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Round robin test on angle of repose: DEM simulation  
results collected from 16 groups around the world

Hidetaka Saomoto<sup>a,\*</sup>, Naotaka Kikkawa<sup>b</sup>, Shuji Moriguchi<sup>c</sup>, Yukio Nakata<sup>d</sup>,  
Masahide Otsubo<sup>e,1</sup>, Vasileios Angelidakis<sup>f</sup>, Yi Pik Cheng<sup>g</sup>, Kevin Chew<sup>h</sup>,  
Gabriele Chiaro<sup>h</sup>, Jérôme Duriez<sup>i</sup>, Sacha Duverger<sup>i</sup>, Joaquín Irazábal  
González<sup>j</sup>, Mingjing Jiang<sup>k,2</sup>, Yohei Karasaki<sup>e</sup>, Akiko Kono<sup>l</sup>, Xintong Li<sup>m</sup>,  
Zhuyuan Lin<sup>n</sup>, Asen Liu<sup>m</sup>, Sadegh Nadimi<sup>f</sup>, Hitoshi Nakase<sup>o</sup>, Daisuke  
Nishiura<sup>p</sup>, Utsa Rashique<sup>q</sup>, Hiroyuki Shimizu<sup>r</sup>, Kumpei Tsuji<sup>s</sup>, Takashi  
Watanabe<sup>t</sup>, Xiaomin Xu<sup>u</sup>, Mourad Zeghal<sup>q</sup>

<sup>a</sup> *Institute of Earthquake and Volcano Geology, National Institute of Advanced Industrial  
Science and Technology, Ibaraki, Japan*

<sup>b</sup> *Construction Safety Research Group, National Institute of Occupational Safety and  
Health, Japan, Tokyo, Japan*

<sup>c</sup> *International Research Institute of Disaster Science, Tohoku University, Miyagi, Japan*

<sup>d</sup> *Graduate School of Sciences and Technology for Innovation, Yamaguchi  
University, Yamaguchi, Japan*

<sup>e</sup> *Institute of Industrial Science, The University of Tokyo, Tokyo, Japan*

<sup>f</sup> *School of Engineering, Newcastle University, Newcastle upon Tyne, The United  
Kingdom*

<sup>g</sup> *Department of Civil, Environmental and Geomatic Engineering, University College  
London, London, The United Kingdom*

<sup>h</sup> *Civil and Natural Resources Engineering, University of Canterbury, Christchurch, New  
Zealand*

<sup>i</sup> *RECOVER, INRAE, Aix Marseille University, Aix-en-Provence, France*

<sup>j</sup> *Machine Learning in Civil Engineering Group, International Centre for Numerical  
Methods in Engineering (CIMNE), Barcelona, Spain*

<sup>k</sup> *School of Civil Engineering, Suzhou University of Science and Technology, Jiangsu  
Province, China*

<sup>l</sup> *Railway Dynamics Division, Railway Technical Research Institute, Tokyo, Japan*

<sup>m</sup> *School of Civil Engineering, Tianjin University, Tianjin, China*

<sup>n</sup> *Department of Earth Science and Engineering, Nanjing University, Jiangsu, China*

<sup>o</sup> *Research And Business Incubation Unit, Tokyo Electric Power Services Co., Ltd.  
, Tokyo, Japan*

<sup>p</sup> *Center for Mathematical Science and Advanced Technology, Japan Agency for  
Marine-Earth Science and Technology, Kanagawa, Japan*

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\*Corresponding author.

*Email address: h-saomoto@aist.go.jp (Hidetaka Saomoto)*

<sup>1</sup>Present affiliation: Public Works Research Institute, Ibaraki, Japan

<sup>2</sup>Former affiliation: Tianjin University, Tianjin, China

<sup>q</sup> *Civil and Environmental Engineering, Rensselaer Polytechnic Institute , New York, The United States of America*

<sup>r</sup> *Civil Engineering Design Division, Kajima corporation , Tokyo, Japan*

<sup>s</sup> *Department of Civil Engineering, Kyushu University, Fukuoka, Japan*

<sup>t</sup> *Disaster Reduction and Environmental Engineering Dept., Kozo Keikaku Engineering Inc. , Tokyo, Japan*

<sup>u</sup> *Department of Engineering, Civil Engineering Division, University of Cambridge, Cambridge, The United Kingdom*

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## **Abstract**

The round robin test (the simultaneous analysis of the same problem) is a method to investigate the variance and sensitivity of results provided by different analysts for a given problem and the reliability of the particular software used by each group participating in the test. A round robin test has been conducted for the traditional numerical method (e.g., finite difference method), but not yet for the discrete element method (DEM). This paper presents the results of the first ever round robin test on the DEM simulation for the angle of repose, involving 16 groups from around the world using different softwares. Within the scope of this round robin test, most groups reported similar simulation results for the angle of repose that differed only by a few degrees from the average of the experimental values, which was initially concealed from participants. There was also good agreement on the degree of variance of the angle of repose. In addition, this paper revealed the recent trends on the interparticle constitutive models and DEM softwares by considering the reports obtained from the participants.

*Keywords:* round robin test, discrete element method, angle of repose, validation, particle, 3D printer

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## 1. Introduction

The discrete element method (DEM) was developed in the 1970s (Cundall, 1971; Cundall and Strack, 1979) and has now become a powerful tool for analyzing the complex behavior of geomaterials featuring particulate assemblies subjected to large deformation and fracturing.

One of the most popular applications of DEM in soil mechanics is to simulate soil element tests, such as the triaxial compression test and the direct shear test. One of the important purposes of simulating soil element tests by DEM is to calibrate the parameters of the interparticle constitutive model by fitting the stress-strain curve obtained from the element tests. After parameter adjustment, the relationship between the microstructure properties, such as particle arrangement, to the macroscopic stress-strain relationship can be discussed. Cheng et al. (2003) created particles that can represent particle fragmentation by bonding about 40 spheres together. They simulated a triaxial compression test using about 400 of these crushable particles. Kikkawa et al. (2013) measured elastic wave velocities of chemical-solidified Toyoura sand using a bender element test and then used the test results to determine the elastic stiffness of contacting DEM particles and the bond stiffness bridging DEM particles. Jiang et al. (2015) proposed an interparticle constitutive model that can account for the rolling and twisting between non-spherical particles and conducted triaxial compression simulations incorporating the proposed model using spherical particles. In their simulation model for triaxial compression tests which included methane hydrate particles, Yu et al. (2016) simulated the stress-strain curve by changing the content of methane hydrate particles inside the simulation model. Otsubo and O'Sullivan (2018)

26 conducted elastic wave propagation tests using particles made of borosili-  
27 cate glass with controlled surface roughness. These were simulated by a  
28 DEM that incorporates an interparticle constitutive model considering sur-  
29 face roughness (Otsubo et al., 2017) and discussed the effect of the particle  
30 surface roughness on the macroscopic shear stiffness. Chew et al. (2022)  
31 conducted DEM simulations for direct shear tests of gravel-rubber mixtures.  
32 The gravel and rubber particles were respectively modeled using clamped  
33 particles of five different shapes.

34 In addition to the soil element test, the DEM simulations coupled with  
35 fluids have been actively studied. Zeghal and El Shamy (2004) simulated  
36 liquefaction by coupling DEM with the Navier-Stokes (NS) equations av-  
37 eraged through porosity. Yamaguchi et al. (2017) modeled a channel bed  
38 with a DEM and simulated the topographic changes in the channel bed  
39 caused by water flowing in the channel. Tsuji et al. (2019) attempted to  
40 simulate the ground collapse due to the deterioration of sewer pipes using  
41 the DEM and the smoothed particle hydrodynamics (SPH) representing the  
42 pore fluid phase. Chen et al. (2022) applied a large-scale DEM simulation  
43 code (DEPTH) to the underwater mixing process for deep-sea mining with  
44 lubrication models.

45 The DEM is applied in engineering to simulate the ballast behavior under  
46 rails caused by railroad loads. Because ballast particles are about 5 cm in  
47 diameter, a simulation model close to the actual condition can be created by  
48 using a high-performance computer. For example, Irazábal et al. (2017) de-  
49 termined the parameters of a bounded rolling friction model to simulate bal-  
50 last particles with spherical particles through a comparison with experimental

51 results. Kono (2018) modeled the accurate ballast shape by combining the  
52 laser measurement and a shape optimization method for clumping proposed  
53 by Matsushima and Saomoto (2002). The ballast particles were then sub-  
54 jected to DEM analysis and compared with the results of cyclic loading tests.  
55 In their analysis of the behaviors of 190,000 ballast particles, Nishiura et al.  
56 (2018) used the quadruple discrete element method (QDEM) in which the  
57 material parameters are directly determined from the macroscopic viscoelas-  
58 tic parameters used in continuum mechanics. In addition to determining  
59 ballast behavior, there are other engineering-oriented applications of DEM  
60 simulations: slope hazards (Nakase et al., 2017); rockfall protection (Kanno  
61 et al., 2021); rock engineering (Duriez et al., 2011; Shimizu et al., 2011; Jiang  
62 et al., 2020); and clay deformation (Lin et al., 2021).

63 The DEM simulations in almost all of the DEM applications described  
64 above have been validated by a single analysis group using a single software.  
65 From this perspective, it is difficult to evaluate the skill of each analyst  
66 and to determine the reliability of the software by referring to these studies  
67 individually. This brings us to the motivation of our study.

68 Round robin test for traditional numerical methods such as the finite  
69 element method have been conducted over the years for different research  
70 fields: seismology (Harris et al., 2011, 2018); rock mechanics (Berre et al.,  
71 2021); coastal hydrology (Horrillo et al., 2015). These round robin tests  
72 indicate that assessing the user-dependency and sensitivity of results and the  
73 reliability of each software is extremely important. It should be noted that  
74 despite the importance of the round robin test, it has never been implemented  
75 for a DEM simulation.

76 We therefore have conducted the first ever round robin test on DEM  
77 simulation for the angle of repose (AOR) under the responsibility of the  
78 TC105 Japanese domestic committee in the Japanese Geotechnical Society.  
79 The objectives of this study are as follows: (1) To clarify the approach taken  
80 by the participants of the round robin test to the simulation of the angle  
81 of repose; (2) To quantitatively analyze the differences between individual  
82 simulation results and experimental results, based on both the average value  
83 and the variance; (3) To discuss the relationship between the differences  
84 from experiments and the modeling techniques especially for particle shape  
85 modeling and interparticle constitutive equation; and (4) To clearly see the  
86 current trend in the DEM software.

## 87 **2. Round robin test for discrete element method**

88 Although the details of the round robin test are found on the website  
89 (TC105 Japanese domestic committee, 2020) and Nakata et al. (2022), we  
90 summarize and describe that information here for the convenience of the  
91 readers.

### 92 *2.1. Outline of round robin test*

93 Figure 1 shows the outline of the round robin test for the AOR. Using  
94 the artificial particles detailed in Section 2.2, the TC105 Japanese committee  
95 (test organizer) conducted two types of experiments for the AOR depicted in  
96 Section 2.3. After obtaining the experimental results, the committee released  
97 the information relating to the particles used in the experiments (material,  
98 shape, mechanical properties) and the two experimental conditions required  
99 for the DEM simulation to the participating groups via the website (TC105

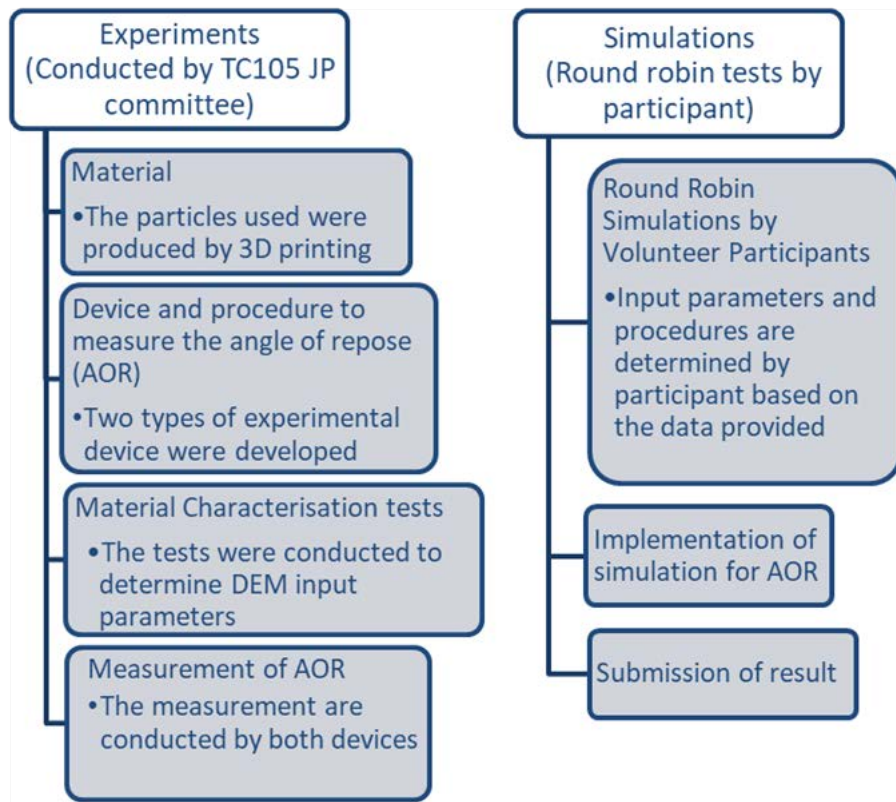


Figure 1: Outline of the round robin test for AOR.



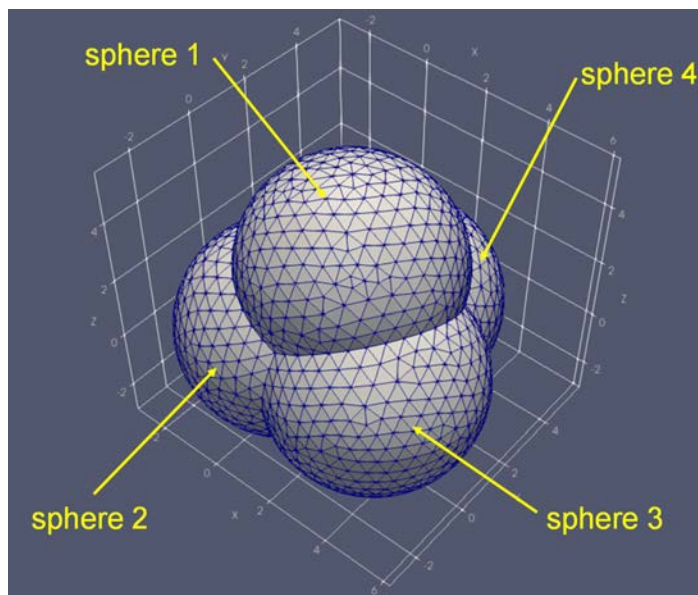


Figure 2: Shape of artificial particles represented by four spheres arranged in a regular tetrahedral form.

100 Japanese domestic committee, 2020). These groups then performed DEM  
101 simulations for the experimental conditions based on their research experi-  
102 ences and perspectives using the information available on the website and  
103 then submitted the simulation results to the committee in accordance with  
104 the report format described in Section 2.5.

### 105 *2.2. Artificial particle used in experiments*

106 Figure 2 shows the shape of the artificial particles, used in the experi-  
107 ment. Each artificial particle was designed with four spheres (spheres 1, 2,  
108 3, and 4) placed at each vertex of a regular tetrahedron. Note that there is  
109 no size distribution for artificial particles used in the experiments. Subse-  
110 quently, the artificial particles were realized with resinous material by using  
111 a 3D printer. The coordinates of each sphere center are expressed as follows:

Table 1: List of characteristics of the artificial particles.

Parameter	Test	Object	Mean	Standard deviation
Static friction angle	Inclined surface test	Resin-resin	35.5°	3.82°
		Acrylic-resin	27.2°	4.26°
Dynamic friction angle	Inclined surface test	Resin-resin	29.36°	2.42°
		Acrylic-resin	16.5°	7.35°
Coefficient of restitution	Drop test	Resin-resin	0.809	0.0115
		Acrylic-resin	0.790	0.0280
Shear modulus	Cyclic uniaxial test	Resin	560 MPa	158 MPa
		for horizontal plane	680 MPa	70 MPa
		for vertical plane	440 MPa	130 MPa
Normal spring coefficient (Normal contact force: 0.1N)	Cyclic uniaxial test	Resin	$6.0 \times 10^4$ N/m	$1.1 \times 10^4$ N/m
		for horizontal plane	$6.9 \times 10^4$ N/m	$0.5 \times 10^4$ N/m
		for vertical plane	$5.2 \times 10^4$ N/m	$0.5 \times 10^4$ N/m

112  $(0, 0, 0)$ ,  $(3.101, 0, 0)$ ,  $(1.551, 0.895, 2.532)$ , and  $(1.551, 2.685, 0)$  for spheres 1,  
 113 2, 3, and 4, respectively (unit: mm). Note that each sphere has the same  
 114 radius (3.101 mm).

115 The material properties of the artificial particles are listed in Table 1.  
 116 The mean values and standard deviations of each parameter were obtained  
 117 by a sufficient number of experiments. In addition to the information listed  
 118 in Table 1, friction angles between the artificial particle material (resin) and  
 119 the surface of the experimental apparatus (acrylic plate) have also been mea-  
 120 sured (Nakata et al., 2022): static friction angle: 27.2 degrees with the stan-  
 121 dard deviation of 4.26 degrees; dynamic friction angle: 16.5 degrees with the  
 122 standard deviation of 7.35 degrees.

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### 123 2.3. Two types of AOR experiment

124 The test organizer prepared two types of AOR experimental setup: Device  
 125 I is a rectangular type (plane strain condition), as shown in Figure 3, and

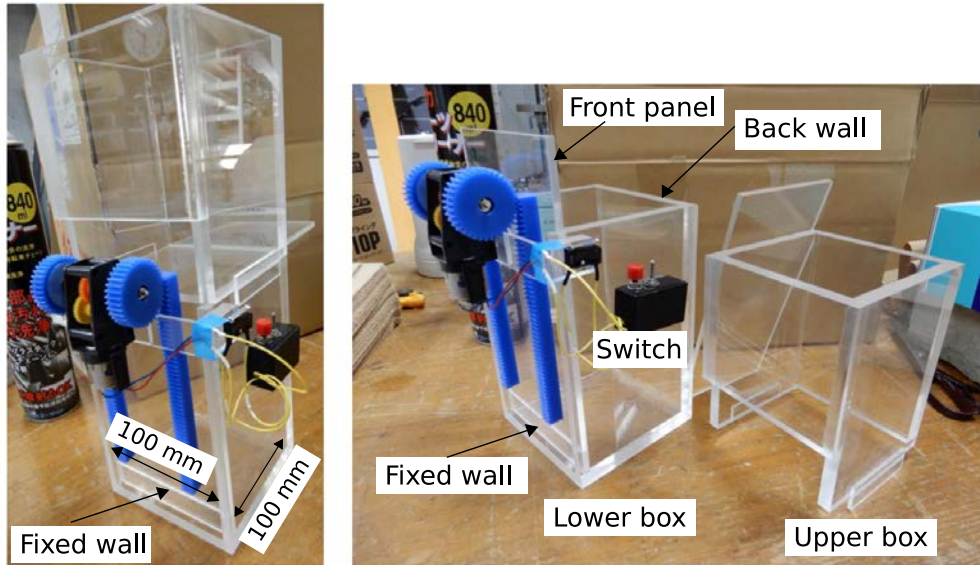


Figure 3: Experimental apparatus for Device I.

126 Device II is a cylindrical type (axial-symmetric condition), as shown in Figure  
 127 4.

128 The Device I apparatus is made of transparent acrylic plates and com-  
 129 prises an upper and a lower box, separated by a horizontal acrylic plate that  
 130 can translate horizontally. The artificial particles (detailed in Section 2.2)  
 131 are initially deposited in the upper acrylic box. During the experiment, the  
 132 artificial particles firstly fall under the action of gravity by translating the  
 133 plate installed between the upper box and the lower box outwards. When  
 134 the particles have come to rest, the front panel of the lower box is pulled  
 135 upwards by an electric motor at a constant speed of 43 mm/s. Almost 2150  
 136 particles were used in those experiment. We can also confirm the size detail  
 137 on the website (TC105 Japanese domestic committee, 2020).

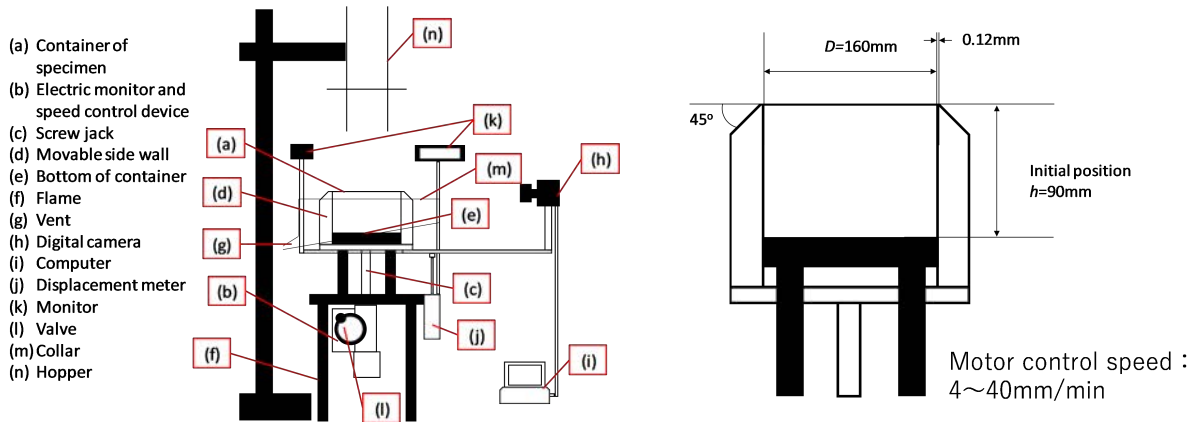


Figure 4: Experimental apparatus for Device II (left: overall view, right: container section where particles are deposited).

138 A schematic illustration of Device II with the cylindrical configuration  
 139 is provided in Figure 4. The container in which the particles are placed [a]  
 140 is enclosed by an acrylic cylindrical wall [d] and a fixed bottom plate [e]  
 141 with a diameter of 160 mm. The cylindrical wall can be moved down at a  
 142 constant speed using an electric motor [b], and the initial height from the top  
 143 of the cylindrical wall to the bottom plate is 90 mm. Two digital cameras  
 144 [h] are placed orthogonally in order to measure the angle of repose. The  
 145 experimental procedure for Device II is as follows: (1) the artificial particles  
 146 are initially deposited in a hopper of 100 mm diameter; (2) the container [a]  
 147 is filled with almost 2700 particles under the action of gravity by translating  
 148 the bottom plate of the hopper.

149 The aforementioned experimental procedure was described in detail on  
 150 the website (TC105 Japanese domestic committee, 2020) prior to the round  
 151 robin test. Therefore, the participants were expected to perform DEM

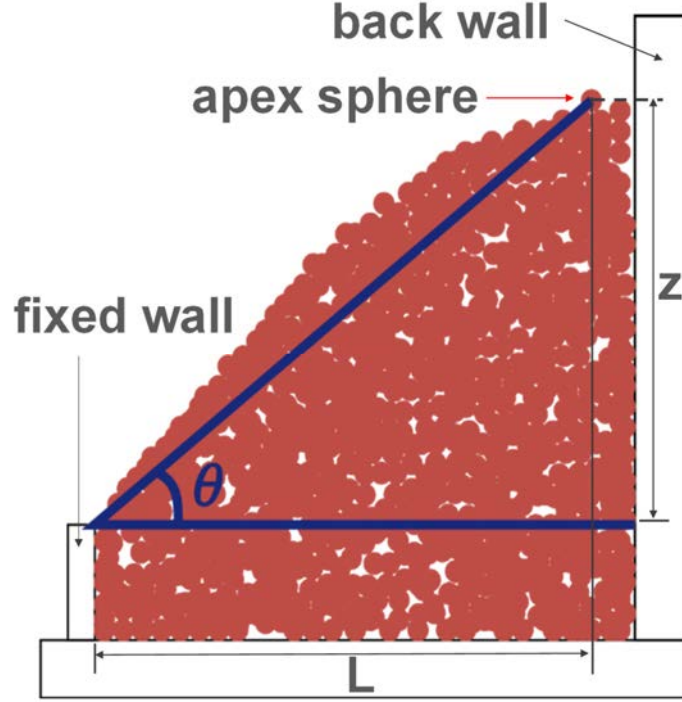


Figure 5: Schematic illustration at the end of DEM simulation for Device I.

152 simulations according to the experimental process for each device.

#### 153 2.4. AOR measurement in experiment

154 Figure 5 shows a schematic illustration at the end of the DEM simulation  
 155 for Device I. The AOR for Device I is uniquely determined using the coor-  
 156 dinate values of the centroid of the apex sphere at the top of the specimen  
 157 (Fig. 5). Using lengths  $Z$  and  $L$  depicted in Figure 5, we have

$$\theta_1 = \tan^{-1} \left( \frac{Z}{L} \right), \quad (1)$$

158 where  $\theta_1$  is the AOR for Device I.

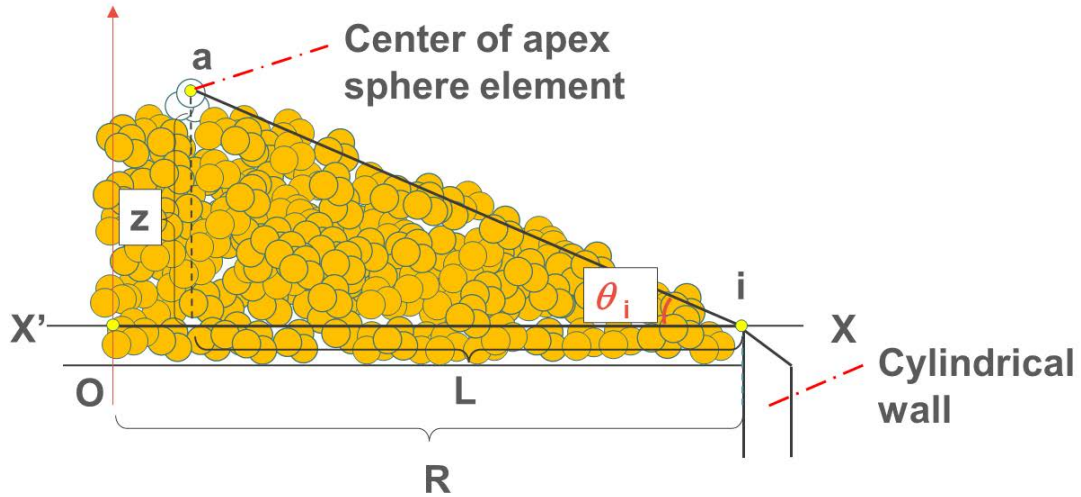


Figure 6: Schematic illustration at the end of DEM simulation for Device II.

159 In the case of Device II, we can use the coordinate values of the apex  
 160 sphere of a particle at the end of simulation to determine the AOR, in the  
 161 same way as described for Device I. Note that there are several possible  
 162 definitions of the AOR for Device II.

163 Figure 6 is a supporting diagram to define the angle of repose in Device  
 164 II, indicating a schematic illustration at the end of the DEM simulation for  
 165 Device II. In general, the xy-coordinate of the sphere located at the top  
 166 (a) does not coincide with the bottom plate center (O). To this end, 360  
 167 measuring points were set on the top of the cylindrical wall at intervals of  
 168 one degree, and the angle  $\theta_i$  was calculated for each line connecting each  
 169 measuring point ( $i$ ) and the top of the sphere element (a). Denoting the  
 170 maximum  $\theta_i$  as  $\theta_{\max}$  and the minimum  $\theta_i$  as  $\theta_{\min}$ , the average of these two  
 171 values can be a representative of angle of repose for Device II. Here, we

172 employ this definition as the AOR for Device II,

$$\theta_{\text{II}} = \frac{\theta_{\text{max}} + \theta_{\text{min}}}{2}, \quad (2)$$

173 where  $\theta_{\text{II}}$  is the the AOR for Device II. Naturally, Eqs. (1) and (2) are ap-  
174 plied to the corresponding DEM simulation results in order to quantitatively  
175 compare the simulation results and the experimentally obtained results.

176 It should be noted that the value of AOR generally depends on the initial  
177 configuration of particles and subsequent packing characteristics. However,  
178 since it is difficult to analyze such effects quantitatively and independently,  
179 we tried to compare the experimental data with simulation results based on  
180 the concept that the effect is one of the uncertainties which causes variation  
181 of the AOR.

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### 182 2.5. Data collection from participants

183 Each participating group is required to submit a spreadsheet containing  
184 the predefined questions prepared by the test organizer and the 3D coordi-  
185 nates of all sphere particles included in tetrahedral particles at the end of the  
186 simulation. The questions in the spreadsheet are designed to gather specific  
187 information, including the following: (1) the software used, (2) the parallel  
188 computation environment, (3) the interparticle constitutive model and its  
189 parameter values, (4) the particle shape and the size used, (5) the method of  
190 creating the initial configuration of particles, (6) the setting of the moving  
191 speed of the boundary wall, (7) the number of simulation trials.

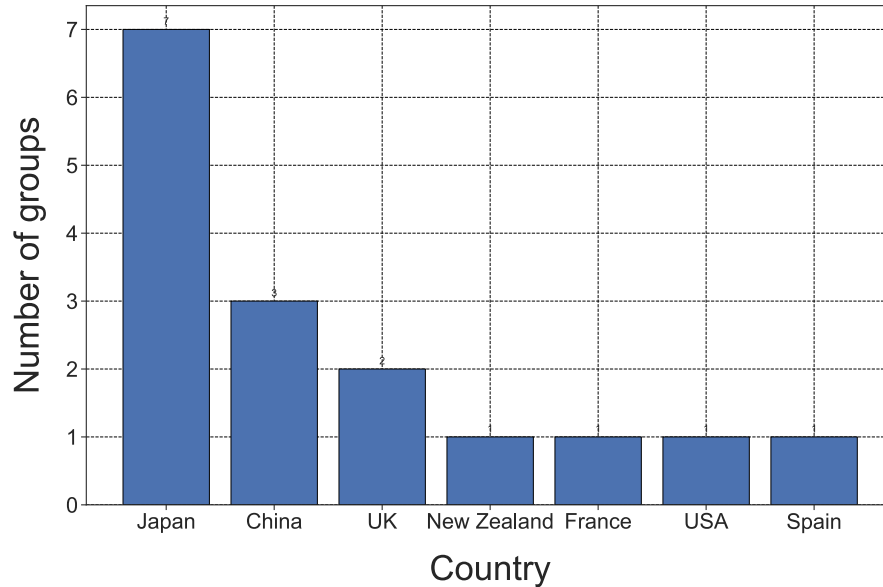


Figure 7: Relationship between the number of analysis groups and country.

192 **3. Results of round robin test**

193 This section summarizes the results of the round robin test where the  
 194 reported AOR values are correlated with the adopted input parameters for  
 195 each analysis group. It should be noted that the results of the round robin  
 196 test are not necessarily general but limited to the specific conditions in the  
 197 experiments, such as boundary conditions, artificially-made particles, and  
 198 low confining pressure.

51, 56

199 *3.1. Number of participation groups by country*

200 The number of groups who participated in the round robin test by country  
 201 is shown in Figure 7. In total, 16 groups from 7 countries participated in the  
 202 round robin test. According to Figure 7, Japan has the largest number of



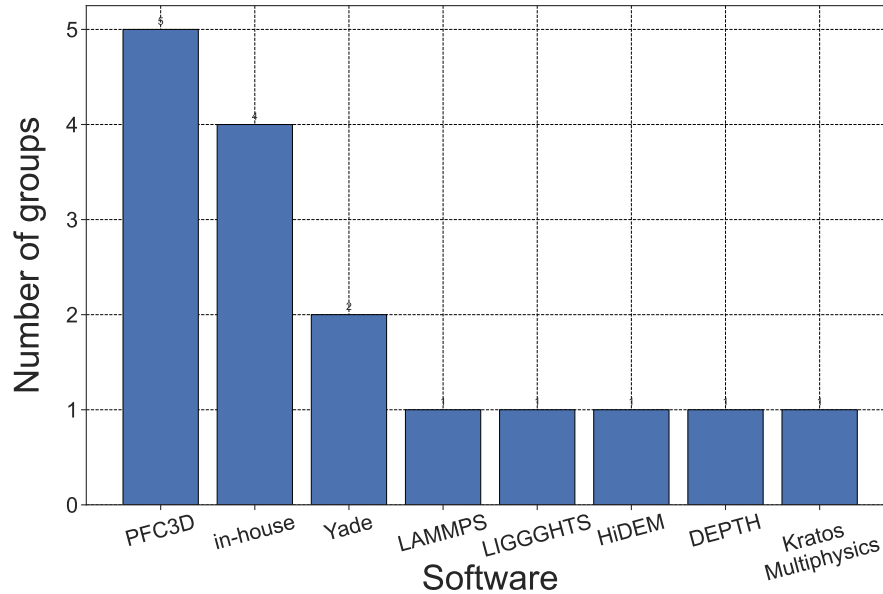


Figure 8: Histogram of software used in round robin test.

203 analysis groups, followed by China and the UK, and France, New Zealand,  
 204 Spain, and the United States are represented by an equal number of groups.

### 205 3.2. Summary for used software

206 The statistical results of the software used in the round robin test are  
 207 illustrated in Figure 8. It can be seen that software most commonly used  
 208 in the round robin test was PFC3D (Itasca Consulting Group, Inc., 2021)  
 209 and in-house software. Yade (Smilauer et al., 2021) was used by two groups.  
 210 Also, LIGGGHTS (Kloss et al., 2012), LAMMPS (Sandia National Laborato-  
 211 ries, 2001; Thompson et al., 2022), HiDEM (Sakaguchi and Nishiura, 2009),  
 212 DEPTH(Chen et al., 2020; Nishiura et al., 2021), and Kratos Multiphysics  
 213 (Dadvand et al., 2010, 2013) were all used by one group.

214 A brief introduction to the various software chosen for the assigned task

215 follows. The PFC3D is a prominent commercial software manufactured by  
216 ITASCA Consulting Group, Inc. and is widely used in discrete element  
217 simulations in the field of geotechnical engineering.

218 Most in-house software is developed independently in university labora-  
219 tories. Note that we did not investigate the details of them used in the round  
220 robin test.

221 Yade is an open-source framework for DEM simulations. Although the  
222 core computation parts are written in C++, the user interface is prepared  
223 with the Python language for easy handling.

224 LIGGGHTS is an open-source discrete element simulator and is an ex-  
225 tension of the molecular dynamics software, LAMMPS (described below). In  
226 comparison with LAMMPS, LIGGGHTS has the following additional fea-  
227 tures: CAD geometry handling, heat conduction, contact force formulation,  
228 and particle arrangement using 3-D meshes.

229 LAMMPS is a classical molecular dynamics simulation code (open-source).  
230 While LAMMPS is designed for molecular dynamics simulations, it comes  
231 with an original granular mechanics package which is to be distinguished  
232 from LIGGGHTS.

233 HiDEM is a Fortran 90/95 based commercial software developed by Japan  
234 Agency for Marine-Earth Science and Technology (JAMSTEC). Further-  
235 more, DEPTH is a commercial software developed from HiDEM that imple-  
236 ments an iterative dynamic load balancer algorithms (Furuichi et al., 2017)  
237 enabling it to run the world’s largest-scale DEM simulation on the massive  
238 parallel computer systems.

239 KRATOS Multiphysics is an open-source framework for building parallel,

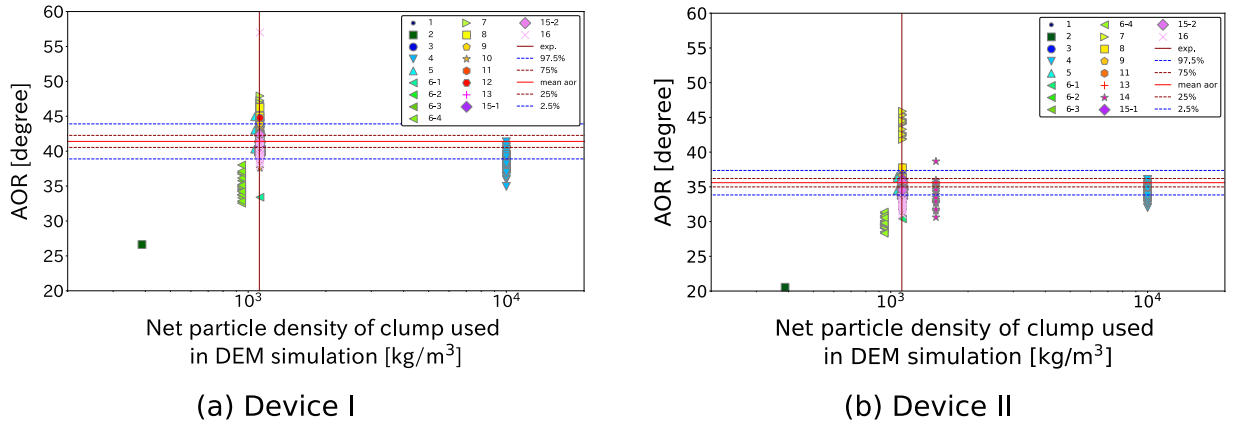


Figure 9: Relationship between AOR experiment results and net particle density used in DEM simulations.

240 multi-disciplinary simulation software including the discrete element method.  
 241 This software features easy coupling of the DEM with other analysis tools  
 242 implemented in KRATOS, such as the DEM and a fluid analysis or the DEM  
 243 and a finite element solid analysis.

### 244 3.3. Modeling for particle shape and mass

245 Figure 9 shows the relationship between the AOR and the density of the  
 246 clumped particle for both Device I (Fig. 9 (a)) and Device II (Fig. 9 (b)).  
 247 In Fig. 9, the vertical axis indicates the value of the angle of repose and the  
 248 horizontal axis indicates the density used in the DEM simulations. The solid  
 249 red line drawn horizontally represents the mean of the experimental AOR  
 250 values, and the dashed dark red and blue lines represent the 75% and 97.5%  
 251 quartiles, respectively. The vertical line with a density close to  $10^3$  indicates  
 252 the density of the material of particles used in the experiments ( $1111 \text{ kg/m}^3$ ).  
 253 Each plot shows the AOR calculated from the DEM simulation results sub-  
 254 mitted by the participants, and the legend indicates the analyst ID (16 groups

255 in total), respectively. Note that the experimental value ( $1111 \text{ kg/m}^2$ ) was  
256 employed in 91% of the total number of simulation runs for Device I (350  
257 runs in total) and in 87% of the total number of simulation runs for Device  
258 II (343 runs in total).

259 Most of the analysis groups used tetrahedron-shaped particles by clump-  
260 ing four spheres as in the experiment, while the particles used by several  
261 other analysis groups had their own user-defined shape or were spherical.  
262 When using a spherical particle shape, which differs from the experimental  
263 one, it is necessary to adjust the interparticle constitutive model reflecting  
264 the particle shape effect which is equivalent to the experimental state in  
265 terms of the rotational motion of the particles and the porosity ratio of the  
266 particle assembly. For example, analysis group 14 used spherical particles  
267 and introduced the rolling resistance of spherical particles to account for the  
268 effect of particle shape. Most analysis groups used the same size particles as  
269 those in the experiment.

270 From the perspective of accuracy, most of the simulation results fell within  
271 the 97.5% quantile of the AOR obtained from the experiments (assuming  
272 normal distribution) irrespective of the device type. Some simulation results  
273 deviated from the experimental values (analysis groups 2 and 4 for Device  
274 I, and analysis groups 2, 4, and 7 for Device II), but these are basically  
275 due to inappropriate parameter settings, **which will be discussed in a later**  
276 **section**. In the case of analysis group 6, the AOR recorded from the DEM  
277 simulations was smaller than the experimental value, because rounded convex  
278 tetrahedral potential particles were employed. These particles interlocked less  
279 than the real, concave tetrahedral particles, a behavior that was expected.

← S4

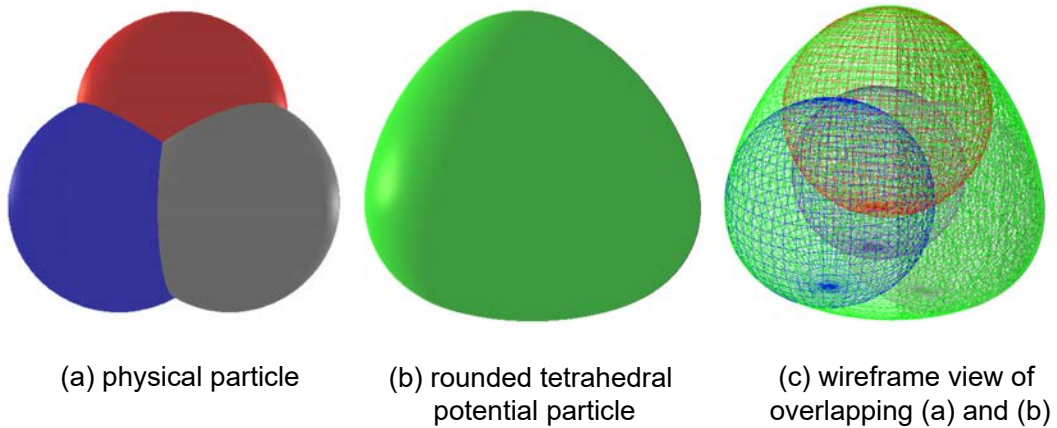


Figure 10: Rounded tetrahedral potential particle shape modeled by analyst 6.

280 Nevertheless, this modeling approach provided a quantification of the effect  
 281 that convexity has on the interlocking capabilities of the analyzed material.  
 282 There were two cases in which the values of density were significantly different  
 283 from the experimental values: analysis group 2, with about  $300 \text{ kg/m}^3$  and  
 284 analysis group 4, with  $10,000 \text{ kg/m}^3$ . The authors guess the analysis group 4  
 285 may aim to reduce the computational cost by increasing the time step in the  
 286 DEM simulation, whereas the intention of group 2 is unclear. The details of  
 287 the inappropriate settings are described in the following discussion section.

S5

288 In the case where the density is set to a slightly smaller value (analy-  
 289 sis group 6) than the experimental value, it seems that the volume of the  
 290 user-defined particle shape (rounded tetrahedral potential particle shape) il-  
 291 lustrated in Figure 10 slightly differs from that of the particles used in the  
 292 experiment, to approximate closely the real inertial characteristics (mass and  
 293 inertia) of the physical particle.

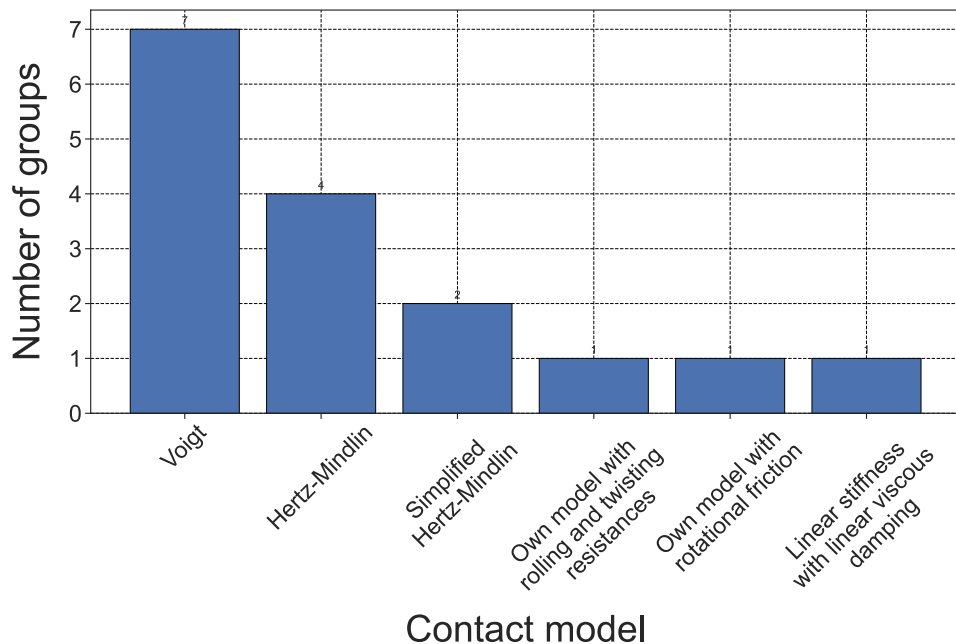


Figure 11: Histogram of interparticle constitutive model.

294 *3.4. Summary for interparticle constitutive model and simulation time step*

295 Figure 11 indicates the histogram of the interparticle constitutive model  
 296 used by the analysis groups. The most-used interparticle constitutive model  
 297 was the Voigt model, followed by the Hertz-Mindlin model. Most of the  
 298 groups that used particles with the same shape as the tetrahedral particle  
 299 used in the experiment adopted the Voigt model or the Hertz-Mindlin model.  
 300 Meanwhile, the groups that used spherical particles adopted interparticle  
 301 constitutive models incorporating rotation resistance corresponding to the  
 302 particle shape effect.

303 Since all the constitutive equations require normal stiffness, we first check  
 304 the setting of the normal stiffness. In addition, because normal directional

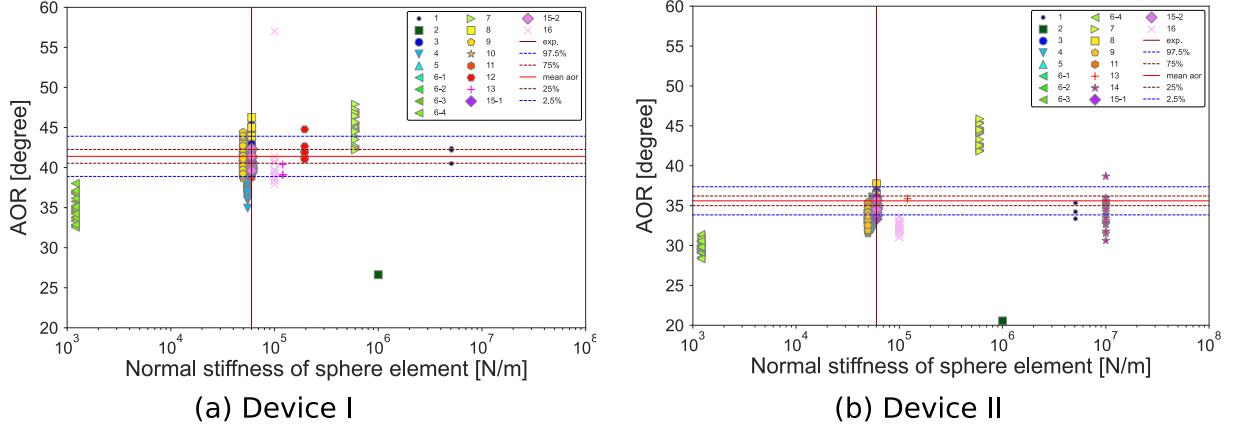


Figure 12: Relationships between AOR experiment results and normal stiffness used in DEM simulations.

305 stiffness is related to the time step setting, normal stiffness is an important  
 306 parameter in this sense.

307 Figure 12 shows the relationships between the AOR and the normal stiff-  
 308 ness for both Device I (Fig. 12 (a)) and Device II (Fig. 12 (b)). The  
 309 horizontal axis shows the normal stiffness used in the DEM simulations. The  
 310 meanings of the vertical axis and legend are the same as described in Fig. 9.  
 311 The normal stiffness for the Hertz-Mindlin contact model varies non-linearly  
 312 with the applied normal force ( $F_n$ ) or overlap ( $\delta_n$ ) between two sphere ele-  
 313 ments in contact. Considering the height of sample ( $\simeq 0.1$  m) and the mate-  
 314 rial density ( $1111 \text{ kg/m}^3$ ), a representative normal force of  $0.1 \text{ N}$  was used to  
 315 estimate the secant normal stiffness ( $K_n$ ) using the following expression:

$$K_n = \frac{F_n}{\delta_n} = \frac{2}{3} (6E^* R^*)^{\frac{1}{3}} F_n^{\frac{1}{3}}, \quad (3)$$

316 where  $E^*$  is the equivalent Young's modulus, and  $R^*$  is the effective radius.

317 The definitions for  $E^*$  and  $R^*$  are respectively as follows:

$$\frac{1}{E^*} = \frac{1 - \nu_i^2}{E_i} + \frac{1 - \nu_j^2}{E_j}, \quad (4)$$

$$\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j}, \quad (5)$$

318 where  $E$  is the Young's modulus,  $R$  is the radius, and  $\nu$  is the Poisson's  
 319 ratio of the two contacting sphere elements of  $i$  and  $j$ . It is noteworthy that  
 320 the setting of the normal stiffness ( $K_n$ ) varies widely among the analysis  
 321 groups irrespective of the device type, ranging from the order of  $1 \times 10^3$  N/m  
 322 to  $1 \times 10^7$  N/m. Although there is a large order of magnitude difference  
 323 in the normal stiffness, most of the simulation results fell within the 97.5%  
 324 quantile in the AOR comparison, regardless of the device type. This result  
 325 suggests that the difference in the normal stiffness may not be so critical to  
 326 the AOR. As the normal stiffness relates the time step of the DEM simulation  
 327 in conjunction with the mass/density of the particle, we also need to check  
 328 the time step used in each simulation run.

329 Figure 13 shows the relationships between the AOR and the normalized  
 330 time step for both Device I and Device II. The normalized time step (hori-  
 331 zontal axis) is a dimensionless quantity defined by  $\frac{\Delta t}{\Delta t_{cr}}$ , where  $\Delta t$  is the time  
 332 step used in the DEM simulation and  $\Delta t_{cr}$  is a critical time step characterized  
 333 by the particle mass  $M$  and the normal stiffness  $K_n$  ( $\Delta t_{cr} = \sqrt{\frac{M}{K_n}}$ ). Note  
 334 that the  $\Delta t$  settings used by each analyst were set in the range of  $10^{-6}$  (s)  
 335 to  $10^{-4}$  (s). Most of the DEM simulations were performed with lower values  
 336 of the time step than the critical time step, whereas analysis groups 1 and 2  
 337 used a large time step that exceeded the critical time step. Almost all the  
 338 analysis groups set  $\Delta t$  within the range of 0.01 to 1.0 times of  $\Delta t_{cr}$ . This



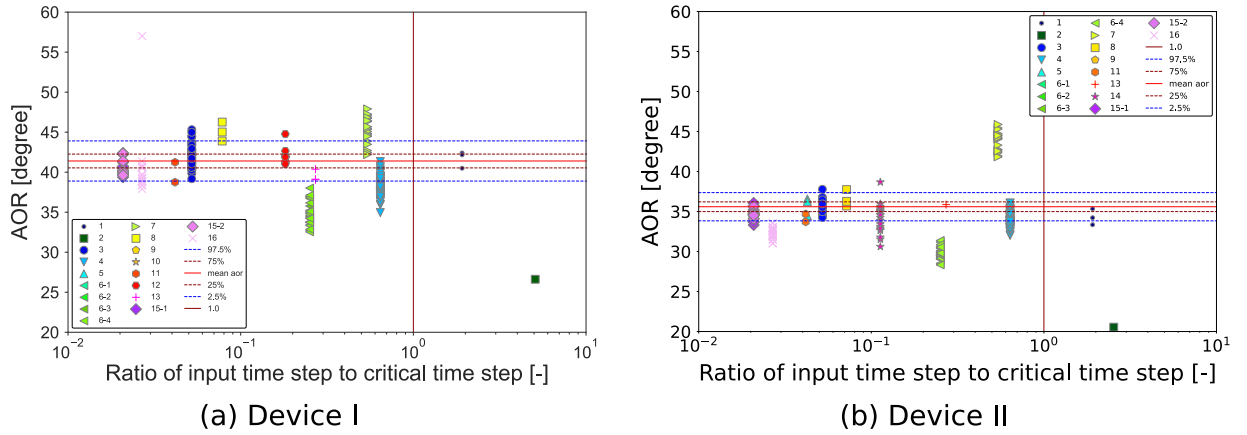


Figure 13: Relationship between AOR experiment results and the normalized time step using the critical time step.

339 suggests that their aim was to improve computational efficiency by setting  
 340 as large a time step as possible while ensuring stable simulation.

### 341 3.5. Summary for friction angle at contact point

342 Figure 14 shows the relationship between the results of the AOR experi-  
 343 ment (on the vertical axis) and the setting of the friction angle at the contact  
 344 point configured by each analysis group (on the horizontal axis). For both  
 345 devices, most of the analysis groups used the interparticle friction coefficient  
 346 corresponding to the mean value of the experiment given as prior informa-  
 347 tion, as listed in Table 1 ( $\tan 35.5^\circ = 0.71$ ). One of the analysis group set  
 348 the interparticle friction coefficient close to 0.5, which may be assumed to be  
 349 the friction angle between the acrylic plate and the resin ( $\tan 27.2^\circ = 0.51$ )  
 350 rather than the experimental value of the interparticle friction angle. The  
 351 intermediate value close to 0.55 corresponds to the mean value of the dy-  
 352 namic friction coefficient obtained from the experiment ( $\tan 29.36^\circ = 0.56$ ).

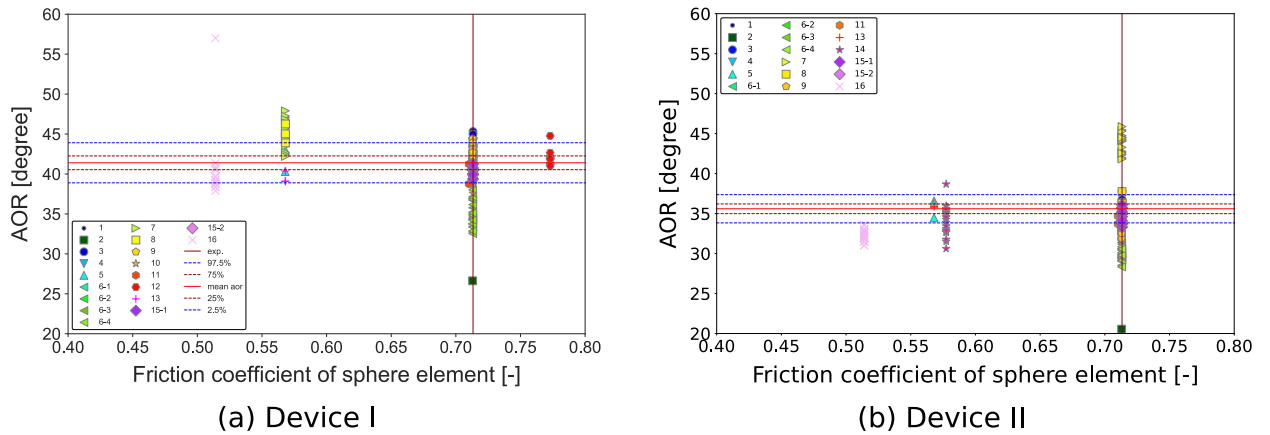


Figure 14: Relationships between AOR experiment results and the friction angle at the contact point used in DEM simulations.

353 It should be noted that while we can find various values for the interparticle  
 354 friction angle, all of them have a certain level of accuracy in terms of corre-  
 355 spondence with the experimental results. For example, the use of a friction  
 356 angle of 0.51 for the interparticle friction angle resulted in no significant dis-  
 357 crepancy with the experimental results irrespective of the device type. This  
 358 fact suggests that a certain level of particle shape modeling, correct parti-  
 359 cle physical properties, and appropriate boundary conditions result in good  
 360 predictions of AOR. The initial configuration of the artificial particles differs  
 361 from each group, but given the small variation in the results, we believe that  
 362 the effect of the initial configuration is small in this round robin test.

### 363 3.6. Comparison with variability between DEM simulations and experiments

364 We compare the results obtained from both the DEM simulations and  
 365 the experiments considering the mean and the variations of the AOR. Note  
 366 that this comparison is possible because we imposed a certain number of

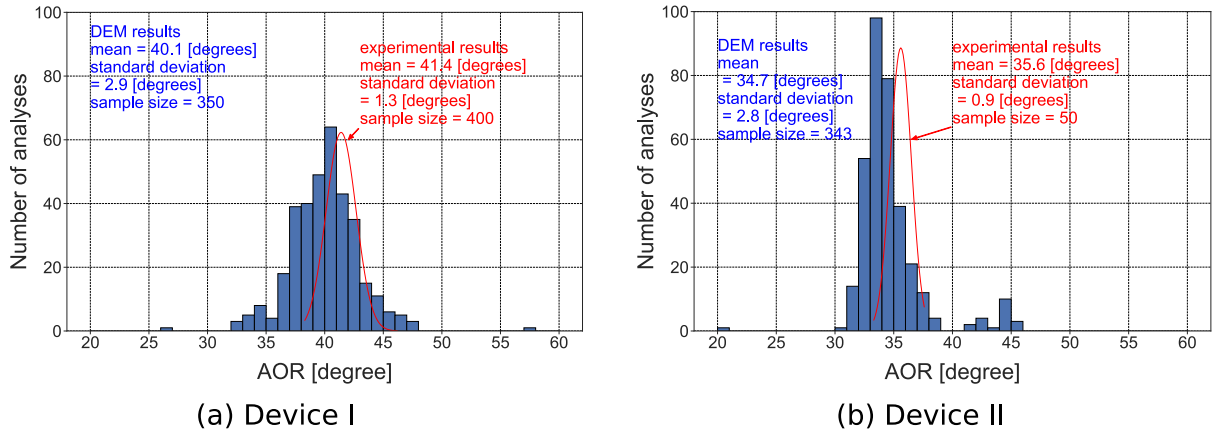


Figure 15: Histogram of AOR based on all simulation results.

367 trials on both the experiments and DEM simulations. Figure 15 indicates  
 368 the histograms of AOR (bar plot) using all DEM simulation results for both  
 369 Device I and Device II. As for Device I (Fig. 15(a)), the mean and standard  
 370 deviation of the histogram (350 samples) are 40.1 degrees and 2.9 degrees,  
 371 respectively, from a normal distribution approximating the histogram. Also,  
 372 the red solid line shows a normal distribution with a mean of 41.4 degrees  
 373 and a standard deviation of 1.3 degrees obtained from the experimental re-  
 374 sults (400 samples). Although the histogram shows a few outliers around 26  
 375 degrees and 57 degrees, it can be seen that the DEM results simulate the  
 376 experimental results with considerable accuracy. In particular, the difference  
 377 between the mean values is 1.3 degrees, indicating that the predictions are  
 378 remarkably accurate. The variance of the DEM simulations is larger than the  
 379 experimental results, but this can be attributed to the normal distribution,  
 380 including the outliers.

381 Likewise, the DEM results for Device II have a mean value of 34.7 degrees  
 382 and a standard deviation of 2.8 degrees, and the corresponding experimental

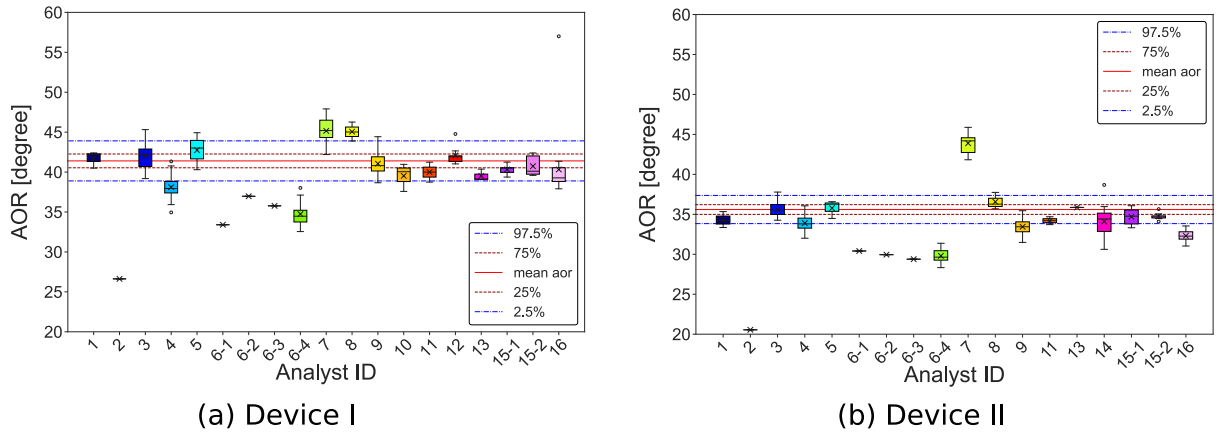


Figure 16: Box plot of AOR simulation results for each participant.

383 values are 35.6 degrees and 0.9 degrees, respectively (Fig. 15(b)). The his-  
 384 togram has a bimodal shape with a small peak around 45 degrees, but the  
 385 reasons for calculating an AOR greater than 40 degrees are largely due to  
 386 the usage of the interparticle constitutive model with an excessive setting for  
 387 rotational resistance.

#### 388 4. Discussion

389 The DEM simulation results submitted by 16 groups from 7 countries  
 390 were classified and statistically analyzed, and most of the simulation results  
 391 were in good agreement with the experimental results. In this section, we  
 392 consider the reason for the outliers from the perspective of the parameter  
 393 settings. After identifying the causes of outliers, we discuss trends in DEM  
 394 software.

395 Figure 16 shows a side-by-side comparison of the DEM simulation results  
 396 for each analysis group (16 groups in total), and the variation of each set of  
 397 DEM simulation results is also represented using a box plot. The horizontal

398 axis indicates the participating group (analysis group) ID and the vertical  
399 axis is the AOR value. The meanings of the solid and dotted lines are the  
400 same as those depicted in Fig. 9. Note that the conventions of the box plot  
401 can be found in Appendix A: they consist of the 25<sup>th</sup> percentile, the 50<sup>th</sup>  
402 percentile, the 75<sup>th</sup> percentile, and outliers.

403 In the case of Device I (Fig. 16(a)), it can be seen that the mean AOR  
404 values submitted by the five analysis groups (ID: 2, 4, 6, 7, 8) are located  
405 outside the 97.5 percentile. In the five cases with outlier results, we can iden-  
406 tify clear reasons for such outlier results in terms of parameter settings, using  
407 convex particle shapes and usage of the interparticle constitutive equations.  
408 The time step used by analysis group 2 is significantly large, as shown in Fig.  
409 13. Due to the use of such a large time step, it can be inferred that a large  
410 penetration occurs at the contact point, thereby resulting in a small value  
411 of the AOR. The particle density used by analysis group 4 is markedly large  
412 (10,000 kg/m<sup>3</sup>), as shown in Fig. 9. Due to the use of large density, it can be  
413 inferred that a large penetration occurs at the contact point, thereby result-  
414 ing in a small value of the AOR. The convex, rounded shape of the potential  
415 particle used by analysis group 6, illustrated in Fig. 10, is likely the reason  
416 for the small value of AOR, as convex particles interlock less than the real,  
417 concave ones. Both analysis groups 7 and 8 used the interparticle constitu-  
418 tive model with rotation stiffness while they employed tetrahedral particles  
419 like those used in the experiment. This result in excessive moment transfer,  
420 which leads to a relatively high AOR. It should be noted that the number  
421 of simulation runs for analysis groups 2 and 4 is only one, respectively. It  
422 is possible that the mean AOR value of the simulation may approach the

← JS

423 experimental one with a larger number of simulations.

424 In the case of Device II (Fig. 16(b)), it can be seen that the mean AOR  
425 values submitted by the four analysis groups (ID: 2, 6, 7, 16) are located  
426 outside the 97.5 percentile. For analysis groups 2 and 7, the reason is likely  
427 the same as that explained for Device I: parameter setting. For analysis group  
428 6, the reason is also likely the same as that explained for Device I: particle  
429 shape (Fig. 10). However, we could not find the reason for the outlier results  
430 of analysis group 16. They used the same interparticle constitutive model  
431 with the parameter set that were used in Device I.

432 From the comparison between the DEM simulations and the experimental  
433 results, it was confirmed that most of the analysis groups calculated AOR  
434 values which were comparable to the experimental results irrespective of the  
435 choice of the interparticle constitutive model. There were three trends in  
436 the interparticle constitutive model: the Voigt model, the Hertz-Mindlin  
437 model and the model with rotational resistance. Most parameters of the first  
438 two models provided as prior information listed in Table 1, meanwhile no  
439 information is available for the models incorporating rotational resistance.

59

440 It should be noted that the difference in the angle of repose between  
441 these models could not be clearly distinguished. Although there were large  
442 differences in the normal stiffness individually, most analysis groups used  
443 appropriate time steps that stabilized the calculations irrespective of the  
444 magnitude of the normal stiffness and particle density. Normal stiffness is of-  
445 ten empirically set to a value different from the measured value, which may  
446 lead to confusion for beginners. The treatise on DEM (O'Sullivan, 2011)  
447 notes that the contact between DEM particles is idealized, and it is difficult

448 to determine the linear stiffness directly from the stiffness of the actual ma-  
449 terial. The treatise also argues that linear stiffness should conceptually be  
450 considered as a kind of “penalty spring”. While the significant difference in  
451 normal stiffness was fortunately not a problem for the prediction of the angle  
452 of repose, the exact normal stiffness should be used for a task like accurately  
453 predicting the elastic wave velocity.

454 As confirmed by our round robin tests, the parameter settings in DEM  
455 simulations are empirical, especially in normal stiffness. It is therefore useful  
456 to establish an expert system or a flowchart for parameter setting in the DEM  
457 simulations. Interestingly, most of the analysis groups did not consider the  
458 standard deviation of each physical property shown in Table 1 when setting  
459 those parameters even though there are certain deviations in the AOR values  
460 from the DEM simulations. This implies that the variation in the particle  
461 configuration had a greater effect on the angle of repose than the variation  
462 in the physical properties.

463 This round robin test allowed us to consider the trend in DEM software.  
464 We found that the use of PFC3D or in-house software is relatively frequent.  
465 Moreover, we found that powerful open source DEM software was also used  
466 (Yade, LIGGGHTS, LAMMPS, Kratos). When introducing DEM software,  
467 ease of installation, documentation, richness of functions, and ease of use  
468 are important considerations, and it was determined that the open source  
469 software listed here meets these criteria. In addition to the popularization  
470 of powerful DEM software, developing software specializing in particle shape  
471 modeling (e.g., Angelidakis et al. (2021)) further promotes the use of DEM  
472 in various engineering fields.

473 Through these round robin tests for the angle of repose, it is reconfirmed  
474 that the parameter settings of the interparticle constitutive model and the  
475 settings of time increments are extremely important. To increase the relia-  
476 bility of DEM analysis, it is necessary to steadily accumulate knowledge on  
477 parameter settings. We believe that these activities will lead to the establish-  
478 ment of verification and validation (V&V) guidelines for DEM simulations.  
479 Finally, we touch on the prospects for future round robin tests in terms of the  
480 problem settings. There are requests to conduct triaxial compression tests  
481 with a certain level of confining pressure, but the problem settings should be  
482 decided carefully, considering the difficulty of the experiment and the abilities  
483 of many software packages to be used in the round robin test.

S/O

## 484 5. Conclusions

485 According to the tabulation of the DEM simulation results for two types  
486 of experimental settings, most simulation cases submitted by participants  
487 agreed with the experimental results with a certain level of accuracy in both  
488 average and variance values for the angle of repose, irrespective of the types  
489 of experiment. For a few cases where the discrepancy with the experimental  
490 results was large, it was concluded that this discrepancy was attributed to  
491 the selected values of modeling parameters, and to the employed modeling  
492 approach (i.e. clumps versus rounded convex particles). In other words, most  
493 of the software used in the round robin test works correctly providing the  
494 proper parameter settings are used. The collected data also revealed trends in  
495 the selection of the interparticle constitutive model (Voigt and Hertz-Mindlin  
496 models) and the DEM software (PFC3D, in-house, and Yade).



497 In future work, we will continue to conduct worldwide DEM round robin  
498 tests under the handling of the TC105 Japanese domestic committee to en-  
499 sure the accuracy of the DEM simulations and the reliability of each type of  
500 DEM software.

### 501 Appendix A. Box plot notation

502 Figure A.1 shows the details of the box plot notation used in Fig 16.  
503 In general, the median differs from the mean and is less sensitive to out-  
504 liers. Hence, the median is useful when the data does not obey the normal  
distribution.

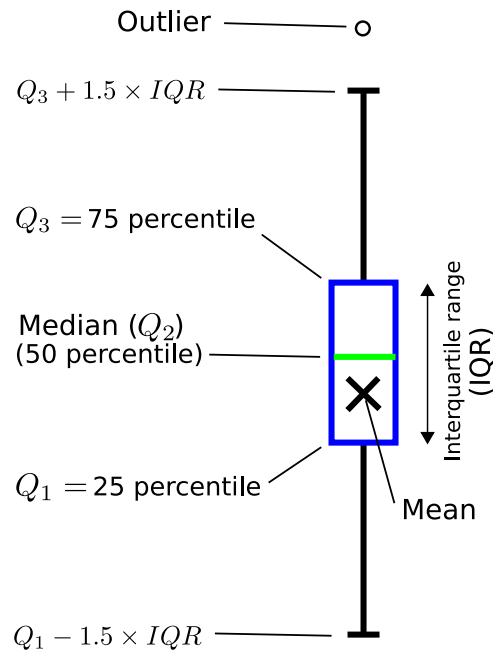


Figure A.1: Box plot notation.

505

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