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A massively parallel multiscale CAFE framework for the modelling of fracture in heterogeneous materials under dynamic loading

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Abstract

This paper presents a novel computational framework for modelling multiscale fracture that can be used to solve engineering problems subject to dynamic loading. The framework simulates, mechanistically, at the mesoscale, the physical processes that lead to brittle fracture. A homogenisation step is used to translate the accumulation of damage from the mesoscale to the macroscale (as a reduced stiffness in the corresponding region of the structure). In order to achieve this, the multiscale framework couples together two open source Fortran packages; the macroscale ParaFEM with the mesoscale CASUP. ParaFEM is a highly parallel finite element analysis library used to model structures at the continuum scale. CASUP is a package that uses cellular automata to simulate brittle fracture in polycrystalline materials. A simple test problem involving a vibrating cantilever beam is used to demonstrate the simulation of dynamic cyclic loading, leading to brittle cracking. In the cellular automata software, there are a range of parameters that can be adjusted, such as the fracture energy and grain size. These are explored to demonstrate how they might affect the predicted structural integrity of the cantilever beam. Parallel performance is investigated using a Cray XC30 supercomputer, showing that the software can make efficient use of tens of thousands of cores. This paper highlights that modelling the physical mechanisms that lead to damage and plasticity could be an attractive alternative to phenomenological constitutive models. This work will be of interest to researchers and practitioners needing more precise predictions or a better understanding of damage propagation under cyclic or impact loading. With further development, this type of framework will enable the insilico design and evaluation of new material microstructures; leading to improved performance of components and devices subject to extreme operating conditions.

Keywords: Multiscale; Parallel; Fracture; Cellular Automata; Finite Element.

1. Introduction

Accurately capturing the physics of structures at multiple scales offers a difficult challenge, both numerically and computationally. Multiscale models often involve the solution to physical phenomena that cannot be modelled using the same methodologies. Traditional continuum methods homogenizing the material properties at engineering length scales, cannot provide the same level of accuracy and fidelity when applied to modelling the physics at the mesoscale (mm to μm). The coupling of different methodologies, to solve each problem and capture the various scales and physics, offers a promising solution to the problem.

The highly heterogeneous nature of fracture and discontinuities in brittle materials makes modelling these phenomena difficult. There are a number of methods in the literature used to capture the fracture and mesoscale physics in structures. Cohesive zone models (CZM) introduced in the late sixties by Dugdale [1] and Barenblatt [2],

based on a [phenomenological](#) traction-separation function, have been popular to capture a range of nonlinear material phenomena, including delamination and cracking in composite structures [3], the effect of embedded particulate on crack trajectory [4] and intergranular fracture in polycrystalline structures [5]. Within CZM models, the crack fronts follow the inter element contours and so they can be computationally expensive, as high levels of refinement are required around crack fronts to obtain mesh independent results. [CZM can be treated extrinsically or intrinsically based on the cohesive zones assumed pre-fracture response, with both methods having numerical challenges \[6\]. One of the requirements for fracture models is to simulate complex three-dimensional fracture, that can be computationally expensive. In general intrinsic approaches are often more easily parallelised, however researchers have developed hybrid approaches \[7\] that maintain the parallel scalability whilst avoiding wave propagation issues common amongst intrinsic methods.](#)

To combat these pitfalls, extended finite element methods (X-FEM) were developed [8]. [These discrete models differ from the constitutive models used in CZM, using local enrichment functions within the elements to capture](#)

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discontinuities. They have been used to model fracture that does not follow the path of inter element surfaces [9]. X-FEM methods require some input via the user, such as crack propagation directions [8] or maximum energy release in crack extension [10]. Researchers have developed coupled XFEM/CZM models to preserve the advantages of both approaches [11]. In general, X-FEM methods have been shown to provide good approximations of fracture, however when applied to multiscale applications the model requires significantly different levels of refinement to capture each of the length scales [12].

Finally and more recently, the use of multiphase field models have been used to study anisotropic crack propagation in polycrystalline materials [13, 14, 15]. The modelling approach, based on the work by Francfort and Marigo [16] in 1998, uses an added variable known as the phase field variable to smear the crack, reducing the numerical difficulties of dealing with discontinuities. Furthermore, mean-field homogenization methods have been used to model damage in carbon-fiber reinforced composites [17].

In comparison to these approaches that broadly characterize the material as a continuum, methods exist in which the microstructure is modelled as a separate domain and embedded within the larger model explicitly. In these models each domain captures the physics at its length scale and the information is passed from domain to domain through various boundary conditions and damage parameters. The level of coupling of multiscale models is categorised into hierarchical [18] in which detail is only passed from the fine scale to the coarse scale, semi-concurrent in which information is passed to either scale [19] and concurrent in which both scales are solved simultaneously and compatibility conditions are used to couple the two [20].

Within these categorisations, researchers have used a range of approaches, including multi level FEM (FE²) [21], coupled FEM to molecular dynamics (MD) [22], using FEM and X-FEM to model different scales within the structure [23] and coupled cellular-automata (CA) and FEM methods [24]. CAFE models have been used to model a range of phenomena, including solidification [25] and recrystallisation [26] and more recently to model damage development and cleavage in quasi brittle materials [27, 28]. A summary of multiscale strategies used for solving fracture problems is provided in Table 1.

In 2015 Shterenlikht and Margetts [24] released a massively parallel CAFE framework for modelling brittle fracture in polycrystalline materials, coupling a general cellular automata library, CASUP, with a highly parallel finite element package ParaFEM. The paper dealt with the incremental loading of a static equilibrium problem, excluding any dynamic effects. The model falls into the category of semi-concurrent multiscale models passing stress fields from the macroscale to the mesoscale and damage parameters back the other way. A key advantage of the framework is its highly parallel implementation. In

2018 Shterenlikht et al [34] highlighted the applicability of coarray Fortran to the CA framework and the scalability it could achieve. This paper describes a new mini-app that uses the framework described in the original article with the CAFE model being adapted to simulate transient, dynamically loaded problems. The paper presents completely novel results, detailing the applications scalability and providing an example test case analysing both the mesoscale and macroscale results.

The paper is structured as follows: Section 2 describes the numerical and mechanistic methodologies of ParaFEM and CASUP respectively, along with an overview of the parallel techniques of both the packages. Section 3 provides the numerical results to a test problem looking at the deformation of a cantilever beam that undergoes brittle fracture. Section 4 gives a detailed breakdown of the time expense and scalability of the application. Finally, Section 5 provides a summary and discussion about the results achieved.

2. Method

The applications are coupled in a segregated manner with it being possible to run each package independently. It is therefore suitable to highlight the numerical methodology and parallel implementation of each of the packages independently.

2.1. Engineering Scale : ParaFEM

The continuum scale of the problem is modelled numerically using FEM. ParaFEM is a FEM toolbox consisting of a series of libraries and mini-apps. The toolbox written in Fortran was specifically developed to be highly parallel and run on a variety of large high performance computing facilities [35]. Each mini-app [36] solves a specific engineering problem, some examples include: heat transfer [37], stochastic finite element modelling [38], geometric nonlinearity [39], material nonlinearity [40], image-based modelling [41] and fluid structure interaction [42].

2.1.1. Numerical Model

The governing equations describing the dynamic equilibrium of a structure, rely on the conservation of momentum. The strong form of the equation for the linear momentum balance is shown in Equation 1.

$$\rho \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b}, \quad (1)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\ddot{\mathbf{u}}$ is the second time derivative of the displacement $\mathbf{u}$, ρ the solid density and $\mathbf{b}$ the body force per unit mass. Multiplying the strong form of the equation by the virtual displacement, $\delta \mathbf{u}$, integrating over the domain, Ω and applying Gauss's diver-

Method	Description	Papers
Continuum/Continuum	Coupled continuum models such as finite element to finite element simulations each modelling a different scale	[29, 30, 19]
Atomistic/Continuum	Molecular dynamics and discrete elements methods are coupled to finite element models	[31, 32, 33]
Mechanistic/Continuum	Mechanistic models such as cellular automata are coupled to finite element models	[24, 34, 27]

Table 1: Summary of general multiscale strategies to solving damage and fracture problems, with example papers.

gence theorem, results in the expression of virtual work, Equation 2. n and the solution at time $n + 1$. The following assumptions are made within the scheme:

$$\begin{aligned} \int_{\Omega} \rho \delta \mathbf{u}^T \ddot{\mathbf{u}} d\Omega + \int_{\Omega} \hat{\boldsymbol{\varepsilon}}^T \boldsymbol{\sigma} d\Omega - \int_{\Gamma} \delta \mathbf{u}^T \mathbf{t} d\Gamma \\ - \int_{\Omega} \rho \delta \mathbf{u}^T \mathbf{b} d\Omega = 0. \end{aligned} \quad (2)$$

In the FEM the arbitrary body is represented by an aggregate of finite elements, linked through their nodes and edges. The displacement in each element is described locally through the element shape functions, $\mathbf{u} = \mathbf{N}\tilde{\mathbf{u}}$, where $\mathbf{N}$ are the element shape functions and $\tilde{\mathbf{u}}$ the local nodal displacements. The relationship between the elemental strains and displacements is given by, $\boldsymbol{\varepsilon} = \mathbf{B}\mathbf{u}$, where $\mathbf{B}$, is the strain-displacement matrix. The fourth order tensor of elastic modulus, $\mathbb{C}$ is used to couple the elemental strains to stresses, $\boldsymbol{\sigma} = \mathbb{C}\boldsymbol{\varepsilon}$. Using the described relationships, the corresponding virtual work expression in its FE form is provided, Equation 3,

$$\begin{aligned} \int_{\Omega} \rho \mathbf{N}^T \mathbf{N} \ddot{\mathbf{u}} d\Omega + \int_{\Omega} \mathbf{B}^T \mathbb{C} \mathbf{B} \tilde{\mathbf{u}} d\Omega - \int_{\Gamma} \mathbf{N}^T \mathbf{t} d\Gamma \\ - \int_{\Omega} \rho \mathbf{N}^T \mathbf{b} d\Omega = 0, \end{aligned} \quad (3)$$

where each expression in the equation can be expressed as a matrix. The mass matrix $\mathbf{M} = \int_{\Omega} \rho \mathbf{N}^T \mathbf{N} d\Omega$, the stiffness matrix $\mathbf{K} = \int_{\Omega} \mathbf{B}^T \mathbb{C} \mathbf{B} d\Omega$ and the external forces on the structure $\mathbf{f}_{ext} = \int_{\Gamma} \mathbf{N}^T \mathbf{t} d\Gamma - \int_{\Omega} \rho \mathbf{N}^T \mathbf{b} d\Omega$. This reduces Equation 3 to Equation 4.

$$\mathbf{M}\ddot{\tilde{\mathbf{u}}} + \mathbf{K}\tilde{\mathbf{u}} = \mathbf{f}_{ext} \quad (4)$$

At the macroscale, the relationship between the stress and strain, the constitutive law, determines the solution to the macroscale problem. The application presented in this article uses a small strain assumption and the material is determined to be isotropic, linear, and elastic. Although, it will be noted later, damage accumulated at the mesoscale results in a reduced stiffness for relevant finite elements, the macroscale analysis is always for small strain elasticity. The transient problem is stepped in time utilising a linear relationship between the solution at time

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \Delta t [(1 - \theta)\dot{\mathbf{u}}_n + \theta\dot{\mathbf{u}}_{n+1}] \quad (5)$$

$$\dot{\mathbf{u}}_{n+1} = \dot{\mathbf{u}}_n + \Delta t [(1 - \theta)\ddot{\mathbf{u}}_n + \theta\ddot{\mathbf{u}}_{n+1}] \quad (6)$$

The variable θ varies between $\frac{1}{2}$ and 1, with $\theta = \frac{1}{2}$ being equivalent of Newmarks $\beta=0.25$ method [43], with average acceleration. The results presented in this work all use a $\theta = \frac{1}{2}$, which is second order accurate in time.

2.1.2. Parallel Implementation

ParaFEM makes use of the message passing interface (MPI) for its parallel communications. The strategy uses an element-by-element technique that spreads both the memory and computational requirements across all the cpus. The problem is distributed evenly across the cpus with each cpu holding only its local information, this avoids building any global matrices that can be memory intensive and time consuming. The preconditioned conjugate gradient (PCG) method is utilised to iteratively solve the system of equations for the FE problem. A ParaFEM *mpi* module is used to hide the low level calls to the MPI routines. This module contains a number of routines that are used to gather and scatter data according to a map that highlights nodes existing on the different cpus. ParaFEM driver programs using this method have shown good scaling on 32,000 cores [44]. Finally, the I/O of ParaFEM involves the master processor reading the data from file and distributing it to each of the processors. This method although can present a bottleneck avoids the writing of a mesh file for each processor that may cause file limit issues as codes attempt to begin using petascale and exascale systems. There is an alternative to this write method. MPI-IO is an extension to MPI and offers capabilities for concurrent reading and writing to a single file from multiple processors. Libraries, such as HDF5, have utilised this extension offering very fast parallel write capabilities.

2.2. Mesoscale : CASUP

The previous section described the model at the engineering scale, the following section will elucidate the methodology used to capture the fracture within a heterogeneous material. Simulating fracture at the mesoscale

can provide an accurate prediction of material strength and its estimated failure point. Polycrystalline materials are composed of many crystals or grains that vary in size and orientation. The composition of these materials at the crystal scale has a significant impact on the material at the macro scale. The highly heterogeneous properties of these crystals can be captured and modelled using CA-SUP, and CA. The CA is a complete digital framework, being discrete in space, time and state. A uniform grid of cells is each assigned a state. Each step the cells state is updated using a series of simple rules. These simple rules often lead to complex physical phenomena at a more global scale within the CA grid. The following subsection will describe how the CA is used to firstly represent a heterogeneous polycrystalline material and secondly how cleavage is modelled.

2.2.1. Grain Growth

Researchers have used a range of methods to represent polycrystalline structures in three dimensions. Voronoi tessellation has been a common method to model these crystal structures [45, 46]. However, the CA uses a different process to represent the individual crystals. A number of random nuclei are placed within the CA domain and the nuclei grow over a number of iterations, to form a polycrystalline structure. Figure 1 provides a two dimensional diagrammatic view of how the grain growth process takes place.

Figure 1: Two dimensional example highlighting the process by which the polycrystalline granular structure is generated within the CA grid. The example shows three grain nuclei(4,8,12) and ignores the grain boundaries.

The entire CA space, or grid is given a value of 0 that represents a liquid state of the cell. Within the grid a random selection of cells are chosen, with each cell representing a different grain number. At this point each grain number is also given a randomly chosen orientation. The grains are subsequently grown from each of the cell nuclei over a number of steps. Each step any liquid cell has a chance of accepting the cell state of a cell in its neigh-

bourhood. A Moores neighbourhood is used, shown in two dimensions in Figure 2.

Figure 2: Two dimensional Moores neighbourhood. The state of the central cell shown in blue, is only dependant on its eight surrounding cells shown in red. In three dimensions the Moores neighbourhood is 26 cells large.

The Moores neighbourhood in three dimensions uses the surrounding 26 cells. This process is repeated until the entire CA grid is full and no cells of a liquid state are left. This simple process can lead to a number of differing polycrystalline structures, shown in Section 3. With each of these cells having a different orientation and preferential cleavage plane. Finally the cells that border two or more grains are considered to be grain boundaries, the cell states are altered once the full domain is populated with grains. As part of the grain growth procedure imperfections can be placed with the structure. The simple nature of the method means this can be done by altering the state of specific cells.

2.2.2. Cleavage

The cleavage process, based on Gilman [47] suggests that the work required for cleavage is based on the surface fracture energy, γ_{hkl} . That is, if the normal stress on the crystallographic plane t_{hkl} multiplied by the distance required to break the atomic bonds, is greater than this surface energy, cleavage will occur. The distance to break the atomic bonds is taken as the atom diameter in the cleavage plane, a_0 . The condition for cleavage to occur is therefore,

$$t_{hkl} \geq \frac{\gamma_{hkl}}{a_0}, \quad (7)$$

where t_{hkl} , the normal stress on the crystallographic plane is related to the stress tensor t^c orientated in the crystals coordinate system through, $t_{hkl} = \mathbf{n}_{hkl} \cdot t^c \cdot \mathbf{n}_{hkl}$. With $\mathbf{n}_{hkl}$ being the normal for the hkl plane. Three crystallographic planes are considered, $\{100\}$, $\{110\}$, and $\{111\}$, with cleavage occurring on the weakest plane. The weakest plane is considered to be the plane that maximises the normal stress, t_{hkl}^{max} .

Within this digital framework this cleavage process is completed through a similar step-by-step process to that described in Section 2.2.1, with the fractured cell growing along a preferential cleavage plane for a number of steps. This preferential cleavage plane differs from grain to grain and is dependant on the initial grain orientation assigned

during the grain growth process. Along with the grain number associated with each cell, they also have a cell state, that describes the current condition of the cell. A full list of cell states is shown in Table 2. They include a fractured and intact grain boundary, an intact cell within a grain and flank or edge cracks along the hkl planes.

Cell State	Value
Intact grain boundary	2
Fractured grain boundary	1
Intact cell	0
100 Flank crack	-1
100 Edge crack	-2
110 Flank crack	-3
110 Edge crack	-4
111 Flank crack	-5
111 Edge crack	-6

Table 2: Possible cell states within the digital framework.

At the start of the simulation almost every cell will exist in states 2 and 0, with some distribution of fractured cells throughout the grid. For cleavage to occur the cleavage criteria, Equation 7, must first be met. This means that the mean stress within the grain must have enough energy to overcome one of the three planes surface energies. If this criteria is met cleavage occurs on the weakest of the three planes. The process to find the weakest plane is shown in Algorithm 1:

Algorithm 1: Algorithm to determine the weakest cleavage plane.

```

 $p_{hkl} = t_{hkl} / \frac{\gamma_{hkl}}{a_0}$ 
 $p^{max} = \max(p_{100}, p_{110}, p_{111})$ 
if  $p^{max} \geq 1$  then
  cleavage on {100} plane
  if  $p_{110} \geq p_{100}$  then
    | cleavage on {110} plane
  end
  if  $p_{111} \geq p_{110}$  then
    | cleavage on {111} plane
  end
end

```

Cleavage occurs through a stepping process, similar to that used to generate the granular structure. An intact cell can change state and become a fractured cell if (i) it is adjacent to a fractured cell, (ii) it lies on the cleavage plane, and (iii) the cleavage criteria is met.

The total number of cleavage steps per time step is dependant on a crack propagation speed, the time step and the cells per unit length. If a material starts with a number of fractured cells, over a number of time steps where the cleavage stress tensor is large enough, cleavage occurs and a number of cleavage planes are generated.

A two dimensional example of the process is shown in Figure 3.

Figure 3: Two dimensional example highlighting the cleavage process. A number of fractured cells exist within the model which propagate along the preferential cleavage planes within the grains (marked with a dashed line). If a crack crosses a grain boundary it will continue to cleave however it will propagate along the new preferred cleavage plane.

It must be noted that this method of modelling cleavage has its simplifying assumptions, the mesoscale nature of the problem means that it exists somewhere in-between molecular dynamics and continuum scale methods. The method has yet to include micro-plasticity that is observed at the crack fronts, during brittle fracture and so critical stresses of the material itself do not correspond exactly to those seen by Gilman [47]. A calibration of the critical stress parameters seen in real materials and those in the applications is required.

This subsection has provided a description of how polycrystalline materials are generated using the CA and how the brittle fracture of these materials takes place. The following sections will provide a summary of the parallel implementation of the CA, before describing the coupled nature of the two methods, CA and FEM for the solution of fracture using a multiscale strategy.

2.2.3. Parallel Implementation

The CA is implemented using coarray Fortran (CAF), that has been part of the Fortran standard since 2008. CAF uses the single program multiple data model, which at runtime creates a series of images that execute the same code. CAF enables remote read and write access from each image, with the execution segments acting on an asynchronous basis. Global barriers exist, named image control statements that are utilised to ensure correct data management and avoid race errors. Using this methodology CASUP has run problems with around 80 billion cells on around 32,000 cores. Detailed description of the implementation of the Coarrays in CASUP can be found in [24, 34].

2.3. Multiscale Modelling : CAFE

The methodologies used to model the macroscale and mesoscale have been described. This section subsequently provides a summary of how the scales and packages interact and the key transfer of data between the two. As

with a number of multiscale modelling approaches [48] localisation and homogenisation techniques are used to couple the two scales, and will be described in more detail. An implementation of the CAFE model is provided in Figure 4, with a description of it below.

Figure 4: CAFE implementation highlighting the key steps, with processes run by both applications in yellow (light), those run by ParaFEM in red (darker) and CASUP in green (darkest). The steps over which the localisation and homogenisation occur are labelled.

The initialisation phase that takes place, sets up the problem. A file based I/O is used to read in the mesh information for ParaFEM, this includes three files, a definitions file containing numerical parameters and material properties, a file containing the element steering arrays and a file containing the nodal coordinates. The master processor reads the file and distributes the steering array and coordinates among the MPI processes. The CA requires only a number of values to define its space and composition. The coordinates of its origin and a vector with the length of each orthogonal side defines the physical dimensions of the grid. The CA grid must overlap the FE if only partly as only CA that are with FE's are involved in the calculation of fracture. The dimensions of the cellular automata and the size of the coarray that computationally represents the CA, is further defined by the average grain size and the mean number of cells per grain. At this phase within the program the grain growth process, described in Section 2.2.1, also takes place, generating the polycrystalline structure within the CA.

The linking between the two applications takes place by coupling clusters of CA that exist within a FE element region to the FE element itself. As is common with multiscale methods the element and cell dimensions are of drastically different sizes and so a large number of CA can exist within each FE. Figure 5 provides a two dimensional example of the clustering and linking within the application. The linking is a quick effective method. A characteristic length is defined by the user, L_c that defines the radius of a sphere whose origin is at the element's centre. Any automata, no matter the cell state, that exists within the element's characteristic length is

Figure 5: An example of the linking process in two dimensions for an embedded CA grid in FE mesh. A automata is associated with an element if it is within its characteristic length, L_c , highlighted in the figure.

assigned to the element. Subsequently, each element contains a collection of automata whose states impact the elements macro properties. After the initialisation and linking phases, the time loop can commence. The solution to the FE problem described in Section 2.1.1 is used to generate the stress tensor for each element. At this point the stress tensor of each element is distributed across the cluster of CA cells that they are associated with. The mean stress of the FE and the CA is equal, however the stress is distributed such that higher stress values lie at crack fronts. Localisation techniques such as these are common amongst multiscale approaches. CASUP then uses the CA stress values to determine whether cleavage will occur, see Section 2.2.2. A homogenisation step takes place to update the macro properties of the material with the effects calculated at the mesoscale. A damage variable is calculated that is a ratio of the number of fractured cells to the total number of cells within the CA cluster or FE.

$$Damage = \frac{\text{fractured cells}}{\text{total cells}} \quad (8)$$

This damage scalar, is used to update the element stiffness. Conceptually as the damage increases the load bearing capacity of the element falls. With the updated Young's Modulus of the element, the stiffness matrix is recalculated. This loop continues until the material fails or the user defined time limit has been reached. Extreme events such as cracks perpendicular to the loading force that result in the element's stiffness falling to zero are not captured by such a model. However, these cases are rare, the heterogeneous grains that have random orientations mean it is unlikely a group of adjoining grains, that impact a finite element's stiffness, have cleavage planes all running in the same direction. The comparison of the simulation with experimental results can be used to calibrate the model, but as a problem tends towards the extreme events, such as that described, the model results will drift away from the experimental values, as is typical with a number of numerical methods.

The application described comes as part of ParaFEM that is available at the git repository under a BSD licence.

The mini-app is labelled xx20 within the “src/program-
s/dev directory.

3. Results

The framework is demonstrated through the use of a simple test problem that considers a cantilever beam undergoing forced vibration that ultimately leads to brittle fracture within the material. The test case aims to highlight the capabilities of the CAFE model with the added capacity to model transient problems and further highlight the key parameters to consider when continuing to develop and use the application.

3.1. Problem Statement

In this problem the brittle fracture of a polycrystalline material undergoing forced vibration is analysed. Firstly a range of loads are applied to identify loading regions over which fracture will occur. After selecting one of these loading factors an in depth analysis provides details of the effect at the mesoscale and macroscale. Figure 6 provides a schematic of the problem test case.

Figure 6: Computational domain of the problem, the boundary conditions are shown on the right without the FE mesh. The CA region is highlighted within the FE domain with a snapshot of a grain structure on the right.

3.1.1. Modelling at the macroscale

The elastic beam has dimensions of $0.01m$, $0.05m$ and $0.01m$ in the x , y and z directions respectively. The CA zone is embedded within the elastic beam at the mid point in the Y direction. The FE continuum has a Young’s modulus of 200 GPa , a density of 7874 kg/m^3 and a poisson’s ratio of 0.3 , which corresponds to the material properties of iron. The beam is fixed at its base and forced with a constant load at its tip. Quadratic 20 noded elements are used throughout the series of tests, using 5000 elements for the initial loading sweeps and approximately 78,000 for the analysis of the fracture case.

The choice of length scale and time scale, for multi-scale methods, can be challenging, and highly problem

dependent [49]. The time scales for cleavage are in the orders of $10^{-6}s$ to $10^{-3}s$ respectively. In comparison engineering time scales can range anywhere from $10^{-1}s$ to 10^4s , when using continuum methods. Within this case a time step of 0.0001 s is used, which means a possible fractured cell will cleave the entire CA zone within one time step. Within this test case the brittle fracture step is only completed once at $0.002s$.

3.1.2. Modelling at the mesoscale

The CA zone is a cube with sides of length $0.01m$. The CA zone is populated with approximately 100×10^6 cells and 1000 grains, which corresponds to 1×10^5 cells per grain, which has been found by Shterenlikht and Margetts [24] to provide grid independent results for a quasi-static analysis. The mean grain diameter is 0.001 m which is a factor of two larger than the average grain size for iron. In this mechanistic methodology the crack propagation speed is set at 1000 m/s . The critical stresses are from Gilman [47], set at 1.05 , 1.25 and 4.9 GPa for the $\{100\}$, $\{110\}$ and $\{111\}$ cleavage planes respectively.

3.2. Initial sweep

The initial loading sweeps, involved ramping up the load to determine the range of load values at which fracture will occur. Figure 7 presents the displacement of the cantilever tip against time. It highlights when cracks are initialised at $0.0025s$ and how differing loads and crack formations, result in different macroscopic profiles of displacement. Figure 8 shows the fracture volume as a percentage of the total number of cells, with the loads corresponding with those in Figure 7.

Figure 7: Displacement time plots for a range of loads. The cut off displacement is shown at $0.08m$ and the crack initiation at $0.0025s$.

The figures highlight that for brittle fracture to occur at the specified time step the load must be approximately $93.8kN$ or above. The displacement time plot for the values below this follow a perfectly elastic response with

Figure 8: The percentage fracture volume for each of the load cases.

no brittle fracture taking place. As the load increases from 93.8kN the percentage of fracture volume increases, however the difference in fracture volume after 125kN is suggested to be due to variation in the grain structure for each of the simulations run. The following section will provide further information into the mini-app and the details of how different scales react.

3.3. Analysis and Discussion

Considering the load, 94kN, the finite element mesh was refined from 5000, 20 noded, hexahedral, quadratic elements to approximately 78,000. This larger test case was run a number of times, with each run on 120 cores. The statistical behaviour of brittle fracture and material properties can be integrated within the miniapp. The polycrystalline structure of the material is randomly generated, and so running the same application on the same machine can result in a range of grain orientations, sizes and shapes. Figure 9 presents the polycrystalline structure formed using the application for a number of the test cases run.

It is clear from Figure 9 that there is an inherent variation within the generation of the polycrystalline structure and hence the cleavage and formation of fracture planes within the structure. Although this variation exists, the localisation techniques tend to smear this variation out on the continuum scale such that the deformation and stress tensors at this engineering scale are similar for all the runs. This variation leads to differing micro crack formations and ultimately differing macro cracks within the structure. The test case was run ten times and Figure 10 shows the micro crack formulations for six of these runs.

It can be seen that the formation of the micro cracks differs from case to case, depending on the initial polycrystalline grain structure and orientation. The colors of the micro cracks represent the plane in which cleavage

Figure 9: Grain distribution from six simulations running on the same machine and the same number of cores, each colour represents a different grain with 1000 grains.

Figure 10: Figures showing the variation in micro crack formulation for the same job. The green and yellow cracks show cleavage in the $\{100\}$ and $\{110\}$ planes respectively.

has occurred. The green represents cleavage in the $\{100\}$ plane and the yellow in the $\{110\}$. There is no cleavage on the $\{111\}$ plane due to the significantly larger cleavage stress required.

Figure 11 highlights how the combination of micro cracks leads to the formulation of a macro crack.

A red band has been drawn on the figure to highlight the orientation and region in which the microcracks have merged to generate a macro crack. The variation in both the effect at the mesoscale and macroscale are shown in Figures 12 and 13 that again show the percentage of fracture volume and the tip displacement respectively.

Figure 12 shows that the percentage fracture volume can range by around 15 % from a maximum of 37 % in analysis (g) to a minimum of 22 % in analysis (d). Comparing this to the micro cracks formed in Figure 10 there is a noticeable difference in density of fracture in

Figure 11: Three views rotated, to show the three dimensional micro cracks generated, the green and yellow represent the the 100 and 110 cleavage planes respectively. A red band has been drawn to highlight the formation of a macro crack.

Figure 12: The fracture volume percentage for the 10 analyses run. The colors associated with the fracture volume are consistent with Figure 13.

Figure 13: The displacement at the tip of the beam for the 10 jobs run. The inset figure highlights the differences in peak deflection for each of the jobs.

significantly. This section has provided an example test case exploring some of the parameters associated with the miniapp, and how it can be used to explore the grain orientation design space.

4. Parallel Performance

Multiscale modelling approaches are well documented in the literature, however they often fail to acknowledge the computational expense. This section highlights the scalability of this application on high performance computing systems.

4.1. Computational Expense

The application was compiled on ARCHER [50], the UK's national computing service, which is a Cray XC30 machine. The nodes are made up of two 12 core E5-2697 Ivy Bridge processors with a clock speed of 2.7 GHz. The compute nodes are linked using the Cray Aries interconnect, with each compute node having 2 non-uniform access (NUMA) regions with 32 GB of memory on each processor. Both packages were compiled using version 8.5.8 of the Cray compiling environment. Profiling information was collected for the simulations using the tracing tool, CrayPAT.

The test case for both the strong and weak scaling is based on that shown in Section 3. Three finite element meshes and three CA grids were generated for the initial analysis and the strong scaling studies. Full details of the FE meshes and CA grids can be found in Table 3.

4.1.1. Performance Analysis

The initial performance analysis considers the breakdown of execution time into the four major components.

Figure 14: From left to right the figures show, (a) the displacement at the macroscale, (b) the cleavage planes inset within the FE model and (c) the FE model, warped by its displacement vector.

Mesh	# Nodes ($\times 10^6$)	# Equations ($\times 10^6$)	# of CA Cells ($\times 10^6$)
A	0.3	1	50
B	2.5	7.7	500
C	20	60	5000

Table 3: Summary of the three FEM meshes and CA grids used for the initial breakdown study and analysing the strong scalability of the application.

These are as follows, the time taken to read in the FE mesh input files (FE mesh input), the time take to initialise CASUP (Initialise CA), the computational time required to solve the FE problem over ten timesteps (Compute FE) and the time taken to solve one timestep, or approximately 10000 steps of the cleavage algorithm (Compute CA).

Figure 15a and 15b present a breakdown of the application using FE mesh C, from Table 3, highlighting the percentage of total execution time and execution times, respectively for a range of core counts. Beginning with the input strategies for both CASUP and ParaFEM it can be seen that CASUP's initialisation method is consistent, up to approximately 100,000 cores. The initialisation process involves a number of steps, including the allocation of the coarray memory space, the mapping between the CA and the FE and the generation of the polycrystalline grain structure. The mapping between the CA and FE uses an all-to-all algorithm and was the most expensive segment within the initialisation process for CASUP. The initialisation of ParaFEM involves the reading of mesh files by the master processor and distribution to the slaves.

(a) The percentage of total execution time spent in the major components of the application.

(b) The execution time for each major component in the application.

Figure 15: The initial cost estimation of the application using Mesh C from Table 3.

From Figure 15a, it can be seen that the initialisation time for ParaFEM is constant up to approximately 25,000 cores before increasing to a significant proportion of the problem execution time, representing around 14% of the solution time on approximately 100,000 cores. For this problem the time spent solving each scale is initially distributed heavily towards the FE before inverting, with the CA taking up approximately 81% on 100,000 cores, whilst the FE represents approximately 3%.

When two packages are coupled sequentially, each existing on different processor, the maximum computational efficiency that can be achieved is 0.5. However, in this case both packages share the same computational resources. The data arrays for each domain are distributed to the available processors. Therefore, each processor contains decomposed data from both domains with mappings link-

ing information that needs to be coupled. The approach means that although the ratio of execution time may vary drastically between the two packages, the computational efficiency is high, with the processors rarely being idle. The following subsections will provide further detail on the strong and weak scaling of the mini-app.

4.1.2. Strong scaling

Figure 16a highlights the speedup of the full application, excluding setup time, whilst Figure 16b presents the speedup of CASUP and ParaFEM independently.

(a) Speedup of the application time excluding the initialisation time for CASUP and the read in time for ParaFEM.

(b) Speedup of ParaFEM and CASUP for each of the three meshes used.

Figure 16: Strong scaling results of the application.

Initial observations from Figure 16a show that this problem achieves good scaling to around 24,000 MPI processes, for Mesh C. Figure 16b shows that for this problem ParaFEM scales well to approximately 5000 equations per core or 400 elements, whilst CASUP scaled well to approximately 410,000 cells per core. A major advantage

of coarray Fortran over typical MPI, is the almost perfect load balancing achieved. The major subroutine for modelling cleavage within the application has a load imbalance of approximately 0.1% across the core counts ranging from 512 to 4096 whilst the major scatter and gather routines within ParaFEM had load imbalances of 9.0% and 5.3% on 512 nodes and 8.1% and 4.8%, on 1024 nodes.

4.1.3. Weak scaling

The weak scaling of the application fixes the amount of work per core. The number of elements per core is fixed at 1000 and the number of cells per core is fixed at 400,000. Figure 17a shows the breakdown of time spent within the compute FEM and compute CA regions of the application and Figure 17b presents the breakdown of the application on 512 nodes.

(a) Percentage breakdown of the computational time, ignoring the initialisation and read in time.

(b) Average percentage of time spent within significant functions for the application run on 512 nodes.

Figure 17: Weak scaling results of the application.

The time step for the weak scaling is constant, so the physical time remains the same for each simulation. Subsequently, it can be seen that the percentage of CPU time spent in each of the regions is consistent from 24 cores to 12288 cores. The size of the problem reaches a maximum at 512 nodes with approximately 50 million nodes in the

FE domain and 5 billion cells in the CA domain. The break down of the application shows that for this test case around 38.8 % of the time was spent on reading FE mesh information and initialising the problem (FEM-IO read and FEM to CA linking). The solution to the FE problem is broken down into time spent in mathematical operations, FEM-math ops. (18.7 %) and time spent in MPI related subroutines, FEM-gather and FEM-scatter (6.9 %).

Figures 18a and 18b present the parallel efficiency of each of the computational stages, solving the FEM problem and iterating the CA, and the increase in the number of PCG iterations and steps required as the problem size grows.

(a) Parallel efficiency of ParaFEM and CASUP, per total number of PCG iterations and steps respectively.

(b) Increase in the number of PCG iterations and steps as the problem size grows.

Figure 18: Weak scaling results of the application.

From Figure 18a it can be seen that CASUP achieves an ideal parallel efficiency to around 1000 cores, and still remains above 75 % on approximately 12,000 cores. ParaFEM in comparison, has a more gradual decline in

parallel efficiency seeing a drop to around 80 % at 1000 cores. Figure 18b shows that the number of PCG iterations and steps for each computational phase increases with MPI processes used. For CASUP this is expected, as the number of steps is based on the cells per unit length and so as the resolution increases, the number of steps must increase to capture the same length of fracture plane. The symmetry of the elemental elastic modulus tensor is maintained throughout the damage process. Therefore, for a set problem size the amount of damage incurred during the problem is not expected to have a significant affect on the convergence of the PCG method. However, as the mesh size increases the number of iteration for the PCG method increases. It has been postulated that for element-by-element decomposition strategies, as used by ParaFEM, the increase in required iterations is due to round-off errors [35]. These round-off errors occur during summation operations at nodes shared by multiple processors, and as more processors are used the affect of the roundoff error increases.

5. Conclusion

This paper has presented, for the first time, a multi-scale modelling framework for dynamic problems (cyclic loading and impact) where the macroscale model of the engineering component accumulates damage computed by the mesoscale simulation of real physical mechanisms that lead to fracture. A mini-app has been written to demonstrate the use of the software for a simple example problem. The problem involves the fracture of an iron bar undergoing forced vibration. The bar includes a region of cellular automata comprising a randomised configuration of grains at the mesoscale. The results show a good qualitative representation of Mode I fracture in a polycrystalline material. Further calibration of the parameters used to model cleavage is required to provide more exact results. The CAFE mini-app scaled well to approximately 24,000 cores.

The computational model presented in this paper sits at levels 2-3 in NASA's technology readiness scale. The primary goal has been to investigate whether such a simulation strategy could work for the modelling of dynamically loaded materials undergoing fracture and failure in a multiscale framework. The calibration and validation of the physical model is still required, however, it is envisaged that this simulation strategy could be used in the future to design and test new materials; leading to improved performance of components and devices subject to extreme operating conditions.

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