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Modelling delaminations using adaptive cohesive segments with rotations in dynamic explicit analysis

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Abstract

Multiple delamination planes can form when a composite structure is subjected to out-of-plane stresses during static over-loading or impact loading. Numerical modelling of such events is often prohibitively expensive because large numbers of cracks can co-exist and interact, and fracture models usually affect the time step size in explicit solutions. Here a new method called Adaptive Mesh Segmentation is proposed, which introduces segmentation ‘on-the-fly’ in meshes of quadratic finite elements with six degrees of freedom per node, without any intervention from the user and without any reductions in time step size for solution stability. Stress singularities are avoided by the use of a modified cohesive zone model. A novel cohesive formulation with rotational degrees of freedom is introduced which increases the resolution of the numerical cohesive zone and allows the use of relatively coarse meshes. Once a critical stress criterion is met, new degrees of freedom are added at element boundaries to model strong discontinuities. A new moment-damage relationship is proposed to link the discontinuity in rotational degrees of freedom with the cohesive zone law which is translational by definition. A method for initiating cohesive tractions and moments with minimal disturbances to the surrounding stress field is also presented.

26 Finally, the model is applied in the analysis of composite delamination benchmarks
27 using relatively coarse meshes and modest model sizes. Considerable improvements
28 in accuracy are observed when compared to conventional methods.

29 *Keywords:*

30 Adaptive Mesh Segmentation, Delamination, Explicit Analysis

31 Nomenclature

32

33	A_{coh}	Area associated with an integration point in a cohesive segment
34	E_{11}, E_{22}, E_{33}	Elastic modulus in material coordinate system
35	$\mathbf{f}_{\text{coh}}$	Cohesive forces obtained from a rotations enabled cohesive segment
36	$\mathbf{f}_{\text{coh-lin}}$	Cohesive forces obtained from a linear cohesive segment
37	$\mathbf{f}_{\text{initial}}$	Nodal forces in a continuum element during segmentation initiation
38	$\mathbf{f}_{\text{coh}}^{\text{Si}}$	Cohesive forces obtained from a cohesive sub-segment
39	G_{12}, G_{23}, G_{13}	Shear modulus in material coordinate system
40	G_{IC}	Fracture energy in Mode I
41	G_{IIC}	Fracture energy in Mode II
42	J	Determinant or Jacobian at an integration point in a cohesive seg-
43		ment
44	K	Penalty stiffness in cohesive law
45	$\mathbf{M}_{\text{coh}}$	Cohesive moments calculated with moment-damage relationship
46	$\mathbf{N}_{\text{rot}}$	Shape functions of a rotations enabled cohesive segment
47	$\mathbf{N}_{\text{quad}}$	Shape functions of a two-dimensional 8-noded quadratic element
48	t	Current time of the simulation

49	t_s	Time during segmentation is initiated at an interface
50	$\mathbf{T}_{\text{coh}}$	Transformation matrix in a cohesive segment
51	u_i	Displacement vector
52	$[\![\mathbf{u}]\!]_{\text{initial}}$	Initial displacement jump calculated during segmentation initiation
53	$\mathbf{U}_{\text{rot}}$	Displacement vector in terms of rotations and translations of corner
54		nodes
55	$\mathbf{U}_{\text{quad}}$	Displacement vector in terms of translations of corner and equivalent
56		virtual mid-side nodes
57	α	Scaling factor for rotational inertia
58	β	Segmentation initiation factor
59	δ	Relative displacement of an interface at an integration point in local
60		coordinate system
61	Δ	Relative displacement of an interface at an integration point in global
62		coordinate system
63	$\sigma_{I,\text{max}}$	Interfacial strength
64	τ	Traction vector calculated at an integration point
65	$\boldsymbol{\tau}_{\text{initial}}$	Initial traction vector calculated during segmentation initiation
66	$\nu_{12}, \nu_{13}, \nu_{23}$	Poisson's ratio in material coordinate system
67	AMS	Adaptive Mesh Segmentation
68	CZM	Cohesive Zone Modelling

69 1. Introduction

70 Fibre reinforced composites have high specific stiffness and strength and are widely
71 used for structural applications in the aerospace industry. In the optimal design of
72 weight-critical structures, calculation of ultimate load and progressive failure is of
73 vital importance. A common manufacturing technique is to use layers (plies) of stiff
74 unidirectional reinforcing fibres embedded in a matrix material. Delamination, where
75 the plies separate from one another, is one of the three main damage mechanism
76 present in the failure of laminated composite materials, along with transverse matrix
77 cracking and fibre failure [1, 2], but is one of the most critical under static, fatigue
78 and impact loading.

79 Cohesive zone modelling (CZM) has become the numerical technique of choice to
80 model delamination failure in composites [3, 4, 5, 6, 7, 8]. CZM represents cracks as
81 strong discontinuities in the displacement field with normal and tangential cohesive
82 tractions that gradually ‘soften’ as damage progresses. This principle, introduced by
83 Dugdale [9] and Barenblatt [10], has become the basis to solve numerous problems
84 in fracture mechanics. Hillerborg *et al.* [11] represented the stress in the crack tip in
85 the form of a traction-separation law and used linear Finite Element (FE) analysis to
86 model crack propagation and crack initiation. The shape of the traction-separation
87 law has little effect on the global load-displacement response of the structure when
88 the interfacial strength and fracture energy are correctly modelled [3, 6].

89 In conventional cohesive zone modelling for composite delamination, potential crack
90 paths are defined ‘a priori’ by inserting cohesive elements (or cohesive surface be-
91 haviour) between plies. However, for large and/or thick composite structures it is
92 often infeasible to define cohesive surfaces between every single ply, so simplifying
93 assumptions must be made which often rely on expensive experimental testing. Also,

multiple cohesive elements through the thickness can make the structure artificially compliant since the cohesive stiffness must always be finite [12].

A versatile technique for modelling strong discontinuities in continuum meshes is the eXtended Finite Element Method (XFEM) [13], which is based on the partition of unity property of the shape functions of finite elements [14]. Following these, methods for modelling discontinuities by standard shape functions alone were developed, which simplify implementation into existing FE software considerably. In the Phantom Node Method (PNM) [15, 16, 17] a fractured element is replaced by two overlapping elements where integration is performed over the volume corresponding to one ‘fragment’ in each element. The ‘cohesive segment method’ proposed by [18] uses the concept of overlapping multiple cohesive segments to model the discontinuity. The Floating Node Method (FNM) [19] is a related technique based on the local re-meshing of finite elements into sub-elements and cohesive segments. Similar methods have also been developed for shell element formulations [12].

Most models described in the literature have been implemented in implicit solution schemes. For modelling high frequency loading events such as impact, a method based on explicit time integration is required. The ‘simplified cohesive segment’ method proposed by the authors [20] uses linear continuum elements in an explicit time integration scheme so that it could easily be implemented in commercial FE solvers. However, since the method is also based on sub-element integration the stable time increment tends to decrease drastically once cracks initiate.

The method presented in this paper is instead based on the automatic insertion of cohesive segments along finite element boundaries and is called *Adaptive Mesh Segmentation* (AMS). In the current work, AMS is demonstrated with linear meshes as well as quadratic meshes with 6 degrees of freedom (DoFs) per node. Besides having a constant time step size and eliminating the need for pre-defined delamination

120 paths, this method addresses a fundamental limitation of the CZM which is the need
121 for having multiple cohesive segments to provide a sufficient number of integration
122 points ‘behind’ every crack front in the model, which usually results in prohibitively
123 fine meshes when linear elements are used. Alternatively, if the variation in displace-
124 ment is modelled using a higher order shape function, multiple integration points
125 can be added within the cohesive segment to model the displacement and traction
126 vector and the fine mesh constraint can be relaxed.

127 The CZM is well known for requiring h -refined meshes within the cohesive process
128 zone to capture crack growth correctly [3]. An alternative is p -refinement; by using
129 higher order basis functions the displacement approximation and the resulting trac-
130 tion field within the cohesive zone can be improved. Quadratic shape functions [21],
131 legendre basis functions [22] and Non-Uniform Rational B-Splines (NURBS) [23] are
132 examples of p -refinements of cohesive models. In the present work a cohesive element
133 formulation with rotational DoFs is developed, enabling quadratic approximations of
134 the elastic displacement field between quadratic continuum elements with 6 DoFs per
135 node. The quadratic shape functions developed by the virtue of rotational degrees
136 of freedom are an order higher than linear shape functions, but retain the advan-
137 tage of being able to be implemented into standard explicit FE 8 noded hexahedral
138 elements. The method is collectively addressed as higher order AMS.

139 The addition of rotational degrees of freedom at nodes is computationally more
140 efficient when compared to addition of mid-side nodes in an element. For instance,
141 the computational cost in an explicit analysis is determined by the cost incurred
142 in a time increment (c_i) and the number of such increments (N_g) required for an
143 analysis. c_i is primarily determined by the continuum element used in an analysis
144 and a compatible continuum element with rotational degrees of freedom is a 48 DOF
145 element (8 nodes with 6 DOFs) and this is less expensive than a 60 DOF element (20

146 nodes with 3 DOFs) [24]. A robust formulation in achieving computational efficiency
 147 is essentially a trade-off between c_i and N_g . With higher order elements, large mesh
 148 sizes and larger critical time step size are possible. Hence N_g and total cost can be
 149 reduced in comparison to a similar analysis with linear elements.
 150 The 48 DOF continuum element formulation [24] is briefly explained in Section 5
 151 and this provides compatibility with the proposed cohesive element formulation.
 152 The first problem in adaptive initiation of cohesive segments is the imbalance of
 153 nodal forces. Adaptive initiation of cohesive segments requires the integration points
 154 to be mapped with a cohesive traction vector through projection of variables from
 155 the surrounding continuum stress field. This ensures the compatibility of the sur-
 156 face traction vector in the initiated cohesive segments with adjoining continuum
 157 elements. Residuals created during initiation cause local force imbalances which in
 158 explicit solutions cause spurious stress waves. Although methods to smear such ini-
 159 tiation errors have been proposed in the past [25] proper minimisation of errors is an
 160 exclusive feature of the proposed model. In one of the existing methods [25], residu-
 161 als are calculated during initiation and applied as a correction force smeared during
 162 crack propagation. In another method [26], peak cohesive tractions across cohesive
 163 elements required to avoid spurious accelerations are calculated and by following the
 164 approach proposed in [25], corrective nodal forces are linearly reduced. However,
 165 these peak cohesive tractions can be larger than the interfacial strength used in a
 166 cohesive law. This artificial change in interfacial strength can affect the global be-
 167 haviour in laminated composite structures [3]. The method proposed here calculates
 168 the traction vector during initiation to ensure nodal equilibrium and corrective forces
 169 are not required. This initial traction vector is always smaller than the interfacial
 170 strength in a cohesive law and hence the behaviour is unaffected. Hence, segmen-
 171 tation initiation always precedes damage initiation. This method is later shown to

172 give smooth initiation in benchmark cases.

173 The second problem in adaptively initiating a cohesive segment occurs when multiple
174 integration points are present at an interface. Delamination propagates when seg-
175 mentation is initiated at all the participating nodes. However, different nodes at this
176 interface can initiate during different time increments and hence the calculation of
177 the initial traction vector that enables nodal force balance at a node of this interface
178 is difficult to perform without causing imbalance in another node *i.e.* the problem
179 is coupled. To solve this problem associated with initiating a cohesive segment with
180 multiple integration points, a ‘sub-segment’ approach, described in Section 4.6, is
181 deployed.

182 The continuity of rotations across the cohesive surfaces is not intrinsic to the cohesive
183 law. Therefore, a new moment-damage relationship is proposed to ensure gradual
184 changes in continuity of rotations across crack surfaces. However, it is shown here
185 that the addition of rotational DoFs is optional and the AMS can also be used with
186 linear elements. All concepts described here are demonstrated and validated through
187 implementation in the explicit finite element solver LS-DYNA [27].

188 Benchmark cases for linear AMS are shown in Section 6.3. In addition to the demon-
189 stration of benchmark cases using higher order AMS (Section 6.4), advantages of ro-
190 tational degrees of freedom (Section 6.4.1) and optimal number of integration points
191 are also investigated (Section 6.4.2).

192 The computational benefits of using higher order elements results in a discretisation
193 where fewer global degrees of freedom are required in the delamination and through-
194 thickness direction, whilst still being able to capture intrinsic composite laminate
195 properties such as bend/twist coupling. A demonstration of this combined benefit
196 with the use of rotational degrees of freedom is shown in Section 7.

197 2. Adaptive Mesh Segmentation

198 This section describes the modelling of displacement discontinuities using *Adaptive*
 199 *Mesh Segmentation* (AMS), which is the framework used here to introduce cohe-
 200 sive behaviour within continuum meshes ‘on-the-fly’, according to physically-based
 201 criteria and without direct user intervention.

202 2.1. Segmentation Procedure

203 Consider the element configuration shown in Figure 1. Let $\mathbf{u}$ and $\mathbf{u}'$ denote the global
 204 and local displacement vectors respectively. Let t_s be the time at which segmentation
 205 is initiated. Before the segmentation, the total number of nodes remains the same
 206 as the initial configuration (at time $t = 0$). Let n be the total number of nodes in
 207 the initial configuration, *i.e.* the ‘parent nodes’. The displacement vectors of the
 208 element can be obtained by scattering global vectors into the corresponding location
 209 of each new element vector,

$$\text{Global displacement vector} = [u_1, u_2, \dots, u_{12}]^T \quad t \leq t_s; \quad (1)$$

$$\text{Displacement vector of Element 1} = [u'_1, u'_2, \dots, u'_8]^T \text{ or } [u_1, u_2, u_3, u_4, u_5, u_6, u_7, u_8]^T; \quad (2)$$

$$\text{Displacement vector of Element 2} = [u'_1, u'_2, \dots, u'_8]^T \text{ or } [u_5, u_6, u_7, u_8, u_9, u_{10}, u_{11}, u_{12}]^T. \quad (3)$$

210 At time $t > t_s$, in order to initiate the split, new ‘segmentation nodes’ are initiated.
 211 It should be noted that segmentation nodes are initiated only at the location of
 212 existing parent nodes. The segmentation can be performed in such a way that all
 213 elements in the mesh can be split relative to each other, but only along the boundaries
 214 of these elements.

215 This method gives the following advantages, namely:

(a) Node numbering before segmentation ($t \leq t_s$); (i) global numbering and (ii) local numbering. The scattering operation is based on equations (1)-(3).

(b) Nodes after segmentation ($t > t_s$); (i) global numbering and (ii) local numbering. The red rhombus represents the segmentation nodes. At the time of initiation, segmentation nodes are initiated from the location of parent nodes. The scattering operation is different from Figure 1 and is based on equations (4)-(7).

Figure 1: Segmentation procedure followed in AMS

- 216 1. Since the crack does not pass through the element, the element volume (and
217 hence its Courant critical time step) are not affected by cohesive segmentation;
- 218 2. The stress mapping after the split from the parent element to the newly formed
219 element containing cohesive segment is less complex and introduces smaller
220 errors in the solution than arbitrary element splitting;
- 221 3. Since the crack does not pass through the integration points of element, fur-
222 ther complexity is avoided. The problem of orienting the crack path has been
223 discussed by other authors. [20].

224 Segmentation nodes, marked in red in Figure 1, are initiated upon reaching a ‘seg-
225 mentation initiation criterion’. This involves re-defining the local mass matrix and
226 ensuring that the stress tensor is compatible with the surrounding stress field so that
227 disturbances are minimised.

228 The mass assigned to new nodes after segmentation and the element mass matrix is
229 described in Section 5.1.

230 Segmentation nodes form a segmentation vector (*i.e.* a plane defined by four points),
231 which together with the global displacement vector models the discontinuities in
232 displacement. At $t > t_s$, the segmentation and global displacement vectors for the
233 example shown in Figure 1 would be,

$$\text{Global displacement vector} = [u_1, u_2, \dots, u_{12}]^T; \quad (4)$$

$$\text{Segmentation vector} = [u_a, u_b, u_c, u_d]^T; \quad (5)$$

$$\text{Displacement vector of Element 1} = [u_1, u_2, u_3, u_4, u_5, u_6, u_7, u_8]^T; \quad (6)$$

$$\text{Displacement vector of Element 2} = [u_a, u_b, u_c, u_d, u_9, u_{10}, u_{11}, u_{12}]^T \quad (7)$$

234 This framework is implemented in the commercial software LS-DYNA through a
235 series of user-defined element subroutines. All parent nodes are updated by the

236 main solver using the internal force vector calculated by the user subroutine. The
 237 time integration for segmentation nodes, once they are initiated, is done completely
 238 within the user subroutine.

239 3. Discretisation Errors in CZM

240 The maximum length of linear cohesive element that can be used in the numerical
 241 cohesive zone based on the material properties is described in [3]. The characteristic
 242 length equations for infinite bodies in mode-I and mode-II are given by,

$$l_{\text{ch,I}} = E'_I \frac{G_{\text{IC}}}{(\sigma_{\text{I,max}})^2} \quad (8)$$

$$l_{\text{ch,II}} = E'_{\text{II}} \frac{G_{\text{IIC}}}{(\sigma_{\text{II,max}})^2} \quad (9)$$

243 where E'_I and E'_{II} are equivalent elastic modulus of the orthotropic material [3].
 244 G_{IC} and G_{IIC} are the fracture energy in Modes I and II. $\sigma_{\text{I,max}}$ and $\sigma_{\text{II,max}}$ are the
 245 interfacial strength in Modes I and II respectively.

246 The characteristic length for slender laminates, with the inclusion of specimen height
 247 h , are proposed in [6] and given by,

$$l_{\text{ch,slender,I}} = \left(E'_I \frac{G_{\text{IC}}}{(\sigma_{\text{I,max}})^2} \right)^{\frac{1}{4}} h^{\frac{3}{4}} \quad (10)$$

$$l_{\text{ch,slender,II}} = \sqrt{E'_{\text{II}} \frac{G_{\text{IIC}}}{(\sigma_{\text{II,max}})^2}} h \quad (11)$$

248 The minimum value from the equations (8)-(11) are multiplied by a factor of 0.5 and
 249 it gives the predicted value of numerical cohesive zone, $L_{\text{NCZ,predicted}}$. By using the
 250 proposed recommendation of minimum three linear elements in the cohesive zone,
 251 the maximum element length that can be used is $\frac{L_{\text{NCZ,predicted}}}{3}$.

252 The restriction on the size of the element can be removed with a higher order element
 253 formulation which gives better approximation of the numerical cohesive zone.

a) Linear Cohesive Elements with two integration points in each dimension

b) Higher Order Cohesive Elements with more than two integration points in each dimension

Figure 2: Schematic representation of the damage progression using CZM in a DCB specimen. Only two-dimensional plane is shown for clarity.

254 Linear cohesive elements with four integration points can be used along with the
255 linear continuum solid element in the analysis of crack initiation and propagation.
256 With linear elements, as shown in Figure 2a, peak load is attained in the Double
257 Cantilever Beam (DCB) test simulation when the first element at the crack tip fails.
258 The traction becomes zero and the crack surfaces are no longer held together by
259 cohesive forces. The entire length of the element experiences discontinuity and the
260 crack tip jumps to node $n+1$ from node n . This failure over the element length in a
261 single time increment creates unbalanced forces over the failed elements and the local
262 disturbance manifests in the forms of oscillations in the global load *vs.* displacement
263 graph.

264 In order to get a good approximation of the numerical cohesive zone, the element size
265 must be reduced. Alternatively, if the displacement field inside the cohesive element
266 can be better resolved but keeping the same element size, the computation can be
267 faster. The proposal is to use rotations at the nodes to obtain a better approximation
268 of displacements inside the cohesive zone and thereby resolve the traction across the
269 surfaces. In such a case, the number of integration points must be increased to obtain
270 the displacements inside the element.

271 The benefits of better resolving the displacement field is schematically explained with
272 the Figure 2b. When compared to linear cohesive elements, higher order cohesive
273 elements give a more realistic approximation of traction across the element length.
274 After the traction at the integration point located at crack tip has become zero, the
275 element does not reach full discontinuity. The cohesive forces are still present by
276 virtue of adjacent integration points in the element, unlike a linear element where
277 crack growth across an element is instantaneous. This can be observed from the plot
278 of the traction-separation law in Figure 2b. In short, the cohesive forces gradually
279 reduce as the crack grows and the presence of unbalanced forces is minimal. It can

280 further reduce the oscillations in the global load vs displacement curve.

281 4. Cohesive Segment Formulation

282 In this section, the cohesive element formulation with translational and rotational
283 DoFs is developed. The displacement field given by the cohesive element can be
284 described in terms of nodal translations and rotations of corner nodes or only as
285 translations of the corner and midside nodes. The former representation is nec-
286 essary during the calculation of cohesive forces from cohesive tractions to ensure
287 compatibility with continuum elements and latter is required while calculating these
288 cohesive tractions, based on the cohesive law, from the displacement jump evaluated
289 with nodal translations. A transformation matrix, $\mathbf{T}_{\text{coh}}$, is defined which uses the
290 coordinates of corner nodes to calculate the coordinates of midside nodes.

291 4.1. Kinematics

292 Consider two surfaces S_A and S_B formed from a single surface S following crack
293 initiation. These two surfaces coincide with each other before crack initiation and
294 separates during crack propagation.

295 As shown in Figure 3a, the nodes a and b are located at the corners. The node c
296 is located mid side on the edge shared by node a and b . The displacement vector,
297 $\mathbf{U}_{\text{rot}}$, in global coordinates is defined with translations and rotations. The cohesive
298 law is defined in terms of translations and it is necessary to convert the rotations
299 to equivalent translation across the surfaces. The transformation for one node c is
300 given by,

$$u_c = \frac{(u_a + u_b)}{2} + \frac{y_b - y_a}{8}(\theta_{zb} - \theta_{za}) + \frac{z_b - z_a}{8}(\theta_{ya} - \theta_{yb}) \quad (12)$$

$$v_c = \frac{(v_a + v_b)}{2} + \frac{z_b - z_a}{8}(\theta_{xb} - \theta_{xa}) + \frac{x_b - x_a}{8}(\theta_{za} - \theta_{zb}) \quad (13)$$

$$w_c = \frac{(w_a + w_b)}{2} + \frac{x_b - x_a}{8}(\theta_{yb} - \theta_{ya}) + \frac{y_b - y_a}{8}(\theta_{xa} - \theta_{xb}) \quad (14)$$

where x_n, y_n, z_n are coordinates of node n . u_n, v_n, w_n are translations of node n and $\theta_{xn}, \theta_{yn}, \theta_{zn}$ are the rotations of node n .

In a similar way, transformation can be carried out for all the eight corner nodes with each having 6 DoFs. This will define the additional nodes at the mid side of every edge and each of these nodes will have three translational DoFs. So, the transformation matrix, $\mathbf{T}_{\text{coh}}$, will be of dimension 48×48 . The transformation is given by,

$$\mathbf{U}_{\text{quad}} = \mathbf{T}_{\text{coh}} \mathbf{U}_{\text{rot}} \quad (15)$$

where $\mathbf{U}_{\text{quad}}$, is the displacement vector defined in terms of translations of corner and mid-side nodes.

The mid surface between Surface S_A and Surface S_B is used to establish the local coordinate system of cohesive segment. The coordinates of Surface S_A , $\mathbf{X}_{\text{quad}}^A$ and Surface S_B , $\mathbf{X}_{\text{quad}}^B$ with mid side nodes, obtained using transformation is used to form the middle surface of cohesive segment given by,

$$\bar{\mathbf{X}} = \frac{\mathbf{X}_{\text{quad}}^A + \mathbf{X}_{\text{quad}}^B}{2} \quad (16)$$

Figure 3: Kinematics in a cohesive segment.

314 4.2. Finite Element Formulation

315 The cohesive segment used for interpolating nodal translations is a two-dimensional
 316 8-noded quadratic element in 3D space. The shape functions are given by,

$$\begin{aligned}
 N_1 &= \frac{1}{4}(1 - \xi)(1 - \eta)(-\xi - \eta - 1) , & N_2 &= \frac{1}{4}(1 + \xi)(1 - \eta)(\xi - \eta + 1) , \\
 N_3 &= \frac{1}{4}(1 + \xi)(1 + \eta)(\xi + \eta - 1) , & N_4 &= \frac{1}{4}(1 - \xi)(1 + \eta)(-\xi + \eta + 1) , \\
 N_5 &= \frac{1}{2}(1 - \eta)(1 + \xi)(1 - \xi) , & N_6 &= \frac{1}{2}(1 + \xi)(1 - \eta)(1 + \eta) , \\
 N_7 &= \frac{1}{2}(1 + \eta)(1 + \xi)(1 - \xi) , & N_8 &= \frac{1}{2}(1 - \xi)(1 + \eta)(1 - \eta) .
 \end{aligned}
 \tag{17}$$

$$\mathbf{N}_{\text{quad}} = \begin{bmatrix} -N_1 & 0 & 0 & \dots & -N_8 & 0 & 0 & N_1 & 0 & 0 & \dots & N_8 & 0 & 0 \\ 0 & -N_1 & 0 & \dots & 0 & -N_8 & 0 & 0 & N_1 & 0 & \dots & 0 & N_8 & 0 \\ 0 & 0 & -N_1 & \dots & 0 & 0 & -N_8 & 0 & 0 & N_1 & \dots & 0 & 0 & N_8 \end{bmatrix}
 \tag{18}$$

318 where ξ and η are isoparametric coordinates. The shape functions for two-dimensional
 319 4 noded element with translations and rotations are given by,

$$\mathbf{N}_{\text{rot}} = \mathbf{N}_{\text{quad}} \mathbf{T}_{\text{coh}}
 \tag{19}$$

320 The tangents are given by,

$$v_{\xi_i} = \bar{X}_{ik} \frac{\partial N_k}{\partial \xi}, \quad v_{\eta_i} = \bar{X}_{ik} \frac{\partial N_k}{\partial \eta} \quad (20)$$

321 where $\mathbf{v}_\xi$ and $\mathbf{v}_\eta$ are not necessarily orthogonal to each other. These vectors are
 322 normalised with their magnitudes to give $\mathbf{e}_1$ and $\mathbf{e}_2$. The normal vector is given by
 323 the cross product between the two tangential vectors, *i.e.*

$$\mathbf{e}_1 = \frac{\mathbf{v}_\xi}{|\mathbf{v}_\xi|}, \quad \mathbf{e}_3 = \frac{\mathbf{v}_\xi \times \mathbf{v}_\eta}{|\mathbf{v}_\xi \times \mathbf{v}_\eta|}, \quad \text{and} \quad \mathbf{e}_2 = \mathbf{e}_3 \times \mathbf{e}_1. \quad (21)$$

324 These vectors are assembled to get the matrix ϕ which maps the displacement into
 325 local coordinate system established by $\mathbf{e}_1, \mathbf{e}_2$ and $\mathbf{e}_3$.

$$\phi = \begin{bmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \end{bmatrix}. \quad (22)$$

326 The area of the cohesive segment corresponding to the integration point is given by,

$$J = |\mathbf{v}_\xi \times \mathbf{v}_\eta|. \quad (23)$$

327 Using the shape functions, $\mathbf{N}_{\text{quad}}$ evaluated at the integration point and nodal dis-
 328 placements $\mathbf{U}_{\text{quad}}$, displacement vector at the integration point in global coordinates,
 329 $\boldsymbol{\delta}$, can be calculated as,

$$\boldsymbol{\delta}(\xi, \eta) = \mathbf{N}_{\text{quad}}(\xi, \eta) \mathbf{U}_{\text{quad}} \quad (24)$$

330 The displacement in local coordinates, $\boldsymbol{\Delta}$, can be calculated using the matrix ϕ as,

$$\boldsymbol{\Delta} = \phi \boldsymbol{\delta} \quad (25)$$

331 The cohesive law is used to obtain the traction, $\boldsymbol{\tau}$, based on displacement vector $\boldsymbol{\Delta}$.

332 The cohesive forces are calculated as,

$$\mathbf{f}_{\text{coh}} = \int_{\xi} \int_{\eta} \mathbf{N}_{\text{rot}}^T \phi^T \boldsymbol{\tau} J \, d\eta \, d\xi. \quad (26)$$

333 where $\mathbf{f}_{\text{coh}}$ is a vector of dimension 48×1 with forces and moments corresponding
 334 to surface S_A and S_B without mid side nodes.

Figure 4: Traction at the time of segmentation. a) Segmentation initiation is performed before reaching the maximum interfacial strength. b) Segmentation initiation is performed after reaching the maximum interfacial strength.

336 The cohesive segments are formed adaptively based on a quadratic stress criterion.
 337 The tractions can be calculated from the stress tensor as,

$$\boldsymbol{\tau} = \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}. \quad (27)$$

338 where $\boldsymbol{\sigma}$ is the stress tensor of the continuum element calculated at the centroid and
 339 $\hat{\mathbf{n}}$ is the unit normal vector to the surface where $\boldsymbol{\tau}$ is calculated. The quadratic
 340 damage criterion is defined as,

$$\sigma_I = \max(\tau_{33}, 0), \quad \sigma_{II} = \sqrt{\tau_{13}^2 + \tau_{23}^2}, \quad (28)$$

$$\beta = \sqrt{\left(\frac{\sigma_I}{\sigma_{I,\max}}\right)^2 + \left(\frac{\sigma_{II}}{\sigma_{II,\max}}\right)^2}. \quad (29)$$

where σ_I and σ_{II} are the normal and resultant interfacial shear stresses, respectively, while $\sigma_I^{\max}$ and $\sigma_{II}^{\max}$ are the tensile and shear interfacial strengths. β is the segmentation initiation factor.

Segmentation initiates when $\beta \geq \beta_{\text{critical}}$, where $0 \leq \beta_{\text{critical}} \leq 1$. When β_{critical} is zero, adaptive mesh segmentation is same as the conventional cohesive zone modelling as the cohesive segments are present from the start of analysis.

The traction calculated based on equation (27) results in considerable deviation from the traction in a cohesive element primarily due to space discretisation error and lack of inter element stress continuity in standard Finite Element solutions. During segmentation initiation, displacement jump or cohesive shift [28] in the form of translations (u_{13}, u_{23}, u_{33}) must be given to the cohesive law such that the tractions during segmentation initiation are compatible with the surrounding elements. The displacement jump which gives traction (τ'_i) is calculated based on penalty stiffness of cohesive law. This initial displacement jump is passed to the cohesive relation located at integration points of an interface that received segmentation initiation and this is similar to Figure 4a. The procedure to calculate this displacement jump is explained in Section 4.5.

If τ'_i is greater than $\tau_{\max}$, interfacial strength, the cohesive law will return to the locus of the fracture energy such that mesh independent results are obtained. However, this scenario will result in large residuals in initiation and must be avoided. β_{critical} ensures that the initiation always occurs before reaching the interfacial strength.

4.4. Errors in Segmentation Initiation

The segmentation initiation criterion is checked at t_{initial} . Following the update of element connectivity based on the segmentation procedure, cohesive segments are formed at the next time step, $t_{\text{initial}} + \Delta t$, where Δt is the stable time increment.

366 Consider a configuration where the cohesive segments are not initiated such that the
 367 semi-discrete momentum equations are defined only with parent nodes at time t . For
 368 all the nodes, n , in the domain Ω at time t ,

$$\mathbf{M}\mathbf{a} = \mathbf{f}_{\text{ext}} - \mathbf{f}_{\text{int}} - \mathbf{f}_{\text{damp}}, \quad (30)$$

369 where $\mathbf{f}_{\text{ext}}$, $\mathbf{f}_{\text{int}}$ and $\mathbf{f}_{\text{damp}}$ corresponds to external global force vector, internal global
 370 force vector and damping force vector. $\mathbf{M}$ is the lumped mass matrix and $\mathbf{a}$ is the
 371 acceleration vector of the nodes. Since a lumped mass matrix is used, the equations
 372 are uncoupled and can be solved directly.

373 If the boundary conditions are imposed as Dirichlet boundary conditions and no
 374 damping is given to the solver, the equation simplifies to,

$$\mathbf{M}\mathbf{a} = -\mathbf{f}_{\text{int}}. \quad (31)$$

375 Let $\mathbf{a}_{\text{new}}$ be the acceleration of nodes that are initiated due to the segmentation
 376 initiation at time t_{initial} . At time $t_{\text{initial}} + \Delta t$, cohesive segments are initiated such
 377 that the acceleration of the new nodes can be written as,

$$\mathbf{M}\mathbf{a}_{\text{new}} = -\mathbf{f}_{\text{int}} + \mathbf{f}_{\text{coh}}. \quad (32)$$

378 When the segmentation initiates, the cohesive segment has a traction less than the
 379 interfacial strength and an elastic response will occur. So, the cohesive force will be
 380 equal and opposite to the nodal force from the continuum element. Any differences
 381 between them, in the elastic regime, will manifest in the form of residue and presents
 382 as oscillations in the global load *vs.* displacement curve of the explicit analysis.

383 The segmentation error during segmentation initiation is defined using internal and
 384 cohesive forces calculated at $t_{\text{initial}} + \Delta t$ and is given by,

$$\mathbf{f}_{\text{error}} = -\mathbf{f}_{\text{int}} + \mathbf{f}_{\text{coh}}. \quad (33)$$

and the norm of the error $\|\mathbf{f}_{\text{error}}\|$ must approach zero upon segmentation initiation. In Menouillard and Belytschko [25], the error is treated as the residual and smeared over successive time increments based on the crack growth. It thus functions as a form of damping, which may impede the crack growth as the acceleration and velocity of the nodes at the crack tip would change based on the residue. By using the initiation method proposed in Section 4.5, smooth initiation can be obtained without the use of damping forces in an explicit analysis.

4.5. Continuity in response at initiation - Balance of nodal forces

The effect of introducing the segmentation is equivalent to a step function [25]. A smooth initiation can be obtained by using nodal forces to initiate the cohesive segments using the proposed approach in mixed mode cases.

For calculating the initial traction, a linear cohesive segment is used. In a linear cohesive segment with closed quadrature integration schemes, such as Newton-Cotes, the location of nodes coincides with integration points. By using the nodal forces, tractions can be calculated and used to initiate the cohesive segments.

The traction obtained at the integration points and the cohesive force calculated can be directly related using equation (34) and they are uncoupled.

The equation for cohesive force using a linear cohesive segment for node n which coincides with integration point ξ_a, η_a is given by,

$$\mathbf{f}_{\text{coh-lin}} = \mathbf{N}_{\text{Lin}}^T(\xi_a, \eta_a) \phi^T(\xi_a, \eta_a) J(\xi_a, \eta_a) \boldsymbol{\tau}_{\text{initial}} \quad (34)$$

where $\boldsymbol{\tau}_{\text{initial}}$ represents the initial traction to be calculated using the proposed approach and $\mathbf{N}_{\text{Lin}}$ corresponds to the linear shape functions of cohesive segment.

$\mathbf{f}_{\text{coh-lin}}$ is a vector of dimension 24×1 .

It is possible to establish the local coordinate system and calculate the area of the linear cohesive segment. The cohesive shift must be given at the time $t_{\text{initial}} + \Delta t$.

409 Let $\mathbf{f}_{\text{initial}}$ be the force from the continuum element, excluding moments, at time
 410 $t_{\text{initial}} + \Delta t$; this force must be equal and opposite to $\mathbf{f}_{\text{coh-lin}}$ at the same time step
 411 to minimise the error norm. By substituting $\mathbf{f}_{\text{initial}}$ in equation (34),

$$-\mathbf{f}_{\text{initial}} = A_{\text{coh}} \boldsymbol{\tau}_{\text{initial}}. \quad (35)$$

412 where A_{coh} is the area of the cohesive integration point. The required traction in the
 413 cohesive element is given by,

$$\boldsymbol{\tau}_{\text{initial}} = -A_{\text{coh}}^{-1} \mathbf{f}_{\text{initial}}. \quad (36)$$

414 This traction is converted to an initial displacement jump, $[[\mathbf{u}]]^{\text{initial}}$, using equa-
 415 tion (37) and passed to the cohesive law with penalty stiffness, K .

$$[[\mathbf{u}]]_{\text{initial}} = \frac{1}{K} \boldsymbol{\tau}_{\text{initial}} \quad (37)$$

416 The displacement jump at subsequent time increments are obtained by adding the
 417 displacement jump at the current time step, $[[\mathbf{u}]]_t$ and the initial displacement jump.

$$[[\mathbf{u}]] = [[\mathbf{u}]]_{\text{initial}} + [[\mathbf{u}]]_t \quad (38)$$

$$\boldsymbol{\tau} = \text{Cohesive law}([[\mathbf{u}]]), \quad (39)$$

418 where $\boldsymbol{\tau}$ is the traction obtained from the cohesive law by passing the displacement
 419 jump.

420 The cohesive law used in the current work is a bi-linear traction separation law
 421 developed at University of Bristol [29].

422 4.6. Cohesive Sub-segments

423 When more than four integration points are present at an interface, initiating a node
 424 and the subsequent inclusion of the initial traction vector corresponding to this node

will cause a nodal force imbalance at the other nodes of this interface.. To facilitate the mapping from the initiated node to multiple integration points, sub-segments are used. A sub-segment is a subset of the cohesive segment and it is formed upon the node initiation with a traction vector uniform across all integration points in the subsegment. Hence, four sub-segments can be present in a cohesive segment corresponding to four nodes.

In the subsequent time increments, variation in the traction field across the cohesive segment is calculated by multiple integration points. This traction field is added together with the uniform traction field corresponding to initial traction vector present in sub-segments. The cumulative traction vector will give the cohesive force of the node present in the cohesive segment.

Hence, the cohesive force of node 1 is given by the cohesive sub-segment 1 and the cohesive segment. In a similar way, an assembly is performed over all the cohesive sub-segments to calculate the cohesive force as,

$$\mathbf{f}_{\text{coh}} = \begin{bmatrix} [\mathbf{I}] & [0] & [0] & [0] \\ [0] & [0] & [0] & [0] \\ [0] & [0] & [0] & [0] \\ [0] & [0] & [0] & [0] \end{bmatrix} \mathbf{f}_{\text{coh}}^{s_1} + \begin{bmatrix} [0] & [0] & [0] & [0] \\ [0] & [\mathbf{I}] & [0] & [0] \\ [0] & [0] & [0] & [0] \\ [0] & [0] & [0] & [0] \end{bmatrix} \mathbf{f}_{\text{coh}}^{s_2} + \dots + \begin{bmatrix} [0] & [0] & [0] & [0] \\ [0] & [0] & [0] & [0] \\ [0] & [0] & [\mathbf{I}] & [0] \\ [0] & [0] & [0] & [0] \end{bmatrix} \mathbf{f}_{\text{coh}}^{s_3} + \begin{bmatrix} [0] & [0] & [0] & [0] \\ [0] & [0] & [0] & [0] \\ [0] & [0] & [0] & [0] \\ [0] & [0] & [0] & [\mathbf{I}] \end{bmatrix} \mathbf{f}_{\text{coh}}^{s_4} \quad (40)$$

where $[\mathbf{I}]$ is a 6×6 identity matrix, $[0]$ is a 6×6 matrix; and $\mathbf{f}_{\text{coh}}^{s_1}$, $\mathbf{f}_{\text{coh}}^{s_2}$, $\mathbf{f}_{\text{coh}}^{s_3}$ and $\mathbf{f}_{\text{coh}}^{s_4}$ are the cohesive force corresponding to the cohesive sub-segment 1,2,3 and 4 respectively.

Figure 5: Cohesive sub-segments to model the initial traction vector calculated upon the initiation of a node when multiple integration points are present in the cohesive segment.

4.7. Moment-damage Relationship - Balance of nodal moments

In the Higher order AMS implementation, equation (26) is used only in the calculation of cohesive forces. The initial traction vector calculated in section 4.5 ensures balance of nodal forces but not nodal moments. This is because an inverse calculation to obtain the three traction components of the initial traction vector from the

447 six internal force terms will not give a unique solution. To ensure continuity in mo-
 448 ments after segmentation initiation and avoid imbalance in nodal moments, a linear
 449 *moment-damage relationship* is proposed, to enable the gradual reduction of moment
 450 transfer (or rotational stiffness) across the cohesive segment as damage evolves.
 451 Consider the continuum elements A and B with the cohesive segment at the time
 452 $t_{\text{initial}} + \Delta t$ where the segmentation is initiated at node n . The moment in this node
 453 at time $t_{\text{initial}} + \Delta t$ is $\mathbf{M}_{\text{initial}}^A$ and $\mathbf{M}_{\text{initial}}^B$ at elements A and B respectively.
 454 During the damage propagation phase, the moment contribution from cohesive seg-
 455 ments can be assumed to change based on the damage variable and ultimately reaches
 456 zero. This assumption is used to obtain the moment damage relationship.
 457 Before crack initiation, the continuity in rotation is given by a balance of moments.
 458 The continuity in rotation is lost when the damage variable, d , reaches unity. Based
 459 on this, the moment contribution given by cohesive elements to continuum elements
 460 A and B at time $t > t_{\text{initial}}$ are,

$$\begin{aligned}
 \mathbf{M}_{\text{coh}}^A &= (1 - d) \mathbf{M}_{\text{initial}}^A \\
 \mathbf{M}_{\text{coh}}^B &= (1 - d) \mathbf{M}_{\text{initial}}^B
 \end{aligned}
 \tag{41}$$

461 where d is the maximum damage in the cohesive segment between continuum ele-
 462 ments A and B at time $t > t_{\text{initial}}$.
 463 The moments in elements A and B at the current time step, $\mathbf{M}_t^A$ and $\mathbf{M}_t^B$, are added
 464 with the moment from cohesive element as,

$$\begin{aligned}
 \mathbf{M}^A &= \mathbf{M}_t^A + \mathbf{M}_{\text{coh}}^A \\
 \mathbf{M}^B &= \mathbf{M}_t^B + \mathbf{M}_{\text{coh}}^B
 \end{aligned}
 \tag{42}$$

465 where $\mathbf{M}^A$ and $\mathbf{M}^B$ are moments returned to the solver at the end of time step.
 466 The continuity of moments after segmentation initiation is reflected in angular ac-
 467 celeration, angular velocity and rotations. Hence, the moment-damage relationship

Figure 6: Cohesive moment as a function of damage variable obtained from the cohesive segment.

468 enables a progressive release in terms of moments and rotations and the interface is
 469 uncoupled when the damage variable becomes 1.

470 5. Continuum Element Description

471 A linear solid element is a 8 node hexahedron with only translational DoFs (u_i, v_i, w_i)
 472 for each node. The element formulation used in the current work is also a 8 node
 473 hexahedron, but it has both translational and rotational DoFs ($u_i, v_i, w_i, \theta_{xi}, \theta_{yi}, \theta_{zi}$)
 474 for each node [24]. While the former is a 24-DoF hexahedron, the latter is a 48-DoF
 475 hexahedron. A higher order element formulation with mid side nodes and quadratic
 476 shape functions would yield 60-DoF hexahedron. Both, 48-DoF hexahedron and
 477 60-DoF hexahedron models a quadratic displacement field.

478 The element formulation is derived and described in [24]. The internal force vector
 479 is calculated directly as the time integration scheme is explicit. The integration is
 480 performed using numerical quadrature with a 14-point integration rule [24]. Despite
 481 the 8-point integration rule being sufficient to calculate the correct volume, the 14-
 482 point integration rule is necessary to eliminate zero energy modes.

483 For dynamic analysis, the mass matrix must be defined. A lumped mass approach

484 is used for the translational DoFs. The rotational inertia along with a factor is used
 485 for rotational DoFs. It is explained in Section 5.1.

486 5.1. Element Mass Matrix

487 For translational DoFs, the mass is calculated from the volume and it is lumped on
 488 the nodes. Let $\mathbf{X}_n(x, y, z)$ be the position vector of node n .

489 The length of the edges are given by,

$$\begin{aligned} l_x &= |\mathbf{X}_2 - \mathbf{X}_1| \\ l_y &= |\mathbf{X}_4 - \mathbf{X}_1| \\ l_z &= |\mathbf{X}_5 - \mathbf{X}_1| \end{aligned} \quad (43)$$

490 where l_x , l_y and l_z are the edge length parallel to x , y and z axes respectively. The
 491 translational mass of the nodes are calculated as,

$$\mathbf{M}_{ii} = \frac{\rho \times l_x \times l_y \times l_z}{8} \quad i = 1, 2, 3, 7, 8, 9 \dots 43, 44, 45 \quad (44)$$

492 where $\mathbf{M}$ is the mass matrix of dimension 48×48 for the corresponding 48-DoF
 493 hexahedron.

494 The rotational inertia is calculated as,

$$\begin{aligned} \text{mass} &= \frac{\rho \times l_x \times l_y \times l_z}{8} \\ I_{xx} &= \frac{\text{mass} \times (l_y^2 + l_z^2)}{12} \\ I_{yy} &= \frac{\text{mass} \times (l_x^2 + l_z^2)}{12} \\ I_{zz} &= \frac{\text{mass} \times (l_x^2 + l_y^2)}{12} \end{aligned} \quad (45)$$

495 The masses corresponding to rotational DoFs are given by,

$$\begin{aligned} \mathbf{M}_{ii} &= \alpha I_{xx} \quad i = 4, 10, 16, \dots 46 \\ \mathbf{M}_{ii} &= \alpha I_{yy} \quad i = 5, 11, 17, \dots 47 \\ \mathbf{M}_{ii} &= \alpha I_{zz} \quad i = 6, 12, 18, \dots 48 \end{aligned} \quad (46)$$

where α is a factor used to scale up the inertia associated with rotational DoFs to get an increase in the time step size for stability. The presence of rotational degrees of freedom will increase the natural frequencies in solid elements and reduce the critical time step [30]. Hence, the factor α is used to selectively scale the inertia and obtain a time step size which is non-prohibitive in using the element formulation. The value of α ranges from 1 to 100 depending on the mass scaling used in the explicit analysis. A more robust method of selecting the optimal value of α is explained in [30] and the selection can be automated with this method, based on element dimensions.

6. Validation and Examples

AMS is demonstrated using linear elements as well as elements with nodal rotations. The concepts of segmentation initiation and initiation based on nodal forces is central to AMS and applicable to both types of elements. AMS as a method can be implemented to different types of elements and two such element types are used in this section.

The results of Linear AMS are shown in Section 6.3 and Higher order AMS in Section 6.4.

6.1. Validation of Cohesive Law

Table 1: Material parameters used to validate the cohesive law implemented

Material	E (GPa)	ν	G_{Ic} (N/mm)	$\sigma_{I,max}$ (MPa)
Isotropic	70.0	0.3	0.2	30

Figure 7: Interface traction *vs.* displacement jump. The blue line is obtained after the initiation of the cohesive segment whereas, the red line is constructed from the initial stiffness.

513 The cohesive law implemented in this paper has been extensively tested in mixed
 514 mode cases. So, the validation here is performed to check whether AMS can repro-
 515 duce the cohesive law. To verify that, two elements, with properties shown in Table
 516 1, are pulled apart as shown in Figure 7. After reaching the critical stress, segmen-
 517 tation nodes are initiated. In this case, only one cohesive segment will be formed
 518 between two elements. Cohesive traction and the displacement from the cohesive
 519 segment are plotted in the graph. The displacement jump at failure marked in Fig-
 520 ure 7 includes the initial displacement jump. The area in the Figure 7 is calculated
 521 as,

$$\text{Area of the triangle} = \frac{1}{2} \times 30 \times 0.0133 = 0.2 \text{ N/mm.}$$

522 In Figure 7, the cohesive segment is initiated adaptively just before reaching the
523 maximum interfacial strength, when damage initiation is impending. At this time of
524 segmentation, the initial displacement jump $[[\mathbf{u}]]_{\text{initial}}$ is calculated with the procedure
525 described in Section 4.5. This initial displacement jump is applied to the cohesive law
526 and the damage evolution, described by linear softening, is calculated by the initiated
527 cohesive segment. The region before segmentation initiation is linear-elastic and this
528 is reconstructed from the initial displacement jump and it is marked in red in Figure
529 7.

530 The total displacement jump at this interface is the summation of the initial dis-
531 placement jump and the displacement jump measured by the cohesive segment after
532 the initiation. At the onset of softening or damage initiation, the total displacement
533 jump is considered elastic. This onset displacement jump is subtracted from the
534 displacement jump at failure (calculated with fracture energy) as well as from the
535 total displacement jump at the interface in the calculation of damage evolution [29].
536 Hence, the damage evolution, modelled with fracture energy and quantified by a
537 damage variable, is unaffected by adaptive initiation.

538 6.2. Benchmark Cases

539 Different test cases such as Double Cantilever Beam (DCB), Three-point End Notched
540 Flexure (3-ENF) and Fixed Ratio Mixed Mode (FRMM) specimens are demonstrated
541 using AMS and the results are compared against analytical solutions given by cor-
542 rected beam theory. The specimen dimensions, shown in Figure 8, and material
543 parameters, mentioned in Table 2, are taken from existing literature [3]. In all the
544 cases, an initial crack length of 35 mm was modelled.

545 The analytical solution used in this paper is based on corrected beam theory [3]. For
546 all the cases shown in Figure 8, experimental results are available in the literature[3].

Table 2: Material parameters for HTA6376/C used in benchmark cases from [3]

E_{11} (GPa)	$E_{22} = E_{33}$ (GPa)	$G_{12} = G_{13}$ (GPa)	G_{23} (GPa)	$\nu_{12} = \nu_{13}$	ν_{23}
120	10.5	5.25	3.48	0.3	0.51

G_{Ic} (N/mm)	G_{IIc} (N/mm)	$\sigma_{I,max}$ (MPa)	$\sigma_{II,max}$ (MPa)	K_I N/mm ³	K_{II} N/mm ³
0.26	1.002	30.0	60.0	10 ⁵	10 ⁵

1- fibre direction 2- transverse direction 3- through thickness direction

547 However, only the analytical solution is compared to show the correlation in a clear
548 way.

549 6.3. Linear AMS

550 In the numerical modelling involving linear AMS, a mesh size of 0.25 mm (600
551 elements) is used in the direction of delamination and a mesh size of 0.5 mm (3
552 elements in each arm of DCB) in the through thickness direction; in total 3600
553 elements were used. A density of 10^{-2} kg/m³ and a time step of size 1.38×10^{-6} s
554 is used in linear AMS. A non-linear strain measure is used in linear AMS. Newton-
555 Cotes quadrature is used for integration points in cohesive elements of linear AMS
556 and a 2×2 quadrature is used. Damping is not applied in the benchmark cases
557 shown in Section 6.3.

Figure 8: Dimensions of different specimens used to demonstrate segmentation

6.3.1. Linear AMS in Mode-I

The initial split length of 35 mm is segmented with a very low interfacial strength and fracture energy. So, the cohesive segments and crack is present from the start of the analysis. This length could have been modelled discretely as a split by duplicating the nodes, but to keep the formulation same for all the benchmark cases, the current method is used.

The significance of the segmentation error defined by equation (33) is illustrated by comparing Figures 9a and 9b. The analysis results of the AMS implementation with linear elements in a DCB model using the procedures described Section 2 is shown in Figure 9b. The AMS is also implemented without the segmentation initiation mentioned in Section 4.3 and initiation based on nodal forces mentioned in Section

(a) DCB load-displacement curves (element size 0.25 mm) obtained with AMS (linear elements) against analytic solution in the absence of segmentation initiation criterion and initiation based on nodal forces.

(b) DCB load-displacement curves (element size 0.25 mm) obtained with AMS (linear elements) against analytic solution.

Figure 9: Load-displacement curves obtained with the DCB test simulation.

569 4.5. The results of that implementation in show in Figure 9a.

570 By comparing the figures, the reduction in the magnitude of oscillations can be
571 easily seen. The load *vs.* displacement curve for the DCB test can be divided into
572 two regions; undamaged response, marked by initial elastic portion, and damaged
573 response, which involves damage propagation. The elastic portion involves damage
574 initiation. The error associated with initiation can be identified with the oscillations
575 in the undamaged response. The initiation based on nodal forces is primarily used
576 to avoid the error and hence reduce oscillation.

577 The oscillations in the damage propagation part have also reduced. In the absence
578 of the proposed segmentation method, errors will propagate from the undamaged
579 response to damaged response. Since the error is avoided in the initiation stage,
580 oscillations have also reduced in damaged response.

581 The shape of the cohesive law [31] and type of solver are variables associated with the
582 oscillations in the damaged response. For the bilinear traction-separation law, if the
583 softening slope is small, the acceleration of nodes and the corresponding oscillations
584 will be reduced. To achieve this, the peak traction can be reduced while keeping the
585 fracture energy same. This technique was used previously [3] as a method to increase
586 the element size within the fracture process zone, but it causes a reduction in the
587 stiffness and the peak load. This technique is not used in the current work, however
588 it is mentioned to show the importance of softening slope on the oscillations in the
589 load *vs.* displacement curve.

590 6.3.2. *Linear AMS in Mode-II*

591 The penetration of arms of ENF specimen is resisted by the use of the cohesive
592 segments with a high penalty stiffness that helps to avoid the penetration. The initial
593 crack length of 35 mm is segmented with cohesive elements of very low fracture energy

Figure 10: 3-ENF load-displacement curves (element size 0.25 mm) obtained with AMS(Linear elements) against analytic solution.

and interfacial strength. From Figure 10, it can be observed that stable initiation of cohesive segments is obtained throughout the initial elastic portion. The peak load is predicted with sufficient accuracy using AMS with linear elements.

6.3.3. Linear AMS in Mixed-mode

The Fixed Ratio Mixed Mode (FRMM) test has both mode-I and mode-II components. The mode ratio is calculated as the ratio between G_I and G_{II} . Based on the fracture energy equations for FRMM, it can be shown that the mode ratio between mode-I and mode-II is 1.33. From Figure 11, it can be seen that stable initiation is obtained in this mixed mode case. This illustrates that the AMS can be applied to wide range of loading cases. The segmentation method follows both the mode-I as well as mode-II in the damage propagation zone.

Figure 11: FRMM load-displacement curves (element size 0.25 mm) obtained with AMS(Linear Elements) against analytic solution.

6.4. Higher Order AMS

To demonstrate the ability of higher order AMS in modelling delamination initiation and propagation, a typical benchmark example of DCB test is chosen. The results are compared against the analytical solution and the numerical modelling result obtained from LS-DYNA using constant stress solid elements (ELFORM - 1) and four integration points cohesive elements (ELFORM - 19). The element formulations in LS-DYNA were chosen to demonstrate the importance of very fine mesh constraints imposed with linear elements.

In the numerical modelling involving higher order AMS and built-in linear elements from LS-DYNA , a mesh size of 1 mm (150 elements) is used in the direction of delamination and a mesh size of 0.75 mm (2 elements in each arm of DCB) in the through thickness direction; in total 600 elements were used. A damping of 10^{-2}

kg/sec is used to dampen the stress oscillations which arises following the failure of cohesive elements. A small magnitude is chosen such that global behaviour is unperturbed.

A critical aspect in the determination of computational cost associated with an explicit analysis is the critical time step size (Δt_{cr}). With larger mesh sizes, a larger magnitude of critical time step size is obtained with higher order AMS and this is presented in Table 3. Δt_{cr} remains same for 0.75 mm and 1.0 mm mesh size in the delamination direction, because the mesh size in the through thickness direction is the limiting dimension and remains constant at 0.75 mm.

A density of 10^{-2} kg/m³ and a time step of size 4.4×10^{-6} s is used in the numerical model with a mesh size of 1 mm in the delamination direction. Furthermore, a mass scaling factor $\alpha = 100$, as mentioned in Section 5.1, is applied to rotational degrees of freedom. A non-linear strain measure is used in higher order AMS. Gauss Lobatto quadrature is used for integration points in cohesive elements of higher order AMS and a 5×5 quadrature is used. Unlike the adaptive modelling performed with Higher order AMS, modelling with linear elements in LS-Dyna is achieved using pre-inserted cohesive elements.

Successful modelling of delamination behaviour with cohesive elements can be estimated with the capability in; (i) modelling of elastic stiffness, (ii) modelling of peak load, (iii) modelling of fracture energy during crack propagation and (iv) modelling the crack propagation with reduced stress oscillations.

The severity of oscillations can be studied with signal-to-noise ratio (SNR). By assuming the analytical solution as signal, SNR can be calculated for the results obtained from numerical modelling.

Table 3: Critical time step size for different mesh sizes used in analysing the DCB example with Higher order AMS (0.75 mm in the through-thickness direction). For reference, the linear AMS time step size for 0.25 mm elements used in Figure 9b is 1.38×10^{-6} s.

Mesh size in the delamination (x) direction (mm)	Critical time step (s)
0.25	1.26×10^{-6}
0.50	2.95×10^{-6}
0.75	4.40×10^{-6}
1.00	4.40×10^{-6}

$$\text{SNR} = 10 \log_{10} \frac{\text{Sum of squared magnitude of signal}}{\text{Sum of squared magnitude of noise}} \quad (47)$$

641 It can be seen evidently from the Figure 12 that the higher order AMS provides good
642 results by satisfying all the points in the four-point criterion; peak load and fracture
643 energy are modelled with a good precision in higher order AMS. Comparison of SNR
644 shows that linear elements produces more oscillations than higher order AMS by a
645 factor of 3.35 (0.652 dB/0.195 dB). The increase in oscillations can be readily linked
646 to the mesh size in the numerical model with linear elements.

647 In higher order AMS, cohesive segments are modelled adaptively whereas linear cohe-
648 sive elements are modelled by pre-inserting them in the mesh. However, results iden-
649 tical to higher order AMS results in Figure 12 can also obtained by pre-inserting ro-
650 tational enabled cohesive segments between compatible continuum elements. Hence,
651 these results are not explicitly plotted in Figure 12.

652 However, the benefits obtained from using higher order AMS need to be discerned

Figure 12: DCB load-displacement curves (element size 1.0 mm) obtained with Higher Order AMS against analytical solution and constant-stress element from LS-DYNA .

further. The improvement in the results could be attributed to multiple factors;
 (i) increase in the integration points in the continuum element, (ii) increase in the
 integration points in cohesive element and (iii) additional degrees of freedom in the
 form of rotations. It is shown in the Section 6.4.1, that the improvement in results is
 primarily due to the rotational degrees of freedom and the benefits of additional inte-
 gration points in a cohesive element can be realised only in the presence of additional
 degrees of freedom such as rotations.

6.4.1. Higher Order AMS - Advantages of Rotational Degrees of Freedom

To further understand the importance of rotations, the following set of numerical
 models are developed with same number of cohesive integration points and compared.

Figure 13: DCB load-displacement curves (element size 1.0 mm) obtained with higher order AMS against different models with same number of integration points in cohesive elements as higher order AMS .

- 663 • Higher order AMS - The results from section 6.4 are used.
- 664 • Higher order AMS without rotational degrees of freedom - This model is same
- 665 as Higher order AMS with the exception of rotational degrees of freedom. In
- 666 the calculation of mid-side nodes using (12) - (14), rotations are set to zero; a
- 667 linear interpolation will be performed.
- 668 • Linear AMS - This model has fully integrated linear continuum elements with
- 669 eight integration points and linear cohesive elements with 25 integration points.

670 It can be observed from the Figure 13 that, despite the presence of same number of
671 cohesive integration points, peak load and fracture energy can be calculated with a

672 good precision and reduced oscillations only using higher order AMS. This can be
673 attributed directly to the presence of additional degrees of freedom in the form of
674 rotations.

675 Comparison of the computational benefits in using higher order AMS over linear
676 elements must be performed using the number of degrees of freedom. However, the
677 benefits in using higher order elements is not just restricted to larger mesh sizes
678 in the delamination direction, but in the through thickness direction as well. This
679 allows modelling a structure with fewer degrees of freedom by using Higher order
680 AMS when compared to linear elements. An example to demonstrate these benefits
681 is shown in Section 7.

682 *6.4.2. Number of Cohesive Integration Points*

683 Various different numerical quadrature schemes have been used in the literature for
684 interface elements [32, 33, 34]. Among quadrature rules such as Newton-cotes (NC)
685 and Gauss-Lobatto (GL), GL is used in the current work as this scheme has been
686 shown to provide improved benefits when large mesh sizes are used [33].

687 In this section, different number of integration points are used in the DCB analysis
688 to determine the optimal number of integration points required; the comparison is
689 shown in Figure 14 . An ' $n \times n$ ' integration scheme means ' n ' integration points in
690 both the dimensions of the cohesive segment.

691 The number of integration points used in the cohesive element with rotations has
692 a significant impact on the crack initiation and propagation. The rotations at the
693 corner nodes are transformed into translations in the mid-side nodes using a trans-
694 formation matrix. The translations describe the crack propagation and the damage
695 calculated based on the cohesive law. By having insufficient integration points, the
696 translations across the interface and the damage may not be calculated accurately.

Figure 14: DCB load-displacement curves (element size 1.0 mm) with 3×3 , 5×5 , 7×7 and 10×10 integration points in cohesive elements used with Higher Order AMS.

It will further influence the moment and damage relationship.

It is necessary to have at least 3×3 quadrature in the cohesive segment to model the quadratic variation. With 3×3 quadrature, significant improvement in results is achieved when compared to linear AMS. For a preliminary analysis, it is possible to start with 3×3 quadrature and the results can be refined with higher order integration schemes.

The 3×3 quadrature is compared against higher order quadrature schemes in Figure 14. As the resolution of the numerical cohesive zone is increased via more integration points, the oscillations in the damage propagation region reduced due to the suppression of unbalanced forces. Significant improvement in results is not obtained

707 after 5×5 quadrature. It can thus be concluded that a 5×5 GL quadrature is suf-
708 ficient to calculate delamination initiation and propagation in the current problem.

709 **7. Homogenisation of Multi-directional Laminates**

710 A continuum element which has rotational DoFs and multiple integration points gives
711 quadratic variation of displacement and can thus model bending and twist within
712 the element which cannot be represented with a linear element formulation. This
713 gives further advantages in the modelling of composites.

714 In the analysis of anisotropic plates, moments and curvatures relationship is repre-
715 sented by a bending stiffness matrix, $\mathbf{D}$. If the matrix is not diagonal, a bending
716 curvature can cause a torsional moment. The off-diagonal terms that can cause such
717 coupling are terms in the last row and column of $\mathbf{D}$ matrix, D_{16} and D_{26} . The 48-
718 DoF hexahedron can model the bend-twist coupling arising out of D_{16} , D_{26} and D_{66}
719 terms.

720 When homogenising a block of plies with linear elements, the bending stiffness will
721 not be captured accurately and ply-by-ply analyses, with more global DoFs are
722 required. The 48-DoF hexahedron can provide a closer approximation to ply-by-ply
723 level results, with a reduced number of DoFs.

724 To homogenise the laminate, 3D lamination parameters are used. For modelling
725 thick composite laminates, 3D lamination parameters were derived in [35], as the
726 conventional lamination parameters use only a 2D assumption. A laminate configu-
727 ration with ‘n’ number of layers can have ‘n’ different ply orientations which makes
728 a large design space. However, with the 4 lamination parameters, the design space
729 reduces to a 4-dimensional space and helps in calculating the stiffness of composites.
730 The homogenisation can also be obtained by using the rotation matrix and the ply
731 orientation. The homogenisation obtained from both of these methods are essentially

Figure 15: Load-displacement curves for unbalanced layup DCB with homogenised higher-order AMS against ply-by-ply and homogenised models in LS-DYNA (ELFORM1)

732 same. However, the use of lamination parameters is an easier method to sample the
733 design space.

734 7.1. DCB with Unbalanced Layup and Higher Order AMS

735 The continuum element used in the current work (48-DoF hexahedron) has more
736 DoFs and integration points than a linear brick element (24-DoF hexahedron). So,
737 it can give better approximation to the field variables. Ply level modelling per-
738 formed using constant stress solid element of LS-DYNA is compared against Higher
739 Order AMS where homogenisation is performed using lamination parameters. It is
740 also compared against linear brick elements with homogenised material properties.

741 For linear elements, the homogenisation is obtained by the conventional method,
742 *i.e.* weighted average of in-plane stiffness terms after transformation to the global
743 reference frame.

744 The layup is chosen such that it will have bend-twist coupling. Since DCB is a
745 displacement controlled test, the arms of the DCB will not experience twist in terms
746 of displacement. However, the nodal forces along the width of the DCB specimen
747 will be different and a planar assumption would be invalid. A width of 10 mm is
748 modelled in all the cases. The layup used is $(45_2, 0_2)_{3S}$.

749 The comparison is shown in Figure 15. Higher order AMS gives very good approx-
750 imation to initial stiffness when compared to the ply-by-ply model. The peak load
751 and damage propagation is captured with sufficient accuracy. The reduction in the
752 oscillations in the damage propagation zone for Higher order AMS when compared
753 to Figures 12 and 14 is due to the modelling of additional elements in the width
754 direction.

755 The homogenised model using constant stress element does not give a good approx-
756 imation to initial stiffness and damage propagation, which clearly defined a require-
757 ment for ply-by-ply level modelling or higher order formulation, in the case of more
758 complex layups.

759 Element sizes for analysing the DCB with unbalanced layup, corresponding to Fig-
760 ure 15, is presented in Table 4. It can be observed from Table 4 that Higher order
761 AMS models the problem with 50 % less number of degrees of freedom and produces
762 a result closer to ply-by-ply level which requires high computational effort.

763 8. Conclusions

764 A novel method for on-the-fly cohesive segmentation of quadratic (48-DoF) hexahe-
765 dral continuum elements has been developed and validated, termed Adaptive Mesh

Table 4: Element size for DCB analysis with unbalanced layup

Model	l_1 (mm)	l_2 (mm)	l_3 (mm)	No. of global DOF
Homogenised model with higher order AMS	1.0	1.0	0.75	49830
Homogenised model with linear elements	0.25	1.0	0.75	99165
Ply-by-ply Model with linear Elements	0.25	0.125	0.125	1.75×10^6

DOF - Degrees of Freedom l_1 - Element length in x -direction (longitudinal);

l_2 - Element length in y -direction (transverse);

l_3 - Element length in z -direction (thickness).

766 Segmentation (AMS). When combined with additional nodal rotation DoFs it can
767 reduce the ‘meshing burden’ and mesh size constraints for modelling delamination
768 failure in composite structures. The method models discontinuity using the standard
769 shape functions and reduces the residuals or errors that arise out of initiating the
770 cohesive segments. Initiation methods based on nodal forces were introduced to cir-
771 cumvent the errors. Test cases are shown in mode-I, mode-II and mixed-mode that
772 demonstrate the applicability of method.

773 The cohesive segment formulation developed for use after initiation specifically aimed
774 to increase the resolution of the numerical cohesive zone via the use of rotational
775 DoFs. When combined with AMS, the mesh size constraint in the cohesive zone has
776 been relaxed. The addition of integration points results in the resolution of cohesive
777 zone. The length of numerical cohesive zone is small when compared to mode-II
778 [3]. Since the cohesive zone length in mode-I delamination is much smaller than
779 in mode-II, mode-I is the critical case for defining the mesh size. The higher order
780 AMS was thus demonstrated with a mode-I DCB test. It was found that the new

781 cohesive segment with a 3×3 quadrature scheme gave a significant improvement
782 in the result, with the benefits of adding further integration points being not very
783 pronounced above a 5×5 quadrature scheme. A 3×3 quadrature scheme can be
784 used for preliminary analysis before refining with more integration points.
785 The introduction of rotational DoFs to the solid elements gives further advantages
786 of using coarse meshes, in that bend/twist coupling effects can still be implemented
787 with homogenized material properties. This is achieved using 3D lamination param-
788 eters. Despite having significantly reduced global DoFs compared to a ply-by-ply
789 level model, good results were obtained for a demonstration case of a DCB with an
790 unbalanced layup.
791 Overall the developments introduced here present a significant step forward for de-
792 lamination failure analysis of large composite structures, where mesh size can be a
793 limiting factor on the use of Cohesive Zone Modelling (CZM) of interface failure.
794 The formulation presented here has been implemented in an explicit dynamic finite
795 element software, so is well suited for simulation of impact and high rate events,
796 which are challenging, but critical cases for the aerospace and automotive industries.

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