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MULTISCALE CAFE FOR FRACTURE IN HETEROGENEOUS MATERIALS UNDER DYNAMIC LOADING CONDITIONS

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Abstract. This paper describes a multi-scale fracture framework, for modelling dynamic fracture in polycrystalline materials. The motivation behind developing such an application is to provide a high fidelity tool to model and capture dynamic structural deformations, at the macro scale, undergoing fracture at the micro scale. The application links two highly scalable applications ParaFEM and CASUP, that model continuum using the finite element method and fracture using cellular automata respectively. Linking the two is done through a initial coupling step assigning the cellular automata to appropriate finite elements. Each time step the application passes data between the two packages, a stress tensor from ParaFEM to CASUP and a damage variable from CASUP to ParaFEM. If the maximum resolved normal stress on any cleavage plane exceeds fracture stress, crack propagation is induced through the material in the cellular automata, and the damage variable changes appropriately, updating the macro properties of the structure, modelled using finite elements. An example test case is shown, considering the degradation of a structure using material with differing critical stresses. The case showed materials undergoing permanent damage without failure and complete failure. Finally the parallel scalability of the application was explored and found to scale to 1000's of cores. Improved fidelity from coupling multiple scales in simulations has a wide range of applications in energy, aerospace and naval industries.

1 INTRODUCTION

Multi scale modelling to capture the physics at scales differing by orders of magnitudes still poses a significant challenge. In the late 1990's a paradigm shift towards simulation based design and predictive modelling lead to the growth in research considering multi scale modelling[1]. The concept of multiscale modelling is broad, involving a range of disciplines such as solid mechanics, materials science, physics, chemistry and fluid mechanics. In particular it has become an established field of work within the area of material science and solid mechanics with a range of methods for coupling molecular dynamics physics with continuum mechanics[2] and multi level finite element methods[3]. However applications capturing the effects of fracture in multiscale methods are limited.[4] is an example of an application doing just that, however there are few others.

Modelling fracture in materials at a single length scale has been researched intensively with scientists using extended finite element methods[5], cohesive zone models[6], multi phase field methods[7] and cellular automata[8] to model crack propagation and cleavage.

This paper describes a mini-app[9] extended from the work by Shterenlikht and Margetts[10] that couples a cellular automata library, CASUP[11], capable of modelling fracture at the meso-scale with an finite element library, ParaFEM[12], capable of capturing detail at the continuum scale. The paper describes the coupling interface at a high level before exploring a test problem involving transient trans granular cleavage of a polycrystalline material.

The paper is ordered as follows, Section 2 describes the method and implementation of the application, Section 3, the results from a simple test problem and the parallel scaling of the application and finally Section 5 discussing the value and impact of the work.

2 METHOD

This section provides an abstract view of the coupling between ParaFEM and CASUP, Figure 1 shows how the key data is passed between the packages.

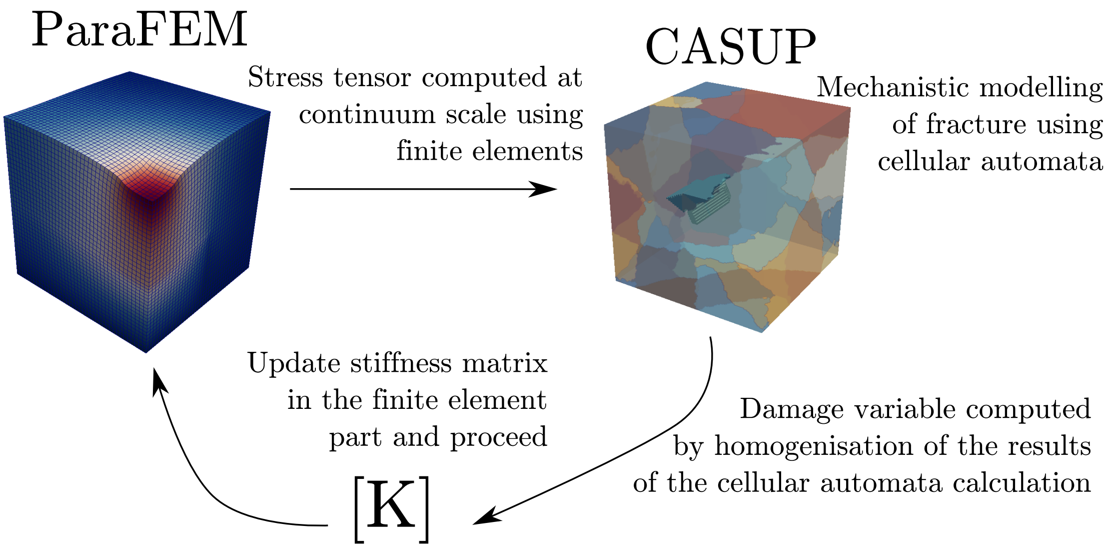

Figure 1: Flow Diagram of a CAFE iteration

At the start of the simulation, both applications are initialised. ParaFEM generates the mesh and CASUP builds the cellular automata grid required. Each time step the partial differential equations describing the continuum in ParaFEM are solved, with the stress tensor passed to CASUP. Based on the stress tensor and a critical stress value defined by the user, CASUP determines whether cleavage will occur. If cleavage occurs a homogenisation process is applied to the cellular automata mapped to a specific finite element. This generates a value for a damage variable that is passed back to ParaFEM for each finite element. The macro properties of the structure are updated. The process repeats until failure of the material occurs or a user specified time limit for the simulation is reached.

2.1 ParaFEM

ParaFEM is an open source parallel application written in Fortran made up of a series of libraries and driver programs[12]. The driver programs each solve a different structural mechanics problem using the finite element method. The library has a range of capabilities including thermomechanical analysis[13], stochastic monte carlo methods[14], fluid-structure interaction[15] and large strain plasticity[16].

In the mini-app developed by the authors for this paper, ParaFEM is solving the transient linear elastic deformation of a solid using the assumption of small strain. Damping is ignored and so Equation 1 represents the governing equation being solved at each time step,

$$\{f\} = [K]\{u\} + [M]\{\ddot{u}\} \tag{1}$$

where f represents an external force vector, $[K]$ and $[M]$ the stiffness and mass matrices respectively, u is the displacement vector and $\ddot{u}$ is the second derivative of displacement in time.

An iterative procedure, the preconditioned conjugate gradient(PCG) method, is used to solve the partial differential equations. Unlike direct solvers, iterative solvers can scale to much higher core counts[17]. Along with this ParaFEM decomposes the mesh on an element by element basis, using the Message Passing Interface (MPI) for communication between processes. This combination of methods has lead to ParaFEM showing good scaling on up to 32,000 cores[12] for various engineering problems.

Table 1 provides a description of the key steps within the mini-app.

Table 1: Summary of key steps in ParaFEM

Routine	**Description**
Initialise	Load the mesh and build the communication matrices
Update [K]	Update the stiffness matrix based on an updated Youngs Modulus
Solve Eqn. 1	Solve the governing equations using PCG method
Recover [σ]	Get elemental stresses and pass to CASUP

Non-linear material behaviour within the structure are induced through the changing macro properties, altered by the interaction with CASUP, and even with such a simple model a range of phenomena can be simulated.

2.2 CASUP

The Cellular Automata library for SUPercomputers (CASUP) is a general purpose cellular automata library written in Fortran making extensive use of 2008 and 2018 coarrays. In the authors mini-app, the CASUP library is used to generate the granular structure be seen in Figure 2, and simulate the transgranular cleavage cracking.

CASUP does not solve a series of governing equations in the classic sense, but uses a series of rules and algorithms to decide if a crack will propagate. Table 2 provides a summary of the important steps within CASUP.

Table 2: Summary of key steps in CASUP

Routine	**Description**
Initialise	Generate initial grain structure in domain
Propagate crack	Using a series of rules, decide if a crack propagates
Calculate D	Calculate the damage scalar
Update E	Use the damage scalar to update the Youngs Modulus

The domain is initialised with each cell being empty, a number of grain nuclei are assigned randomly within the domain and allowed to grow, until the entire domain is represented by either a grain or grain boundary. Typically the CA cells are much smaller than the representative FE size, such that every element occupies a space covering a cluster of CA cells. Every time step the FE stress tensor is passed to CA where it is redistributed over the cluster of cells attached to this FE. This is a classical localisation step of any multi-scale technique. Any CA cell in which the maximum resolved normal stress on $\{100\}$ or $\{110\}$ planes exceeds the material fracture stress (which is a function of the surface energy [10]) becomes failed. A number of CA cells can fail in a single CA iteration, together all failed cells form a micro-scale crack. The damage scalar is calculated based on the proportion of failed cells to live cells within a finite element. This value is used to update the stiffness of each finite element.

3 CASE STUDY DESCRIPTION

The problem involves the forced vibration of a cantilever beam, with only a specified region containing the cellular automata. Figure 2 provides a diagrammatic view of the problem test case.

The beam is $5mm$ in height with a $1mm^2$ cross sectional area. At the center of the beam a $1mm^3$ volume of cellular automata cells exist, as shown in Figure 2. The structure has a Youngs modulus of 200 GPa, a density of 7874 kg/m^3 and Poissons ratio of 0.3, which corresponds to Iron. There are approximately 135,000 isotropic, quadratic hexahedral finite elements within the structure. The cellular automata volume is made up of around 625 grains with $1e5$ cells per grain.

The beam is forced in time, $f(t)$, at a frequency of $w = 1000\ rad/s$, which excites only the first mode of vibration within the structure. The beam is vibrated for an initial period of 0.05 seconds without any cracking present. A crack is subsequently initialised

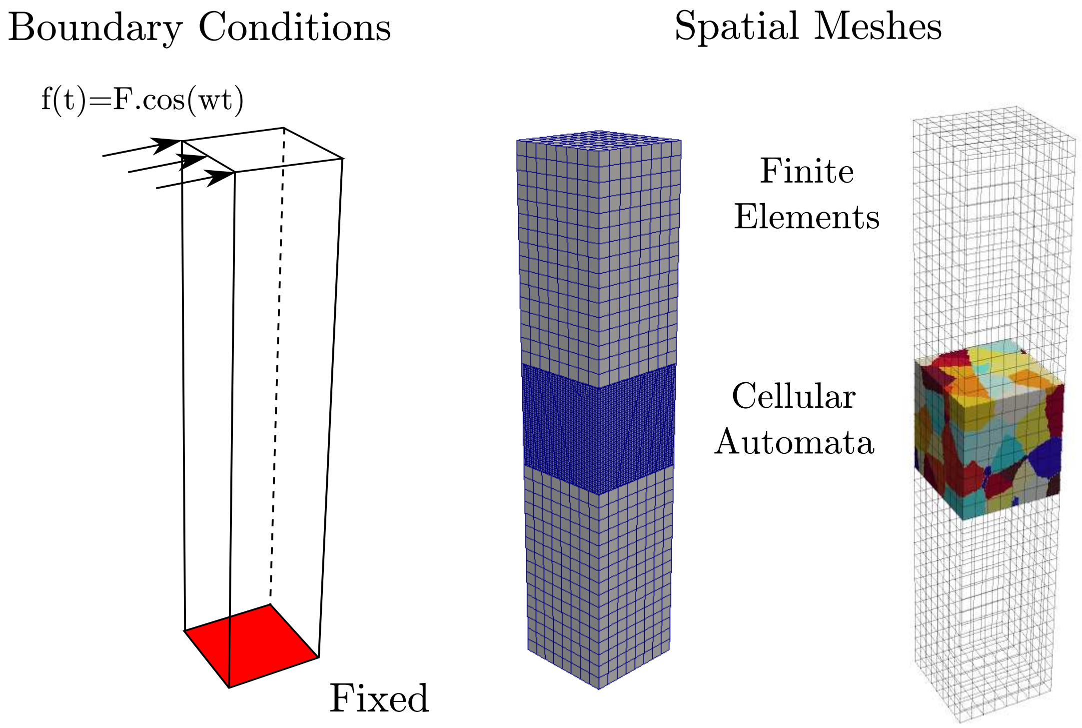

Figure 2: Problem setup

at $x = z = 0$ and $y = 0.5mm$, which corresponds to a point at the edge of the cellular automata zone and half way up the y axis. Two theoretical materials are chosen to highlight the capabilities of the framework, with the critical stresses or cleavage plane stresses differing by an order of magnitude. The length scale of the cellular automata is set such that each timestep a crack can propagate $0.2mm$ or $1/5$ of the model.

4 RESULTS

4.1 Test case

The deflection of the tip of the beam is plotted against time for two materials in Figure 3. Mat_A has incurred some permanent damage and Mat_B has undergone catastrophic failure.

When the crack is initiated in Mat_A some permanent damage occurs, seen by the divergence from the elastic response. Within the cellular automata a micro crack was seen to propagate to the grain boundary but not develop further. Further more the material continues to sit within the response of the elastic regime suggesting the material has not failed but just endured some permanent plastic damage in part of the structure.

However, in the bottom plot clear failure can be seen. After the crack has been initiated the beam continues to deflect in its first mode for approximately 1 period. There is some micro cracking present and so the results diverge from the purely elastic response. At the point of maximum deflection, when the material stress is at its highest, a large level of

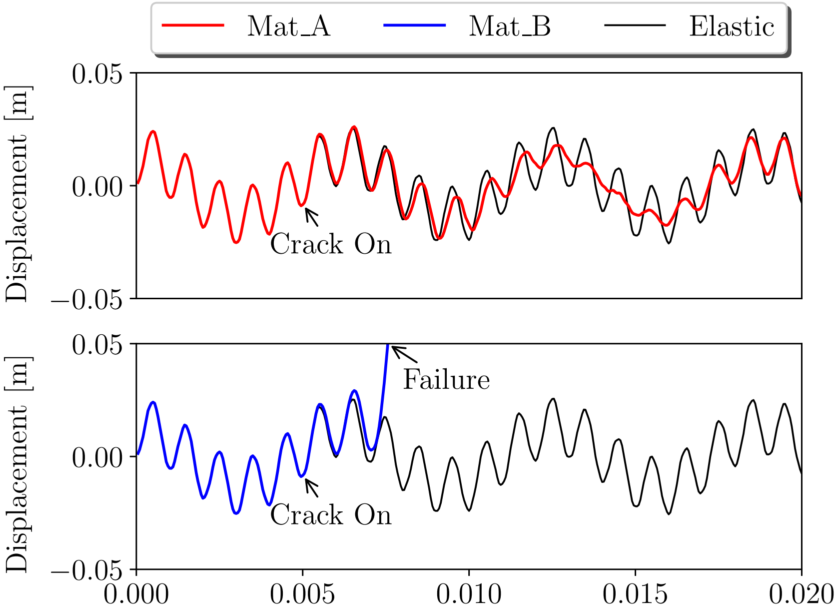

Figure 3: Tip Displacement

crack propagation takes place and the large number of micro cracks rapidly form a macro crack. This completely reduces the strength of the structure, which can be seen by the sharp increase of tip displacement. Although the simulation will not crash the solution is no longer physically realistic.

Figure 4 shows the finite element models of the beam for two positions. The top set of figures represents the displacement of the elements in x,y and z under tension, and the bottom half under compression.

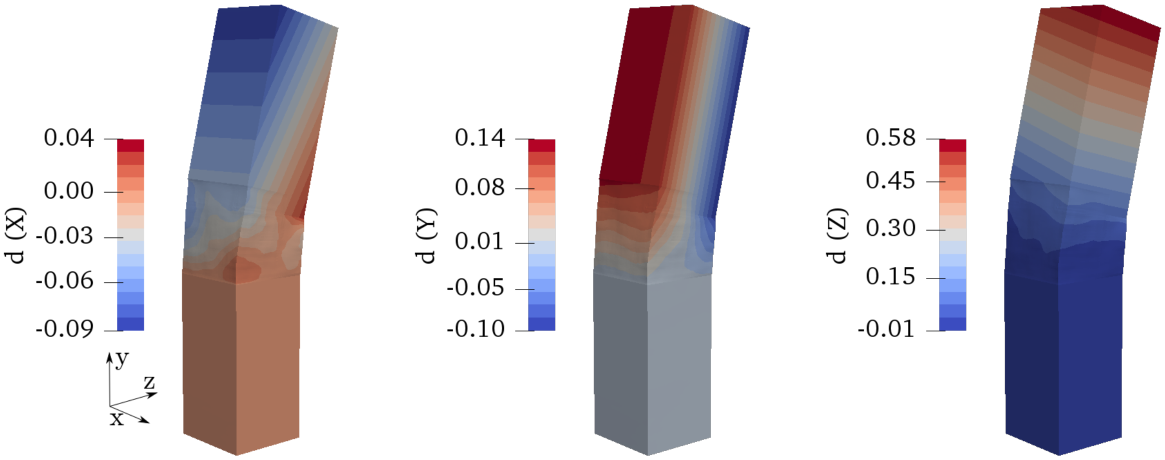

Figure 4: Displacement of cracked zone under tension in X, Y and Z direction

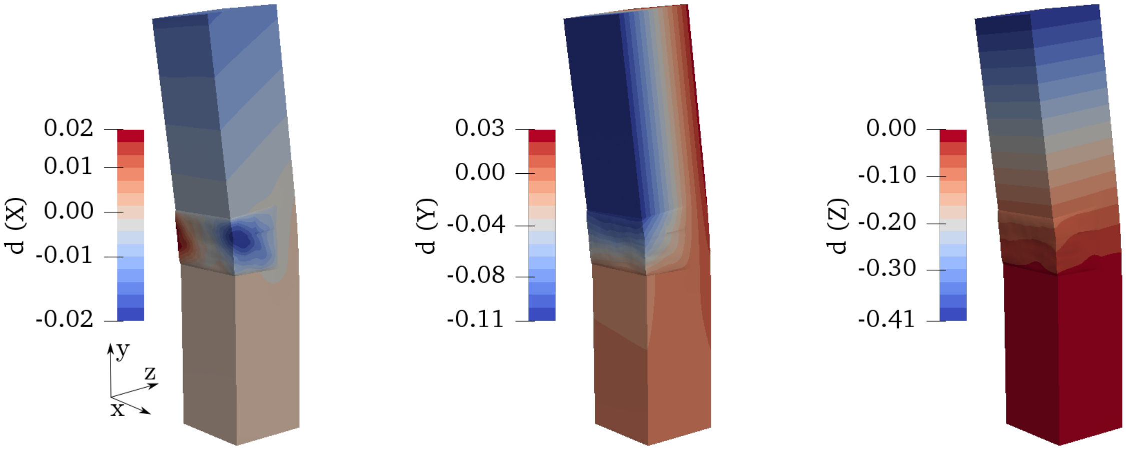

Figure 5: Displacement of cracked zone under compression in X, Y and Z direction

The deformation patterns look similar to a bar under tension with necking. A clear region of failure can be seen, with the contours showing how the material is now reacting. One image of particular note is the bottom left, when the material is under compression, it can be seen that the the material is being forced out at the edges, with relatively concentrated regions of displacement in the failed region.

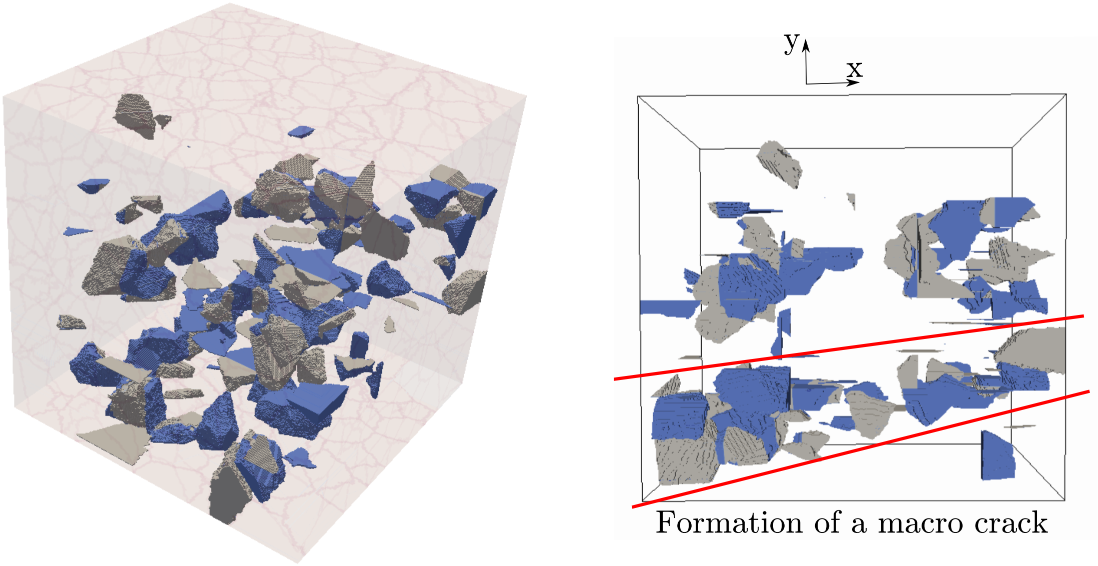

Figure 6: Typical crack formations(left) and cracking viewed in x-y plane(right)

An image of the typical crack formation within the cellular automata zone is shown in Figure 6. The grey and blue represent cracks on the {100} and {110} planes, which have the lowest critical stresses of the material. A number of flat micro cracks can be seen. It was noticeable from the 3D view of the model that the micro cracks formed in a distinct band in the x-y plane, joining up to form macro-cracks The banding seen in Figure 6, right, seems counter-intuitive, with the major displacement occurring in the out of plane direction. However it is consistent with the formation of shear bands.

4.2 Scaling

One important issue with multiscale modelling is that capturing the different scales such as the crack growth and macro deformation, can be computationally expensive[18]. It is important that applications such as these scale to high core counts to keep simulation times reasonable.

The strong scaling of the application has been tested using 10 time steps. Approximately 23 million nodes were used in the finite element mesh, corresponding to just over 63 million equations to be solved. The cellular automata contained approximately 62.5 million cells. Figures 7 and 8 show the speed up of application in terms of total execution time and then the speed up achieved by the "Solve PCG" routine per iteration, the most time consuming operation within this problem.

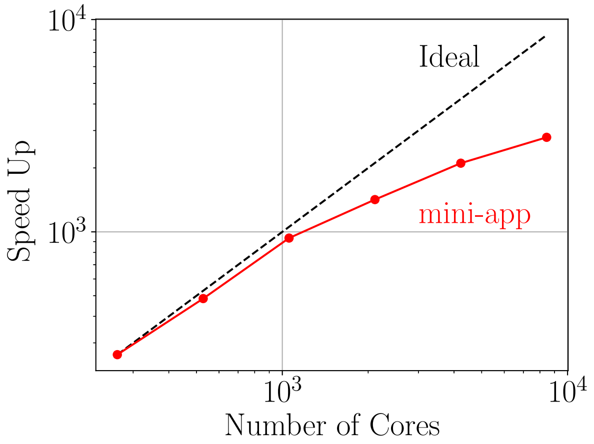

Figure 7: Total simulation time

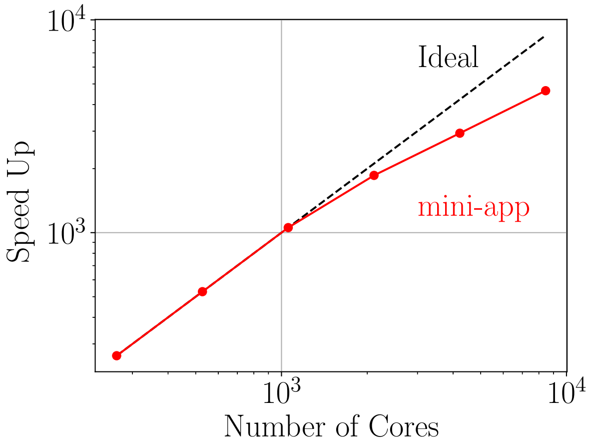

Figure 8: "Solve PCG" solution/iteration

It can be seen that the application scales well on 1000's of cores. In the timing data(not presented here) it was noticed that the scalability of CASUP dropped before that of ParaFEM which the authors believe to be due to a lack of work per core. It should be noted that the scaling tests of the application were run excluding the IO operations.

5 CONCLUSION

The paper has presented a multiscale framework for modelling transient transgranular cracking in heterogeneous materials.

The simple test case that has been used for initial testing, has highlighted a number of parameters that can be considered when modelling at multiple length scales. Time and length scales pose a challenging task when modelling multiscale processes. Careful calibration of theses parameters along with critical material stresses may be required on a material by material and model by model basis. However once completed the application offers a powerful tool for huge parameter sweeps across 1000's of cores, for material optimisation purposes, and to model different materials such as composites that are prevalent in aerospace and the energy industries[19].

The authors consider that the application currently lies at level 3 in terms of technology readiness levels with further work into exploring the parameter space and validation with experimental data to move the project forward. A range of modern 3D imaging techniques exist that can provide experimental data for validation and verification[20].

The authors plan to explore the parameter space in more detail, including considering the impact of the length scale, number of grains and their sizes, on failure under dynamic loading conditions.

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