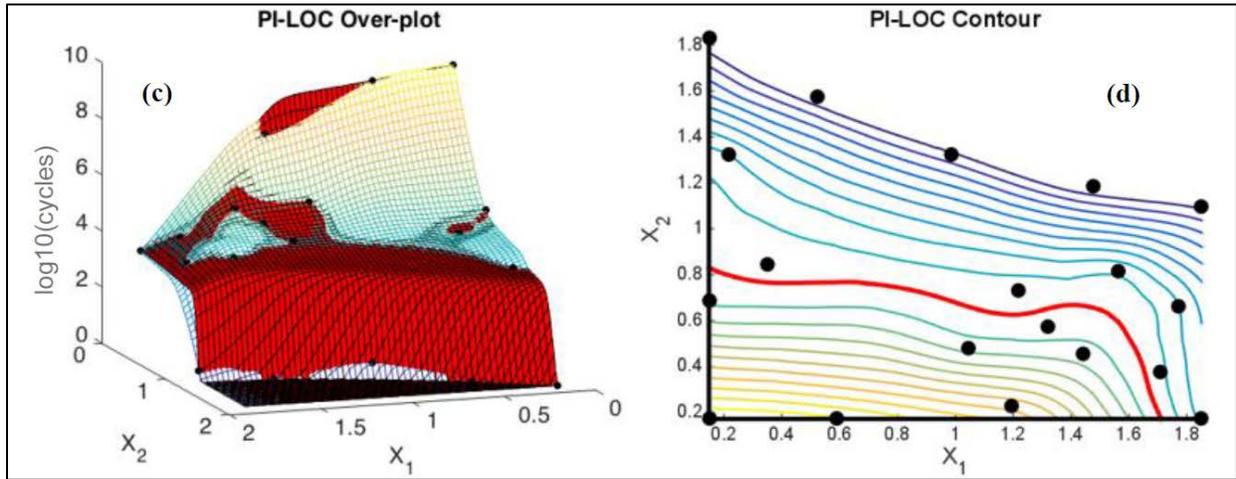


Figure 7. Example of Physics Informed LOC-Kriging Predictions.

Table 2. Life Model Performance Comparison for Root-Mean-Square Error, Maximum 1 Sigma Standard Deviation, and Integral of the Mean-Square-Error.

Metric	Stationary Kriging	PI LOC-Kriging	Improvement
RMSE	1.15	0.582	49.3%
Max One Sigma	0.636	0.467	26.6%
Integral MSE	0.194	0.129	33.7%

## 6 Simulating Short Crack Growth in Grain Scale Models

While the previous work focused on taking a phenomenological approach to develop models where damage mechanisms can interact, the present research thrust investigated the possibility of using microscale models and short crack growth for physics based models. In collaboration the PI, Ravi Chona, and Prof. Spear during her 10 week summer visit; three tasks were undertaken to assess the feasibility of the microscale approach. While much progress was made, there is a great deal of work that remains. The top priority is to identify the most significant microstructural feature(s) and statistics that must be represented faithfully in order to predict crack initiation and small crack growth in polycrystalline materials. Second, the ability to computationally grow small microstructural cracks requires an accurate set of rules that dictates the evolution of the crack shape and rate, as well as meshing algorithms that can follow this crack.

### 6.1 Task 1: Machine learning.

This first task sought to answer the question: Can machine based learning be used to help understand the relationship between microstructural parameters and small crack growth?. Machine based learning methodology was initiated in collaboration with Prof. Spear's group to address microstructurally small fatigue crack growth rules. This information will be used to identify input and output parameters for mining a combined 3D experimental/numerical data set. After an extensive literature review and much discussion among the group, the following seven microstructural features were selected to be used as input parameters of the machine learning framework:

- 1) Distance to nearest grain boundary.
- 2) Direction to nearest grain boundary.
- 3) Crystal orientation of the current grain.
- 4) Misorientation angle of the nearest grain boundary.
- 5) Angle between the local crack-plane normal and the nearest grain-boundary normal.
- 6) Taylor factor of the current grain.
- 7) Difference in Taylor factor across the nearest grain boundary.

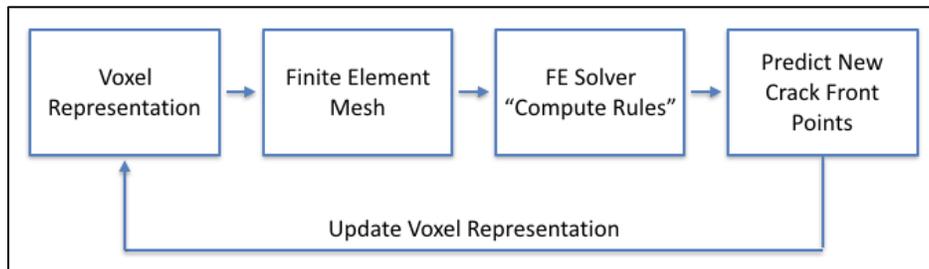
Going forward, each of these parameters are to be assessed at discrete points along a known 3D crack front. The corresponding output parameters will be growth rate and direction for each of the discrete points. Parameters 1-5 relate to intrinsic, geometrical features of the microstructure with respect to the crack geometry. Parameters 6 and 7 take into account the local micromechanical response of the microstructure due to applied loading conditions and will be extracted from crystal-plasticity simulations that incorporate high-fidelity representations of the crack geometry.

### 6.2 Task 2: Computational Crack Growth in a Polycrystal

This task investigated the development of a computational framework to predict arbitrary 3D crack growth in a polycrystalline material. A proof-of-concept was exercised on a synthetic polycrystal using an image based approach. In general, there are two requirements to enable accurate prediction of 3D crack-shape evolution: 1) an accurate set of rules for evolution of the crack shape, including local rate and trajectory, and 2) a computational framework that is flexible and robust enough to represent accurately the shape of the evolving crack surface throughout the material domain of interest. Brian Phung, worked on augmenting an image-based (i.e., voxel-based)

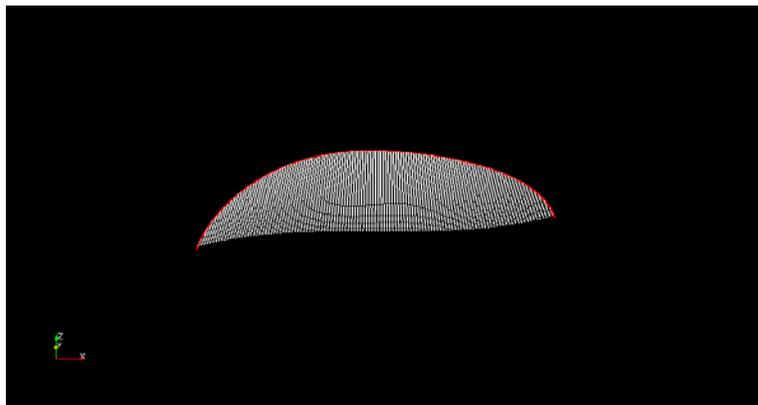
methodology for the prediction of arbitrarily complex 3D crack growth within polycrystalline materials. To our knowledge, no framework exists that can predict, with high fidelity, the evolution of 3D traction-free surfaces through polycrystalline materials. For instance, the software FRANC3D 2 represents cracks explicitly and with high fidelity, but is unable to do so for polycrystalline materials (based on testing conducted over the summer). An image-based method enables explicit, high-fidelity, crack representations in polycrystals using conformal finite-element (FE) meshes. However, the method was developed for the express purpose of replicating experimental observations and not for predicting crack growth.

The existing image-based method was modified to enable prediction of arbitrary 3D crack shapes within a polycrystalline material. An overview of the algorithm for the method is shown in Figure 8. A voxel representation of an arbitrary microstructure is obtained synthetically or reconstructed from experimental scans. The voxels are arranged on a structured 3D grid. The voxel representation is converted into a tetrahedral FE mesh using the software DREAM.3D. Due to a special voxel-identification scheme the FE mesh includes traction-free surface along the 3D crack surface. An FE solver then executes the FE analysis, and a wrapper uses the FE results to assess the crack-growth rule as specified by the user. Upon assessing crack-growth along the 3D crack front, the framework then predicts the new crack front, updates the voxel representation, and repeats the procedure.

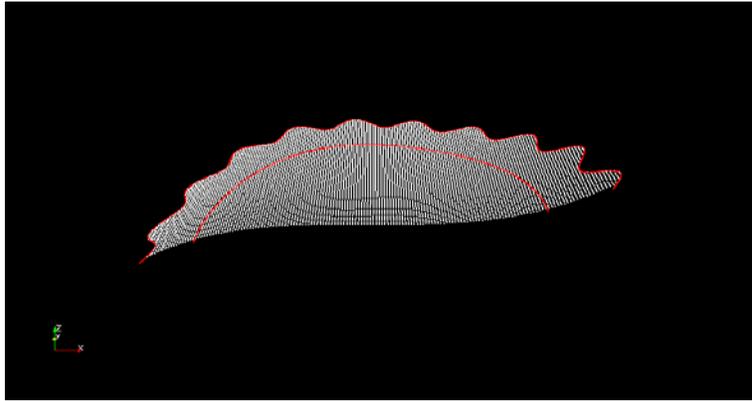


**Figure 8. Algorithm of Proposed Image-Based Method for Predicting Arbitrary Crack Growth.**

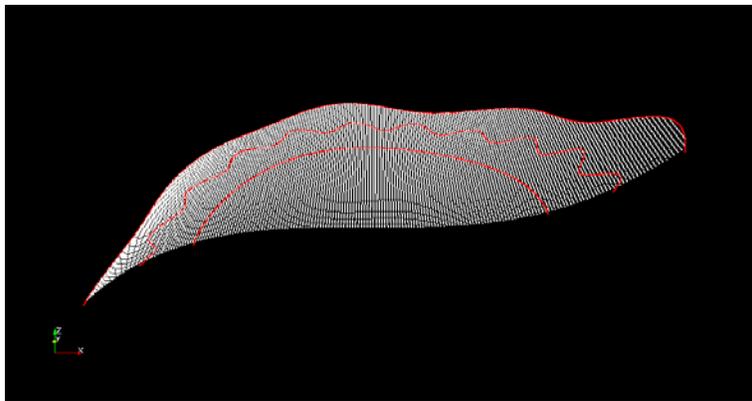
The above algorithm was implemented to perform a proof-of-concept simulation. The initial crack surface is shown in *Figure 9*. The predicted crack surface after one iteration of the algorithm is shown in *Figure 10*. Finally, one last iteration was performed, and the last predicted crack surface is shown in *Figure 11*. *Figure 12* shows the three crack fronts, which span multiple grains within the microstructure.



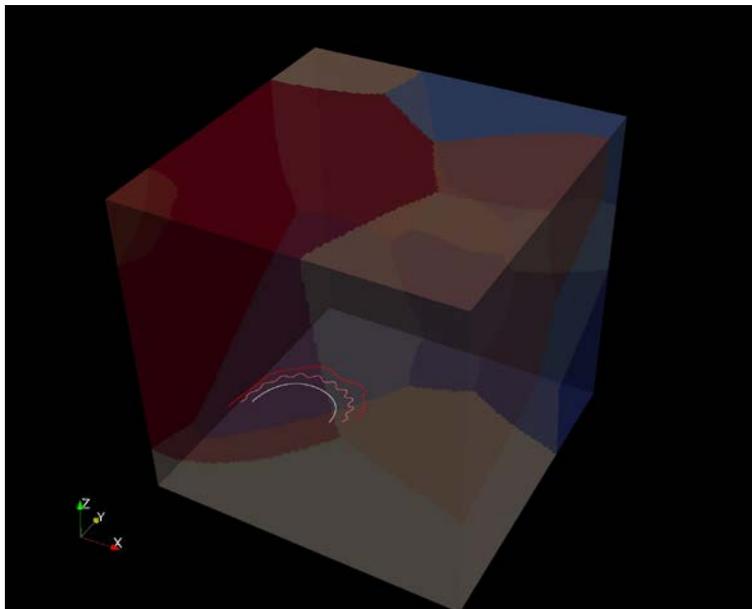
**Figure 9. Initial Crack Surface.**



**Figure 10. Crack Surface Following First Crack-Growth Increment.**

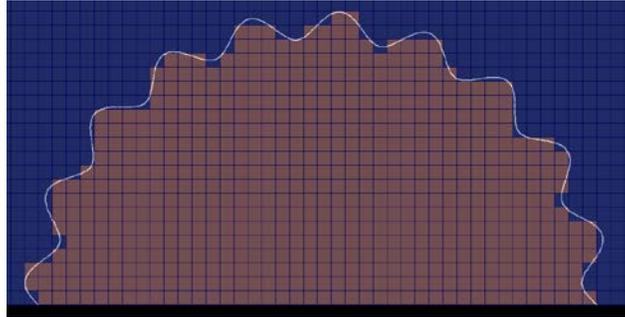


**Figure 11. Crack Surface Following Second Crack-Growth Increment.**



**Figure 12. Predicted Crack Fronts within a Synthetic Polycrystal.**

Despite its novelty and robustness, there are limitations of the proposed image-based approach. The first limitation is that the crack representation is highly dependent upon voxel spacing. This effect can be observed in *Figure 13*. Specifically, the image depicts the first predicted crack front (i.e. *Figure 10*) in white and a coarse voxel spacing below. The maroon voxels are determined to be part of the crack surface, which results in a poor description of the curved crack front. This effect can be minimized with high voxel density and/or Laplacian smoothing. However, these adjustments could lead to intractable computational time and/or significant approximation errors.



**Figure 13. Limitations of Method Include Large Dependencies on Voxel Spacing.**

Another issue is the need to maintain history dependence in the material between each mesh. The framework currently treats each iteration of crack growth as an independent FE model, and material-state history dependence or internal state variable mapping between each model has not yet been implemented. It is anticipated that traditional material-state mapping algorithms will lead to solution errors in regions of high gradients, e.g., along the crack front.

In light of the above limitations, the research team met with DREAM.3D developers at AFRL (Drs. Mike Groeber and Sean Donegan) to discuss possible solutions. Together, the group proposed the development of a DREAM.3D extension that can leverage the topological data structure within DREAM.3D instead of relying on an image-based description. The anticipated result of the new proposed approach would be a more accurate crack-surface representation that does not require material-state mapping, as remeshing will not occur. This approach will enable truly arbitrary crack evolution while maintaining material-state history in an efficient manner. This remains the topic of ongoing research by Phung.

### **6.3 Task 3: Representative Volume Element size for crack growth**

Task 3 focused on the size that must be polycrystalline model should be to remove boundary and loading condition artifacts. It has been shown that the microstructural neighborhood of a crack can have a significant influence on the behavior of the crack throughout the microstructurally small regime. Thus, it is the goal of many researchers to capture, both experimentally and computationally, the 3D microstructural features surrounding a small crack. One method used to make 3D microstructural measurements at AFRL is serial sectioning. This method involves measuring the 2D microstructure of a sample on a single plane, removing material to access a new plane of the sample, and measuring the microstructure of the new plane. After collecting data from planes throughout the sample, software is used to stitch the data together to create a 3D representation of the microstructure. Consequently, the time required to complete the measurements increases dramatically with increasing volume of interest. Similar to

microstructural measurements, the time required to perform a numerical simulation of a microstructure is significantly influenced by, among many factors, the number of grains included in the model. Without having a good rule of thumb for how many grains should be included in the model, researchers are left to either greatly underestimate the volume of influence for a cracked domain, or to spend exorbitant computational time resolving all of the possible microstructural features within a specified volume. Thus, having a priori knowledge of how large the microstructural neighborhood of interest would help to guide both experimentalists and modelers who seek to study microstructurally short cracks.

During the ten-week program spent at AFRL, M.S. student Karen DeMille initiated a study to answer the critical question: How much material (quantified in terms of grain diameters) should be included above/below and ahead of a short crack to ensure that the crack-front fields have achieved convergence? The objective of the study was to provide a closed-form approximation for the smallest values of  $d_1$  and  $d_2$ , the distances ahead of and above/below, respectively, a mode-I crack front such that crack-front fields are guaranteed to be converged. The values for  $d_1$  and  $d_2$  are provided in terms of average grain diameter.

Currently, two types of volume elements are used in computational mechanics. The first of these types of elements is the Representative Volume Element (RVE). According to Drugan and Willis, an RVE is “the smallest material volume element of the composite for which the usual spatially constant ‘overall modulus’ macroscopic constitutive representation is a sufficiently accurate model to represent mean constitutive response”. The second type of volume element is the Statistical Volume Element (SVE), which is any finite volume element smaller than the RVE and larger than the characteristic microstructure size.

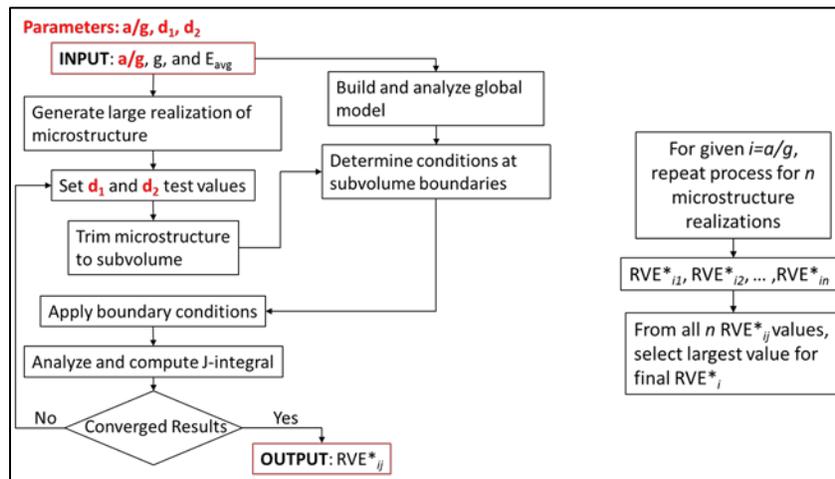
A type of volume element for microstructurally short cracks was proposed using a definition that is similar to a traditional RVE but asserts convergence of local, microstructure-sensitive metrics rather than a global, macroscopic one. The volume element, which we call RVE\*, is to be the smallest polycrystalline volume containing a crack, where the local crack-front parameters, such as the J-integral, are converged for a specified set of boundary conditions. Determination of RVE\* guarantees not only that enough microstructure is included in the volume to represent the influence of far-field loading on the crack, but that the influence of geometrical edge or boundary effects on the crack-front fields is minimized. A number of assumptions must be made in the determination of RVE\*. In this work, we assume a semi-circular surface crack oriented in a nominally mode-I configuration. Grains are represented as cubes, and it is assumed that RVE\* can be reasonably determined based on a linear-elastic response of the polycrystal. Grain orientations are represented implicitly by varying the elastic moduli. Finally, it is assumed that RVE\* can be determined based on a static crack analysis meaning fatigue loading and crack growth are not considered in this first iteration of the research.

The value of RVE\* depends upon the applied boundary conditions, and several sets of boundary conditions are being investigated in the present work. One set represents a material volume extracted from an infinite medium (with the exception of the surface containing the crack). Another set will represent a stand-alone volume of material with free surfaces, much like the small-scale specimens used, for example, for in-situ synchrotron studies. Finally, a set of boundary conditions somewhere in between the above limiting cases will be used. The boundary conditions are based on fatigue tests conducted by Dr. Reji John at AFRL/RXCM. The specimens of interest are made

of Ti-6242S and have width, height, and thickness dimensions of 10 mm, 25 mm, and 2.1 mm, respectively. The specimens are FIB notched and subjected to a maximum nominal stress of 800 MPa and stress ratio of  $R = 0.05$ .

Using the assumptions indicated above, the algorithms for determining  $RVE^*$  are shown in Figure 14. In both figures, the indices  $i$  and  $j$  correspond to distinct instantiations of the crack size and microstructure, respectively. As shown on the left in Figure 14, a single value of  $RVE^*$  is predicted for a given normalized half-crack length of interest,  $a/g$ , average grain size,  $g$ , and average elastic modulus,  $E_{avg}$ . Based on these parameters, a global model is first generated and analyzed to provide the boundary conditions on the local, microstructural model. The algorithm then generates a 3D microstructural realization with a semi-circular surface crack. Elastic moduli are assigned to the grains using a sampling method that accounts for the variability in the elastic response of each grain. The algorithm then iteratively adjusts the size of the cracked volume (viz.,  $d_1$  and  $d_2$ ) until the computed J-integral values have converged to an acceptable tolerance over the entire crack-front domain. Each time the microstructural volume is adjusted, the boundary conditions are updated using the displacement values computed from the global model. Once the J-integral values are converged along the entire crack front, the corresponding values for  $d_1$  and  $d_2$  represent  $RVE^*$  for a given  $a/g$  and a single microstructural instantiation.

As depicted on the right in Figure 14, the aforementioned algorithm must be executed multiple times to achieve a limiting value of  $RVE^*$  for a given  $a/g$ . For example, if  $a/g$  is small such that the crack front samples very few grains, then multiple microstructural instantiations should be analyzed to ensure that the possible range of grain orientations is sampled by the crack front. Doing so will better ensure that the limiting microstructural instantiation is identified and that the most conservative value of  $RVE^*$  is selected.



**Figure 14. Left: algorithm for generating a single value of  $RVE^*$  using FE analysis.**

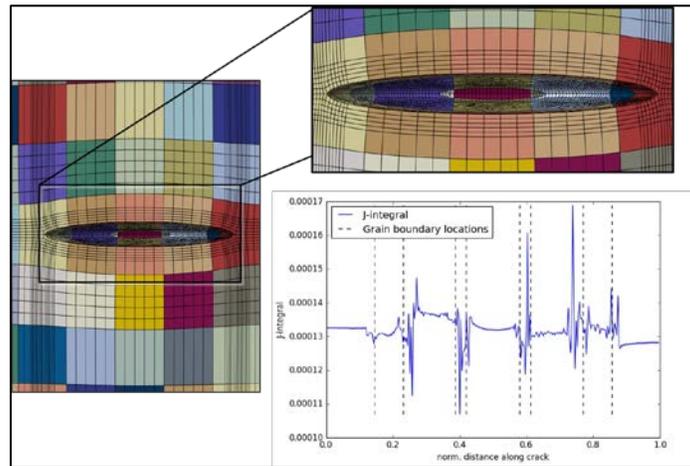
As part of preliminary work for the  $RVE^*$  study, an existing crack-analysis software, FRANC3D 2, was assessed to gauge feasibility of using it to analyze microstructurally small cracks. The software is capable of remeshing an uncracked FE model to include an explicit representation of a 3D crack. The cracked model is then analyzed using an FE solver, like ABAQUS. Using results

from the FE analysis, FRANC3D then computes local crack-front parameters, e.g. stress intensity factors (SIFs) or J-integral values.

While FRANC3D is a robust tool for analyzing crack geometries embedded within a single material domain, it was concluded from the assessment that FRANC3D is not suitable for meshing and analyzing cracks that span multiple material domains. It is postulated, after talking with Dr. Bruce Carter of Fracture Analysis Consultants, that topological challenges arise in meshing a crack geometry that intersects internal material boundaries (i.e. grain boundaries). Thus, it was decided during the summer that the algorithm shown in Figure 14 will not incorporate FRANC3D. Rather, the algorithm consists of a set of Python scripts that automatically generate cracked models using ABAQUS.

Figure 15 shows an example of simulation results for one of the idealized microstructures containing a crack front that spans nine distinct grains, where the colors shown represent grains of varying elastic moduli. The FE model was generated automatically using a Python script that takes  $a/g$  and  $E_{avg}$  as input. The model was then analyzed using ABAQUS, and the J-integral was calculated along the entire crack front.

Near-term work will focus on identifying an expression for RVE\* for the Ti-6242S samples of interest to Dr. Reji John. Longer-term work will focus on deriving an expression for RVE\* for the two other types of boundary conditions described earlier.



**Figure 15. Idealized Polycrystal with semi-circular surface crack, shown with exaggerated deformation. Colors correspond to different grains. J-integral calculated along the crack front ( $N/\mu m$ ).**

## References

1. Miner, M. "Cumulative Damage in Fatigue", *Journal of Applied Mechanics*, vol 12, pp. A159-A164, September 1945.
2. Penmetsa, R. C., Hill, R. R., Ahner, D. K., and Russel, B. D., "Capturing Uncertainty in Fatigue Life Data," *International Journal of Reliability and Safety*, Vol. 9, No. 1, 2015
3. Clark, D. L., Bae, H., & Penmetsa, R. C., "Locally-Optimized Covariance Kriging for Engineering Design Exploration", *AIAA SciTech 2015*, Kissimmee, FL, AIAA-2015-1372

**APPENDIX A  
PERSONNEL**

Air Force Employees:

Personnel	Degree	MY	Remarks
Ravi Penmetsa	PhD	0.7	PI 10/1/2013-2/14/2016
Joseph Hollkamp	PhD	1.0	SME - Vibrations and fatigue
Brian Gockel	PhD 2016	1.3	SME - Material Science
Ravi Chona	PhD	0.5	ST, SSC Director & PI 2/15/2016-9/31/2016

Collaborators/ Visiting Scientist

Personnel	Institution
Ali Gordon	University of Central Florida
Thomas Bouchenot	University of Central Florida
Raymond R. Hill	Air Force Institute of Technology
Darryl K. Ahner	Air Force Institute of Technology
Brent D. Russell	Air Force Institute of Technology
Ha-Rok Bae	Wright State University
Daniel L. Clark	Wright State University
Koorosh Gobal	Wright State University
Ashley D. Spear	University of Utah
Karen DeMille	University of Utah
Brian Phung	University of Utah
Patrick O'Hara	UTC
Ricardo Perez	UTC

## **APPENDIX B LIST OF PUBLICATIONS**

Published in Peer-Reviewed Journals:

Penmetsa, R. C., Hill, R. R., Ahner, D. K., and Russel, B. D., “Capturing Uncertainty in Fatigue Life Data,” *International Journal of Reliability and Safety*, Vol. 9, No. 1, 2015

Conference Proceedings & Technical Reports:

Hollkamp J.J., Perez R.A., and Spottswood S.M., "Design Sensitivities of Components using Nonlinear Reduced-Order Models and Complex Variables," *Proceedings of IMAC-XXXV*, Garden Grove, Ca, Feb 2017.

Gordon, A. P., Bouchenot, T., and Penmetsa, R. (2015) “A Microstructurally-Informed, Continuum-Level Life Prediction Model for Thermo-Acousto-Mechanically Fatigue Ti-6242S and IN617” *AIAA SciTech 2015*, Kissimmee, FL, January 5th-9th.

Sedlack, M., Jasmin, A., Lavandera, P., Gordon, A. P., and Penmetsa, R. (2015) “Design and Evaluation of a Test Device for Thermal-Acoustical-Mechanical Fatigue Experiments” *AIAA SciTech 2015*, Kissimmee, FL, January 5th-9th.

Jasmin, A., Sedlack, M., Lavandera, P., Gordon, A. P., and Penmetsa, R. (2015) “Design and Assessment of a Test Platform for Advanced Simulation of Cyclic Thermo-Acousto-Mechanical Loading” *TMS 2015 144th Annual Meeting & Exhibition*, Orlando, FL, March 15th-19th.

Gordon, A. P., Nunez-delPrado, Jones, N., and Penmetsa, R. C., (2015) “Life Prediction of Ti-6242S and IN617 under Thermo-Acousto-Mechanical Fatigue” *TMS TMS 2015 144th Annual Meeting & Exhibition*, Orlando, FL, March 15th-19th.

Gordon, A. P., Jones, N., Nunez delPrado, A., Penmetsa, R., and O’Nora, N. “A Microstructurally-Informed Life Prediction Model for Combined Thermal-Acoustical-Mechanical Fatigue” *Propulsion – Safety and Affordable Readiness (P-SAR) Conference*, Baltimore, MD, March 30th – April 2nd.

Gordon, A. P., O’Nora, N., Bouchenot, T., Ambrose, J., Jones, N., and Penmetsa, R. C. “A Thermoviscoplasticity Model for Ti-6242S under Creep-Fatigue Conditions”. *SciTech 2016 (Accepted)*, American Institute of Aeronautics and Astronautics, San Diego, CA, January 4th-8th, 2016.

Clark, L. D., Bae, H., Gobal, K., and Penmetsa, R., “Engineering Design Exploration Utilizing Locally Optimized Covariance Kriging,” *2016 AIAA SciTech Conference*, San Diego, CA. Under review for publication in the *AIAA Journal*.

Clark, D. L., Bae, H., & Penmetsa, R. C., “Locally-Optimized Covariance Kriging for Engineering Design Exploration”, *AIAA SciTech 2015*, Kissimmee, FL, AIAA-2015-1372

Hollkamp J.J., and O'Hara P.J., "Using Complex Variables to Estimate the Derivatives of Nonlinear Reduced-Order Models," AIAA-2016-1707, 57<sup>th</sup> AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference, San Diego, CA, Jan 2016.