# 1 Career 2016

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## 1.2 Tasks

### 1.2.1 T.3 Things to do Haneesh:

1. ~~Email Wenqiang and ask for input to construct the current achievements for the section~~ [~~(iii) Results from Prior NSF Support~~](#h.3pm0x94ma1o7)~~.~~
2. ~~Prepare Task Biographical Sketch for Max.~~
   1. ~~Read Biographical sketch requirements from GPG~~
3. Move broader impacts.
4. Wavy DCB
5. The VRF method works.
6. Introduction to Phase field modeling.
7. Simulations with new mechanisms.
8. Take images from your own paper.
9. Send email to Douglas asking for the Letter from Larry.
   1. Send last years letters.
10. Send the CMMI program information to Priscilla.
11. Contact Sci-Toons
12. Contact Leadership Alliance
13. Read the ARO proposal.
    1. Introduction to Phase field modeling.
    2. Assign new simulations to Weilin

Read previous CAREER proposal.

1. Simulations that shown that the VRF method works.

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### 1.2.2 T.1 Things to do Kaushik:

*(Strike out completed tasks)*

### 1.2.3 Finish section Anticipated difficulties.

* 1. ~~Make sure that the arc-length and continuation methods would be relevant and useful as we have suggested.~~
  2. ~~Read and understand about dynamic relaxation (DR). Similarly check if DR would be relevant and useful as we have suggested.~~
  3. Fill in the XX (missing info) as much as possible at this stage. You can complete filling in the missing info after we have added the preliminary results section.

~~1.2.4 Scaling of the computational time with the no. of CPUs.~~

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### 1.2.5 T.2 Things to do Max:

1. While preparing the *Facilities and Equipment* and the *Budget* fill in the CPU missing numbers in section \label{sec:AD} in ProjectDescription.tex. We need current and requested CPU numbers.

a. ~~Cover Sheet~~: ~~(~~priscilla and Douglas will handle this~~)~~

b. Project Summary

c. ~~Table of Contents~~ (automatically generated)

d. Project Description

Broader Impacts

e. References

~~f. Biographical Sketches~~

g. Budget and Budget Justification

h. ~~Current and Pending Support~~ (priscilla and Douglas will handle this)

i. Facilities, Equipment, and Other Resources

j. Special Information and Supplementary Documentation

#### 

Data Management Plan

~~Postdoctoral Mentoring Plan.~~ (Let’s not ask for a postdoctoral scholar)

**d. Project Description**

### 1.2.6 Biographical Sketch-Guidelines

* + – Two pages
  + – Senior personnel – *Haneesh Kesari*

## *1.3 Introduction*

As we continue to build higher, travel faster, and live more sustainably, we also must search for new materials that are lighter, stronger, and tougher. While strength–or the ability to bear the largest load–may appear to be the most crucial property, in many cases, toughness is actually more desirable. Specifically, in applications in which safety or reliability is paramount (e.g., bridges, turbine engines in aircrafts, or XXX), the best material is the one whose ability to carry loads is minimally affected by damage or wear-and-tear accumulated through use. For example, no matter how strong a bridge is, it would not be reliable if it were to fail catastrophically without any warning signs. Rather, small amounts of cracking or deformation of its components should not drastically reduce the bridge’s load carrying capacity. Consequently, the damaged components can be identified, and either be replaced or repaired before they lose complete functionality.

A material’s ability to impede the growth of cracks or defects is captured by its toughness properties. When a crack is created in a tough material, such as ductile steel, that material’s ability to carry loads is not drastically reduced. Furthermore when the crack does propagate through the material, it does so in a steady, controlled manner. On the other hand, the load carrying capacity of brittle materials, like glass, is highly affected by the presence of defects or flaws. While these materials tend to be strong, they typically fail through abrupt, catastrophic fracture during which cracks propagate in an uncontrolled manner.

In most engineering materials, from steels to ceramics, strength and toughness are mutually exclusive. That is, there are few materials that are both strong and tough. The PI believes that this is a critical bottleneck for aerospace, transportation, and energy production technologies (see Section BROADER IMPACTS). Recently, however, it has been shown that some structural biomaterials (SBs) possess both high strength and high toughness. In many cases, SBs are heterogeneous, and consist of a ceramic and an organic phase mixed together in intricate 3D patterns at the micrometer scale. The way that these two phases are interlaced–what is known as the SB’s architecture–is extremely complex compared to architectures typically seen in engineering composites, such as XXX. Some examples of architectures seen in SBs are the brick-and-mortar arrangement of ceramic tablets in shells, and the interlocking helices in the club-like appendage of the mantis shrimp (see Figure XXX). Since these SBs are characterized by the numerous, intricately arranged interfaces between the ceramic phases, we refer to them as interface dense SBs, or *id*-SBs.

While *id*-SBs are often composed of >95% brittle ceramic material by volume, they have been shown to possess extraordinary toughness properties while being able to maintain both strength and stiffness. For example, the total energy dissipated during the fracture of nacre has been shown to exceed that of its constituent ceramic material, aragonite, by three orders of magnitude. The apparent correlation between the SBs’ intricate architectures and their extraordinary mechanical properties has motivated many studies that investigate the connection between architecture and properties. Are specific architectural designs are the key to overcoming the tradeoff between strength and toughness? And if so, what are the mechanisms through which toughness is attained through these designs?

A portion of the toughness enhancement in *id*-SBs has been explained using classical mechanisms such as crack bridging, frictional pull-out of fibers or lamellae, or plastic dissipation at the interfaces caused by failure of sacrificial bonds (REF artful interfaces in biological materials, Fratzl 2011). These mechanisms reduce the stress concentration at the tip of a crack and also dissipate energy during crack growth, making it more difficult to propagate cracks. Theoretical mechanics models for *id*-SBs that incorporate these toughening mechanisms predict enhancements to toughness properties (e.g., work of fracture) of up to several hundred percent (REF barthelat vincent, currey, Kamat/ballarini 2000). However, they often do not amount to the toughness enhancements that are observed experimentally (REF currey). The PI believes that this is because it is not clear which architectural parameters are the most critical for enhancing toughness, since the mechanisms through which toughening occurs are still not well-understood. There could be a large number of toughening mechanisms operating in SBs that are not included in the models. However, it is also possible that what is being witnessed is not a myriad of well-understood mechanisms operating in concert, but rather a completely new mechanism.

The theoretical mechanics models currently used to explain toughening of *id*-SBs typically use <10 parameters to describe the architecture of the material. Many *id*-SBs, however, are far more complex. For example, the architecture of compact bone consists of an assembly of cylindrical fibers, known as osteons (see Figure XXX). Each osteon is made up of many concentric layers, and each layer is composed of collagen fibers in a particular geometric arrangement. In order to describe this architecture, the elastic properties of the constituent materials, and the toughness properties of the interfaces between fibers, layers and osteons we would need several hundred parameters! Even far simpler *id*-SB architectures like the crossed-ply layup in the shell of the queen conch, *strombus gigas*, possess at least several dozen architectural parameters. Due to the sheer complexity of these architectures is it impossible to predict all of the toughening mechanisms *a priori*, or to identify which mechanisms account for the majority of the toughness enhancement. Furthermore, the architectures of *id*-SBs often contain features whose sizes are continuously distributed from the centimeter to the micro- or even nanometer scale. That is, there is no clear separation between the characteristic size of the *id*-SB and the sizes of its architectural features. This “omni scale” attribute of *id*-SBs means that the mechanics of different features cannot be analyzed separately and then combined to yield the overall behavior of the *id*-SB. Rather, the entire architecture must be modeled and analyzed at once.

The PI believes that one of the main reasons that the toughening mechanisms are not well understood is because currently there are no methods that allow one to “see” inside the material as it fails. This is because quantifying the extent to which different mechanisms are operating in an *id*-SBs requires information about the deformation and damage behavior of the interfaces, which is quite challenging to obtain experimentally. Since these interfaces are 3D, complex and internal to the material, it is difficult to directly visualize them. In the past, information about the interfaces’ geometry was obtained by taking multiple cross-sections of an *id*-SB and making inferences about the 3D geometry from these 2D slices (REF). While this method can be used to obtain geometric information, it cannot be used to obtain information about the deformation or failure behavior of the interfaces during mechanical tests. This is because cross-sectioning an id-material could change the extent to which certain toughening mechanisms can operate. Recently, micro-CT scanners have been used to visualize the interfaces of *id*-SB while mechanical tests were being performed. While this method appears promising, for researchers without direct access to a micro-CT scanner, investigating toughening mechanisms in *id*-SBs this way would be prohibitively expensive. Furthermore, some studies have revealed that the high energy x-rays emitted by CT scanners can embrittle the proteinaceous interfaces of *id*-SBs. This embrittlement may affect the extent to which some toughening mechanisms can operate in the material. This makes it difficult to determine which mechanisms are most important to an *id*-SB in its natural state. However, the fact that such expensive resources are being used to visualize the deformation and failure of interfaces in *id*-SBs highlights the importance of this information to the material-mechanics community.

Recent efforts to understand toughening mechanisms in *id*-SBs have used computational mechanics models in place of experiments. The primary advantage of performing virtual experiments is that it is very easy to “see” inside the material and identify the mechanisms through which toughness is attained. However, since these virtual experiments are still only models for the real materials, the spectrum of toughening mechanisms that they can capture is in some way limited. For example, some computational mechanics models, such as XXX, require that the trajectory of crack growth be specified as an input. These models are therefore unable to capture toughening due to crack deflection and branching caused by the material’s architecture. In order to capture a greater diversity of mechanisms, the assumptions underlying a computational model should be very basic. Recently, molecular dynamics simulations (REF buehler) and large-scale computational micromechanics simulations (REF begley and CZM) have been used to identify new toughening mechanisms in *id*-SBs. These methods, however, are extremely computationally expensive and therefore have not been used to model some of the more complex id-SB architectures that possess omni-scale features.

The PI proposes to develop and use a computational tool based on variational regularized fracture (VRF) (see Section XXX) to investigate toughening mechanisms in *id*-materials. By comparing results generated using a preliminary version of this tool to experiments on *id*-SBs (see Section XXX), the PI believes that the proposed method has sufficient generality to serve as an investigative tool. Compared to existing computational tools (e.g., XXX), the assumptions underlying the proposed method are very basic and therefore it is able to capture a greater diversity of mechanisms. In the proposed computational tool the constituent materials fail in a brittle manner. Therefore failure events are restricted to two categories: 1) brittle failure of the ceramic phase, or 2) brittle failure of the interface. However, prior knowledge of crack trajectories is not assumed, and cracks within the material are allowed to evolve freely. This is a stark contrast to methods like XXX in which both the constituents’ failure behaviors and the anticipated crack paths are required as inputs. Hence, the proposed computational tool can be used to predict the direction of crack growth based on a material’s mechanical properties, architecture and loading (see Section XXX). Most importantly, in VRF cracks and interfaces are not modeled explicitly. This feature makes VRF very efficient for analyzing materials, like *id*-SBs, that possess complex internal interfaces develop complex crack patterns. This computational efficiency makes VRF well suited to analyzing materials with omni-scale architectures, or architectures without a clear separation of length scales.

However, VRF is not without its own host of problems. The origin of many of the problems with the VRF stem from the fact that currently it is not well-developed from a solid mechanics perspective. Before the VRF can be regarded as a valid theory of fracture, several key mechanics issue must be addressed. These problems are a) fracture should only occur through tensile stresses, b) crack growth in brittle materials should progress in an unstable manner, and c) cracks must remain spatially localized, i.e., damage should not spread in thick bands. The first aim of the proposed research (see Section XXX) is to address these three key issues with VRF. The majority of the proposed effort focuses on resolving the “non-localization” problem, (c), since our preliminary work suggests that this is a fundamental flaw in the currently used VRF theory. In Section XXX we outline the steps that will be used to identify the cause of the non-localization problem and subsequently reformulate the VRF theory to resolve this problem.

While the PI’s long term career goal is to develop a VRF computational tool capable of capturing the failure mechanisms of id-SBs such as bone and conch shell, the complexity of these materials makes them ill-suited for the development phase. Rather, after correcting the fundamental issues in the current VRF theory, the PI first plans to a) demonstrate the utility of the VRF tool in discovering new toughening mechanisms (see Section XXX) and then b) predict the failure behavior and toughening mechanisms of a relatively simple *id*-SB (see Section XXX).

First, the PI proposes to use the computational tool built on the corrected VRF theory to discover new toughening mechanisms in materials with wavy interfaces. Interestingly, wavy interfaces are a prominent motif in *id*-SBs, such as woodpecker beaks and the cranial bones of rams (see Figure XXX). The SBs that contain wavy interfaces are predominantly subjected to impact or cyclic loads and must remain intact in order to perform their mechanical functions. This suggests that this type of interface could be a key ingredient for enhancing the toughness of these materials. In Section XXX we present preliminary research in which we study the failure process of 2D wavy interfaces using two simple geometries using the computational VRF tool presented in Section XXX. We found that the wavy interface increases the toughness of the material and that the magnitude of this increase is related to the amplitude and wavelength of the undulations. Most importantly, we discovered a novel toughening mechanism that precipitates this toughness enhancement. We propose a continuation of this research on wavy interfaces that focuses on extending our analysis to 3D wavy interfaces and to include more architectural parameters to describe the shape of the wavy undulations (see Section XXX for details). The proposed extension is motivated by theoretical models (REF ortiz) that suggest that the toughness of a wavy interface is further enhanced by increasing the complexity of the undulations. Through this component of the proposed effort the PI hopes to validate the power of the VRF computational tool as a way to discover new toughening mechanisms in *id*-materials.

Next, the PI proposes to use the VRF computational tool to investigate toughening mechanisms in a relatively simple id-SB. The PI has chosen the skeletal elements, known as spicules, of the Euplectella aspergillum sponge as the model *id*-SB to investigate (see Section XXX). This *id*-SB is ideal for the initial investigations due to its architectural simplicity (<30 parameters), and the brittle nature of its constituent materials. Furthermore, the PI already has experience studying the architecture and mechanical properties of this SB (REF Monn2015, Monn2016 submitted). Briefly, the spicules are hair like fibers that are composed of roughly 25 concentric silica cylinders. The fibers are up to 10 cm long and 50 $\mu$m in diameter with the individual silica cylinders being roughly 200-XXX nm thick. The areas between the silica cylinders are extremely thin (~5 nm) and are filled with a proteinaceous material. Initial mechanical tests of the spicules suggest that these proteinaceous interfaces are weak compared to the silica cylinders (see Section XXX). In order to evaluate the predictive power of the VRF computational tool, the PI proposes to compare toughness properties obtained from a virtual mechanical test of a spicule to those obtained through mechanical tests. In Section XXX, the PI presents preliminary results of the measured force-displacement response of a spicule loaded in three-point bending using a custom built testing stage. In order to measure the toughness properties of the spicules, the custom-built testing stage must first be modified so that notches can be cut into the spicules prior to testing. An initial design of one component of this testing stage is shown in Figure XXX. Due to the spicules’ size (roughly that of a human hair), notches cannot be cut using conventional tools, such as diamond saws, or razor blades. The PI proposes to use focused ion beam (FIB) milling to cut the notches in the spicules. In order to ensure that the notch cutting procedure does not affect the measured toughness, it must be tuned so that ion implantation is minimized and very sharp (<100 nm) notch tip radii can be achieved. A pilot study of FIB notching was conducted (see Section XXX) using a preliminary design of the testing stage. The details of the proposed experiments are presented in Section XXX. In order to compare the measured toughness of the spicules to that predicted by the VRF computational tool, a virtual spicule must be constructed. To model a spicule, its architectural parameters (i.e., the radii of the concentric silica layers) must be measured. The PI has already developed a procedure for imaging and measuring the layers in a spicule (see Section XXX) (REF Monn 2015). A preliminary 2D model of a spicule has been developed in order to begin to identify toughening mechanisms and the effect of layer number and thickness on the toughness (see Section XXX). The PI plans to construct a 3D model of a spicule using the measurements of the silica layers to compare to the physical tests (see Section XXX). Specifically, the PI will use the results of the experiment (i.e., the force-displacement response, and measure toughness properties) to calibrate the spicule model. Then, the spicule model will be used to investigate whether any mechanisms exist that increase the spicules’ toughness properties. Through this component of the proposed effort, the PI will show the power of coupling VRF with mechanical tests to identify mechanisms that enhance toughness properties in *id*-SBs.

Based on the knowledge gained through the investigation of the spicules and the wavy interfaces, the VRF computational tool will be used to develop new architectural designs that possess similar toughening mechanisms as those observed in these model systems. When developing the new, *id*-SB inspired designs, we want to determine the values for the architectural parameters that correspond to the material with the greatest toughness. Due to the sheer number of parameters, however, performing a full parametric study of the effects they have on the material’s toughness would be impossible. Furthermore, due to the size and dimensionality of this parameter space, it could be difficult to even determine sets of parameters that produce even modest enhancements to toughness. Therefore, it would be valuable to have reduced-order analytical theories that, although coarse, could model the toughening mechanisms in *id*-materials. While these theories would be less precise the computational tool, they could be used to quickly identify a region in the parameter space in which significant toughness enhancements can be attained. After using a reduced-order model to identify the region in the parameter space over which to search for beneficial architectures, the computational tool could be used to arrive at near-optimal designs with high precision (see Figure XXX). The PI proposes to use continuum mechanics theories and asymptotic analysis to derive suitable micromechanics theories to provide a rough characterization of the parameters’ effects on toughness. Preliminary efforts toward developing a micromechanics theory of toughness for id-materials with wavy interfaces are presented in Section XXX. The PI will use a similar procedure to derive a continuum mechanics theory for characterizing the parameters’ affects on the toughness of spicules as well. The details of how these reduced-order continuum theories will be used to supplement parametric studies using the VRF computational tool are provided in Section XXX. The goal of this component of the proposed effort is to develop guidelines for designing bio-inspired *id*-materials that contain a combination of concentric layers and wavy interfaces. Specifically we will identify the architectural parameters that produce *id*-materials with the greatest toughness. Possible implications of the utility of the VRF computational tool paired with the continuum reduced-order models for the development of new engineering materials are discussed in Section XXX.

The overarching goals of this project is to ascertain whether VRF theory is a valid theory of fracture and can subsequently be used to explore the relationship between toughness and architecture in *id*-materials. And to subsequently show that the VRF computational tool can be used to design bio-inspired materials with enhanced toughness properties. We divide the proposed effort into 4 Aims that each have several associated Tasks.

**Aim 1)** Formulate a new VRF theory by addressing the three major shortcomings of the current VRF theory: 1) stability of crack growth in brittle materials, 2) crack growth in both tension and compression, 3) non-localization, or broadening, of cracks.

**Task 1)** Stability

**Task 2)** Broadening effect

**Task 3)** Compression-tension split

**Aim 2)** How does microarchitecture affect toughness (discovery tool)

**Preliminary results:**

**Task 1)** relate toughness properties and microarchitectural parameters for wavy interfaces (TAKE INFO FROM ARO PROPOSAL)

**Aim 3)** Mechanical characterization of SBs’ toughness properties. Relating mechanism and response in a model system: spicules

**Task 1)** Experimental measurement of G\_c and WoF

**Task 2)** Make 3D VRM framework and spicule model

**Task 3)** compare to virtual and physical experiments of this SB

**Aim 4)** develop ROMs connecting architecture and toughness and use the ROMs along with the VRF tool to determine the best designs

**Task 1)** develop ROM for spicule toughness

**Task 2)** use ROMs for wavy interfaces and spicule to find regions in parameter space corresponding to “good” designs

**Task 3)** use the VRF computational tool to determine the optimal or at least “best” designs for these two specific types of architectures

EXTRA INFO:

~~The toughening mechanisms that have been identified already are often very specific to a particular~~ *~~id~~*~~-SB architecture. It is surprising that a toughening mechanism, which accounts for the majority of the observed toughness enhancement, is not shared among a broader class of~~ *~~id~~*~~-SBs. While it is true that each~~ *~~id~~*~~-SB architecture is unique, they share many common features, such as XXX. Therefore, it seems only natural to presume that there must exist some general toughening mechanism that would be shared amongst many different~~ *~~id~~*~~-SBs. This kind of common mechanism would be similar to how dislocation motion is a common failure mechanism in metals. For this reason, the PI believes that there are important toughening mechanisms that are common to most~~ *~~id~~*~~-materials that are still undiscovered. The PI’s long term goal is to study the mechanisms through which the architecture of~~ *~~id~~*~~-SBs enhance their toughness properties.~~

~~Synthetic variants of~~ *~~id~~*~~-SBs have been produced in an attempt to systematically investigate the connection between architecture and toughness. New fabrication methods, such as ice templating and slip casting, have been developed in order to produce these synthetic~~ *~~id~~*~~-materials. Recently, a parametric study of toughness properties was performed on a synthetic nacre. This~~ *~~id~~*~~-material consisted of alumina tablets arranged in a brick-and-mortar architecture separated by thin layers of poly(methyl methacrylate); a weak, compliant polymer. The aspect ratio of the tablets and extent to which adjacent tablets overlapped (see Figure XXX) were varied and the material’s toughness properties were measured. It was found that the energy dissipated during fracture (i.e., the work of fracture) could be changed by tuning these architectural parameters. Specifically, with the right choices of aspect ratio and tablet overlap, the work of fracture could be enhanced by up to XXX% over that of monolithic alumina.~~

Main problems with the method:

1. Broadening
2. How the parameter in the model should be chosen, ~~E, \nu,~~ cG\_c, ell\_0, g(\phi), ad-hoc.
3. Irreversibility;
4. Compressive and Tensile.

Long term research goals.

1. Extending the analysis to take into account finite deformation, Dynamics effects, Non-linear material behavior

1. *Brittle interface fracture may be an insufficient model.* Plastic, Viscoelastic,or Viscoplastic behavior at the interfaces may a key features in the energy absorption mechanisms.

Specific research objectives

## 1.4 Motivation.

*As long as a branch of knowledge offers an abundance of problems, it is full of vitality.*

–David Hilbert

The goal of the proposed project is to generate new knowledge (experimental and theoretical) and computational capabilities for the discovery, understanding, and modeling of new toughening and strengthening mechanisms in *id*-brittle materials. As elaborated in section~\cite{NewMechanicsinIdMaterials}, experimental investigations on biological and bioinspired *id*-brittle materials show that there is high probability that these materials hide some very ingenious, hitherto unknown, mechanisms. The discovering of such mechanisms would in itself constitute valuable new scientific knowledge. However, the new mechanisms would also create plentiful new opportunities for the development of new mechanics theories. The PI himself plans to dedicate as part of his career in development such new mechanics theories. However, the new knowledge generated by this project is expected to be sufficiently broad and rich to stimulate/galvanize and aid/facilitate the generation of new knowledge by the wider mechanics community.

At his most optimistic, the PI hopes that these new opportunities to model new mechanisms/phenomena will re-vitalize and re-invigorate the theoretical mechanics community. The development, study, refinement, and expansion of the modeling and the mathematical aspects of such theories is expected to be an expansive and an enriching scientific endeavor.

However, it is likely that the reader might wonder as why the PI has selected to focus his career on *interface dense brittle materials. Surely, there must be other materials classes with similar or even greater potential for the discovery of new mechanisms, and consequent development of new mechanics theories.*

Well

it is might be useful to discuss as to why the PI plans to focus on the particular class

1. Technological progress strongly depends on our ability to meet humanity’s ever growing need for energy. Recently, this has led us to explore a number of new and innovative directions both in the production and the storage of energy. For example, solar energy production capacity in the United States has grown by nearly 700% in the last five years alone (REF SEIA). However, a number of energy production technologies, such as hydroelectric, natural gas, and coal implicitly rely on turbine engines. This is likely to hold true even for some of the next generation of energy production technologies, such as nuclear fusion, concentrating solar power, and ocean thermal energy conversion (OTEC).
2. The thermodynamic efficiency of gas turbine engines (GTEs) is increased with increasing turbine inlet temperatures. Therefore, in the case of GTEs it is important to use materials that are capable of withstanding high temperatures yet still have high strength, stiffness and toughness. Traditionally, Nickel-based superalloys have been used to fabricate the hot components (such as the turbine blades and combustion chamber) of the GTEs, as they are some of the most lightweight and tough materials capable of withstanding very high temperatures (up to 1500 degrees). However, in order to further enhance the GTE’s efficiency the temperatures in the hottest parts of the engines are being raised even further. This is made possible by applying ceramic-based thermal barrier coatings (TBCs) to the surfaces of the superalloys. While ongoing research continues to raise the temperature capability of TBCs, the temperature capability of the Ni-based alloys has mostly remained flat. To compensate for this discrepancy between temperature capabilities, currently the superalloy components are cooled using air circulation systems to allow them to operate alongside the higher temperature capable TBCs. However, adding the cooling systems significantly reduces the specific power produced by the GTEs.
3. Therefore, there is a search for a new class of materials that can replace the Ni-based superalloys. Such materials should be capable of operating at higher temperatures than Ni-based superalloys without the need for any additional cooling, and have equal or better specific mechanical strength and toughness. Research into finding a replacement for Ni-based superalloys has been going on for decades, primarily along two lines: (i) Mo-based and Nb- based alloys and (ii) ceramic matrix composites (CMCs). It appears that CMCs are winning that race, as is evidenced by the significant investments made into CMCs by a major engine manufacturer, and the recent demonstration of engines that use both stationary and rotating CMC components in the hot-section.
4. Ceramics are as strong as superalloys while being lighter and being able to withstand higher temperatures and corrosive environments. However, they are brittle and are prone to fracture during thermal or mechanical shock loading. Therefore, to increase the toughness, the ceramic materials are made into composites (e.g., CMCs). However, there are still many hurdles that stop us from taking advantage of the tremendous potential of CMCs.
5. The first generation of CMCs simply involved dispersing one ceramic phase in the form of particles or fibers in another ~~different or same~~ ceramic phase ~~that acted as the matrix~~. It was found that only when the dispersed phase was in the form of very long fibers was there a substantial increase in the toughness of the CMC. Leading from that, currently, CMC parts are created additively. First, ceramic fibers are laid flat or woven together to form sheets/plies. Then a preform~~/mold/scaffolding~~ in the shape of the final part is created by stacking the plies one on top of another. ~~Among several other processing steps~~ The preform is then infiltrated with the ceramic matrix phase to get the final part. The primary architectural design in such cases is within the plane of each ply. Since, in the stacking direction, at the most, the plies can be simply rotated in-plane with respect to each other. Due to this reason, these CMCs are typically termed 2D CMCs. One of the primary hurdles that is stopping us from taking advantage of CMC is that 2D CMC parts are invariably weaker–by almost an order of magnitude–in the out-of-plane direction and are prone to delamination failure. There are currently attempts to circumvent this problem through the use of sophisticated 3D architectures. These architectures are constructed using a variety of new fabrication techniques such as slip casting, ice templating, robo-casting, and weaving techniques adapted from the textile industry. For example, consider the case of integral ceramic textile structures (ICTSs). The fiber preforms of these CMCs are created using 3D textile weaving methods that produce interlaced in-plane and through-thickness fibers. The fibers in ICTSs that bridge multiple plies enhance out-of-plane toughness properties and alleviate the delamination problems characteristic of 2D CMCs.~~For example consider the case of ICTS.~~
6. The new 3D architectures are highly complex and are radically different from the 2D CMC designs. Many of them are inspired from architectures seen in structural biomaterials (SBs), which also in many cases are composites consisting of ceramic tablets, fibers or layers glued together using an organic/polymeric phase. Some examples of SBs with these types of 3D architectures are bone, the nacreous layer in abalone shell, and the club-like appendage of the mantis shrimp. While these SBs are often composed of >95% ceramic material by volume, they have been shown to possess extraordinary toughness properties while being able to maintain both the strength and stiffness of the constituent ceramic material. For example, the total energy dissipated during the fracture of nacre has been shown to exceed that of its constituent ceramic material, aragonite, by three orders of magnitude. The incredible toughness in SBs arise from the large number of interfaces and intricate architecture of these interfaces. It is believed that the tremendous amount of interfacial area and the interfaces’ intricate 3D geometry is the key to the structural biomaterials’ incredible toughness, damage tolerance, and energy dissipation. Some of the enhancements to the SBs’ toughness properties have been explained using classical toughening mechanisms such as crack bridging, frictional pull-out of fibers or lamellae, or plastic dissipation at the interfaces caused by failure of sacrificial bonds (REF artful interfaces in biological materials, Fratzl 2011). All of these mechanisms reduce the stress concentration at the tip of a crack in the material, and consequently make it more difficult to propagate cracks. Models for SBs that incorporate these toughening mechanisms predict enhancements to toughness properties (e.g., work of fracture) of up to several hundred percent (REF bathelat and Kamat 2000). However, they do not account for the toughness enhancements that are observed experimentally. One explanation for this is that there could be a large number of other toughening mechanisms operating in SBs that are not included in the models. It is also possible that what is being witnessed is not a myriad of well-understood mechanisms operating in concert, but rather a completely new mechanism. While these mechanisms can be used to explain the observed enhancements of toughness properties, they cannot be used to predict the anticipated toughness of a new design based on the architecture alone. This is because, in general the link between architecture and toughness is not well-understood. This type of predictive power would allow the deliberate design of CMCs as opposed to merely mimicking the architectures of SBs with enhanced toughness properties. In this case the architectures of the SBs could serve as a starting point from which the architecture is tuned to give rise to even greater toughness enhancements.
7. The large amount of interfacial area and its intricate 3D nature provide a large amount of design freedom. The SBs intelligently take advantage of this design freedom by coupling old toughening mechanisms or precipitating completely new ones to substantially enhance their toughness, compared to the toughness of their constituents. When creating the next generation of interface dense CMCs (id-CMCs), this large amount of design freedom provides us with not only an incredible opportunity but also a daunting challenge. Because, the large design freedom makes it prohibitively time consuming and expensive to to figure out the optimal, or even satisfactory, small-scale architecture design by simply performing a large number of experimental parametric studies. Therefore, to leverage the power of 3D id-CMCs we must develop a better way to predict toughness from information about a CMC’s small-scale architecture and constituent material properties alone.
8. The PI plans to take up this challenge as his long term career objective. In order to intelligently take advantage of the design freedom afforded by the 3D, interface dense designs, it is necessary to first understand the mechanisms through which interfaces and their geometry enhance the large scale toughness. Then it is necessary to consolidate that knowledge to create a computational tool that will enable one to connect small-scale architecture parameters and the large-scale toughness in *id*-materials. In line with this long term objective, the specific research objective of the proposed project is as follows:  
     
   (i) Understand the mechanisms underlying how the small-scale interface architecture can enhance large scale toughness, and (ii) develop a computational mechanics method that captures such mechanics and can be used for designing the next generation of *id*-materials.

Proposed

### As evidenced by structural biomaterials, intelligently taking advantage of the the almost unlimited degrees of freedom in -architectures is the key to creating CMCs with incredibly high damage tolerance and notch-insensitivity. The additional design free in the With the introduction of this micro-architecture design comes the problem of being able to reliably connect the large-scale mechanical properties to those of the constituent phase and the micro-architecture parameters.

The properties of the CMC critically of course depend on the properties of the constituent phases, but what is very in very interesting is that the depend in a nonlinear fashion on the small-scale geometry of the architectures of phases.

## 1.5 Anticipated difficulties and our plan to handle them.

*Computational expense:* One of the undesirable attributes of the VRF simulations is that they are computationally very expensive. The simulations reported in sec. XX are based on simplified models of SB architectures–they are 2D in nature and contain only 3-5 weak interfaces. Despite that those simulations tooks XX hours to complete. They involved XX dof FE meshes and were run on XX CPUS in parallel. More realistic computational models of the SBs architectures shown in Fig. XX are expected to require far more dofs. For example, a 2D model of the architecture shown in Fig. XX is expected to contain anywhere between XX to YY dofs. The PI’s lab has access to considerable computational resources (see Facilities and Equipment). However despite that, it is possible that performing the planned VRF simulations of more realistic SBs architectures can pose some computational and data management difficulties. This is especially anticipated when using the VRF tools to perform virtual experiments, as we plan to do in Tasks XX and YY. This is because, in the virtual experiments, the analyst will likely have to run a VRF simulation repeatedly to study the effect of small changes in the problem parameters on the manner in which the crack patterns evolve and affect the energy absorption capacity of the material. Though it greatly depends on the stamina and patience of the analyst, from past experiences, the PI believes that a VRF simulation will be useful as a discovery tool only if it takes less than a day in real time to complete.

In order to be prepared for the anticipated computational difficulties we have allocated funds in the budget to procure additional computational and data storage/manipulation resources. The PI’s lab currently has access to XX cpus. We have requested funds to procure XX additional cpus and purchase usage time on external computational clusters with priority access. We are confident that by performing parallel computations using the increased no. of cpus we would be able perform the planned VRF simulations described in Tasks XX–YY.

*Convergence of the nonlinear solver*: The results shown in sec. XX were obtained by linearizing equations XX and YY and then solving them simultaneously using the Newton-Raphson (NR) method. In general we found it very difficult get the the NR iterations to converge. Many of the times we were able to get the iterations to converge by sufficiently refining the FE mesh. However, in some cases no amount of mesh refinement helped. Thus, if ignored, the unreliable nature of the nonlinear solver in our simulations can pose a considerable threat to the project’s success.

Based on our preliminary investigation, we believe that the convergence problems may be due to mechanical instabilities in the problem; which are similar to the buckling and snapping type instabilities seen in nonlinear structural mechanics problems. This is because, in the VRF simulations the non-convergence problems often preceded situations in which we were expecting the occurrence of instabilities, such as abrupt crack growth, kinking, or branching. Convergence problems due to instabilities is a well studied issue in non-linear finite elements analysis and is often handled by using the arc-length/continuation methods instead of the Newton-Raphson method. If the arc-length methods do not resolve the convergence then we will use the method of Dynamics Relaxation. In dynamic relaxation the XXXXXXXXX.

As per DR, the solution to XX--YY corresponding to quasi-static loading is approximated with the solution to a dynamic version of the equations XX-YY with artificial damping. Let the discretized version of XX--YY be

Intellectual merit

1. Understanding the mechanics and physics of fracture is of great scientific and engineering importance.

Incorporate the first figure that shows that VRF gives correct results..

VRF theory shows tremendous potential for revitalizing fracture mechanics by opening up a new paradigms for understanding and modeling fracture. The VRF theory-based numerical methods are ideally positioned to galvanize revolutionary developments in the computational design of high-toughness materials. However, the VRF theory is insufficiently developed from a solid mechanics perspective. Several fundamental mechanics issues need to be resolved before VRF theory can be considered a valid theory of fracture. Resolution of these fundamental issues is expected to be quite challenging and hence require a long-term, concerted effort involving techniques from many sub-fields of mechanics and applied mathematics. However, even a partial resolution of the identified issues could lead to revolutionary developments in theoretical and computational solid mechanics. The proposed CAREER is aimed at addressing a very important issue in the VRF theory, which we have termed the “non-localization problem”. This issue is foremost among those that need to be resolved before VRF can be considered a valid theory of fracture. Furthermore, the scope of this problem is ideally suited for the time frame of the STIR project.

***Previous and related work***

*Experimental–(Max)*

1. *Barthelot.*
2. *Christine Ortiz*
3. *Espinosa*
4. *Ravichandran wood*

*Theoretical–(Haneesh, Wenqiang)*

1. Shuman Xia
2. Huagian Gao
3. Kaushik Bhattachary
4. Zhigang Suo
5. Askan Vaziri

*Computational–(Kaushik, Welin)*

1. XFEM, Cohesive zone methods.
2. Bourdin
3. ~~Borden~~
4. Self.
5. Pablo Zaviretti
6. Allan Bower
7. ~~Outline current method for making CMCs (ply layup)~~
8. ~~What are limitations of this method? (limited scope of tuneable design parameters, low toughness when loaded out of plane)~~
9. Are there any examples of people making new 3D architectures already? How did they arrive at their designs?
10. These next generation CMCs are limited by 1) fabrication complexity and 2) lack of design tools
11. Fabrication has been stepped up recently (ice templating, MM 3D printing, etc), however there is no robust design tool to predict the effective toughness of a CMC from its microarchitecture.
12. These were mostly chosen arbitrarily not deliberately because there is no way currently to relate the architecture to the expected toughness
13. We want to develop this tool.
14. However, with such a large design space, where do we start?
    1. A theoretical framework to determine the based places to look
    2. Couple this with looking to tough composites in nature. What do their architectures look like? We have seen that synthetic variants of these composites display the similar enhancements to toughness → not a bad place to start.

# 

## 1.6 Societal and Technological impacts

Such materials will have a wide impact on society by leading to improvements and innovations in a variety of industrial sectors. For example, they will improve fuel efficiencies and safety standards in the transportation (automobile and aviation) and energy sectors.

Main Goal: Next generation of superior structural materials: *light weight, high strength, high toughness*.

used in: GTE combustion chamber (blades; both rotor and stator are too complex), re entry heat shield and steering panels, brake disks, slide bearings for pumps (must be corrosion resistant and tough), nuclear reactor components

The hurdles is the fabrication direction are slowly being overcome. Eq., ICTM. Freeze casting. Slip casting. Multi-material 3D printing. Laser volume engraving. However, the lack of robust and effective design tools is still lacking.

Possible

1. CMC have traditionally been constrained by fabrication techniques and the lack of robust design tools.
2. So to make the next generation of CMCs we need a robust design tool guided by the understanding of the relationship between the CMCs structure and its mechanical properties

1. Fabrication is stepped up. However, design tools are lacking. Because there is heterogeniety, and failure mechnaics can span multiple length scales and quite difficutlt to correlate to the small-scale design-geometry of the composite.
2. However, the increasing severity of operating conditions in future aerospace transportation renders the menu of available materials vanishingly small, and in many cases limits the choice to a very few high-temperature ceramics.1
3. Since ICTS are heterogeneous at all length scales, and there are multiple failure mechanisms that are often coupled, detailed understanding of the ensemble properties are needed.
4. Potentially, in addition to enhancing the toughness properties, the large design freedom also make it possible to simultaneously tune other properties, such as stiffness and strength (are there examples of this?).