Guidelines:

1. Please strikethrough lines that you have completed.
2. Prepare all write-up in latex.

Haneesh, To do:

1. ~~Where is Kaushik's manuscript?~~
2. Facilities equipment and other resources, add it into the main document–assign to Max.
3. Comment on Kaushik's write up.
4. Three page biographical sketch
5. Prepare comments on Weilin's Write up
6. Talk to Priscilla, whether we will be submitting the proposal as an email or through grants.gov.
7. Ask Priscilla if we need "Contract Facilities Capital Cost of Money"
8. Prepare comments on Max's suture literature.

Proposed research:

1. Handing broadening
2. Dynamics of phase field modeling ---done by Borden, implementation is still open however
3. Plasticity----
4. Parallelization----also an implementation problem.
5. Analytical modeling of the instabilities-----this is a good problem.

1. Figure Woodpecker, and Motivation, 1 page
2. Objectives ½ page
3. Scientific approaches: 2 pages,
4. Relationship to competing research, (XFEM, CZM, damage mechanics, allan bowers paper) ¾ page
5. Effort ¼ page
6. (e)+(g) ¾ page
7. (h) ¼ page
8. Uncertainties 1/2

Kaushik, To do:

1. ~~Compose a paragraph that explains the advantages of the phase field method in comparison to other methods, such as XFEM and cohesive zone methods. This paragraph should not be overly technical. This should be aimed at someone who does not know FEA but knows fracture mechanics. In order for composing this paragraph you might have to briefly explain XFEM and Cohesive zone methods for a general audience.~~

2. ~~Add in Cottreal and Rice's Crack kinking, Rice's Crack curving, and Hakim and Karma's papers in a project literature subfolder.~~

Regularized Variational Fracture Modeling
~~Overview of computational fracture methods~~

Introduction

Computational modeling of crack initiation and propagation continues to be an active area of research in ~~the fracture mechanics community~~.

1. ~~Here I think you should say something about the classical approaches about modeling fracture initiation and propagation.~~

   a. ~~What was the primary contribution of Griffith? Something along the lines of *He established the necessary condition for a crack to initiate. However, Griffiths condition is not the sufficient condition*. May be take a look at section 7.3.1 in Ercan Gu ̈rses thesis document (VariationalFracture).~~

   b. ~~What were some of the seminal studies on figuring out the actual crack path, i.e. the direction in which a crack propagates?~~

   c. ~~What was the contribution of Cotterell and Rice. Their paper on crack kinking is highly cited. What is the primary contribution of Cotterell and Rice's work? What criterion did Cotterell and Rice use in deciding the kink angle?~~

   d. ~~Rice also worked on crack curving. What were his primary results? What criterion did Rice use in deciding the crack path, the direction of crack propagation?~~

   e. ~~List some of the classical criteria for deciding the direction of crack propagation, e.g.,~~
      i. ~~maximum hoop stress, ([XX])~~
      ii. ~~maximum XX, ([XX])~~
      iii. ~~minimum YY, etc., ([XX])~~
      iv. ~~maximum strain energy density criteria~~
      v. ~~principal of local symmetry,~~ $K_{\mathrm{II}} = 0$

~~(see section 10.1.8 in Ercan Gu ̈rses thesis document (VariationalFracture) to get started. He talks about the~~

1. ~~configurational force~~
2. ~~maximum circumferential stress(hoop stress)~~
3. ~~averaged maximum circumferential stress criteria~~
4. ~~maximum principal stress criteria.~~

~~Ensure that (1-4) also tell us in which direction the crack propagates rather simply when the crack propagates.~~

f. ~~What is Dr. Rubinstein's primary contribution with regard to predicting the direction of crack propagation? He has a number of papers on fracture. However, we only need to focus on the papers that are related to the criteria used for deciding the direction of crack propagation. You can start with the paper in the literature subfolder AsherRubinstein. Add the Dr. Rubinstein papers that you review in the same folder AsherRubinstein.~~

~~Regularized Variational Fracture Modeling~~

g. ~~Introduce the variational modeling of fracture as a generalization of the idea of Griffith. Here we want to grow the crack such that the total energy of the system always decreases. In the mathematical community variational fracture is studied as a global minimization problem. That is, the goal is to find the crack path as a whole and the corresponding displacement field that globally minimize the total mechanical energy of the system. We, however, do not take that point of view. In our model, the crack is grown in a sequence of infinitesimal increments, with the direction each increment chosen to reduce the total energy as much as possible. Thus, the system always moves is in the direction of local energy gradient.~~

h. ~~Write the un-regularized form of the functional. State that it is very difficult to perform the local minimization of the functional due to the surface and volume integrals.~~

i. ~~Introduce the regularized version of the functionals. Cite the papers that give the numerical implementation (Blaise Bourdain, Borden, Karma's Papers).~~

~~One of recent developments in computational fracture mechanics has been the emergence of phase field methods to predict crack paths in elastic materials. This method was introduced by Francfort and Marigo (see [5]) and its numerical implementation was addressed by Bourdin et al. (see [2]). In this method, the total energy (E_t) is considered as the sum of bulk (E_b) and surface (E_s) energies given as,~~

$$E_t = E_b + E_s \cancel{,}$$

~~where~~

$$E_b = \int_\Omega g(\phi)\psi\left(u,\nabla u\right)d\Omega$$

~~and~~

$$E_s = \int_\Omega G_b\left(\ell_0\|\nabla\phi\|^2 + \frac{\phi^2}{\ell_0}\right)d\Omega$$

~~whose notation are you following?~~

~~The symbol u is the displacement field, ψ (u, ∇u) is the elastic strain energy, G_b is the bulk fracture toughness, φ is a scalar damage variable, g(φ) is a degradation function ,l_0 is the length scale parameter of the model and $\| \cdot \|$ is the Euclidean-2 norm. The damage variable φ introduces fracture into the model and it is bounded between 0 and 1. The solid is unbroken when φ = 0 and is completely broken when φ = 1.~~

The crack growth law arise naturally as part of the variational formalism.

j. State that as per Hakim and Karma, the criteria for the crack initiation and direction of crack propagation in the RVFM are.

$$G = G_c \qquad (1)$$

$$G_\theta = G_{\theta c} \qquad (2)$$

where,

$$G_\theta := \frac{dG}{d\theta}$$

You need to explain how the above criteria in RVFM, eqs. (1) and (2), as derived by Hakim and Karma are the same the ones supported by Rubinstein.

Preliminary Results

In a number of cases the RVFM predicts the crack path that is observed in experiments and is analytically predicted using the XXXXX fracture criteria in simple LEFM problems.

1. The crack initiates at the loading predicted by the Griffith criteria. (Plate with an edge crack). You can take this result from the manuscript.
2. In simple problems, RVFM produces the crack trajectories as those predicted by the XXXX criteria. For each for the shear loading of XXXXX
3. Comparison with experimental results. Three hole.

In comparison to comparable computational methods the RVFM has the following very attractive features. (i) There is no need to remesh the solid after each crack increment. (ii) It can handle a variety of complex crack patterns, such as branched and intersecting cracks (find picture from Bordens, and Blaise Bourdain's papers). (iii) There is no need for a priori knowledge about the general shape and topology of the crack pattern. (iv) No special treatment is needed for handling cracks patterns in 3D solids.

The primary drawback of RVFM is the computational cost. The size of the finite elements, h, need to be smaller (typically $< 1/10$) than l_0, the regularization parameter. The parameter l_0 dictates the region over which the crack is smeared out. For that reason l_0 needs to be much smaller ($< 1/10$) than the smallest of the characteristic geometric parameters of the crack. In sharp notches the notch tip radius is at least 1/50 of the solid dimensions. Thus, for accurate calculation typical RVFM simulation typically contain 0.1–1 million elements. However, we do not perceive this as a significant drawback For example the simulations reported in section X were based on FE meshes that contained 500,000 elements. This was possible because the computational simulations being developed by the PI's group are capable of running on several CPUs in parallel. The PI has access to significant computational resources at Brown. See section XX for details.

A number of computational techniques have been developed and are routinely used to model fracture. These can broadly be classified into (i) Finite element (FE) based, (ii) Boundary element (BE) based, (iii) Singular integral equation based, (iv) Molecular Dynamics and Statics based. Compared to the

Finite element based computational methods provide some useful advantages ovre. Over the past years several computational techniques have been developed to model crack growth in materials. The most popular of these are

(i) Cohesive zone method (CZM) [10, 3],
(ii) Extended finite element method (XFEM) [4] .
(i) Use of Singularity elements.

(iii) Element deletion methods.
(iv) Virtual Internal Bond method.

1. CZM is based on finite element analysis. Crack growth is modeled by allowing the adjoining elements ahead of the crack tip to separate. As the elements separate, tractions act on the mating faces of the element as per a pre assigned traction separation law (cohesive zone law). When the separation reaches a critical value, the mutual traction vanishes and the element are taken to have completely separated and are now part of the opposing crack faces. As the RVFM, in CZM there is no need for remeshing the domain after each growth increment. Furthermore, its is also possible to handle branched and intersecting cracks. However, the CZM has the following drawbacks in comparison to the RVFM:

    a. *Mesh sensitivity:* crack trajectory depends critically on the size of the finite elements, especially in regions close to the crack propagation.
    b. Need of *a priori* knowledge of crack growth direction: The crack can only growth in the directions in which the modeler has chosen to allow adjoining pairs of elements to separate. So, insufficient *a priori* knowledge about the crack growth direction can cause the CZM to predict incorrect crack paths. Allowing all pairs of adjoining elements to separate is not a viable solution, since that substantially changes the bulk mechanical behavior of the solid.

2. The XFEM is also based in finite element technology. In XFEM the standard finite element basis functions are enriched ("extended") by including basis functions that allow displacement fields to be discontinuous across elements. As in RVFM, in the XFEM too there is no need for remeshing. Also as in the RVFM, there is no critical need of *a priori knowledge* of the crack growth. As in the RVFM, it is also capable of handle branched and intersecting cracks through some modifications. However these modifications are not straightforward since they include adding different types of basis function depending on the the topology of the crack patter, e.g. on the number of branches

3. , to model the displacement discontinuity introduced during crack propagation discontinuous enriched elements are used. Introduction of these enriched elements can considerably increase the condition number of the linear system of equations being solved, thus, making the system of linear equations ill-conditioned which leads to serious convergence problems (see [6]). Hence, it is often necessary to come up with strategies to prevent ill-conditioning while using XFEM (see [11, 9]). Modeling complex crack patterns such as crack branching with high accuracy is not feasible with these methods (see [8]).

Advantages of the RVFM:

(i) It has been demonstrated that this model has the capability to model the formation and evolution of complex crack patterns such as crack branching and … with high accuracy in a straightforward manner (see [1]).

(ii) It has also been shown to produce accurate crack paths for classical fracture mechanics problems such as mode-II failure (see [7]). NO

1. Not clear.
2. Not enough details,
3. what constitutes as "accurate"
4. Refer to a section of

(ii) The length scale parameter l_0 eliminates the dependence of crack path on element size (see [7, 1]). ~~Crack initiation in this model follows the Griffith criterion and the propagation direction is a consequence of minimization of total energy E_t.~~

Advantages of the Regularized Variational Fracture Model.

1. The formulation can be

Max, To do:

	Cover page	1
A	Table of contents	1
B1	Statement of Disclosure Preference (ARO Form 52 or 52A) B-1	1
B2	Research and Related Other Project Information B-2	1

C	Project Abstract C-1	1
D	Project Description (Technical Proposal) D-1 - D	10
E	Biographical Sketch E-1 - E	2
F	Bibliography F-1 - F	3
G	Current and Pending Support G-1 - G	1
H	Facilities, Equipment, and Other Resources H-1 - H	1
I	Proposal Budget I-1 - I	
	Budget	1
	Justification	1
J	Contract Facilities Capital Cost of Money (DD Form 1861)(Commercial Organizations only) J-1	1
K	Appendices	0
		25

1. Edit *ProjectDescription_ARO.tex* in this Project Description folder so that

   a. ~~all the sections shown in the above table and in this document show up on different pages.~~
   ~~(An alternative is to have all the sections in different folders, as different .tex files. And then assemble them by combining the respective pdf documents, as we did with the NSF proposal. It is your choice. Having all the sections in the same file might be easier for this proposal.)~~

   b. ~~Ensure that the margins are 1 inch all around~~
   ~~(I think I have already have this fixed, however, please double check this.)~~
   The text was slightly off center (about ⅛ inch). I have reduced this offset to 1/16 of an inch. I can't figure out how to fix it completely without removing your fancy headers. It is the fancyhdr package that is causing the problem.

   c. ~~The font is set to Times New Roman 12 pt.~~
   ~~(I think I have already have this fixed, however, please double check this.)~~
   If we want TRUE times new roman, we need to compile with XElatex, as TNR is not native to Latex. The package you are currently using (\usepackage{times}) is currently obsolete. for best results people seem to recommend \usepackage{mathptmx}. this uses Times Roman as a font with a Times Roman approximation for the math environment. There are VERY slight differences between Times Roman and Times New Roman. I think these are not noticeable. I have changed to this package.

   Sounds great Max.

   d. ~~Fix the page numbering such that the numbering for each section starts anew, and is in the format shown in this document.~~

   e. ~~After adding in all the sections, ensure that the table of contents also shows up and is numbered appropriately as shown in this document~~
   Cannot get the numbering to show the full page range. after trying to get this to work for ~3-4 hours I have just included their table of contents document (which is allowed).

   f. ~~Check that the References section also shows up with the appropriate the page numbering.~~

   g. ~~Add toggle switches in the document, one for each section. The idea is to use the different toggle (e.g. if else construct) switches to selectively compile the different sections. (I think you did this when you you were preparing the solutions for the *continuum mechanics* course.)~~

h. ~~download the forms highlighted in blue in the above table.~~

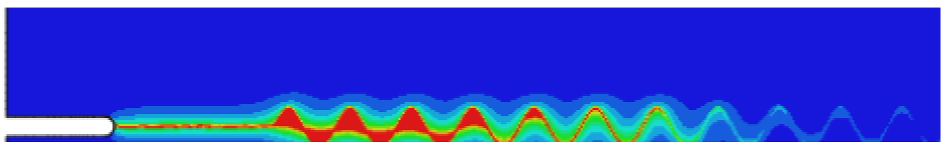
i. ~~Add the necessary latex code in *ProjectDescription_ARO.tex,* so that the pdfs of the above downloaded forms can be added at the correct location in the final document. Ensure that their page numbering follows the stipulated format.~~

1. ~~Do you know of any biological materials that have wavy interfaces that are believed to enhance their toughness. Nacre seems to be a good example of a lamellar material. However, I have not know of any biological materials where the toughness increases due to the wavy, or non-planar nature of the weak interfaces. Take a look at the *Weilin, To Do* section. We have simulations showing the enhancement of work of fracture with a sinusoidal interface. However, are there any biological materials that derive their toughness from a similar mechanism?~~ Teeth consist of two distinct regions. The outer region of the tooth is composed of highly mineralized enamel. This material is brittle and very hard. The inner material is dentin, which is still mineralized but is much tougher. The interface between these two materials is known as the enamel-dentin junction (EDJ). This EDJ is hypomineralized and has been described as a localized region of organic material. In images, the EDJ appears to be very thin and a sharp transition between the dentin and enamel regions. The enamel has a rod-like microstructure that is arranged perpendicular to the EDJ. When these rods impinge on the EDJ they create small "tufts" or roughness on the surface. In 3D this roughness has been described as a "scalloped" interface. Studies have shown that the toughness of the EDJ is very large, however I wonder whether they were actually measuring the effective toughness and that the toughness amplification is in fact due to the scalloped structure. I have added references to a subfolder titled Teeth Literature in the literature folder of the google drive. The "tufted" nature of the EDJ can be seen in Figure 2a of DeCarlo2008.pdf, Figure 2 of Lawn2009.pdf, and the inset of Figure 2 of Ritchie2005.pdf.
   The only other material I can think of **might** be antler. However, this carries some modeling assumptions with it. Specifically, see Figure 5K of antler_Ritchie2010 in the same subfolder as the teeth papers. I'm wondering if we could justify modeling the anti-plane transverse fracture of bone/antler as a wavy interface. In this mode you have a collection of roughly circular osteons embedded in a softer matrix. If the osteons are closely spaced then it seems like you will have thin layers of soft materials between closely packed hard materials which could act like a wavy/rough weak interface between two layers ina blurred out sense. Again, I think this is more of a stretch than the EDJ or wavy nacre tablets (see "Tablet-level origin of toughening in abalone shells and translation to synthetic composite materials").

1. Add text in the Project description addressing the following
   • Describe organization and names of other parties funding this work. If "none", say so.
   • Provide statement of environmental impact and resource use. If "none", say so.
   • Provide statement regarding use of ozone-depleting substances. If "none", say so.

Weilin, To do:

Figure. 1



Read the necessary papers and answer the following questions:

1. What was the primary contribution of Griffith?
2. What were some of the seminal studies on figuring out the actual crack path, i.e. the direction in which a crack propagates?
3. What was the contribution of Cotterell and Rice. Their paper on crack kinking is highly cited. What is the primary contribution of Cotterell and Rice's work? What criterion did Cotterell and Rice use in deciding the kink angle?
4. Rice also worked on crack curving. What were his primary results? What criterion did Rice use in deciding the crack path, the direction of crack propagation?
5. Ask Kaushik for the JMPS paper by Hakim and Karma, and read it. We will read it when we meet.

1. Prepare a section detailing the Wavy crack simulations that you performed. The latex label of this section should be *SinusoidalInterfaceSec*.

   The figure from your simulations is shown above. You stored these simulation results in the folder: "*/WeilinD/Reports/20160110_phase_filed_fracture"*.

   I prepared a presentation based on your simulation results. This presentation is titled "Jan12_16.pdf", and you can find it in the folder "*/WeilinD/Reports/20160110_phase_filed_fracture*".

   Your section can have the following structure:

   a. *Preamble:* Open with the main results from your simulation, e.g., *changing the geometry of the interface increases the work of fracture.*
      i. ~~Has this result been shown by other researches? There is experimental evidence for this, however, however, has shown computationally or theoretically that the work of fracture (WOF, $\mathcal{W}$) can be enhanced by making the interface sinusoidal? If yes, then please refer to those papers (add references). For example, consider this paper [1]~~

~~ii.~~ ~~Do our simulations say more than any simulations that have been reported in literature? If yes, then please comment on that. It appears unlikely that we are the first ones to perform these type of simulations.~~

~~iii.~~ ~~Is our model more capable than the models used to perform the simulations that are reported in literature? If yes, then please comment on how. For example, our model can handle scenarios where the crack moves out of the interface and into the bulk, and back into the interface again. That is, our model can simultaneously span both the interface and the bulk. Can the other models handle these scenarios?~~

~~The idea is to bring out how our simulations are more informative than any previous simulations, and how our computational model is more informative than the model used to perform the simulation presented in literature. Since otherwise why should anyone be interested in either our results or model?~~

b. ***The model problem.***

~~*i.*~~ ~~*geometry of the problem*: two elastic solids, their dimensions, notch dimensions, geometry of the interface, amplitude, wavelength. Add a schematic as Figure~\ref{SinusoidalInterfaceFigSchematic}.~~ ~~**The schematic can show the region surrounding the interface crack region.**~~

~~*ii.*~~ ~~*Kinematics*: small displacement and small strain,~~

~~*iii.*~~ ~~*Constitutive law*: linear elasticity~~

~~*iv.*~~ ~~Loading: tensile~~ ~~**Is the loading displacement controlled or load controlled?**~~

~~*v.*~~ ~~Simulation: Describe how the simulation was performed.~~

c. ***The results:***

~~i.~~ ~~*For small amplitudes* the crack is confined the the interface. Is the crack propagation smooth with the loading, or are there any instabilities? This can be ascertained by plotting the crack arc-length as a function of the loading parameter. The instabilities will show up as discontinuities in this plot.~~

~~ii.~~ ~~Is the work of fracture greater than that for an equivalent straight crack? Have you performed the simulation with the straight crack? If no, then please perform the simulation now.~~

~~iii.~~ ~~*For large amplitude*: the crack leaves the interface and ventures into the solid. Is the crack propagation smooth with the loading, or are there any instabilities? Is the work of fracture greater than the straight cracks and the small amplitude cracks?~~

iv. Does the work of fracture keep increasing with the amplitude, or does it increase and then decrease with amplitude? Or does it increase and then remain flat with amplitude

~~v.~~ ~~Have you performed a simulation without the weak interface? Right now the simulation is for heterogenous fracture. The top and bottom solids have a certain fracture toughness whereas the interface has a different fracture toughness. What happens when you make the fracture toughness of the interface equal to the fracture toughness of the top and bottom solids.~~

vi. ~~What do you think is the maximum fracture toughness that is achievable? Do, you think the fracture toughness of the weak interface can be greater than the fracture toughness of the bulk solid, composing the top and the bottom bodies?~~

The upbound toughness of weak interface should be around the value of bulk material. The simulation by setting the interface and bulk properties to be the same shows that the fracture toughness (work of fracture) is around 1.3 J/m^2, although the simulation did not converge at last.

vii. ~~Support your arguments by pointing to the figures.~~
~~Figure~\ref{SinusoidalInterfaceFigCrackPropagation}~~

1. ~~Figure (a) show snapshot of crack remaining at the interfaces for small A.~~
2. ~~Figure (b) show snapshot of crack jumping out of the interfaces for large A.~~
3. ~~Figure (c) Show the load-displacement curves for different A.~~
4. ~~Figure (d) shown the Work of fracture as a function of the A.~~

~~Zoom in to the crack region. See e.g. Figure 1. That is the crack trajectory should be very clear. The region around the crack is not that important.~~

~~The subfigures in figure 2 of your write *SinusoidalInterfaceSec.pdf* are not arranged as per the above guidelines (e.g. subfigures © and (d) should in the positions of (a) and (b), respectively.)~~

~~The subfigures showing the crack propagation in Figure 2 of your write *SinusoidalInterfaceSec.pdf* should show a closed up version as described above (highlighted in orange) and exemplified in Figure 1~~

d. Next steps: What should be the natural next steps in these computational simulations?

i. by how much can the fracture toughness be enhanced?

1. By how much can the fracture toughness be enhanced by changing the A/\lambda ratio

2. By how much can the fracture toughness be enhanced by changing \lambda.

e.

i. Decrease λ. In the current simulations, we keep λ constant and vary A. This was primarily done in order to make the simulations computationally feasible. However, the questions is how does W change with the length scale of the interface geometry. Say the amplitude and wavelength are scales as $A = \alpha\lambda$. The question is how does, W depend on α and λ. This would require very computationally expensive simulations. These computationally expensive simulations will be performed as part of the proposed research.

2. ~~Find the paper by *Francois Barthelat* where they etch weak interfaces in glass using a laser system. They show that the toughness of the wavy crack depends on the amplitude of the waves. I think this paper this paper was published in either *nature* or *nature materials*.~~
   a. ~~Read the paper and summarize here the main points from the paper.~~
   b. ~~Perhaps we should we should include one figure from this paper.~~

3. Find one more experimental paper which shows that making the interface wavy can enhance the work of fracture.
4. ~~All your wavy crack research results have been moved from ***20160110_phase_filed_fracture*** to ***ARO/ResearchResults***~~

1. Zavattieri, P. D., Hector, L. G., Jr, and Bower, A. F. "**Determination of the Effective Mode-I Toughness of a Sinusoidal Interface between Two Elastic Solids**" *International Journal of Fracture* 145, no. 3 (2007): 167–180. doi:10.1007/s10704-007-9109-y, Available at http://link.springer.com/article/10.1007/s10704-007-9109-y

Miscellaneous

3. Find experiments that show that the *work of fracture* can be modulated through design of the lamellar solid. The design would entail ordering of the lamella, stiffness ratio of the lamella, interface strength, lamella strength, relative thickness ratio of the lamella. Preferably brittle solids. Avoid brick mortar structures.