



Title	Development of a GPGPU-parallelized FDEM based on extrinsic cohesive zone model with master-slave algorithm
Author(s)	Maeda, Yutaro; Ogata, Sho; Fukuda, Daisuke et al.
Citation	Computers and Geotechnics. 2024, 166, p. 105942
Version Type	AM
URL	<a href="https://hdl.handle.net/11094/93482">https://hdl.handle.net/11094/93482</a>
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1      **Development of a GPGPU-parallelized FDEM based on Extrinsic**  
2      **Cohesive Zone Model with Master-Slave Algorithm**

3

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20 **Abstract**

21 This paper proposes a novel general-purpose graphic-processing-units (GPGPU) parallel  
22 computing approach to an extrinsic cohesive zone model (ECZM) - based combined finite-  
23 discrete element method (FDEM) for simulating rock fracturing. The proposed GPGPU-  
24 parallelized ECZM-FDEM incorporates a master-slave algorithm as an alternative to the  
25 complex adaptive remeshing process, which is usually used in ECZM but has prevented it from  
26 being parallelized using GPGPU. Numerical experiments of the Brazilian test and uniaxial  
27 compression test of rocks are conducted to compare the proposed ECZM-FDEM with a  
28 GPGPU-parallelized FDEM using the intrinsic cohesive zone model (ICZM-FDEM). Results  
29 show that the proposed method can not only overcome the accuracy degradation of calculated  
30 stresses and deformations that is inevitable in ICZM-FDEM but also reasonably simulate rock  
31 fracturing. Moreover, the proposed GPGPU-parallelized ECZM-FDEM achieves a maximum  
32 relative speed-up of 13 times over GPGPU-parallelized ICZM-FDEM due to efficient contact  
33 calculations and larger stable time steps. Thus, the proposed ECZM-FDEM is more physically  
34 sound and more computationally efficient compared with ICZM-FDEM, which may contribute  
35 to the further developments of FDEM.

36 **Keywords:**

37 Rock fracturing, 2-D FDEM, Extrinsic Cohesive Zone Model (ECZM), Intrinsic Cohesive Zone  
38 Model (ICZM), GPGPU parallel computation

39

40

41 **1. Introduction**

42 Reasonable numerical modelling of rock fracturing process is necessary for a variety of  
43 geotechnical applications in civil, mining, and energy fields. Recently, hybrid numerical  
44 methods that incorporate the advantages of both continuous-based and discontinuous-based  
45 methods have received significant attention. The combined finite-discrete element method  
46 (FDEM) (Munjiza, 2004) is one of the most popular hybrid methods, which combines the finite  
47 element method (FEM) and the discrete element method (DEM), and has been applied to various  
48 rock fracture problems (e.g. An et al., 2017; Elmo and Stead, 2010; Fukuda et al., 2019; Guo et  
49 al., 2016; Hamdi et al., 2014; Knight et al., 2020; Lisjak et al., 2014; Lisjak et al., 2018;  
50 Mahabadi et al., 2012; Rock field, 2023; Vlachopoulos and Vazaios, 2018; Yan et al., 2022a).  
51 FDEM is based on the explicit time integration scheme and can simulate the deformation  
52 process of continuous rocks, the transition process from a continuum to a discontinuum (i.e.,  
53 fracture initiations and propagations in rocks), and the contact process between material surfaces  
54 including newly created macroscopic fracture surfaces (i.e., discontinuous deformation process).  
55 Thus, FDEM is suitable for the simulations of various engineering applications involving in  
56 highly non-linear problems which are characterized by the series of complex rock fracturing  
57 processes. Historically, two representative FDEM codes, i.e., open-source "Y-code" (Munjiza,

58 2004) and commercial "ELFEN code" (Rock field, 2023) were developed. Since then, various  
59 FDEM codes have been developed including "HOSS" code (e.g. Knight et al., 2020; Rougier et  
60 al., 2014), "Irazu" code (e.g. Geomechanica, 2023; Lisjak et al., 2018), "MultiFracS code" (Yan  
61 et al., 2022a, 2022b), "Solidity" code (e.g. Guo et al., 2016; Latham et al., 2012), "Y-Geo" code  
62 (e.g. Mahabadi et al., 2012; Tatone and Grasselli, 2015), and the authors' "Y-HFDEM code" (e.g.  
63 Liu et al., 2015; Fukuda et al., 2019, 2020a) in alphabetical order among others, and the  
64 applications of these codes to rock fracture problems have been reported (see Knight et al., 2020  
65 for a comprehensive review on the history of recent FDEM developments).

66 To model rock fracturing process, almost all the FDEM codes, except for ELFEN, in the  
67 recent literature utilizes the cohesive zone model (CZM) (Barenblatt, 1962; Dugdale, 1960) by  
68 separating the boundaries or inside of continuum elements and inserting cohesive elements at  
69 separated portions. In CZM, rock fracturing is modeled by the softening of cohesive tractions  
70 acting on the initially zero-thickness cohesive elements according to their relative opening and  
71 sliding, i.e., traction-separation law. Note that ELFEN models material softening by degrading  
72 tensile strengths associated with the increments of inelastic extensional strains under the  
73 assumption that quasi-brittle fracture is mainly extensional in nature, and thus does not use CZM  
74 (Klerck, 2000; Klerck et al., 2004). In ELFEN, when the degraded tensile strength reaches zero,  
75 a discrete fracture is introduced. For CZM implementations, there are three main approaches:  
76 Intrinsic CZM (ICZM), Extrinsic CZM (ECZM) (Fukuda et al., 2020b; Pandolfi and Ortiz,

77 2002; Papouli et al., 2003; Zhang et al., 2007), and discontinuous Galerkin-based CZM  
 78 (DGCZM) (Nguyen, 2014). Note that the so-called universal CZM (UCZM) has been proposed  
 79 and implemented in HOSS code. However, since the details of the UCZM have not been  
 80 publicly available in the journal papers, UCZM is not reviewed here. Hereafter, we only focus  
 81 on reviewing ICZM, ECZM and DGCZM. Although all these approaches are the same in terms  
 82 of the post-peak behavior in the traction-separation law, they are different in terms of the timing  
 83 of inserting the cohesive elements and corresponding implementations.

84

85 Table. 1. Classification of FDEM codes according to parallelization and CZM scheme.

Parallelization schemes		CZM schemes	
		ICZM-based	ECZM-based
CPU-based	MPI	Lukas et al., 2014 (Y-based) Lei et al., 2014 (HOSS <sup>※</sup> )	—
	Shared Memory	Xiang et al., 2016 (Solidity)	—
GPGPU-based		Lisjak et al., 2018 (Irazu)	
		Fukuda et al., 2019 (Y-HFDEM)	
		Liu et al., 2019 (Y-based)	—
		Liu et al., 2021, 2022(Y-based)	
		Yan et al., 2019, 2022a (MultiFracS)	

※ UCZM is also available.

86

87 In ICZM, cohesive elements are inserted at all boundaries of continuum elements from the  
88 start of the simulation even if no damage has occurred. Since there is no need to update mesh  
89 connectivity (i.e., adaptive remeshing) during the simulation, it is easy to implement parallel  
90 computation schemes to enhance computing performances. In fact, the majority of the existing  
91 FDEM codes are based on ICZM (hereafter, ICZM-FDEM), and have been actively accelerated  
92 by parallel computations. Table. 1 lists the FDEM codes that have incorporated various parallel  
93 computations up to present, including FDEM codes based on ECZM (hereafter, ECZM-FDEM)  
94 which are to be discussed later in this section. As shown in Table 1, various parallel schemes  
95 have been implemented for ICZM-FDEM. Among them, the CPU-based parallelization  
96 schemes are implemented for FDEM using multiple CPUs, which includes FDEM based on  
97 relatively large-scale parallel computations using message-passing interface (MPI) (Lei et al.,  
98 2014; Lukas et al. 2014) and relatively small-scale parallel computations using shared memory  
99 programming such as OpenMP (Xiang et al., 2016). However, since the CPU-based  
100 parallelization requires multiple CPU cores, a massive computing system such as a  
101 supercomputer with enormous resources are needed to achieve high performance parallel  
102 computing. On the other hand, several cases of FDEM parallelization have incorporated general-  
103 purpose graphic-processing-units (GPGPU), which have many cores within a single GPGPU  
104 card and can be installed in a personal computer (PC) or a workstation (e.g., Fukuda et al., 2019;

105 Lisjak et al., 2018; Liu et al., 2019; Liu et al., 2021, 2022; Yan et al., 2022a). GPGPU-based  
106 parallelization has the advantages of a relatively lower-cost setup and cheaper energy  
107 consumption as compared to CPU-based parallelization. With this background, the ICZM-  
108 FDEM based on GPGPU parallel computation has been actively developed. However, ICZM-  
109 FDEM has a serious drawback since an artificial elastic response constrained by a finite stiffness  
110 (i.e., cohesive penalty) must be introduced to reasonably handle the continuous deformation  
111 process of rocks before any crack initiations. This drawback makes the stable time step  $\Delta t$  in the  
112 ICZM-FDEM analysis become much smaller than that in the explicit FEM without cohesive  
113 elements. Moreover, it causes the problem of increasing the bulk compliance of the modelled  
114 rocks since the cohesive elements can open/slide even in the intact/continuous deformation  
115 regime (see the discussion in Fukuda et al., 2020b in the case of rock dynamics problems).  
116 Furthermore, because the cohesive elements are inserted in the whole domain from the  
117 beginning of the simulation, one controversial issue arises: when should the contact processing  
118 (i.e., the contact detection and contact force calculation) by DEM be initiated for the continuum  
119 elements located inside the solid body? One of the solutions is the brute-force contact activation  
120 approach (BCAA), in which the contact is processed for all separated continuum elements from  
121 the start of the simulation and which is used in many ICZM-FDEM codes. However, Fukuda et  
122 al. (2021) and Mohammadnejad et al. (2020) pointed out BCAA was not only physically  
123 unreasonable but also required enormous computational costs, which may still be too much even

124 with the parallel computation. On the contrary, the adaptive contact activation approach  
125 (ACAA) utilized by Guo (2014) and semi-ACAA (Fukuda et al., 2021) only activate the contact  
126 processing at locations where the cohesive elements are completely/partially broken (i.e.,  
127 physical cracks appear). Through this way, the shortcomings of BCAA mentioned above are  
128 solved, and ACAA and semi-ACAA can succeed in reducing the computational cost  
129 significantly compared to BCAA. In summary, ICZM-FDEM has the extremely attractive aspect  
130 of easy parallelization but also suffers from the drawbacks mentioned above.

131 One solution to these problems inherent in ICZM-FDEM is ECZM-FDEM, in which, the  
132 cohesive elements are inserted on the boundaries of the continuum elements only when and  
133 where the given failure criteria are satisfied. In this sense, ECZM-FDEM is simply a pure FEM  
134 without any cohesive elements at the intact/continuous deformation regime of rocks. Therefore,  
135 the problems of too small stable time step and increasing bulk compliance inherent in ICZM-  
136 FDEM never occur. Moreover, because the contact calculations are unnecessary inside the solid  
137 body before the cohesive elements are inserted, the concept of BCAA does not appear in ECZM-  
138 FDEM, while only ACAA or semi-ACAA is applicable. Thus, the excessive computation costs  
139 inherent in ICZM-FDEM are overcome in ECZM-FDEM. However, the developments and  
140 applications of ECZM-FDEM are extremely limited to present and most of them are based on  
141 the complex adaptive remeshing required when inserting cohesive elements during the  
142 calculation in ECZM-FDEM (e.g. Fukuda et al., 2020b; Rock field, 2023) including ECZM-

143 based pure FEM (Fukuda et al., 2020b; Pandolfi and Ortiz, 2002; Papouli et al., 2003; Zhang  
144 et al., 2007). For example, Fukuda et al. (2020b) implemented a three-dimensional (3-D)  
145 ECZM-FDEM and applied it to model the dynamic tensile fracture tests of rocks utilizing  
146 sequential Fortran 90. However, the remeshing algorithm used in that code is sequential and it  
147 has been challenging or impossible to directly extend it to the GPGPU parallelization. Even in  
148 the reported cases of ECZM-based pure FEM, only MPI parallel implementations (Espinha et  
149 al., 2013; Dooley et al., 2009) have been reported. In sum, as shown in Table. 1, there are no  
150 applications of GPGPU parallel computation to ECZM-FDEM till this moment.

151 In addition to ECZM for the possible solution to the inherent issues in ICZM-FDEM,  
152 DGCZM "weakly enforces the continuity of the displacements across cohesive elements at the  
153 undamaged state which are active in ICZM-FDEM" using two control parameters  $\theta_{DG}$  and  $\alpha$   
154 (refer to Nguyen, 2014 for the explanation of these two parameters), and thus the GPGPU  
155 parallel implementation of DGCZM is very easy as that of ICZM. However, there has been no  
156 research on the application of DGCZM to FDEM, and thus further research is needed. Besides,  
157 as implied by the point "weakly enforce the continuity", a slight reduction in the precision of  
158 modelling the continuous deformation process using DGCZM is inevitable compared to ECZM  
159 although DGCZM may bring about a significant improvement over ICZM for the modelling of  
160 the continuous behavior.

161 In view of the literature review above, it should be significantly valuable if GPGPU-

162 parallel ECZM-FDEM can be developed with any relative ease. To achieve it, this study  
163 attempts to extend the concepts proposed in Cai et al. (2023), Dooley et al. (2009), Maeda et al.  
164 (2022) and Woo et al. (2014 & 2019) to GPGPU parallel computation. Dooley et al. (2009)  
165 proposed a 2-dimentional (2-D) ECZM-based pure FEM in MPI parallel computing framework,  
166 in which all boundaries of continuum elements are physically separated as those in ICZM at the  
167 onset of the simulation. In this method, all nodes at the same location (hereafter “detached  
168 nodes”) are conceptually tied with each other, which includes not only the initial FEM nodes  
169 but also these nodes generated from the insertion of cohesive elements. Suppose a FEM node  
170 “ $i$ ” before the insertion of any cohesive elements is detached into a group of  $N$  detached nodes  
171 “ $i_0 \sim i_{N-1}$ ” (hereafter “node group”) generated after the insertion of cohesive elements. One  
172 detached node is then considered as the representative node, i.e. master node (M-node) while  
173 the all other detached nodes are set as copy nodes, i.e. slave nodes (S-nodes) in each node group.  
174 After that, pure FEM simulation can be achieved by assembling the masses and nodal forces of  
175 all S-nodes in the same node group into the corresponding M-node and solving the equations of  
176 motion for this M-node. In this way, the cohesive elements can be completely dormant before  
177 any crack initiation. Dooley et al. (2009) further demonstrated that the cohesive elements could  
178 be adaptively inserted/activated by updating the relation between M-node and S-node (M-S  
179 relation) “ $i_0 \sim i_{N-1}$ ” in the same node group. Unfortunately, the updating algorithm of the M-S  
180 relation (hereafter M-S algorithm) was not sufficiently described in Dooley et al. (2009)

181 although it was the most crucial part of the proposed method. Later, Woo et al. (2014 & 2019)  
182 proposed a method very similar to ECZM, which was called as the selective activation of ICZM.  
183 As in Dooley et al. (2009), this method constrains the detached nodes belonging to the same  
184 node group to a representative node (multi-point constraints, i.e., MPCs) to realize a calculation  
185 accuracy equivalent to pure FEM. Then, the MPCs surrounding the continuum element  
186 boundary where fracture is "likely" to occur are released. However, this method has not been  
187 parallelized. In addition, neither Dooley et al. (2009) nor Woo et al. (2014 & 2019) focused on  
188 FDEM. More recently, Cai et al. (2023) and Maeda et al. (2022) extended the M-S algorithm  
189 originally proposed by Dooley et al. (2009) to FDEM to develop ECZM-FDEM for rock  
190 mechanics applications. However, only sequential computations are implemented in both Cai et  
191 al. (2023) and Maeda et al. (2022) while a GPGPU parallel implementation of ECZM-FDEM  
192 based on the M-S algorithm has not been achieved yet. In view of the background reviewed  
193 above, this paper proposes a GPGPU-parallelized ECZM-FDEM on the basis of the M-S  
194 algorithm in Cai et al. (2023), Dooley et al. (2009) and Maeda et al. (2022) without adaptive  
195 remeshing and implements it in Y-HFDEM code to simulate rock fracturing process.

196 The remaining of this paper is organized as follows. Section 2 describes the methodology  
197 and numerical implementation of GPGPU-parallelized ECZM-FDEM with the M-S algorithm.  
198 Section 3 verifies the GPGPU-parallelized ECZM-FDEM by applying it to simulate the rock  
199 fracturing process in the conventional laboratory tests. The obtained results are discussed

200 through various comparative studies between the GPGPU implementations of both 2-D ICZM-  
201 FDEM (Fukuda et al., 2019) and 2-D ECZM-FDEM with M-S algorithm. Section 4 concludes  
202 the achievements of this study and points out the issues for future study.

203

204 **2. GPGPU-based ECZM-FDEM with Master-Slave Algorithm**

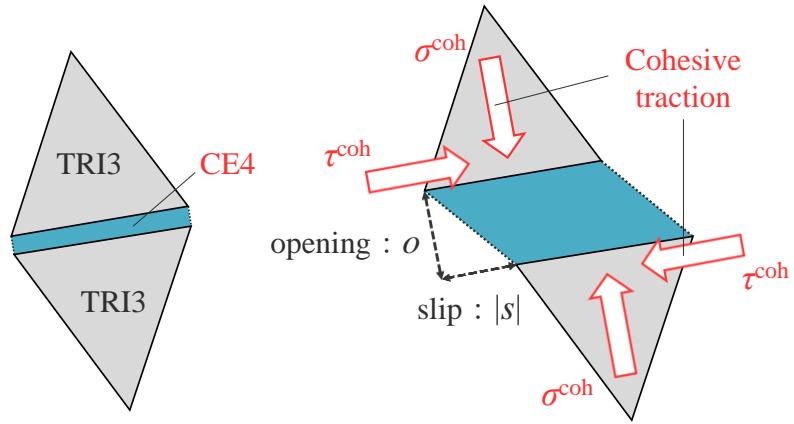
205 2.1. ECZM-FDEM with Master-Slave Algorithm

206 In this study, the GPGPU-parallelized ECZM-FDEM is realized in Y-HFDEM code (Liu et  
207 al., 2015; Fukuda et al., 2019) by newly incorporating the powerful algorithm that can fully  
208 consider the features of ECZM without complicated adaptive remeshing. This is achieved by  
209 utilizing the GPGPU-parallelized ICZM-FDEM utility which is already available in Y-HFDEM  
210 code (Fukuda et al., 2019). This paper only focuses on 2-D problems and its 3-D extension is  
211 considered as our future task. Although all simulations in this paper are conducted under the  
212 plane strain condition, it should be emphasized that the proposed M-S algorithm is applicable  
213 under both the plane strain and the plane stress conditions. The tensile and compressive stresses  
214 are regarded as positive and negative, respectively, which holds true throughout the paper unless  
215 otherwise stated.

216 FDEM has to deal with the following three important processes in order to simulate rock  
217 fracturing, (i) continuous deformation of the intact rock, (ii) transition from continuum to  
218 discontinuum (i.e. fracture initiation and propagation) and (iii) contact between solid surfaces

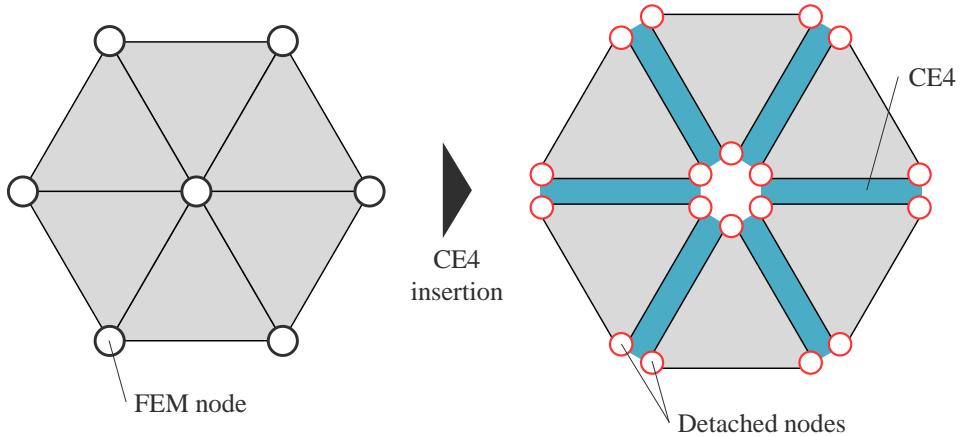
219 including newly generated discontinuities upon rock fracturing. FDEM models the three  
220 processes (i)~(iii) through continuum mechanics, non-linear fracture mechanics based on CZM  
221 (Barenblatt, 1962; Dugdale, 1960) and contact mechanics (Munjiza, 2004), respectively. The  
222 difference between the traditional ICZM-FDEM and the proposed ECZM-FDEM with M-S  
223 algorithm (hereafter, MS-ECZM-FDEM) lies mainly in the handling of CZM and the process  
224 of assembling nodal forces from S-nodes to their M-nodes, which will be explained below.

225 In MS-ECZM-FDEM, the nodal masses and nodal forces are calculated through the  
226 computation of the aforementioned processes (i)~(iii) in each time step. The core idea of MS-  
227 ECZM-FDEM is that the all the continuum elements (which are 3-node triangle elements  
228 (TRI3s) in this study) are already detached by the insertion of initially zero-thickness 4-node  
229 cohesive elements (CE4s) at the onset of the simulation which is exactly same as the ICZM-  
230 FDEM (see Figs. 1 and 2). Thus, the proposed developments can be easily implemented into  
231 any existing ICZM-FDEM codes such as open source Y-code (Munjiza, 2004) and GPGPU-  
232 based Y-HFDEM code (Fukuda et al., 2019). The nodes generated upon the insertion of CE4s  
233 are “detached nodes” as mentioned in Section 1. In addition, Fig. 3 shows the concept of “node  
234 group” mentioned in Section 1, which consists of the detached nodes originally belonging to the  
235 same FEM node before the insertion of CE4.



236

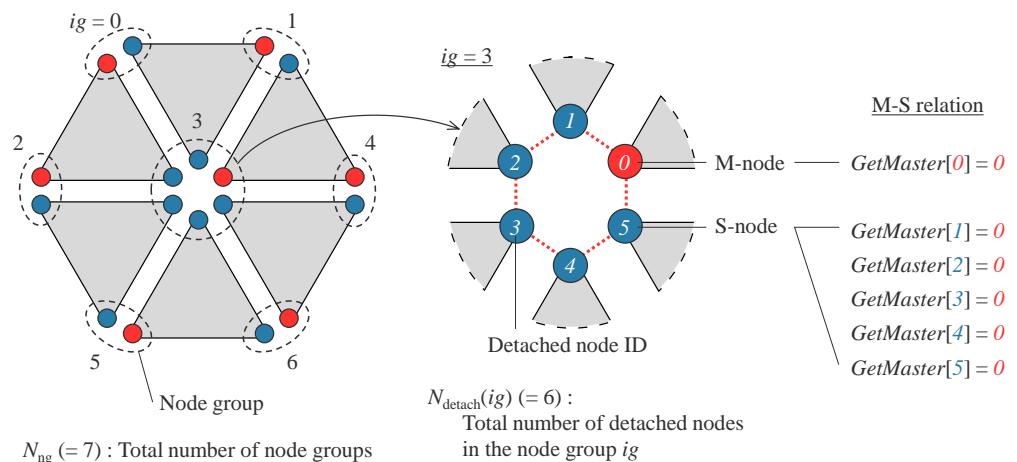
237 Fig. 1. Topological relation of TRI3s and CE4 (left) and overview of cohesive tractions with  
238 respect to opening and slip of CE4 in CZM (right).



239

240 Fig. 2. The concept of detached nodes.

241



242

243 Fig. 3. The concept of node groups and M-S relation.

244

245 With these concepts in mind, we first explain how the aforementioned processes (i) and

246 (iii) are modelled in the framework of MS-ECZM-FDEM while the treatment of the process (ii)

247 is provided later. Let us first explain the case that the target problem only consists of multiple

248 discrete bodies “without any fractures”, in which each discrete body is purely continuous and

249 only the continuous deformation of TRI3s in each discrete body (process (i)) and the contact

250 between the discrete bodies (process (iii)) are involved. Since all nodes are detached in the MS-

251 ECZM-FDEM, let  $N_{\text{detach}}$  be the total number of detached nodes in the target system. It should

252 be noted that  $N_{\text{detach}}$  is the same as the total number of nodes in the case of ICZM-FDEM. Let

253 us consider a single node group “ $ig (= 0, 1, 2, \dots, N_{\text{ng}}-1)$ ” where  $N_{\text{ng}}$  is the total number of node

254 groups in the system, and  $N_{\text{ng}}$  is exactly same as the total number of FEM nodes before the

255 insertion of CE4s. The node group  $ig$  consists of  $N_{\text{detach}}(ig)$  detached nodes where  $N_{\text{detach}}(ig)$  can

256 be readily available from any existing ICZM-FDEM codes. To realize the pure continuous

257 deformation within each discrete body, we apply the following M-S algorithm. In each node

258 group  $ig$ , a single detached node is considered as the M-node while all other detached nodes in

259 the same node group  $ig$  are assigned as the S-nodes to the M-node of  $ig$  (see Fig. 3). In terms of

260 implementations, we first introduce a key data structure for the M-S node relation named

261 “*GetMaster[i]*” for each detached node  $i (= 0, 1, 2, \dots, N_{\text{detach}}-1)$  which literally stores the

262 information of the M-node of the detached node  $i$  (see Fig. 3). The following rules are then  
263 assigned. If a detached node  $i$  satisfies the condition “ $GetMaster[i] = i$ ”,  $i$  is the M-node.  
264 Otherwise, if a detached node  $i$  satisfies the condition “ $GetMaster[i] = j (j \neq i)$ ”,  $i$  is the S-node  
265 whose M-node is  $j$ . The construction of “ $GetMaster$ ” is the key to the successful implementation  
266 of MS-ECZM-FDEM. For the stage involving with no fracturing, “ $GetMaster$ ” can be readily  
267 constructed using the existing ICZM-FDEM code. In addition, at the onset of the FDEM  
268 simulation, initial and current nodal coordinates as well as initial nodal velocities are set to be  
269 same between a M-node and their S-nodes in each node group. For the aforementioned process  
270 (i), this study assumes that each TRI3 obeys the isotropic hyper-elastic solid with viscous  
271 damping (see. Eqs. (2) and (3) in Fukuda et al., 2020a) under plane-strain condition and Cauchy  
272 stress tensor  $\sigma_{ij}$  is computed in each TRI3. Then,  $\sigma_{ij}$  is converted to the equivalent nodal force  
273  $\mathbf{f}_{int}$  [N], and  $\mathbf{f}_{int}$  is assembled to each detached node in the TRI3. When each TRI3 is processed,  
274 lumped nodal mass  $\mathbf{M}$  [kg] is also computed and is assembled to detached nodes in the TRI3. It  
275 must be noted that, at this stage, the assembling of nodal force is processed on the basis of each  
276 detached node and we can directly utilize the existing ICZM-FDEM code without any  
277 modification. For the aforementioned process (iii), the contact between two discrete bodies are  
278 handled by that between the elements, i.e., TRI3s in this study, used to discretize the two discrete  
279 bodies based on the potential contact force theory proposed by Munjiza (2004). When any  
280 overlap between two TRI3s is detected, the exact overlapping shape is computed.

281 Correspondingly, the repulsive normal contact forces are computed based on the contact  
 282 potential, which is determined from the overlapping area (see Munjiza (2004) for full detail),  
 283 along with the contact friction force based on the Coulomb type friction law. Then, the computed  
 284 contact force is converted to the equivalent nodal force  $\mathbf{f}_{\text{con}}$  [N], which is assembled to each  
 285 detached node by directly utilizing the existing ICZM-FDEM code without any modification. If  
 286 any external load (such as water pressure or gravity) is involved in the target problem, the  
 287 equivalent nodal force  $\mathbf{f}_{\text{ext}}$  [N] is assembled to each detached node in the same way.

288 Finally, using the aforementioned M-S relation “*GetMaster*”,  $\mathbf{M}$ ,  $\mathbf{f}_{\text{int}}$ ,  $\mathbf{f}_{\text{ext}}$  and  $\mathbf{f}_{\text{con}}$  of  
 289 detached nodes are assembled to their M-nodes, and the resultant equation of motion only for  
 290 each M-node is solved in the explicit time integration scheme as given by Eq. (1):

$$291 \quad \mathbf{M} \frac{\partial^2 \mathbf{u}}{\partial t^2} = \mathbf{f}_{\text{ext}} - \mathbf{f}_{\text{int}} + \mathbf{f}_{\text{con}} \quad (1)$$

292 where  $\mathbf{u}$  [m] is the nodal displacement and  $t$  [s] is the time. After the update of nodal information  
 293 for M-nodes, the updated nodal velocity and current nodal coordinates of each M-node are  
 294 copied to their S-nodes for the following timesteps to utilize the existing ICZM-FDEM code  
 295 without any modification. In this way, the processes (i) and (iii) can be simulated as if no active  
 296 CE4s exist in the system and each discrete body behaves as pure continuum as that in pure FEM.  
 297 Using this approach, the issue of the increase of the bulk artificial compliance in the ICZM-  
 298 FDEM can be completely overcome. Moreover, since the CE4s become completely dormant at  
 299 this stage (Hereafter, these dormant CE4s before the onset of crack initiations are simply called

300 “dormant CE4s”), we only need to consider TRI3s on the surface of each discrete body as  
 301 potential contact candidates subjected to the contact detection. Thus, the concept of BCAA  
 302 utilized in FDEM literature can be completely avoided. As long as each discrete body is intact  
 303 without any fracturing, the M-S relation “*GetMaster*” does not need to be updated. The  
 304 important remaining tasks are “how the dormant CE4s are activated to model the crack  
 305 initiation”, “how the M-S relation *GetMaster* is updated upon crack initiation” and “how the  
 306 ECZM is implemented in FDEM” in the framework of GPGPU computing, which are explained  
 307 in the remainder of this section.

308 The activation timing of the dormant CE4s is determined based on the normal and shear  
 309 tractions acting on the boundary of two TRI3s where the target dormant CE4 is located. Note  
 310 that the dormant CE4 is exactly the line element coinciding with the boundary of the TRI3s.  
 311 Thus, we interpolate the Cauchy stress tensor  $\sigma$  on the boundary of TRI3 by taking the average  
 312 of those in the surrounding two TRI3s. Let  $\mathbf{n}$  denote the outward unit normal vector of the  
 313 boundary of TRI3, the normal traction ( $\sigma_n = (\sigma \mathbf{n}) \cdot \mathbf{n}$ ) and shear traction ( $\tau_n = \|\sigma \mathbf{n} - \sigma_n \mathbf{n}\|$ ) acting  
 314 on the boundary can be calculated. When these values reach either the given tensile strength or  
 315 Mohr-Coulomb shear strength set at the boundary of TRI3, tensile or shear failures occur,  
 316 respectively, and the dormant CE4 is activated. The failure criteria are presented as follows:

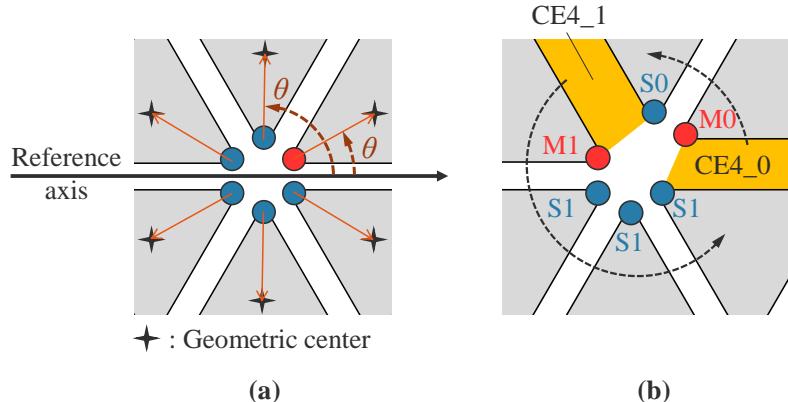
$$\begin{cases} F_1 \equiv \sigma_n - f_t \\ F_2 \equiv |\tau_n| - \langle c - \sigma_n \tan \phi \rangle \end{cases} \quad (2)$$

318 where  $f_t$  [Pa],  $c$  [Pa] and  $\phi$  [degree] are tensile strength, cohesion, and internal friction angle of

319 a CE4, respectively. Through Eq. (2), crack initiation, i.e., the activation of the dormant CE4, is  
320 assumed to occur when either  $F_1 \geq 0$  or  $F_2 \geq 0$  is satisfied.

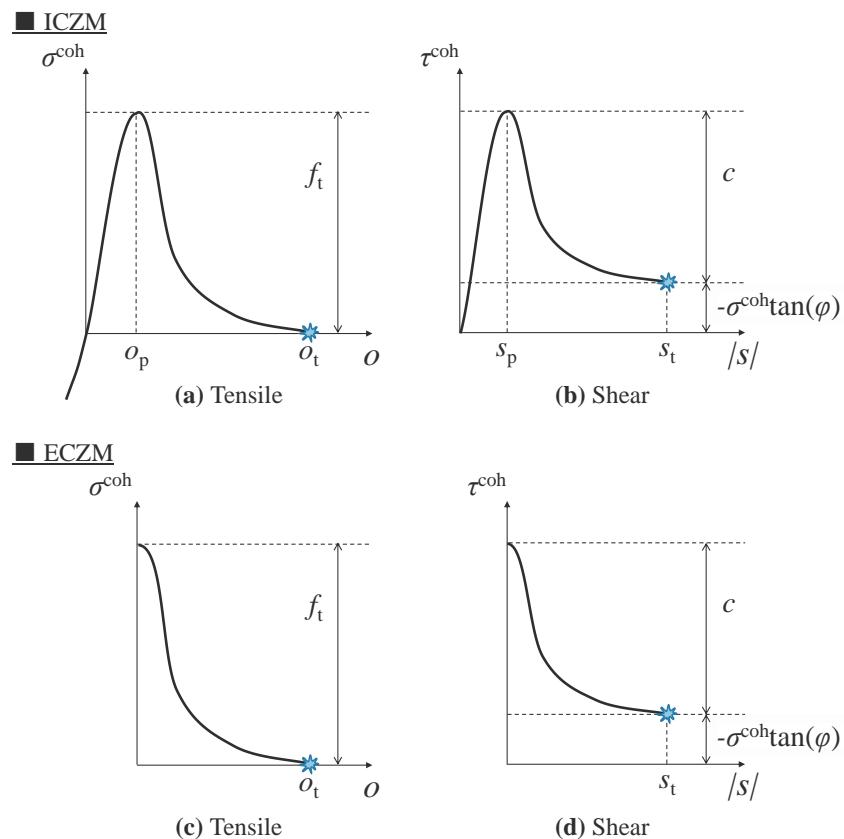
321 Once any dormant CE4s are activated, the M-S relation “*GetMaster*” must be adaptively  
322 updated. We follow the M-S algorithm introduced by the authors (Maeda et al., 2022). As  
323 depicted in Fig. 4, the counterclockwise search around the reference axis pointing the positive  
324  $x$  direction is performed for the node group  $ig$  ( $=0, 1, 2, \dots, N_{ng}-1$ ). The detached nodes in each  
325 node group are sorted counterclockwise based on the geometric center of TRI3s to which each  
326 detached node member in the same node group belongs. Starting the search from one of the  
327 dormant CE4s (CE4\_0 in Fig. 4) which has just satisfied the aforementioned failure criteria, the  
328 first encountered detached node immediately after passing across the CE4\_0 is considered as  
329 the first M-node (M0 in Fig. 4). Then, before the searching passes across the other activated  
330 CE4 (CE4\_1 in Fig. 4), all the encountered detached nodes are assigned to S-nodes (S0 in Fig.  
331 4) to M0. Then, in the similar manner to M0, the first encountered detached node immediately  
332 after passing across the CE4\_1 is considered as the second M-node (M1 in Fig. 4). In this way,  
333 any number of activations of the dormant CE4s which satisfy the failure criteria in the  
334 corresponding time step can be handled with ease. Besides, this computation can be localized  
335 to each node group. Thus, by updating the M-S relation in each node group, very complex  
336 topological change due to fracturing can be automatically traced without using complex  
337 adaptive remeshing as in Fukuda et al. (2020b) (see Fig. 3 therein) and corresponding data

338 structure for manipulating remeshing, which makes the parallelization of the algorithm very  
 339 easy. Thus, the advantage of the applied M-S algorithm is not only limited to the localization of  
 340 processing by avoiding remeshing but also its ease of implementation and saving memory usage.

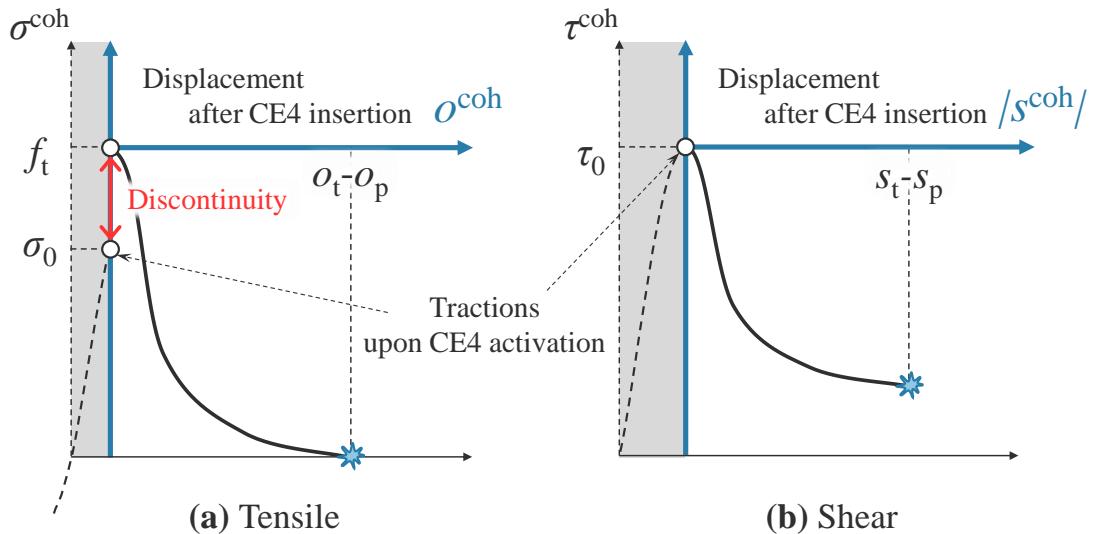


341  
 342 Fig. 4. M-S relation construction by counterclockwise search. (a) before failure (b) after failure.

343



344  
 345 Fig. 5. Tensile/Shear traction-separation law. (a)(b) ICZM (c)(d) ECZM.



346

347 Fig. 6. Tensile/Shear traction-separation law of a conventional ECZM in case only the shear

348 failure criterion is met ( $F_1 < 0$  and  $F_2 \geq 0$ ).

349

350 The final important task for the successful implementation of the MS-ECZM-FDEM is

351 how the ECZM is implemented. Before explaining that, one technical challenge must be pointed

352 out. Figure 5 (a)(b) and (c)(d) show the traction-separation laws for CE4 in the case of ICZM

353 and ECZM, respectively, where  $\sigma^{coh}$  [Pa] and  $\tau^{coh}$  [Pa] are normal and shear cohesive tractions,

354 respectively, according to the relative displacements of the two faces constituting a CE4 ( $o$  [m]:

355 opening amount of CE4 in which opening is positive and  $|s|$  [m]: sliding amount of CE4) (Fig.

356 1). On one hand, in the case of ICZM, pure mode I, pure mode II and mixed mode I-II fracturing

357 can be modeled with ease (see Mahabadi et al., 2012; Fukuda et al., 2019) although the artificial

358 compliance increase becomes the issue due to the existence of artificial elastic regime, i.e.  $o < o_p$

359 and  $|s| < s_p$  where  $o_p$  and  $s_p$  [m] are the “artificial” elastic limits of  $o$  and  $|s|$ , respectively (Munjiza

360 et al., 1999). On the other hand in the case of ECZM, Fig. 5 (c)(d) can be correct only when the  
361 dormant CE4 is activated with both  $F_1 \geq 0$  and  $F_2 \geq 0$  being simultaneously satisfied in Eq. (2).  
362 However, depending on the loading type in each target problem and due to the nature of  
363 unstructured mesh utilized in almost all the modern FDEM codes, the simultaneous satisfaction  
364 of the conditions  $F_1 \geq 0$  and  $F_2 \geq 0$  is very rare, and the cases “ $F_1 \geq 0$  and  $F_2 < 0$ ” and “ $F_1 < 0$  and  
365  $F_2 \geq 0$ ” are rather encountered frequently. In fact, in most of the previous research using ECZM-  
366 based FEM (Cai et al., 2023; Dooley et al., 2009; Zhang et al., 2007), the cohesive tractions at  
367 the activation on a CE4 are set to the input strength values regardless of the failure modes.  
368 Figure 6 shows the softening curves of a conventional ECZM where only the shear failure  
369 criterion is met by  $\tau_n = \tau_0$  ( $F_1 < 0$  and  $F_2 \geq 0$ ). In such a case, as shown in Fig. 6, although the  
370 normal traction  $\sigma_n = \sigma_0$  upon the CE4 activation is less than the tensile strength, the normal  
371 cohesive traction starts from the tensile strength, and thus a time-discontinuity in the stress state  
372 before and after CE4 activation should occur. This time-discontinuity should also occur in the  
373 case where only the tensile failure criterion is met ( $F_1 \geq 0$  and  $F_2 < 0$ ). Particularly, the time-  
374 discontinuity may be significant in the case that the normal traction  $\sigma_0$  is a compressive stress  
375 when CE4 is activated due to shear failure only. Dooley et al. (2009) assume that shear failure  
376 does not occur in such a compressive stress field, which, however, is not a reasonable  
377 assumption for the rock engineering applications targeted in this study. Note that Fig. 5 (a)(b)  
378 and (c)(d) in this paper are similar to Fig. 1(d) and (e), respectively in Cai et al. (2023). However,

379 Cai et al. (2023) did not consider this time-discontinuity in their ECZM-FDEM at all. Based on  
 380 this consideration, the following approach is taken as a remedy for alleviating this time-  
 381 discontinuity issue although further study is needed for completely solving this issue. To this  
 382 end, the traction-separation law (Fig. 5 (a)(b)) utilized in the ICZM-FDEM implementation is  
 383 utilized. In the ICZM, to calculate  $\sigma^{\text{coh}}$  and  $\tau^{\text{coh}}$ , the constitutive laws based on the tensile and  
 384 shear softening laws, i.e. tensile/shear softening curves, are applied according to Eqs. (3) ~ (9)  
 385 (e.g., Fukuda et al. (2019)). Note that in this traction-separation law, three integration points are  
 386 adopted in each CE4 and the contribution of the integration points to the nodal forces is set  
 387 according to Munjiza (1999) (See Eqs. (19) and (20) therein):

$$388 \quad \sigma^{\text{coh}} = \begin{cases} \frac{2o}{o_p} f_t & \text{if } o \leq 0 \\ \left[ \frac{2o}{o_p} - \left( \frac{o}{o_p} \right)^2 \right] f(D) f_t & \text{if } 0 \leq o \leq o_p \\ f(D) f_t & \text{if } o_p \leq o \leq o_t \end{cases} \quad (3)$$

$$389 \quad \tau^{\text{coh}} = \begin{cases} \left[ \frac{2|s|}{s_p} - \left( \frac{|s|}{s_p} \right)^2 \right] \times \langle f(D)c - \sigma^{\text{coh}} \tan \phi \rangle & \text{if } 0 \leq |s| \leq s_p \\ \langle f(D)c - \sigma^{\text{coh}} \tan \phi \rangle & \text{if } s_p \leq |s| \leq s_t \end{cases} \quad (4)$$

$$390 \quad f(D) = \left[ 1 - \frac{\alpha + \beta - 1}{\alpha + \beta} \exp \left( D \frac{\alpha + \gamma \beta}{(\alpha + \beta)(1 - \alpha - \beta)} \right) \right] \times \left[ \alpha(1 - D) + \beta(1 - D)^\gamma \right] \quad (5)$$

$$391 \quad o_p = \frac{2h f_t}{P} \quad (6)$$

$$392 \quad s_p = \frac{2h c}{P} \quad (7)$$

393 
$$G_{fI} = \int_{o_p}^{o_t} \sigma^{coh}(o) do \quad (8)$$

394 
$$G_{fII} + W_{res} = \int_{s_p}^{s_t} \{ \tau^{coh}(|s|) \} d|s| \quad (9)$$

395 where  $o_t$  [m] and  $s_t$  [m] are the critical values of  $o$  and  $|s|$ , respectively;  $\langle \rangle$  is Macaulay brackets;

396  $h$  [m] is the representative length of a CE4;  $P$  [Pa] is the cohesive penalty;  $G_{fI}$  [ $J/m^2$ ] and  $G_{fII}$

397 [ $J/m^2$ ] in Eqs. (8) and (9) are the Mode I and Mode II fracture energies consumed during the

398 generation of tensile and shear failures, respectively;  $W_{res}$  [ $J/m^2$ ] is the amount of work per area

399 of CE4 given by the residual stress term in the Mohr-Coulomb shear strength model illustrated

400 in Eq. (9);  $f(D)$  [-] ( $0 \leq f \leq 1$ ) is the softening function that determines the softening curve and

401 approximates the experimental stress-displacement curves obtained from the literature (Evans

402 and Marathe, 1968);  $D$  ( $0 \leq D \leq 1$ ) [-] is the damage variable indicating the damage degree of CE4;

403  $\alpha, \beta, \gamma$  [-] are the parameters that determine the curve shape of softening curves. Note that the

404 states with  $o \leq o_p$  or  $0 \leq |s| \leq s_p$  represent the artificial elastic state with  $D = 0$ , those with  $o_p \leq o \leq o_t$ ,

405  $s_p \leq |s| \leq s_t$  represent the damaged state (strain softening state with  $0 < D < 1$ ) where a CE4 can be

406 regarded as a micro fracture, and the state with  $o_t \leq o$  or  $s_t \leq |s|$  indicates the CE4 is broken with  $D$

407 = 1, deactivated, and turned into a macro fracture, and TRI3s surrounding the CE4 are treated

408 as the surface of the discrete bodies. Besides, when the above-mentioned damage variable  $D$  is

409 computed, the tension-induced damage  $D_o$  [-] and the shear-induced damage  $D_s$  [-], are

410 computed as follows:

411 
$$D = \min \left( 1, \sqrt{D_o^2 + D_s^2} \right) \quad (10)$$

412 
$$D_o = \min\left(1, \frac{o - o_p}{o_t}\right) \text{ if } o_p \leq o \leq o_t, \text{ otherwise } 0 \quad (11)$$

413 
$$D_s = \min\left(1, \frac{|s| - s_p}{s_t}\right) \text{ if } s_p \leq |s| \leq s_t, \text{ otherwise } 0 \quad (12)$$

414 No damage recovery is assumed to occur, and the damage variable  $D$  adopts the maximum value  
 415 between the previous steps and the current step. In addition, the unloading process (decrease in  
 416  $o, |s|$ ) and reloading process (increase in  $o, |s|$ ) during material softening ( $o_p \leq o \leq o_t, s_p \leq |s| \leq s_t$ ) are  
 417 also modeled by the following equations (Camacho and Ortiz, 1996; Fukuda et al., 2019).

418 
$$\sigma^{\text{coh}} = \frac{o}{o_{\max}} f(D) f_t \text{ if } 0 \leq o \leq o_{\max} \text{ and } o_{\max} > o_p \quad (13)$$

419 
$$\tau^{\text{coh}} = \frac{|s|}{s_{\max}} \langle f(D) c - \sigma^{\text{coh}} \tan \phi \rangle \text{ if } 0 \leq |s| \leq s_{\max} \text{ and } s_{\max} > s_p \quad (14)$$

420 where  $o_{\max}$  [m] and  $s_{\max}$  [m] are the maximum values of  $o$  and  $|s|$ , respectively, which the CE4  
 421 experiences during the FDEM simulation.

422 Based on the above ICZM-based formulation, the countermeasure adopted by Maeda et al.  
 423 (2022) is applied in this study. The boundary tractions  $(\sigma_n, \tau_n) = (\sigma_0 \text{ (Eq. (15))}, \tau_0 \text{ (Eq. (16))})$   
 424 acting on the dormant CE4 upon the activation timing, when the failure criterion (Eq. (2)) is  
 425 satisfied, are stored as shown in Eqs. (15) and (16), respectively:

426 
$$\sigma_0 = \min(\sigma_n, f_t) \quad (15)$$

427 
$$\tau_0 = \min(|\tau_n|, \langle c - \sigma_n \tan \phi \rangle) \quad (16)$$

428 Next, we define the following nominal opening/sliding displacements for the newly activated  
 429 CE4 based on the boundary tractions  $(\sigma_0, \tau_0)$  as follows:

430 
$$o^{\text{nominal}} = \frac{2h\sigma_0}{P} \quad (17)$$

431

$$s^{\text{nominal}} = \frac{2h\tau_0}{P} \quad (18)$$

432 Then, the effective opening/sliding ( $o, s$ ) of the activated CE4 used in softening functions of  
 433 cohesive tractions are defined as the sum of the nominal opening/sliding displacements ( $o^{\text{nominal}}$ ,  
 434  $s^{\text{nominal}}$ ) and actual geometrical opening/sliding displacements ( $o^{\text{coh}}, s^{\text{coh}}$ ) which occur after the  
 435 CE4 activation as shown in Eqs. (19) and (20):

436

$$o = o^{\text{nominal}} + o^{\text{coh}} \quad (19)$$

437

$$|s| = |s^{\text{nominal}} + s^{\text{coh}}| \quad (20)$$

438 It should be noted that the values of ( $o^{\text{coh}}, s^{\text{coh}}$ ) at the activation timing of the dormant CE4 are  
 439 zero because the CE4 has no gap. Then, these ( $o, |s|$ ) are used in the above Eqs. (3) ~ (14). This  
 440 approach is expected to alleviate the time-discontinuity issue to some extent and a similar  
 441 concept has been used in the literature (e.g. Woo et al., 2019 and Fig.4 therein). However, with  
 442 this approach, it must be noted that, upon the activation of CE4s, the effect of cohesive penalty  
 443  $P$  takes part in the FDEM simulation and thus the stable time step becomes almost same as that  
 444 in ICZM-FDEM since then while the time step can be taken relatively larger before the first  
 445 CE4's activation. Furthermore, it is essential to emphasize that the complete elimination of the  
 446 time-discontinuity in local nodal forces before and after the activation of CE4s remains a  
 447 challenge. As discussed by Chen et al. (2019), the core issue lies in the reliance on failure  
 448 judgments based on the stress states extrapolated from bulk elements (TRI3s in the present  
 449 implementation), while the nodal forces contributed by the interpolated stresses and cohesive  
 450 tractions remain independent. In their comprehensive review, Chen et al. (2019) examined the

451 existing methods aimed at mitigating or resolving this time-discontinuity issue and concluded  
452 that these methods are too exceedingly complex to implement. Correspondingly, they proposed  
453 a promising node-based approach aiming to achieve continuous transitions, in which, both the  
454 failure judgment and cohesive force calculation are performed directly at each node. However,  
455 it is worth noting that the application of the node-based approach is limited to simple crack  
456 patterns, e.g., progressive debonding or delamination in composite structures and thus cannot  
457 be readily applied to address the complex fracture problems involving with shear failures under  
458 compressions within the framework of the Mohr-Coulomb shear failure model. Consequently,  
459 the resolution of this problem within our model is a subject for future research. Additionally,  
460 another time-discontinuity issue arises when a cohesive element reaches complete damage ( $D$   
461 = 1) under a compressive stress field, i.e., transitioning from a state governed by the penalty of  
462 the cohesive elements to one governed by the contact penalty associated with contact interaction.  
463 This challenge is encountered in all CZM-based FDEM in spite of ICZM or ECZM. As a  
464 potential solution of to address this issue, Deng et al. (2021) proposed a smooth transition  
465 approach by assigning individual normal stiffness to each contact couple. However, our current  
466 paper only focuses on the implementation of MS-ECZM in the framework of GPGPU although  
467 we appreciate the time-discontinuity issue, which is regarded as a top priority of our future  
468 development. The computed cohesive tractions ( $\sigma^{\text{coh}}$ ,  $\tau^{\text{coh}}$ ) are converted to the equivalent nodal  
469 force  $\mathbf{f}_{\text{coh}}$  [N], which is assembled to each detached node by utilizing the existing ICZM-FDEM

470 code with very minor modification according to Eqs. (15) ~ (20), and further assembled to their  
471 M-nodes. Thus, upon fracturing, the resultant equation of motion for M-nodes is given as Eq.

472 (21):

473 
$$\mathbf{M} \frac{\partial^2 \mathbf{u}}{\partial t^2} = \mathbf{f}_{\text{ext}} - \mathbf{f}_{\text{int}} + \mathbf{f}_{\text{con}} + \mathbf{f}_{\text{coh}} \quad (21)$$

474 After the nodal information is updated for M-nodes, the nodal velocity and current nodal  
475 coordinates are copied to their S-nodes for the following timesteps to fully utilize the existing  
476 ICZM-FDEM code.

477 2.2. GPGPU parallel implementation

478 As mentioned in Section 2.1, the proposed MS-ECZM-FDEM can utilize the existing  
479 ICZM-FDEM code including the ICZM-based GPGPU-parallelized Y-HFDEM code with very  
480 minor modification. The only notable differences lie in the treatment of the judgement of the  
481 failure (Eq. (2)) and resultant update in the M-S relation (Fig. 4 (b)). Moreover, the processing  
482 of the update in the M-S relation is highly localized and suitable for parallel computation while  
483 it is challenging to parallelize the adaptive remeshing used in Fukuda et al. (2020b), Pandolfi  
484 and Ortiz (2002) and Yamamoto et al. (1999) especially in terms of GPGPU parallelization. This  
485 section implements the proposed algorithm through the GPGPU parallel computation using  
486 computing unified device architecture (CUDA) C/C++. The GPGPU parallel computing uses  
487 the following abstractions: threads, blocks, and grids (Fig. 7). In the GPGPU devices, parallel  
488 processing is performed in many threads using kernel functions. The threads are just execution

489 units of kernel functions, and each thread performs operations similar to sequential computation.

490 The blocks are the groups that manage several threads and allow memory sharing and

491 synchronization among the threads within a block. Furthermore, the grids are the groups of

492 blocks. This hierarchical management of threads enables parallel processing. Figure 8 shows

493 the flow chart of the proposed MS-ECZM-FDEM with GPGPU parallel computing. In Fig. 8,

494 the blue letters are the specific processes for the MS-ECZM-FDEM while the rest processes are

495 the same as those used in the ICZM-based GPGPU-parallelized 2-D Y-HFDEM code. Therefore,

496 the proposed MS-ECZM-FDEM can be realized by simply adding the processes shown in blue

497 in Fig. 8 to the existing ICZM-FDEM codes. For the part which is common with the ICZM-

498 FDEM, the interested readers are referred to the detailed explanations in Fukuda et al. (2019)

499 and only the newly implemented portions are explained here. In Fig. 8, the process enclosed by

500 the dashed line is the parallel computation in the GPGPU device. First, before entering the

501 parallel computation by the GPGPU devices, the angle  $\theta$  between the reference axis and the

502 vector connecting each detached node and the geometric center of the TRI3, to which it belongs,

503 are calculated for all the detached nodes, which in each group is sorted in the counterclockwise

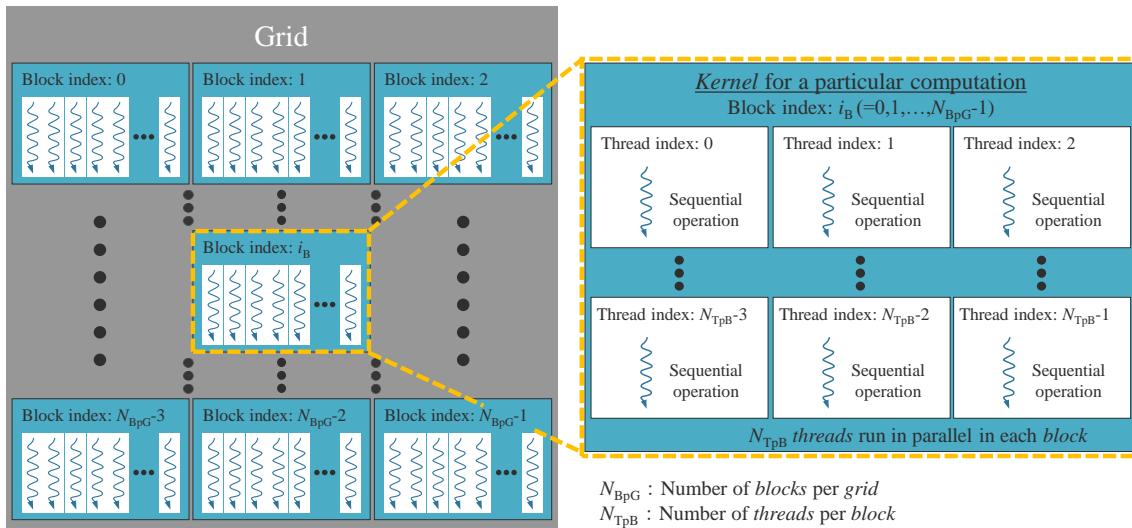
504 manner in order of decreasing  $\theta$  (Fig. 4 (a)). After this sorting, the initial M-S relation

505 “*GetMaster*” (Fig. 3) is constructed by simply selecting the detached node with the smallest  $\theta$

506 as M-node while other detached nodes as S-nodes to this M-node in each node group. Note that

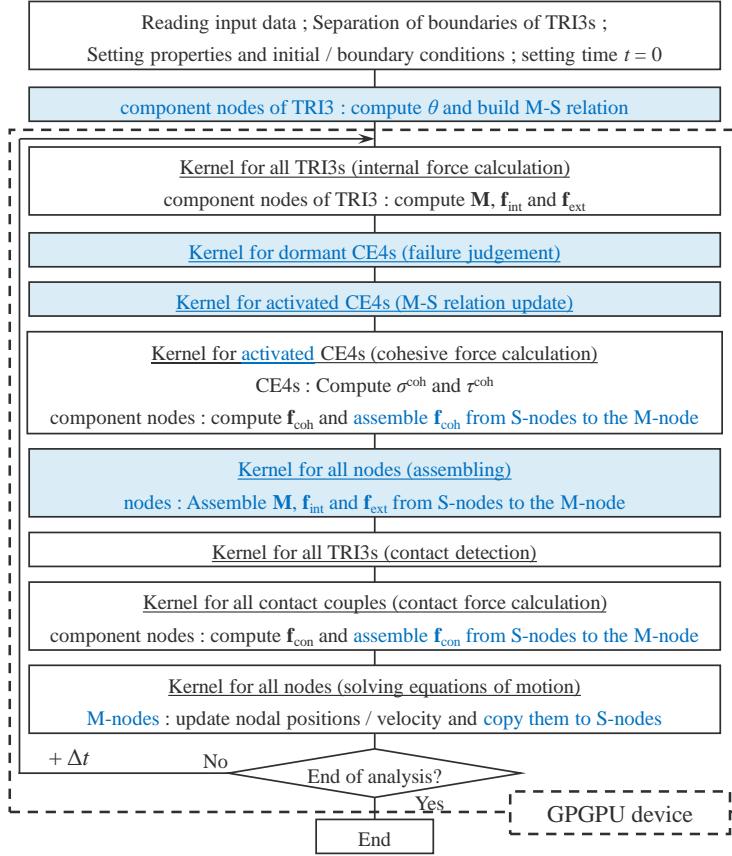
507 these processes are handled in a host computer and processed by sequential computations only

508 once at the onset of the simulation, which takes negligible computational time. The information  
 509 of the relation between the sorted detached node IDs in each node group and *GetMaster* are  
 510 transferred to the global GPGPU memory, and the subsequent computations are completely  
 511 processed on GPGPU except for the output timing when the computed data from the GPGPU  
 512 are transferred back to the host computer to generate the output files for visualization by the  
 513 opensource software Paraview (Ayachit, 2015).



515 Fig. 7. The concept of GPGPU programming. (Fukuda et al., 2019).

516



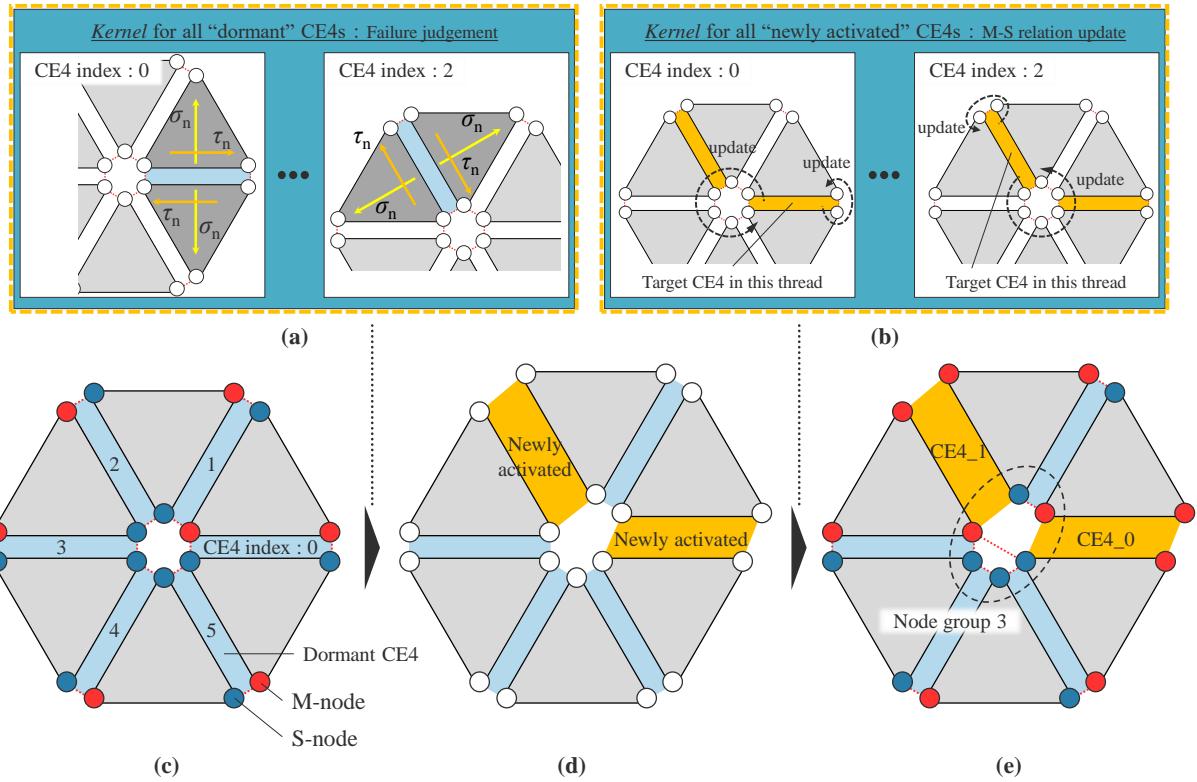
517

518 Fig. 8. Flow chart of proposed MS-ECZM-FDEM with GPGPU parallel computing.

519

520 As shown in Fig. 9, after calculating the Cauchy stress tensor  $\sigma_{ij}$  (for computing  $\mathbf{f}_{int}$ ) from  
521 the parallel processing of each TRI3s, the boundary stress tractions ( $\sigma_n, \tau_n$ ) acting on all the  
522 dormant CE4s are computed in parallel by assigning each CUDA thread to each dormant CE4  
523 and failure judgment based on the boundary tractions (Eq. (2), Fig. 9 (a)). Note that, during the  
524 computations, an 1-dimentional (1-D) integer array “*i1CE4IDs*” and an 1-D Boolean array  
525 “*b1CE4states*” are prepared to store all the dormant and active CE4 IDs and state (active or  
526 dormant) of the CE4s, respectively. When any newly activated CE4s are identified, *i1CE4IDs*  
527 is sorted using *b1CE4states* as key in parallel following the parallel radix soring algorithm

528 (Satish et al., 2009) in the way that all the dormant CE4s' IDs are placed in the heading part of  
 529 the *i1CE4IDs* array. In this way, the load balance between each CUDA thread in each CUDA  
 530 block can be maximized for judging the failure of dormant CE4s and computation of cohesive  
 531 tractions ( $\sigma^{\text{coh}}$ ,  $\tau^{\text{coh}}$ ) for active CE4s.



532  
 533 Fig. 9. The GPGPU parallel computation processes for CE4s in MS-ECZM-FDEM. **(a)** failure  
 534 judgement, **(b)** M-S relation update, **(c)** before failure judgement, **(d)** after failure judgement  
 535 and **(e)** after M-S relation update.

536  
 537 For the update in the M-S relations “*GetMaster*”, each CUDA thread is assigned to each  
 538 newly activated CE4s that has just satisfied the failure judgement in this step. Note that each  
 539 newly activated CE4 consists of two node groups and thus each thread partially updates the M-

540 S relations in each node group. Figure 9 (b)(d)(e) shows the updating process of the M-S  
541 relations when two adjacent CE4s (CE4\_0 and CE4\_1 in Fig. 4 (b)) sharing the node group ( $ig$   
542 = 3 in Fig. 3) are newly activated, which is the same as shown in Fig. 4 (b). For the node group  
543 No. 3, the threads for CE4\_0 and CE4\_1 partially update the M-S relation of the node group No.  
544 3. For the thread processing CE4\_0 when processing the node group No. 3, the first detached  
545 node, i.e., the right red node in the node group No. 3 is considered as an M-node and the  
546 counterclockwise search registers all the detached nodes until passing over other newly and  
547 already activated CE4s (CE4\_1 in this case). Likewise, for the thread processing CE4\_1 when  
548 processing the node group No. 3, the first detached node, i.e., the left red node in the node group  
549 No. 3 is considered as an M-node and the counterclockwise search registers all the detached  
550 nodes until passing over other newly and already activated CE4s (CE4\_0 in this case). Therefore,  
551 the M-S update can be processed completely in parallel.

552 After computing the nodal masses and nodal forces for each detached node based on  
553 ICZM-FDEM manner, they are assembled from the S-nodes to their M-node through *GetMaster*,  
554 which is processed by assigning CUDA thread to each node group. Then, the nodal coordinates  
555 and nodal velocities of the M-nodes are updated based on the equations of motion (Eq. (1) for  
556 intact regime and Eq. (21) after fracture initiation) by assigning CUDA thread to each M-node.  
557 Finally, the updated information is copied from the M-nodes to their S-nodes through *GetMaster*  
558 by assigning CUDA thread to each node group.

559

560 **3. Validation of GPGPU-parallelized MS-ECZM-FDEM**

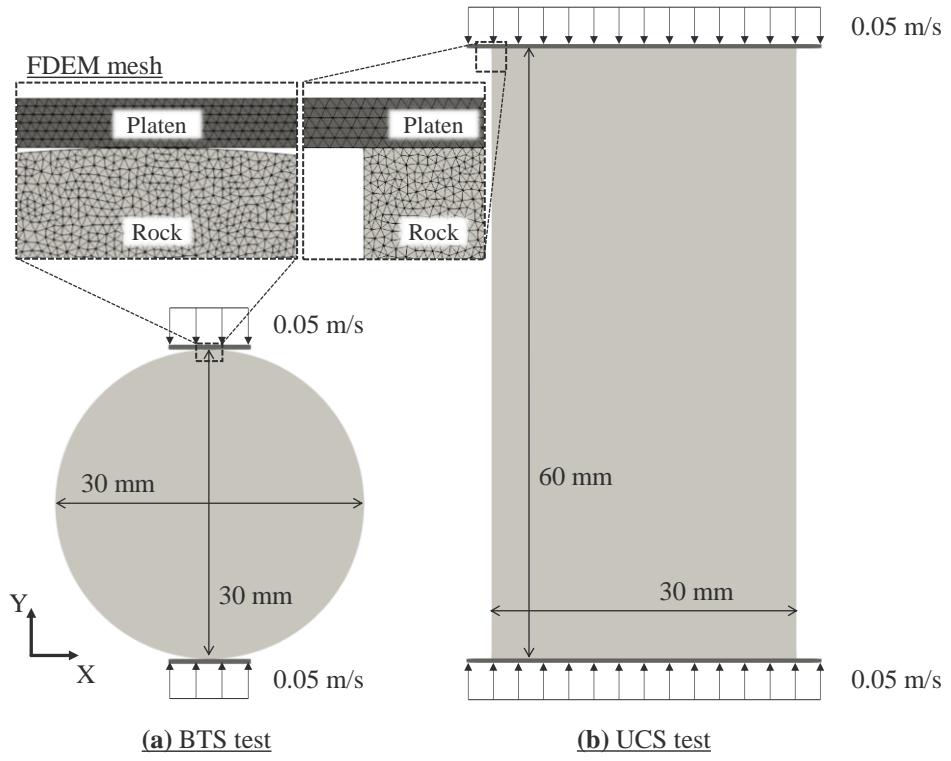
561 Numerical experiments of the fundamental laboratory rock mechanics tests, i.e., Brazilian  
562 tensile strength (BTS) and uniaxial compressive strength (UCS) tests under quasi-static loading,  
563 are conducted to validate the GPGPU-parallelized 2-D MS-ECZM-FDEM code developed in  
564 Section 2. In the remainder of this section, the MS-ECZM-FDEM is simply called as ECZM-  
565 FDEM. The results from the modellings of the BTS and UCS tests using GPGPU parallelized  
566 ECZM-FDEM and ICZM-FDEM codes are compared in terms of (I) accuracy of continuous  
567 deformation, (II) stable time step and (III) contact activation timing. It is important to note that  
568 this paper is not intended to delve into the evaluation of computational efficiency comparison  
569 between GPGPU parallelization and sequential computation since it has already been  
570 extensively discussed in our former publication (Fukuda et al., 2019). Instead, this paper focuses  
571 on the comparison between the GPGPU-based 2-D ECZM-FDEM and ICZM-FDEM codes,  
572 which should provide sufficient insights into their computational performance.

573 3.1. Overview of numerical models for BTS and UCS tests

574 Figure 10 shows the 2-D FDEM models for modelling the BTS and UCS tests. The  
575 diameter and height of the models are 30 [mm]  $\times$  30 [mm] for the BTS test and 30 [mm]  $\times$  60  
576 [mm] for the UCS test, respectively. These FDEM models are discretized by TRI3s using  
577 unstructured mesh and average element size  $h$  for both models is 90 [ $\mu\text{m}$ ]. The number of TRI3s

578 included in the BTS and UCS tests are 187,061 and 475,810, respectively. Siliceous mudstone  
579 is considered as a target rock. The input parameters for the FDEM simulations for the BTS and  
580 UCS tests are set as shown in Table. 2 assuming this rock is isotropic and homogeneous. The  
581 density, Young's modulus, Poisson's ratio, tensile strength, cohesion, and internal friction angle  
582 are set based on Aoyagi et al. (2018) while other parameters are determined based on trial and  
583 error. Dynamic relaxation scheme (Munjiza, 2004) is used to approximately achieve the quasi-  
584 static condition and correspondingly damping coefficient  $\eta = 2h\sqrt{\rho E}$  (see. Eqs. (2) and (3) in  
585 Fukuda et al. (2020b)) is assigned to each TRI3. The constant velocity of 0.05 [m/s] is assigned  
586 to each of the upper and lower platen and apparent strain rates are 3.3 [1/s] for BTS test and 1.7  
587 [1/s] for UCS test. The time step  $\Delta t$  is set to be 1.0 [ $\times 10^{-9}$  s/step]. It is known that a higher  
588 loading rate has a significant effect on the simulation results under quasi-static conditions such  
589 as the BTS and UCS tests (Mohammadnejad et al. (2020)). However, the loading rate set in this  
590 study has been confirmed to be appropriate because the stress-strain curve for the UCS test in  
591 Fig. 15, which is described below, does not show any fluctuation observed in Mohammadnejad  
592 et al. (2020). Furthermore, as a method of determining whether the loading rate setting can  
593 reasonably simulate quasi-static loading conditions, it is widely accepted that, if the ratio of total  
594 kinetic energy to total strain energy of a rock specimen is less than 0.05 at intact regime, the  
595 response obtained from the analysis does not include dynamic effects (Rojak et al., 2021;  
596 Siswanto et al., 2016). From the preliminary simulation, we confirmed that the above energy

597 ratio through all the simulations in this analysis is much smaller than 0.05 and thus we  
598 considered that the loading rate is adequately small (Maeda et al., 2022).



599  
600 Fig. 10. Numerical models for FDEM simulations of (a) BTS and (b) UCS tests.  
601

602 Table. 2. Input parameters for FDEM simulations of BTS and UCS tests.

Parameter		Value
Density	$\rho$ [kg/m <sup>3</sup> ]	1840
Young's modulus	$E$ [GPa]	1.82
Poisson's ratio	$\nu$ [-]	0.17
Tensile strength	$f_t$ [MPa]	1.83
Cohesion	$c$ [MPa]	4.81
Internal friction angle	$\varphi$ [°]	26
Mode I fracture energy	$G_{fI}$ [J/m <sup>2</sup> ]	16
Mode II fracture energy	$G_{fII}$ [J/m <sup>2</sup> ]	160
Cohesive penalty	$P$ [GPa]	182
Normal contact penalty	$P_{n\_con}$ [GPa]	18.2
Friction coefficient of rock-platen surfaces	$\mu_{fric}$ [-]	0.1
Friction coefficient of rock fracture surfaces	$\mu_{fric}$ [-]	0.5

603 3.2. Verification and validation of GPGPU-parallelized ECZM-FDEM through comparative

604 study

605 For comparison purpose, three different types of FDEM simulations, i.e., “ECZM-FDEM”,

606 “ICZM-FDEM”, and “FDEM without CZM”, are considered using the same numerical model

607 set up in Section 3.1. The reason why “FDEM without CZM” is also considered is that each

608 discrete body (rock and loading plates in the current case) behaves as purely continuum without

609 any fracturing and thus can be considered as a benchmark for checking the precision of the

610 FDEM computation for the continuous deformation of the rock at the intact regime, in which

611 the rock behaves purely in FEM manner. Note that “FDEM without CZM” is achieved by

612 deactivating the failure judgement (see Section 2.1 and Eq. (2)) in the ECZM-FDEM to verify

613 that the developed GPGPU-based ECZM-FDEM code works well without the activation of  
614 dormant CE4s by setting extremely large strength parameters.

615 In addition, different contact activation schemes, i.e., BCAA and (semi-)ACAA, are  
616 possible for ICZM-FDEM as mentioned in Section 1 while (semi-)ACAA is only possible for  
617 “ECZM-FDEM”. To facilitate a fair comparison between ICZM-FDEM and ECZM-FDEM, a  
618 case of ICZM-FDEM with semi-ACAA is considered. It is worth noting that, in the literature  
619 related to FDEM developments and applications, ICZM-FDEM with BCAA, not semi-ACAA,  
620 is currently the most widely used approach. In this section, four cases in Table. 3 are considered  
621 for the following investigations. Figure 11 shows the difference between Case 2 (BCAA) and  
622 Cases 1, 3 and 4 for the case of BTS and UCS test models at the beginning of the FDEM  
623 simulations. The red area in Fig. 11 is the activated area for contact calculations (i.e. contact  
624 detection and contact force calculations), and the blue area is the part in which the contact  
625 calculations are initially deactivated. As shown in Fig. 11, the difference between the cases with  
626 BCAA (Case 2) and the semi-ACAA (Cases 1 and 3) is that the all the TRI3s are subjected to  
627 the contact calculations from the onset of the simulations in the BCAA while only the TRI3s on  
628 the rock-platen surfaces and those surrounding the CE6s just entering the shear softening regime  
629 are subjected to the contact calculations in the case of semi-ACAA. Please refer to Fukuda et al.  
630 (2021) for the detailed discussion of the BCAA and semi-ACAA. Since the ECZM does not  
631 involve with fracturing until first crack initiation occurs, it is evident that the BCAA concept is

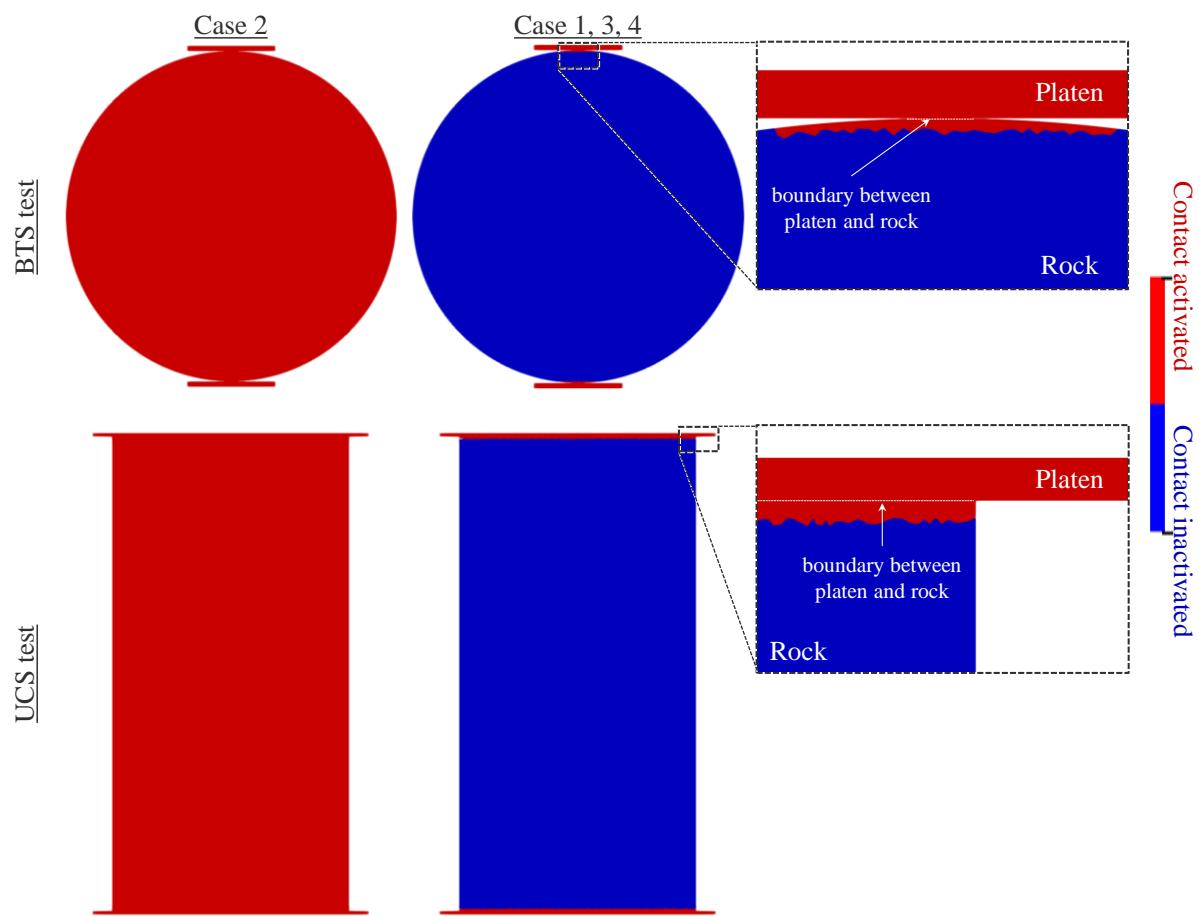
632 just unreasonable and not needed at all. Note that the because of no fracturing involved in Case

633 4, no adaptive contact activation is needed. The GPGPU-parallelization is applied in all cases.

634

635 Table. 3. Definition of four cases considered for the comparison.

	<b>FDEM Type</b>	<b>Contact activation scheme</b>	<b>TRI3s subjected to contact detection</b>
<b>Case 1</b>	ECZM-FDEM	Semi-ACAA	TRI3s on the rock-platen surfaces and newly created fractures
<b>Case 2</b>	ICZM-FDEM	BCAA	All the TRI3s in the system
<b>Case 3</b>	ICZM-FDEM	Semi-ACAA	TRI3s on the rock-platen surfaces and newly created fractures
<b>Case 4</b>	FDEM without CZM	Activated at the onset of the FDEM simulation	TRI3s on the rock-platen surfaces



636

637 Fig. 11. Illustration explaining the different contact activation scheme in four cases in Table. 3.

638

639 Figure 12 shows the fracture process simulated from the BTS tests in the Cases 1, 2 and 3,

640 which shows the spatial distribution of the damage state  $D$  in Eq. (10) at each loading stage with

641 respect to nominal axial strain. The nominal axial strain  $\varepsilon_a$  is defined by the total axial

642 displacement of both platens divided by the diameter of the rock disc. The contours in Fig. 12

643 represent the logarithm of the damage variable  $D$ , i.e.  $\log_{10}D$ , and  $\log_{10}D \geq -3$  is visualized. A

644 common trend observed in all cases is that microcracks of the order of  $-3 \leq \log_{10}D \leq -2$  occur

645 near the loading platens, and the macroscopic fractures ( $\log_{10}D = 0$ ) that lead to the failure of the

646 specimen progress vertically in the central part of the specimen. Although the final failure

647 patterns are slightly different in each case, the characteristics of the resultant failure trends are

648 consistent with those from the typical BTS tests of rocks. Thus, the GPGPU-implementation of

649 adaptively activating dormant CE4s in the framework of MS-ECZM-FDEM is verified, and the

650 result of Case 1 shows the almost similar fracture process as the conventional ICZM-FDEM

651 (Cases 2 and 3). From the results of the Case 2 (ICZM-FDEM with BCAA), it is noticeable that

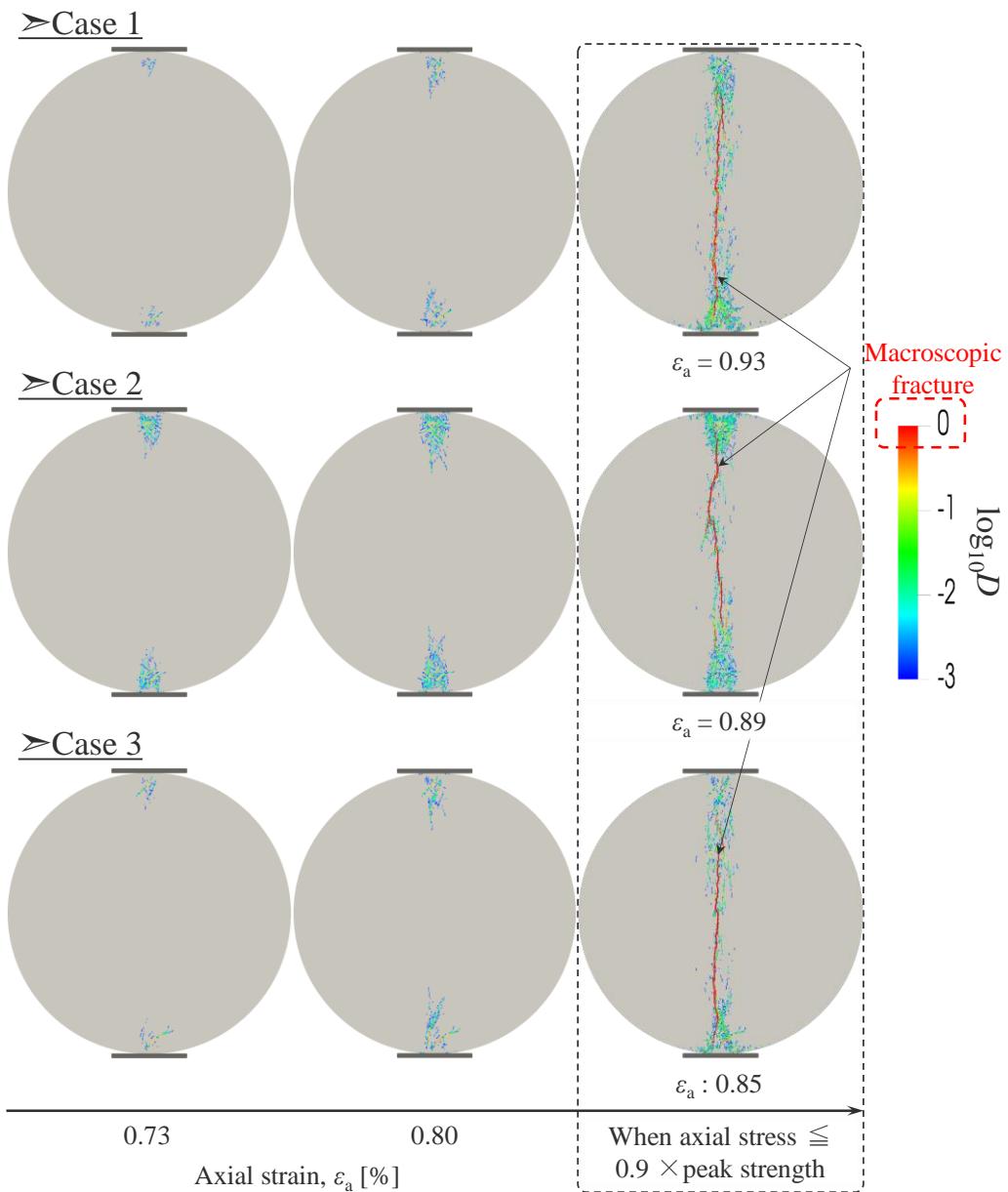
652 more microcracks are observed near the loading platens compared to those of the Case 3 (ICZM-

653 FDEM with semi-ACAA). The difference between the two cases may be due to the dual-force

654 (i.e., the combination of cohesive traction and contact force) in the BCAA, which acts on the

655 inside of the rock part even in the intact regime as discussed by Fukuda et al. (2021). This may

656 enhance the micro-cracking. In contrast, Case 1 (ECZM-FDEM with semi-ACAA), which can  
 657 avoid this dual-force issue, shows similar microcracks as Case 3.



658

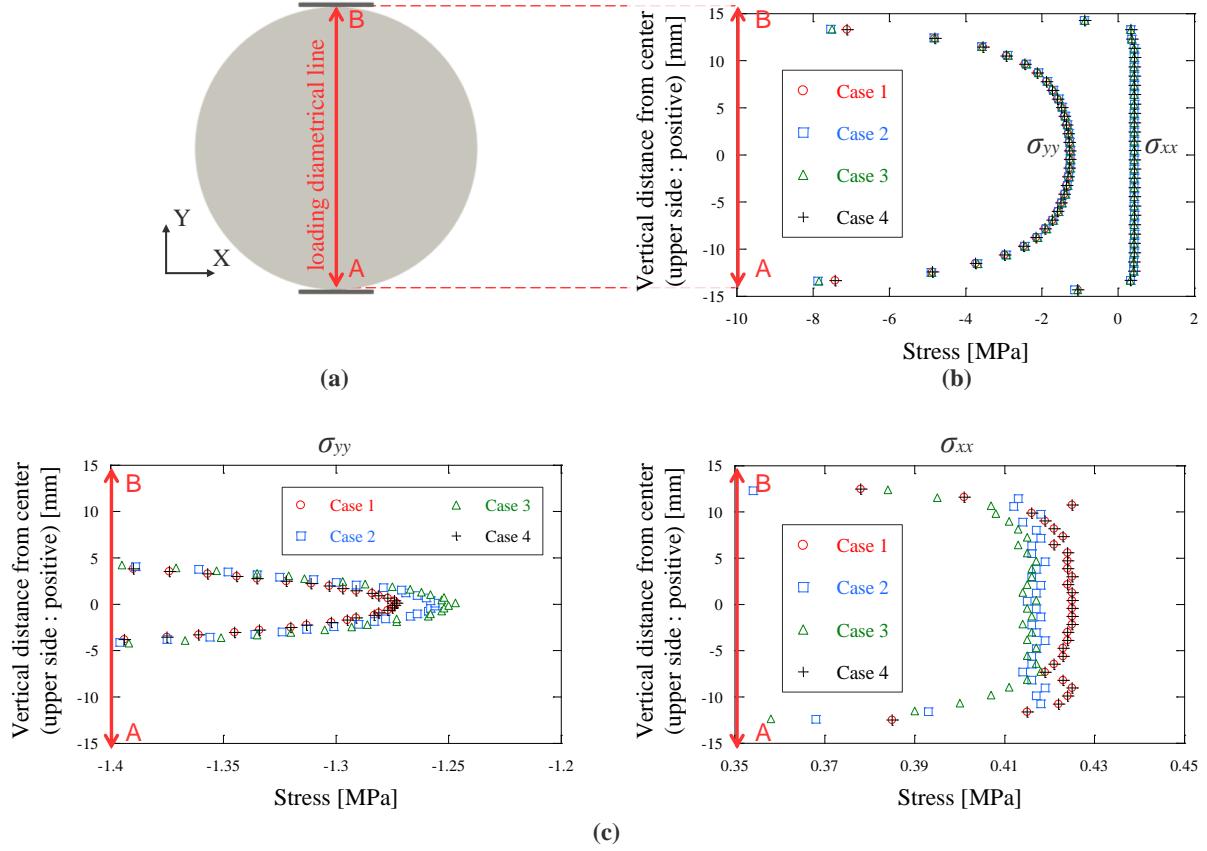
659 Fig. 12. Comparisons of fracture processes in BTS test for Cases 1, 2 and 3 in Table. 3.

660

661 Figure 13 plots the stress distribution along the loading diametrical line at a time when the  
 662 nominal axial strain (contraction: positive) is small with the level of 0.2 % for Cases 1-4. Figure

663 13 (a) shows the observation line for stress monitoring. Figure 13 (b) plots the  $\sigma_{xx}$  and  $\sigma_{yy}$  along  
664 the observation line while Fig. 13 (c) shows an enlarged view of Fig. 13 (b). Since this stage  
665 corresponds to intact rock well before the failure stage, the stress distribution in Cases 1-3  
666 should agree that in Case 4 (FDEM without CZM). In fact, the results of Case 1 (ECZM-FDEM)  
667 in Fig. 13 (b) clearly show that both  $\sigma_{xx}$  and  $\sigma_{yy}$  are in perfect agreement with the benchmark  
668 Case 4 (FDEM without CZM). On the other hand, the results of ICZM-FDEM, i.e., Cases 2 and  
669 3, show some deviation from FDEM without CZM. This deviation is clearly due to the  
670 deterioration of the accuracy in computing continuous deformation and stress calculation by  
671 inserting active CE4s at the onset of the simulation in the ICZM. To quantitatively evaluate these  
672 deviations, the average values of  $\sigma_{xx}$  for the TRI3s existing within a range of  $\pm 5$  mm from the  
673 center of the specimen, and the average values of  $\sigma_{yy}$  for the TRI3s existing within a range of  $\pm 1$   
674 mm from the center of the specimen are calculated for Cases 1~4, and the deviation of the  
675 average stress [%] of Cases 1~3 against the benchmark Case 4 is investigated. For Cases 2 and  
676 3, i.e., ICZM-FDEM, this deviation for  $\sigma_{xx}$  is found to be 1.6 % for BCAA and 2.0 % for semi-  
677 ACAA, respectively, while 1.4 % for BCAA and 1.8 % for semi-ACAA for  $\sigma_{yy}$ . In contrast, Case  
678 1 (ECZM-FDEM) shows no deviation for both  $\sigma_{xx}$  and  $\sigma_{yy}$ . Thus, it can be concluded that the  
679 ICZM-FDEM involves with approximately 1.4~2 % deterioration of stress calculation accuracy,  
680 and the advantage of ECZM-FDEM is evident.

681



682

683 Fig. 13. Comparisons of stress distributions along the loading diametrical line of the specimen  
 684 in FDEM simulations of BTS test between Cases 1, 2, 3 and 4 defined in Table. 3. **(a)** Schematic  
 685 of loading diametrical line, **(b)** Stress distribution along the loading diametrical line, **(c)**  
 686 Enlarged view of  $\sigma_{yy}$  (left) and  $\sigma_{xx}$  (right) in **(b)**.

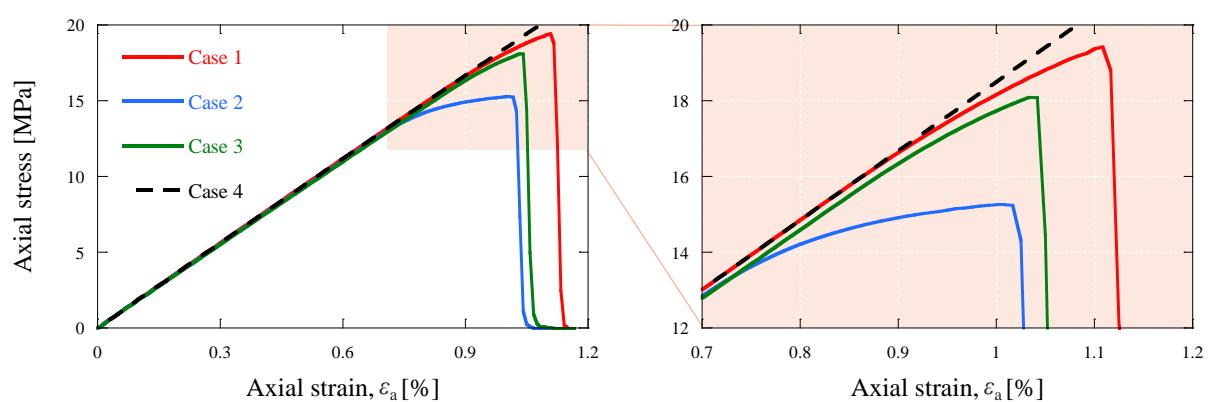
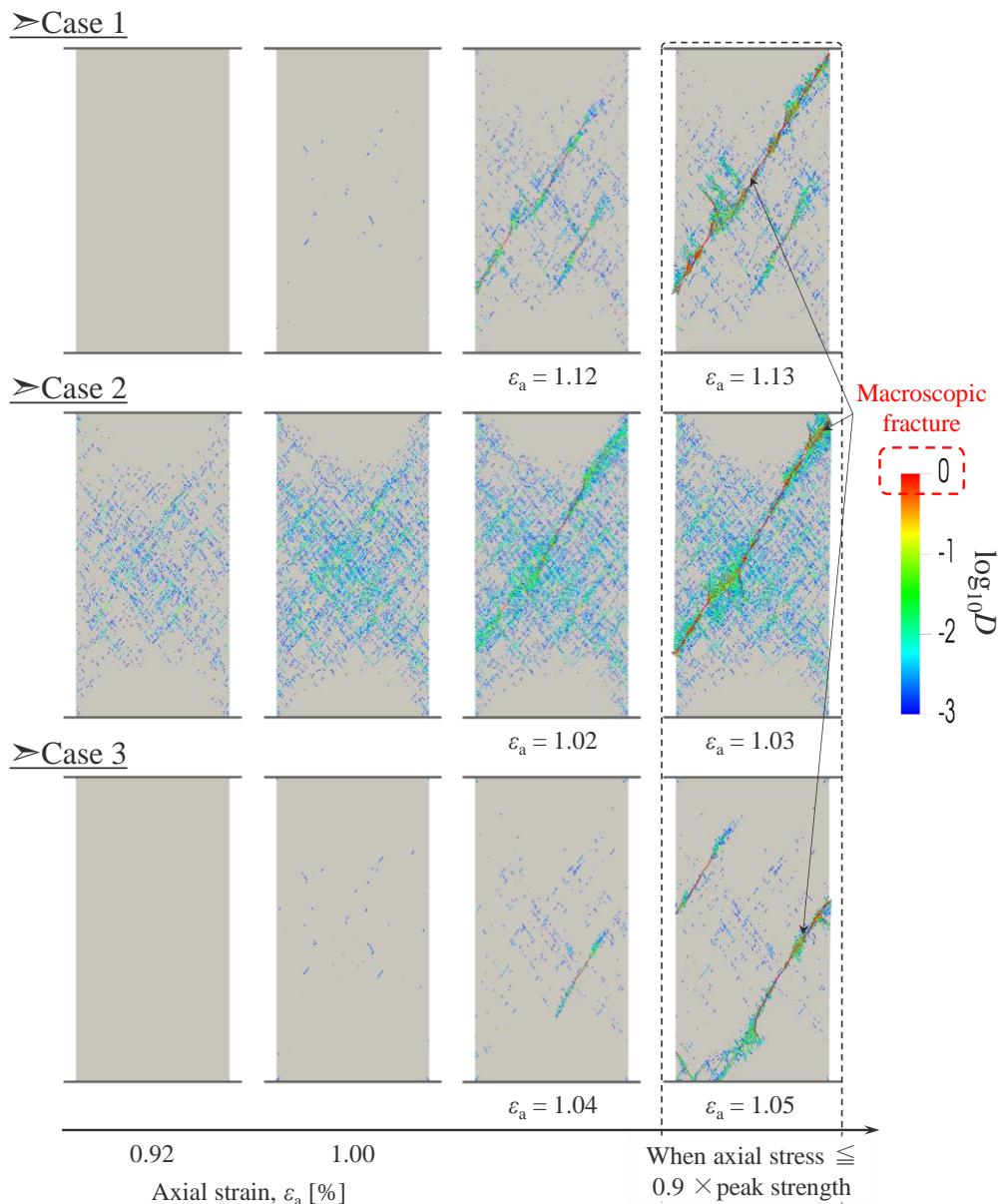
687

688 Figures 14 and 15 show the fracture process and axial stress-strain curve for Cases 1, 2 and  
 689 3 in UCS test for selected axial strain levels. In Fig. 15 (contraction: positive), dotted line  
 690 indicates the stress-strain line for benchmark Case 4 to verify the initial continuous behavior of  
 691 Cases 1~3 at intact regime. Note that the apparent axial strain  $\varepsilon_a$  in these figures is obtained by  
 692 dividing the total displacement at the upper and lower platens by the height of the specimen.

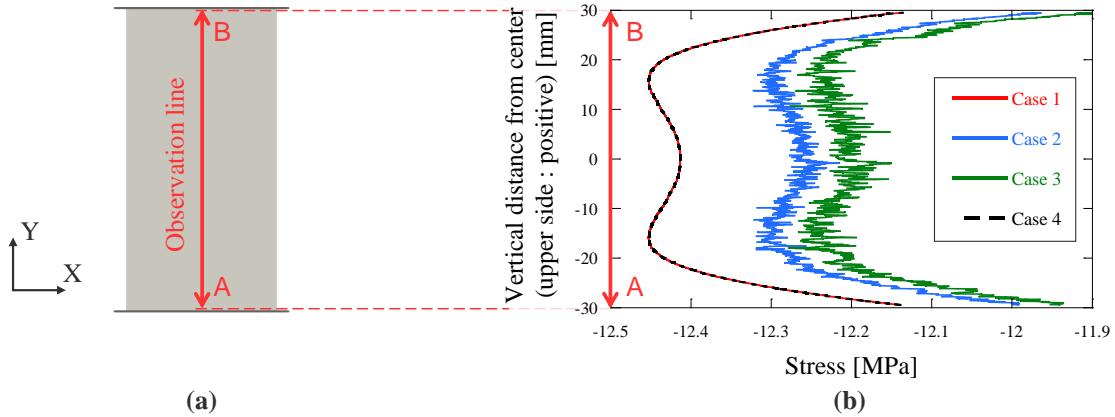
693 The contour in Fig. 14 represents the spatial distribution of  $\log_{10}D$  for  $\log_{10}D \geq -3$ . For the intact  
694 deformation regime before the commencement of non-linear behavior near the peak in the  
695 stress-strain curve (Fig. 15), Cases 1-3 show more or less good agreement with FDEM without  
696 CZM. However, if these three cases are compared in terms of tangent modulus at the 50 % peak  
697 strength, the corresponding deviations of Cases 1 (ECZM), 2 (ICZM with BCAA) and 3 (ICZM  
698 with semi-ACAA) against Case 4 are 0 %, 1.2 % and 1.7 %, respectively, which again shows  
699 the advantage of ECZM-FDEM in improving the precision of continuous deformation at the  
700 intact regime. In addition, to check the precision of continuous deformation at the intact regime  
701 from the viewpoint of the stress distribution, Fig. 16 shows the stress distribution for  $\sigma_{yy}$  along  
702 the loading line at a time when the apparent axial strain  $\varepsilon_a$  is small with the level of 0.67 % for  
703 Cases 1-4. Figure 16 (a) shows the observation line for stress monitoring. Figure 16 (b) plots  
704 the  $\sigma_{yy}$  along the observation line. The figure shows that, as in the stress-strain curve, Case 1  
705 (ECZM-FDEM) is in perfect agreement with the benchmark Case 4 (FDEM without CZM),  
706 while Cases 2 and 3, i.e., ICZM-FDEM, deviate from the benchmark Case 4. Furthermore, an  
707 obvious difference in curve shape is observed between ECZM-FDEM and ICZM-FDEM: while  
708 the curve shape of ECZM-FDEM is smooth, that of ICZM-FDEM is highly fluctuated,  
709 indicating a clearly discontinuous stress distribution, even at intact regime. This can be due to a  
710 geometrical inconsistency in the mesh, in other words, a physical gap caused by the relative  
711 displacement of CE4s between TRI3s even for the continuous deformation regime in the ICZM.

712 The geometric inconsistency causes local numerical instability. These results for stress-strain  
713 curve and stress distribution confirm the high accuracy of the calculations in ECZM-FDEM at  
714 intact conditions. These results for stress-strain curve and stress distribution confirm the high  
715 precision of the calculations in ECZM-FDEM at intact regime. To the best of knowledge of the  
716 authors, there are not any valid theoretical solutions or benchmark analyses available for  
717 delineating any arbitrary fracture initiation, propagation, and interaction in heterogeneous rocks.  
718 Consequently, it is very challenging, if not impossible, to compare the accuracy between the  
719 simulations from ECZM-FDEM and ICZM-FDEM after the onset of fracturing. However, it is  
720 anticipated that the less noisy stress distribution from ECZM-FDEM should result in more  
721 rational crack initiation and propagation.

722



727 Table. 3.



728

729 Fig. 16. Comparisons of stress distributions for  $\sigma_{yy}$  along the observation line of the specimen  
 730 in FDEM simulations of UCS test between Cases 1, 2, 3 and 4 defined in Table. 3. (a) Schematic  
 731 of observation line, (b) Stress distribution for  $\sigma_{yy}$  along the observation line.

732

733 In the pre-peak stage of Fig. 15, it can be observed that all Cases 1-3 show a nonlinear  
 734 behavior accompanied by a decrease in slope near the peak, which is due to the transition from  
 735 continuum to discontinuum by the commencement of softening of CE4s, which is evident from  
 736 Fig. 14 when  $\varepsilon_a = 0.92$  [%]. Similar to the trend observed in the BTS test, the amount of  
 737 generated microcracks at the same level of  $\varepsilon_a$  varies between each case, and only ICZM (BCAA)  
 738 shows more significant number of microcracks (see the results of  $\varepsilon_a = 0.92$  [%] ~1.00[%]). Again,  
 739 this could also be attributed to the effect of dual-force, which may enhance the local  
 740 noise/fluctuation in stress, and much rapid decrease in the stiffness of bulk rock. For the failure  
 741 process in Fig. 14, at the third axial strain level from the left, Cases 2 and 3, i.e., ICZM-FDEM

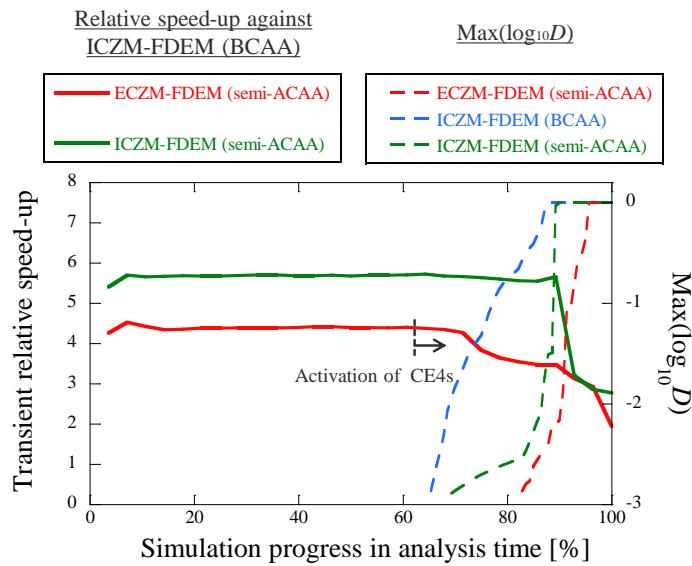
742 show localized fracture growth from a single location, while Case 1 (ECZM-FDEM) shows  
743 fracture growth from multiple locations. Again, since CE4s can open/slide even at intact regime  
744 in the ICZM-FDEM, if a CE4 is softened, the CE4's deformation in ICZM can strongly  
745 enhances the deformation direction of surrounding CE4s than the case of ECZM. Consequently,  
746 fracturing around the softened CE4 may easily occur, propagate, and localize, along the  
747 deformation direction of the softened CE4s in the ICZM. On the other hand, in ECZM-FDEM,  
748 dormant CE4s cannot open/slide at the intact regime and the failure criteria for the  
749 commencement of softening (Eq. (2)) are based on the stress fields. Thus, if a CE4 is softened,  
750 stress concentration occurs in the surrounding TRI3s, leading to the satisfaction of the failure  
751 criteria in surrounding TRI3s' boundary (i.e., dormant CE4). In this process, the normal/shear  
752 stresses on surrounding dormant CE4s due to stress concentration does not necessarily  
753 correspond to the deformation direction of the softened CE4. In other words, the deformation  
754 direction of the softened CE4 does not directly affect the surrounding CE4s. Therefore, the  
755 deformability or localization along the direction of the softening CE4 is less likely to occur  
756 compared to ICZM-FDEM. This explanation is also supported by the fact that, at the peak stage  
757 of Fig. 15, the peak strength and the strain at that time in Case 1 (ECZM-FDEM) are higher than  
758 in Cases 2 and 3. ICZM-FDEM can be considered as a model in which the failure progresses  
759 more easily than ECZM-FDEM, due to the aforementioned numerical instability caused by  
760 geometric inconsistency and localization of fracturing. In contrast, the ECZM-FDEM has more

761 stable nature, the rock model based on ECZM-FDEM behaves much stronger than ICZM-  
762 FDEM. For the resultant failure patterns, all Cases 1~3 in Fig. 14 show the formation of a shear  
763 band, and its inclination is of the same degree, which also verifies the developed ECZM-FDEM  
764 code and validates its applicability. However, it is evident that the calibrated input parameters  
765 in the ICZM-FDEM cannot be directly used in the ECZM-FDEM.

766 Furthermore, the computational speeds among Cases 1, 2 and 3 are compared, although it  
767 is difficult to simply compare because of the different timing of the fracturing in each case. To  
768 this end, by keeping the time step  $\Delta t = 1.0 [\times 10^{-9} \text{ s}]$ , the concept of  $t_{250}$ , which indicates the  
769 runtime required for completing every 250 [ $\mu\text{s}$ ] (=250,000 timesteps) of the above FDEM  
770 simulation of the UCS model, is introduced and it is monitored for these three cases. Since the  
771  $t_{250}$  for Case 2 (ICZM-FDEM (BCAA)) is the longest, it is used as the reference. Then, transient  
772 relative speed-up is defined as  $(t_{250} \text{ for ICZM-FDEM (BCAA)})/(t_{250} \text{ for ECZM-FDEM (semi-}$   
773  $\text{ACAA})$  and  $(t_{250} \text{ for ICZM-FDEM (BCAA)})/(t_{250} \text{ for ICZM-FDEM (semi-ACAA})$  for Cases  
774 1 and 3 against Case 2, respectively. Figure 17 shows the comparison of transient relative speed-  
775 up with respect to the simulation progress in analysis time, in which 0 % and 100 % is adjusted  
776 to  $t = 0 \mu\text{s}$  and  $t = 7000 \mu\text{s}$ , respectively. To check how the damage state  $D$  in the rock part in  
777 the above UCS model affects the computational performance, this figure also shows the  
778 evolution of the maximum damage  $D$ , i.e.  $(\max(\log_{10}D))$ , among all the CE4s for each case.  
779 Firstly, the ICZM-FDEM (semi-ACAA) shows approximately six times relative-speed up

780 against ICZM-FDEM (BCAA) during the early stages of the FDEM simulation of UCS model  
781 before the onset of damaging. Then, this relative speed-up ratio reduces close to 1 when  
782  $\max(\log_{10}D) = 0$  is satisfied which is due to significant number of TRI3s newly added to the  
783 contact force calculation. This behavior is very similar to what is reported to dynamic UCS  
784 modelling in Fukuda et al. (2021). On the other hand, the ECZM-FDEM (semi-ACAA) shows  
785 approximately four times relative speed-up against ICZM-FDEM (BCAA) before the onset of  
786 damaging. Therefore, ECZM-FDEM (semi-ACAA) is less computationally efficient than the  
787 ICZM-FDEM (semi-ACAA). This is attributed to the unique processing in the MS-ECZM-  
788 FDEM such as the failure judgement, update of M-S relation and assembling the information of  
789 S-nodes to their M-nodes. The ECZM-FDEM (semi-ACAA) code has still the potential for  
790 improvements in terms of the computational efficiency. For instance, there is room to enhance  
791 the performance of the current code in the context of failure judgment. Currently, this judgment  
792 is conducted against all TRI3 boundaries, irrespective of the stress levels. It is possible to further  
793 enhance the computational performance by implementing an algorithm of processing the failure  
794 judgment only for the boundaries whose stress levels are closer to satisfy the failure criteria.  
795 This is regarded as another task for future study. With the increase in the number of activated  
796 CE4s due to damaging, the computational efficiency of ECZM-FDEM (semi-ACAA) becomes  
797 closet to that of ICZM-FDEM (semi-ACAA) since less failure judgement is needed and more  
798 contact force calculation becomes the most computationally demanding part of the FDEM

799 calculations. Then, the performance of the ECZM-FDEM (semi-ACAA) becomes closer to that  
 800 of ICZM-FDEM (BCAA) after the point of maximum ( $\log_{10}D$ ) = 0. Therefore, it can be  
 801 concluded that the ECZM-FDEM (semi-ACAA) is slightly slower than that ICZM-FDEM  
 802 (semi-ACAA) as long as the same time step  $\Delta t$  is used. The total runtime is identified as 17,209  
 803 [s], 13,141 [s] and 67,976 [s] for ECZM-FDEM (semi-ACAA), ICZM-FDEM (semi-ACAA)  
 804 and ICZM-FDEM (BCAA), respectively. However, since the ECZM-FDEM (semi-ACAA)  
 805 does not involve in any CE4s before the onset of the fracturing, the stable time step for the  
 806 ECZM-FDEM (semi-ACAA) can be taken larger than that for the ICZM-FDEM (semi-ACAA).  
 807 Thus, this factor is investigated in Section 3.3 in more detail.



808  
 809 Fig. 17. Transient relative speed-up of ECZM-FDEM (semi-ACAA) and ICZM-FDEM (semi-  
 810 ACAA) against ICZM-FDEM (BCAA), and change of  $\max(\log_{10}D)$  using UCS test model.

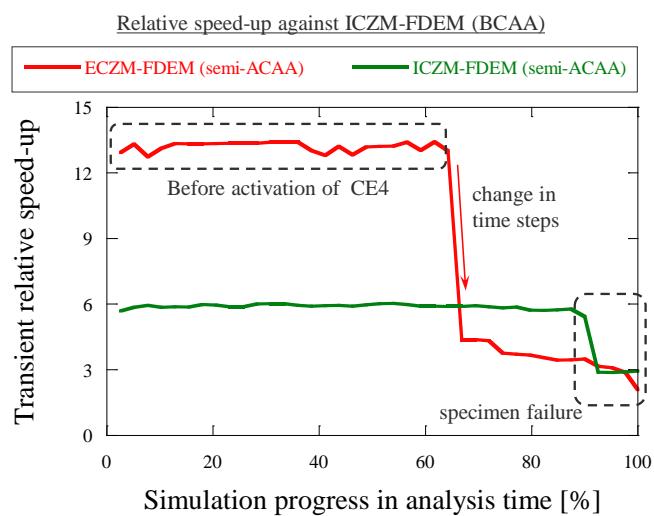
811

812 3.3. Effect of stable time step on computing performance

813 According to our estimation of the maximum stable time step based on the material  
814 properties and mesh geometries (Mohammadnejad et al., 2020) and preliminary analyses using  
815 various values of time step  $\Delta t$ , it was identified that the stable time step  $\Delta t_{\text{crit}}$  for the ICZM-  
816 FDEM (semi-ACAA) and ICZM-FDEM (BCAA) can be taken approximately  $2.0 [\times 10^{-9} \text{ s/step}]$   
817 for the entire simulation. On the other hand,  $\Delta t_{\text{crit}}$  for the ECZM-FDEM (semi-ACAA) can be  
818 taken approximately  $6.0 [\times 10^{-9} \text{ s/step}]$  as long as no CE4s are activated by the crack initiation,  
819 i.e., in the intact regime. Note that in the preliminary analyses of this study, it was confirmed  
820 that, if the values of  $\Delta t$  were set larger than  $\Delta t_{\text{crit}}$  for each case, the FDEM calculations showed  
821 the spurious mode soon after the onset of the simulation, resulting in unrealistic stress level ( $>$   
822 GPa) at various locations. However, to deal with time-discontinuity due to the activation of  
823 dormant CE4s in the ECZM-FDEM (semi-ACAA), cohesive penalty's effect takes part in the  
824 FDEM simulation, which results in the stable time step becomes more or less same as that in  
825 the ICZM-FDEM with semi-ACAA and BCAA since the crack initiation occurs. By taking this  
826 advantage of larger stable time step of ECZM-FDEM (semi-ACAA) in the intact regime, the  
827 comparison of transient relative speed-up is made similar to Fig. 17. To that end, ECZM-FDEM  
828 (semi-ACAA) simulation is conducted using  $\Delta t = 6.0 [\times 10^{-9} \text{ s}]$  and  $\Delta t = 2.0 [\times 10^{-9} \text{ s}]$  before and  
829 after the first activation of CE4, respectively, while the constant  $\Delta t = 2.0 [\times 10^{-9} \text{ s}]$  is used for  
830 ICZM-FDEMs with semi-ACAA and BCAA. Here, the runtime  $t_{180}$  required to calculate for

every 180 [ $\mu$ s] is considered in the above-mentioned UCS model and is monitored. In the case of ECZM-FDEM (semi-ACAA) before the first activation of CE4,  $t_{180}$  is equivalent to  $6.0 [\times 10^{-9} \text{ s}] \times 30,000$  timesteps. On the other hand,  $t_{180}$  is equivalent to  $2.0 [\times 10^{-9} \text{ s}] \times 90,000$  timesteps for ICZM-FDEMs with semi-ACAA and BCAA as well as for ECZM-FDEM (semi-ACAA) after the first activation of CE4. Note that the first activation of CE4 is observed between 720,000 steps and 750,000 steps in the case of ECZM-FDEM (semi-ACAA). Since the  $t_{180}$  for Case 2 (ICZM-FDEM (BCAA)) is the longest, it is again used as the reference. Then, transient relative speed-up is defined as  $(t_{180} \text{ for ICZM-FDEM (BCAA)})/(t_{180} \text{ for ECZM-FDEM (semi-ACAA)})$  and  $(t_{180} \text{ for ICZM-FDEM (BCAA)})/(t_{180} \text{ for ICZM-FDEM (semi-ACAA)})$  for Cases 1 and 3 against Case 2, respectively, which is shown in Fig. 18. The horizontal axis in Fig. 18 is the simulation progress in analysis time, in which 0 % and 100 % is adjusted to  $t = 0 \mu\text{s}$  and  $t = 7000 \mu\text{s}$ , respectively. Figure 18 clearly shows that the relative speedup of ECZM-FDEM (semi-ACAA) against ICZM-FDEM (BCAA) is about 13 times before the first activation of CE4. This relative speed-up of ECZM-FDEM (semi-ACAA) against ICZM-FDEM (BCAA) is about 3 times faster than the case in which the constant  $\Delta t$  is used in ECZM-FDEM (semi-ACAA) as shown in Fig. 17 since the value of  $\Delta t$  used in ECZM-FDEM (semi-ACAA) is taken to be 3 times larger than that used in ICZM-FDEM. After the first activation of CE4 and the reduction in  $\Delta t$ , the relative speed-up of the ECZM-FDEM (semi-ACAA) decreased to about 4 times against ICZM-FDEM (BCAA), which is lower than that of ICZM-FDEM (semi-ACAA) against

850 ICZM-FDEM(BCAA) and similar to the trend in Fig. 17. Then, the total simulation time is  
 851 identified as 4,527 [s], 5,246 [s] and 29,953 [s] for ECZM-FDEM (semi-ACAA), ICZM-FDEM  
 852 (semi-ACAA) and ICZM-FDEM (BCAA), respectively. Thus, the total runtime of ECZM-  
 853 FDEM (semi-ACAA) with variable  $\Delta t$  becomes the smallest among the three cases. Thus, if the  
 854 simulation time for the intact regime occupies relatively larger part of the entire simulation,  
 855 which tends to be true for many quasi-static loading scenarios especially for hard rocks such as  
 856 granite, ECZM-FDEM (semi-ACAA) can achieve better performance than ICZM-FDEM  
 857 thanks to the larger stable time step. Therefore, not only the improvement of the calculation  
 858 precision in the intact deformation regime but also the improvement of the computational  
 859 efficiency is achieved by introducing the proposed GPGPU-based ECZM-FDEM while the  
 860 obtained fracture pattern can be still reasonable.



861  
 862 Fig. 18. Transient relative speed-up of ECZM-FDEM (semi-ACAA) with variable time step and  
 863 ICZM-FDEM (semi-ACAA) against ICZM-FDEM (BCAA), and change of  $\max(\log_{10}D)$  using  
 864 UCS test model.

865

866 **4. Conclusions**

867 In this study, GPGPU-parallelized 2-D ECZM-FDEM was proposed by applying the M-S  
868 algorithm as an alternative method for the complex adaptive remeshing traditionally adopted in  
869 ECZM-FDEM. The proposed MS-ECZM-FDEM algorithm was explained in detail and  
870 implemented in the GPGPU-parallelized Y-HFDEM code. Then, the developed code was  
871 applied to numerically model the BTS and UCS tests of siliceous mudstone under quasi-static  
872 loading for verification and validation. Furthermore, the results from the numerical modellings  
873 of the BTS and UCS tests using GPGPU-parallelized ECZM-FDEM and ICZM-FDEM were  
874 compared against each other in terms of several aspects, which are summarized below:

875 • During the continuous deformation stage, the accuracy of ICZM-FDEM is compromised  
876 against FDEM without cohesive elements by 1.6 % ~ 2.0 % and 1.4 % ~ 1.8 % for the  
877 distribution of normal stresses ( $\sigma_{xx}$ ,  $\sigma_{yy}$ ), respectively, inside the specimen in the BTS  
878 modelling, and by 1.2 % ~ 1.7 % for the tangent modulus in the stress-strain curve in the  
879 UCS modelling. However, ECZM-FDEM showed no degradation in accuracy compared  
880 with FDEM without cohesive elements. Moreover, for the spatial stress distribution before  
881 fracturing in the UCS modelling, ECZM-FDEM showed a smooth distribution while  
882 ICZM-FDEM showed a noisy and disturbed distribution.

883 • In terms of the stable time step, ECZM-FDEM can set the time step in the intact regime

884 about three times larger compared to ICZM-FDEM with the cohesive penalty being 100  
885 times of Young's modulus of the rock. Furthermore, by taking advantage of larger stable  
886 time step in ECZM-FDEM, the total runtime of ECZM-FDEM became smaller than that of  
887 ICZM-FDEM in the case of modelling the UCS test. This study targeted at the soft rock  
888 and the relative speed-up in the total runtime was about 6 times faster. It is expected, if hard  
889 rock is modelled, a much more significant times of relative speed-up can be achieved the  
890 runtime spent in modelling the intact regime of the hard rock is much longer.

891 • As for the contact activation, ECZM-FDEM removes the need for the BCAA, which has  
892 been prevalent in the ICZM-FDEM community but extremely computationally intense.  
893 Instead, ECZM-FDEM implements the more computationally efficient semi-ACAA and  
894 ACAA for the contact activation. It is confirmed that a relative speed-up of about 13 times  
895 of ECZM-FDEM based on the semi-ACAA can be achieved against ICZM-FDEM based  
896 on BCAA in the intact regime together with the improvement about the aforementioned  
897 stable time step. However, after the crack initiation, the stable time step of ECZM-FDEM  
898 becomes more or less same as that of ICZM-FDEM due to the effect of larger cohesive  
899 penalty to deal with time-discontinuity issue inherent in ECZM.

900 Thus, the proposed GPGPU-parallelized ECZM-FDEM with the M-S algorithm is  
901 confirmed to provide effective and valuable improvements over the conventional GPGPU-  
902 parallelized ICZM-FDEM for the numerical modelling of rock fracturing process. However,

903 only 2-D model is considered in this study and further study is need to extended the proposed  
904 GPGPU-parallelized ECZM-FDEM with the M-S algorithm to 3-D model in order to reasonably  
905 model rock fracture problems. Although the proposed counter-clockwise searching around each  
906 node group cannot be directly used in the 3-D case, the M-S algorithm adopted this study is  
907 expected to pave the way to realize the 3-D implementation of GPGPU parallelized ECZM-  
908 FDEM.

909

910 **Acknowledgement**

911 This work was partially funded by JST FOREST Program (Grant Number JPJFR216Y, Japan)  
912 and JSPS KAKENHI (Grant Numbers 22H01589, 20K14826), and JFE 21<sup>st</sup> Century Foundation,  
913 Hitachi Global Foundation, JGC-S SCHOLARSHIP FOUNDATION to S.O., and JSPS  
914 KAKENHI (Grant Number 22K04996) to D.F. Their support is gratefully acknowledged.

915

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1062

1063                   **Nomenclature**

1064                   Abbreviations

1065   1-D                   1-dimentional

1066   2-D                   2-dimentional

1067   3-D                   3-dimensional

1068   GPGPU               general-purpose graphic-processing-units

1069   MPI                   message-passing interface

1070   PC                   personal computer

1071   CUDA                   computing unified device architecture

1072   FEM                   finite element method

1073   DEM                   discrete element method

1074	FDEM	combined finite-discrete element method
1075	CZM	cohesive zone model
1076	ICZM	intrinsic cohesive zone model
1077	ECZM	extrinsic cohesive zone model
1078	DGCZM	Galerkin-based cohesive zone model
1079	UCZM	universal cohesive zone model
1080	ICZM-FDEM	intrinsic cohesive zone model - based combined finite-discrete
1081		element method
1082	ECZM-FDEM	extrinsic cohesive zone model - based combined finite-discrete
1083		element method
1084	BCAA	brute-force contact activation approach
1085	ACAA	adaptive contact activation approach
1086	M-node	master node
1087	S-node	slave node
1088	M-S relation	relation between M-node and S-node
1089	M-S algorithm	updating algorithm of the M-S relation
1090	MPCs	multi-point constraints
1091	TRI3s	3-node triangle elements
1092	CE4s	4-node cohesive elements

1093 BTS Brazilian tensile strength

1094 UCS uniaxial compressive strength

1095