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# IMPLEMENTATION OF A COHESIVE ZONE MODEL INTO THE OPEN SOURCE FINITE ELEMENT SOFTWARE ParaFEM

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## ABSTRACT

Cohesive elements have proven to be an excellent approach in computational fracture mechanics. Nevertheless, massively parallel computations are required in order to capture damage patterns and evolution meticulously in Carbon Fibre Reinforced Composites (CFRCs). Commercial packages do not exhibit satisfactory scalability in massively parallel computers. Thus, it is essential to implement cohesive elements in suitable codes for large scale simulations. The steps that need to be carried out in order to implement a Cohesive Zone Model (CZM) into the open source finite element (FE) package: ParaFEM (http://parafem.org.uk) are presented. These steps are: (1) a study on the CZM existing in ABAQUS and its key parameters, (2) the generation of a fortran ABAQUS User Element subroutine (UEL) of that particular CZM, (3) the integration of the latter into the source code of ParaFEM as a Cohesive Interface (zero geometrical thickness) Element Subroutine, (4) verification of its accurate functionality with the aid of well established benchmark problems, (5) and finally the culmination of scalability tests and direct comparison between the two programs. The work will be of interest to researchers wishing to perform very large analyses with cohesive elements using supercomputers.

***Keywords:*** *Cohesive Element Subroutine; Modelling of Microstructure; Modelling Damage; Carbon Fibre Composites; Large Scale Simulation*

## 1. Introduction

The motivation of the work is to enable accurate microstructural simulations to be carried out in composite damage evolution. Composites exhibit a very convoluted response under loading due to the complexity and certain randomness that can be found in their microstructures [1]. Moreover, the interaction of their various damage mechanisms with one another is inordinately important as well. Despite the fact that there are available tools, both analytical and numerical, that can be employed in order to simplify their analysis macroscopically through various homogenization procedures [2] and multiscale approaches [3], these are not fully capable of predicting damage evolution and fracture under various loading conditions.

The systematic application of advanced composite materials in the sensitive aerospace sector (transportation) is probably only inhibited by the lack of serious computational models for the latter. Obviously, physical testing is far more expensive compared with computational modelling and testing. It is a fact that the use of these more efficient materials in contrast to the conventional heavy materials that are currently being used will enact a safer, inexpensive air travel and ultimately will have a beneficial impact on the environment as well.

Cohesive elements have been extensively employed inside FE software in order to predict damage initiation and progression in composite materials. Nevertheless, the use of cohesive elements increases the size of problem that needs to be solved. Thus, they have been used sparingly in areas where fracture is expected to occur, i.e. with pre-defined crack paths. As computational power increases with the introduction of new generations of supercomputers, it is advantageous to possess tools capable of exploiting this potential. A massively parallel and scalability study on damage initiation and evolution in laminate structures can be found in [4], where the exact mesoscale solution was investigated by employing parallel iterative solvers based on the LaTIn mixed domain

decomposition algorithm. Commercial packages such as ABAQUS do not scale well on parallel supercomputers and here we investigate the use of cohesive elements in the open source parallel software ParaFEM [5]. The implementation steps of a well established CZM into this open source software are given below. ParaFEM uses MPI for message passing and has been proven to scale on up to 64,000 cores for problems with >1 billion unknowns [6]. The purpose of this research is to improve the particular CZM, rendering it into a computational tool that will be able to capture damage in a more realistic and physical manner. More specifically, the simulation of damage initiation and propagation in CFRCs emphasizing mixed-mode failure conditions for large models where all the material interfaces include cohesive elements.

## 2. The CZM

The chosen CZM is the same as the one used in ABAQUS [7], [8]. This particular traction separation law has been proven to effectively capture the mechanics and physics of damage initiation and propagation in CFRCs [9], [10]. More specifically, in the implemented model the damage is assumed to initiate when a Quadratic Nominal Traction Criterion is met. $t_n$, $t_s$, $t_t$ indicate the current tractions in the *normal, first shear* and *second shear* directions respectively while the superscript *C* indicates user-defined critical values at damage initiation.

$$\left\{\frac{\langle t_n \rangle}{t^C{}_n}\right\}^2 + \left\{\frac{t_s}{t^C{}_s}\right\}^2 + \left\{\frac{t_t}{t^C{}_t}\right\}^2 = 1 \tag{1}$$

The Macaulay brackets < > imply that compressive forces do not contribute to failure initiation in the normal direction. The recorded traction values and recorded separation values when the quadratic criterion is met are defined as $t_n{}^o$, $t_s{}^o$, $t_t{}^o$ and $\delta_n{}^o$, $\delta_s{}^o$, $\delta_t{}^o$ respectively.

After damage onset, that is after the damage initiation criterion is met, a damage evolution law defines the stiffness degradation of the cohesive element due to damage propagation. It can be represented with a damage scalar variable D, valued between 0 and 1. D = 0 indicates no damage, whereas D = 1 indicates fully developed damage. D is the averaged (mixed mode), overall damage progression state. The mean traction components $\bar{t}_n$, $\bar{t}_s$, $\bar{t}_t$ represent the predicted elastic traction-separation behaviour for the current strains without damage based on user-defined penalty stiffness.

$$t_n = \begin{cases} (1-D)\bar{t}_n & \text{for } \bar{t}_n \geq 0 \\ \bar{t}_n & \text{for } \bar{t}_n < 0 \end{cases} \qquad \text{(no damage due to compressive forces)} \tag{2}$$

$$t_s = (1-D)\bar{t}_s \tag{3}$$

$$t_t = (1-D)\bar{t}_t \tag{4}$$

Now, the fracture energy $G_c$ is the required energy for the formation of a new surface due to fracture and can be employed to define the damage evolution. It is represented by the area under the traction-separation graph (Figure 1). Since in CFRCs the fracture energies along the two shear directions are equal, the Benzeggagh-Kenane ($\eta$ = *BK exponent*) damage evolution description can be employed to describe the mixed-mode fracture energy [9]. $G_n$, $G_s$, $G_t$ indicate the work done (dissipated energy) thus far in the *normal, first shear* and *second shear* directions respectively while the superscript *C* indicates their user-defined critical values at full degradation.

$$G_C = G_n{}^C + \left(G_s{}^C - G_n{}^C\right)\left\{\frac{G_s + G_t}{G_n + G_s + G_t}\right\}^\eta \tag{5}$$

A linear softening (damage evolution) law is adopted.

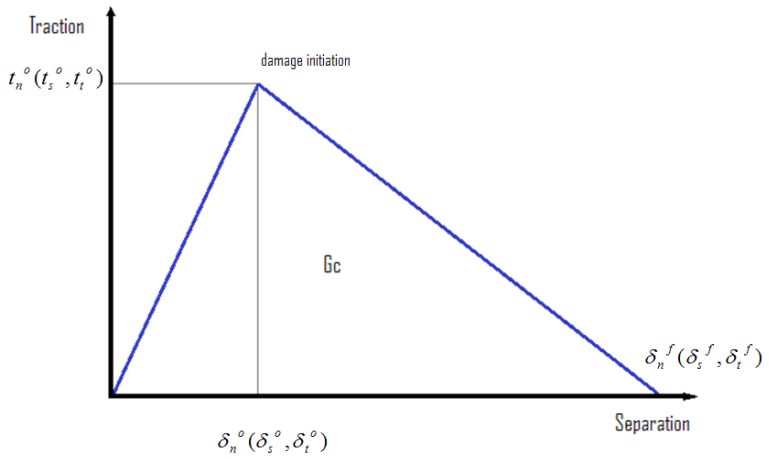


Figure 1: Mixed Mode – Linear Softening Law.

The linear damage evolution, D can be expressed as such:

$$D = \frac{\delta_m^f(\delta_m^{\max} - \delta_m^o)}{\delta_m^{\max}(\delta_m^f - \delta_m^o)} \tag{6}$$

where $\delta_m^f = 2G^C / t_m^o$ (effective displacement at full degradation) (7)

$$t_m^o = \sqrt{\langle t_n^o \rangle^2 + t_s^{o2} + t_t^{o2}} \quad \text{(effective traction at damage initiation)} \tag{8}$$

$$\delta_m^o = \sqrt{\langle \delta_n^o \rangle^2 + \delta_s^{o2} + \delta_t^{o2}} \quad \text{(effective displacement at damage initiation)} \tag{9}$$

The $\delta_m^{\max}$ variable is employed in order to record the damage state of the interface averting the latter to return to its undamaged state during unloading (maximum value of the effective displacement attained during loading history).

## 3. Method

The first step that needs to be carried out before the implementation of the above CZM into ParaFEM is the generation of an UEL incorporating this cohesive material response. Two different UELs must be programmed for linear 3D meshes. A linear 'wedge' interface cohesive element and a linear 'brick' interface cohesive element. 2D interfaces between hexahedral elements are 'bricks' and 2D interfaces between tetrahedral elements are 'wedges'. The thickness of these cohesive elements can be specified as unity. Therefore, the computed strains from the nodal forces can be equal to the displacements. The actual geometrical thickness of these elements in a FE Model is zero despite the fact they are solid elements. Thus, the geometry of the FE model can remain unaffected.

The second step is the validation of the precision and correctness of these UELs via well established benchmark tests. Based on the work of Camanho & Dávila [8], the original benchmark tests that were undertaken for the validation of the cohesive capabilities of ABAQUS are being adopted. These are: a double cantilever beam (DCB) test, an end notched flexure (ENF) test and a mixed-mode bending (MMB) test. These tests can assess the functionality of the UELs under pure normal decohesion, pure shear decohesion and mixed-mode decohesion respectively. The newly generated numerical results are being compared with the original numerical and experimental results included in [8].

The third step that needs to be carried out is the integration of the UELs into the source code of ParaFEM as a fortran subroutine. The benchmark tests should once more be modelled, this time in ParaFEM, and compared with all the data obtained in step 2, thus confirming the accurate functionality of the new features of ParaFEM.
As a last step, scaling tests must be performed between ABAQUS and ParaFEM. The DCB test is selected as the benchmark test. The test must be run numerous times with a varying mesh/cohesive-elements density, by altering the computational resources employed (number of running cores) and therefore, evaluating the performance of the two solvers (ABAQUS & ParaFEM) on a particular computer based on the overall simulation time. The results of the aforementioned benchmark and scalability tests will be presented in the conference.

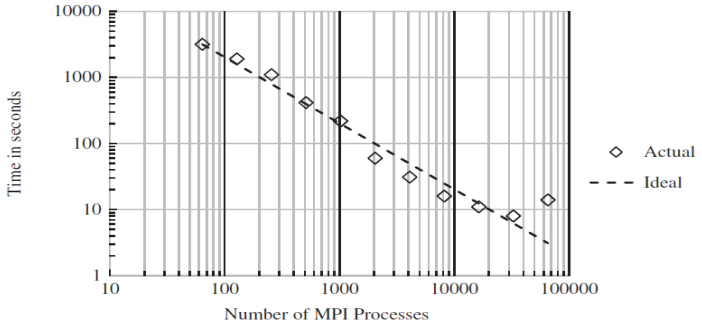


Figure 2: A typical Scaling Graph of a linear problem in ParaFEM (125 million equations: Cray XE6) [6].

## 4. Discussion

The implementation procedure presented earlier is part of a greater research plan. Its purpose is to improve the particular CZM, rendering it into a computational tool that will be able to capture damage in a more realistic and physical manner on a very large scale. Simulation of real and artificially generated microstructures on large scale has not yet been attempted. Thus, three different interfaces will be modelled (matrix/fiber, matrix/matrix & fiber/fiber) with cohesive interface elements. The mesh geometry along with the diverse interfaces parameters are of special interest and therefore crucial for the delivery of meaningful results from the simulations.

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