Material-Modeling Support for *PFC*:
Questions & Answers

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Itasca Webinar (December 14, 2017)

Q&A (January 12, 2018)

QUESTION 1

Are you going to post the recorded webinar on your website?

A: The webinar will be posted to the Itasca website, along with the webinar slides (in PDF format) and this question & answer document. A link to these materials will be sent to all webinar registrants.

Also, I have a question regarding the webinar. Is it possible to perform a thermal analysis using *PFC* to a bonded material? And monitor the thermal cracks that occur to the material during thermal cycles?

A: Yes, it is possible to perform a thermal analysis upon a *PFC* bonded-particle material by using the thermal module in *PFC* --- see the *PFC* help file: Additional Features: Thermal Calculation. The thermally induced cracks can be monitored with the crack-monitoring feature in the Material-Modeling Support package (see page 35 in the fistPkg25 memo).

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Thermal Calculation

The thermal module of *PFC* allows simulation of transient heat conduction and storage in materials consisting of *PFC* particles, as well as development of thermally induced strains and forces. The thermal material is represented as a network of heat reservoirs (associated with each mechanical body) and thermal contacts (associated with each mechanical contact). Heat flow occurs via conduction in the active thermal contacts that connect the reservoirs. Radiative and convective heat transfer are not included in the present formulation. Thermally induced strains are produced in the *PFC* material by modifying the particle size. Mechanical contact models may also account for thermally induced forces.

The following paper describes modeling of thermally-induced damage with *PFC*.

Bonded-particle modeling of thermally fractured granite

T.S. Wanne*, R.P Young

QUESTION 2

The webinar indicated that for tension test, stresses can be measured:

1. from the walls;

2. using measurement sphere.

My question is that are these two stresses equivalent?

The direction of the stress from the wall will be in the direction of the tensile load, like a typical physical tensile test of material.

The direction of the stress from a measurement sphere is unknown. So, such a stress would not be considered as the "tensile stress" defined in a typical physical test.

We are simulating the tensile test of a plant fibre and thinking about monitoring the stress using measurement spheres. But is this stress considered as the conventional tensile stress?

A: The measurement sphere computes an average stress tensor acting on the particles with centroids that lie within the sphere. The measurement procedure is described in the *PFC* help file at General Components: Measure: Measured Quantities. This is the stress tensor, so it is independent of direction. If the tensile test axis of pull is aligned with the global z-direction, then the tensile stress would be sigma_zz.

Stress

Stress is a continuum quantity and, therefore, does not exist at each point in a particle assembly, because the medium is discrete (see figure below). In the discrete *PFC* model, contact forces and particle displacements are computed. These quantities are useful when studying the material behavior on a microscale, but they cannot be transferred directly to a continuum model. Averaging procedures are necessary to make the step from the microscale to a continuum. The average stress $\bar{\sigma}_{ij}$ in a measurement region of volume V is computed as ([Christoffersen1981]):

$$\bar{\sigma} = -\frac{1}{V} \sum_{N_c} \mathbf{F}^{(c)} \otimes \mathbf{L}^{(c)} \tag{6}$$

where N_c is the number of contacts that lie in the measurement region or on its boundary, $\mathbf{F}^{(c)}$ is the the contact force vector, $\mathbf{L}^{(c)}$ is the branch vector joining the centroids of the two bodies in contact, $\otimes$ denotes outer product, and compressive stress is negative by convention. Note that the underlying assumptions behind the formula above are based on a static analysis. Alternative computations may be desired for dynamic situations (for example, see [Fortin2003]).

QUESTION 3

I have a question about material modeling:

I want to model the injection of a fluid into some soil. As I understood fluids can be modeled with CFD extension in *PFC*. Is there a webinar or guide through this? Is this possible to create contact (like PBond) between injected fluid and existing soil? Can this thing (injection of a fluid into soil) be modeled with *PFC*?

A: There are many different ways in which fluid-particle interaction can be modeled, and each approach is suitable for a particular class of problems. These issues are discussed in the introduction to the CFD module for *PFC* (see Additional Features: CFD module for *PFC3D*5.0). The built-in module is not suitable for modeling the injection of fluid into soil. I am not aware of a simple scheme to model this with DEM; however, one of the schemes described on the following slide might be suitable for your purposes.

You ask about creating a bond between injected fluid and existing soil. If the fluid was modeled as many small frictionless particles, then one could bond such fluid particles to soil particles.
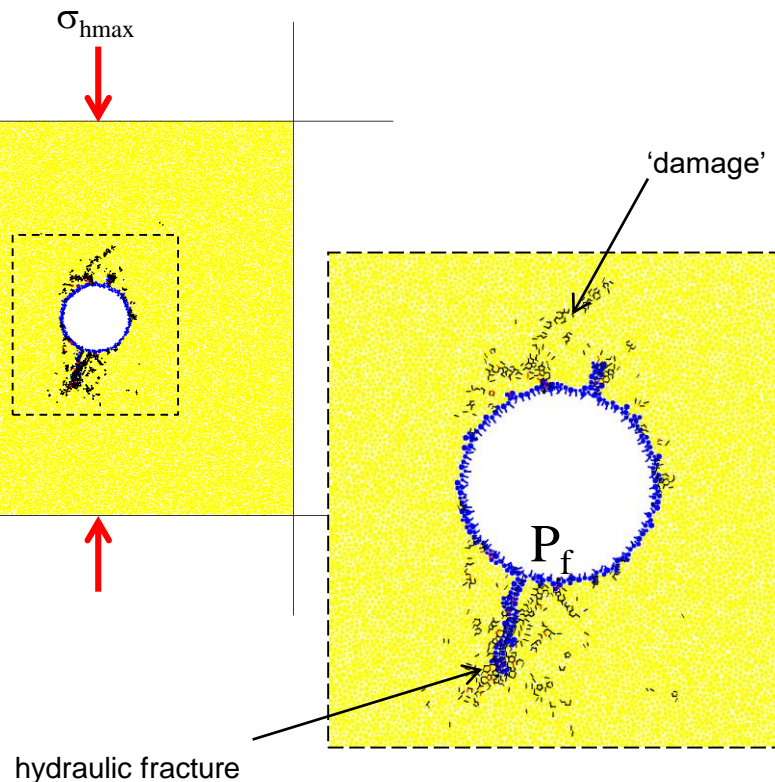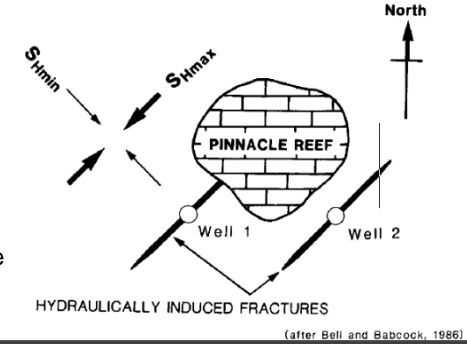
Hydraulic fracture

Induced hydraulic fracturing occurs as a result of artificially increasing the pore fluid pressure in a rock body. There are many possibilities of incorporating the effects of a fluid in a DEM model, two of which are shown here.
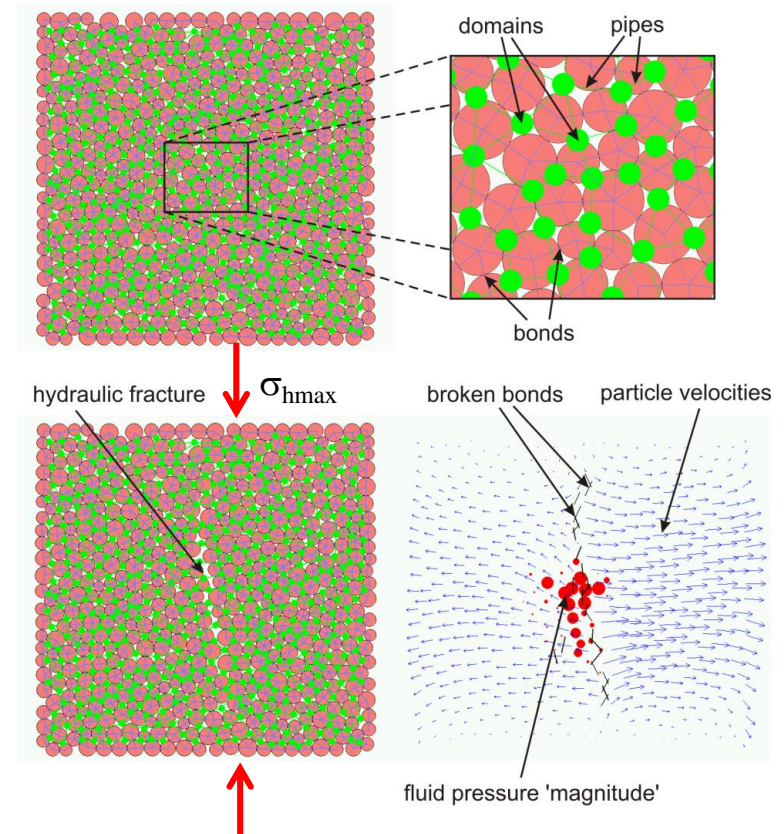
Map view of a subsurface oil-bearing pinnacle reef. Well 1 can be connected to the reef oil reservoir by hydraulic fracturing since the local stress regime causes fractures to propagate NE and SW. Fractures originating in well 2 will miss the target (Bell, 1990).

Pressurised hole in a 2D DEM model
The pressure inside a hole is gradually increased while a remote, or 'regional', stress is held constant. Fluid does not enter the pore-space in this approach. Fluid is only present in the hole and fractures connected with it. Although this approach is simple, many questions could be addressed, such as the impact of anisotropy and/or pre-existing fractures on hydrofracture geometry/aperture.

σ_{hmax}

'damage'

P_f

hydraulic fracture

Fluid coupling in 2D DEM model
Flow pathways are parallel-plated channels, or pipes, at contacts (aperture of channel proportional to normal force). Reservoirs, or domains, are connected via pipes and reservoir pressures are updated via fluid calculations.

domains   pipes

bonds

hydraulic fracture σ_{hmax} broken bonds   particle velocities

fluid pressure 'magnitude'

QUESTION 4

I believe that during the webinar Mr. Potyondy pointed out that the source codes of the *PFC* files will also be available. I only received the PDF files. I would be really great full if you share the link to examples source codes.

A: I presume that by "source codes," you mean the data files that comprise the material-modeling support package. All of this material can be downloaded from the link: www.itascacg.com/material-modeling-support.

QUESTION 5

Is this presentation going to be available on the Itasca website? I would be very interested in getting access to the presentation.

Do you have a copy of the material for today's webinar?

A: The webinar itself (which is a video recording) and the presentation slides (in the form of a PDF file) can be obtained from the Itasca website, I presume that this material will be accessible from the Material-Modeling Support page: www.itascacg.com/material-modeling-support
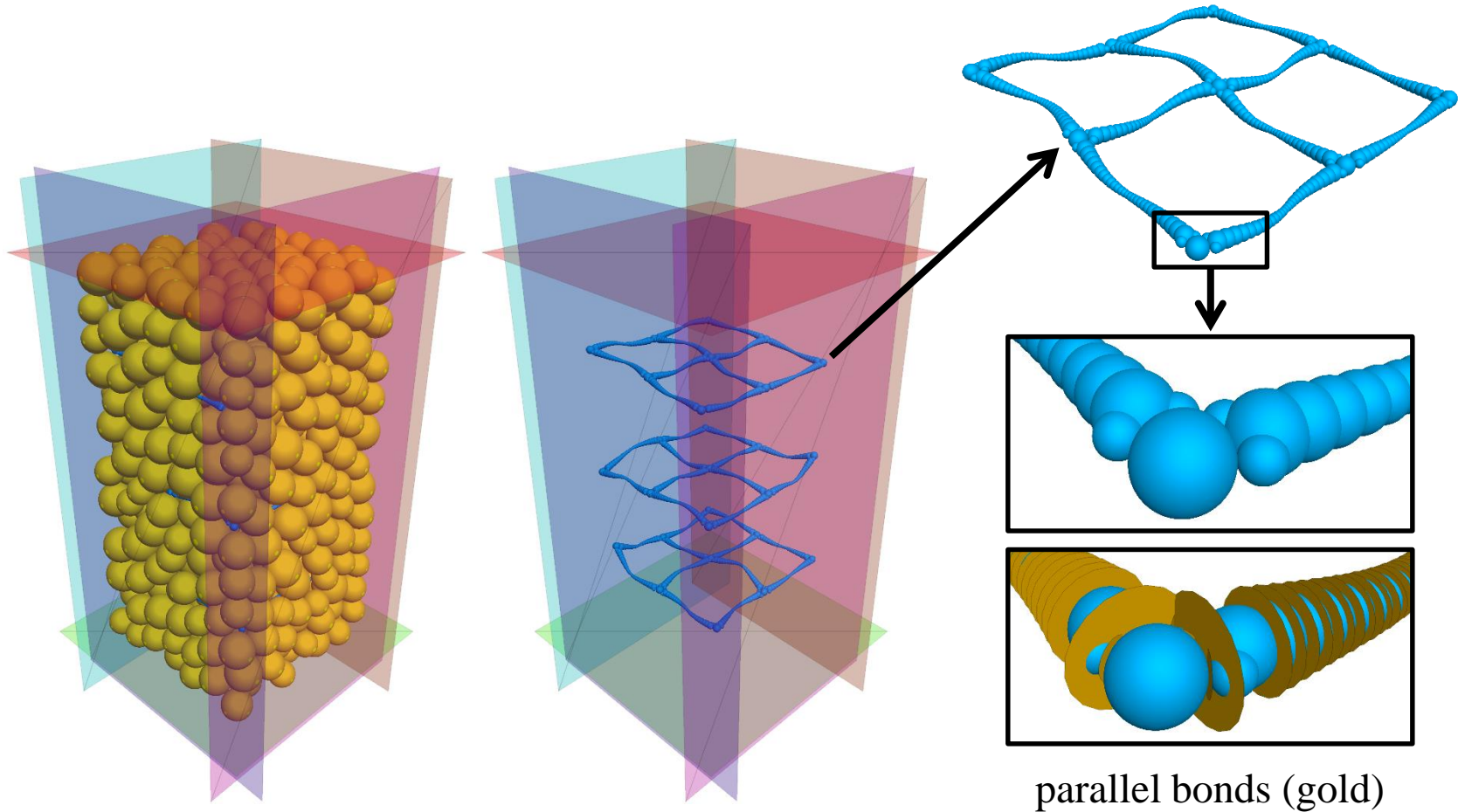
QUESTION 6

I would like to thank you very much for the presentation last week which was very useful. Additionally I would like to ask if you have a software that could show good contribution for geogrid in soil stabilization and reinforcement ...especially for road applications. I am now search about such a finite element program which can help me in the design.

A: Itasca has recently developed a pavement-design package that works with *PFC3D*. The package capabilities are summarized on the next slide, along with the link at which the package can be obtained. The geogrids can be modeled as strings of parallel-bonded balls, which interact with the granular particles in which they are embedded. Please contact me directly (my email is on the front page of this document) to learn more about this package and its capabilities, and related documentation in the form of papers and talks.

Pavement-Design Package*

Supports creation and triaxial testing of synthetic unsaturated granular material containing geogrid, measure resilient modulus for grid and no grid.

parallel bonds (gold)

granular material
(balls or clumps and
hill contact model)

geogrid
(strings of overlapping bonded spherical balls)

QUESTION 7

First of all, thank you for sharing this. Unfortunately, I couldn't make it yesterday, but have some questions and was wondering if I could still ask questions.

A: I am always willing to answer questions about *PFC* modeling, and in particular, about bonded-particle modeling. You can send such questions directly to me at the email address on the first page of this document.

QUESTION 8

Thanks for packaging up those items; the webinar was quite instructive. I noticed in the packing phase that the porosity did not monotonically decrease in at least one case (though I forget which one). This indicates that some part of the material genesis procedure is causing the material to dilate in some fashion. Is this considered an accurate representation of the dilative/contractive behavior of granular soils under various loading scenarios? As a geotechnical earthquake engineer, this has interesting implications for modeling liquefaction behavior in soils; I'm curious if and how Itasca has been applying this.

A: You need to be more specific, for me to answer this question. The boundary-contraction procedure of material-genesis begins with a cloud of overlapping particles and allows them to rearrange under zero friction. Then the boundary walls are moved under servo control so that the desired material pressure is achieved. Send me a question via email, and we can discuss this further, especially the part about how Itasca models liquefaction in soils --- this is typically done using a special constitutive model in the *FLAC* and *FLAC3D* codes.

QUESTION 9

A. Is it possible to establish different boundary conditions in the package?

   I'm interested in learning about infinite boundary condition and flexible boundary condition made of particles instead of spheres.

B. Do you know how to maintain constant confining pressure for particulate boundary?

A: The boundary conditions cannot be modified within the package. *PFC* itself provide a periodic boundary condition, such that when a particle exits one side of the domain it begins to appear on the opposite domain side --- see the {domain command}.

The `periodic` condition applies periodic boundary conditions. When the ball or clump centroid falls outside of the model domain, they are translated back to the opposite side of the model. To ensure that contacts are created as if the model was continuous,

A flexible boundary comprised of a chain of *PFC2D* particles can be developed, and has been used to apply a pressure boundary condition during rock-cutting tests in which a cutter is moved across the surface of a bonded-particle assembly (see figure below). A rock-cutting environment was provided along with *PFC2D* 4.0 (Emam and Potyondy, 2010), but has not been recreated for *PFC2D* 5.0. If a few days of funding could be obtained, then it could be recreated for *PFC2D* 5.0. An algorithm has also been developed to apply pressure to the surface of a *PFC3D* bonded-particle model (Potyondy, 2012). With a few days of effort, it could also be implemented to work with *PFC3D* 5.0. Please contact me directly, if you are willing to pay for a few days of my time to implement either of these schemes for *PFC 5.0*.
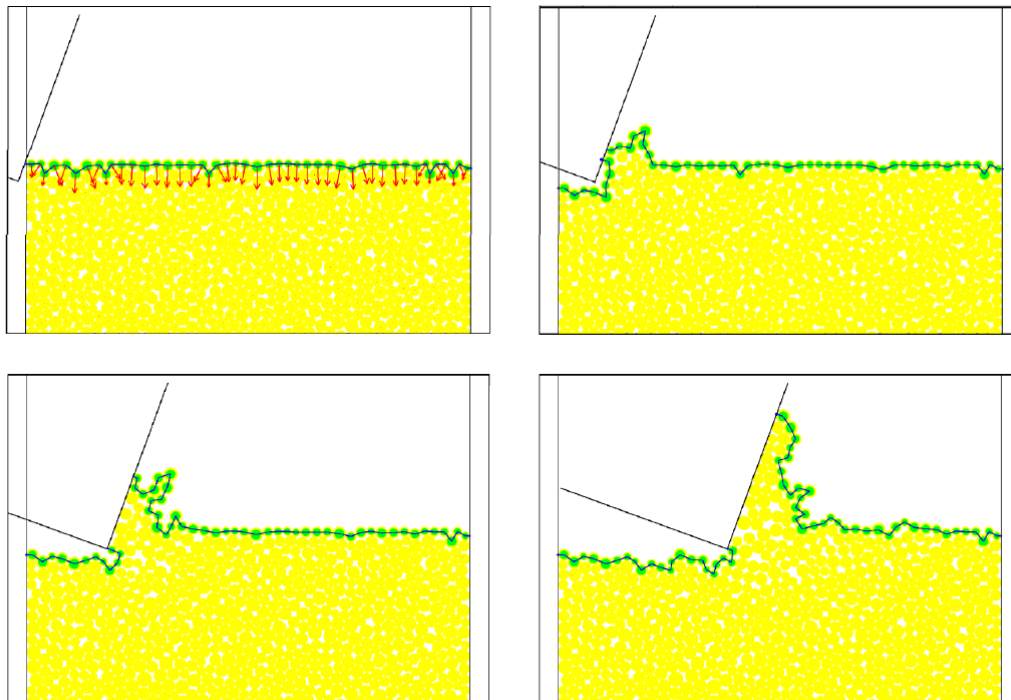
Figure 2   Particles and spanning chains with 10-MPa confining pressure for cutter displacements of 0, 10, 20 and 40 mm (applied external forces shown in upper-left image)

REFERENCES

Emam, S., and D. Potyondy (2010) "PFC2D Rock-Cutting Procedures," Itasca Consulting Group, Inc., Minneapolis, MN, Technical Memorandum ICG7156-L, April 8, 2010.

Potyondy, D. (2012) "*PFC3D* Pressure Boundary Condition," *PFC3D* Example on Itasca website, Itasca Consulting Group, Inc., Minneapolis, MN, Technical Memorandum ICG7233-L, January 30, 2012.

Please contact me directly to obtain these memos.

QUESTION 10

Is the strain rate selected in the compression test equal to the standard compression rate/sample height?

A: The strain rate used in the simulated compression test is many orders of magnitude larger than the standard rate used in physical experiments. The reason for this, and suggested ways to select the appropriate strain rate are discussed in the section {5.4 Loading Rate} in the fistPkg25 memo. The first paragraph is given below.

5.4   Loading Rate

The response of a real material and a DEM model are sensitive to loading rate. In most cases, we choose a loading rate that is slow enough to insure a quasi-static response. The quasi-static response is the response obtained when the test has been conducted under quasi-static conditions, which means that the loading has been slow enough that the system has time to adjust to the force redistribution that accompanies each nonlinear event (slip or bond breakage). This response could be obtained by performing a strain-controlled test, whereby the loading velocity is set to zero after each nonlinear event until the system reaches a new state of static equilibrium. In this way, we would trace out the stress-strain curve up to the peak, and the peak value would correspond with the quasi-static response. One can ensure that such a response has been obtained by conducting a strain-controlled test at a series of constant loading velocities, and demonstrating that the response is the same for all loading velocities below some critical velocity.

QUESTION 11

Currently, I want to use *PFC3D* to simulate a rubber strip tension test. When tensile test, the strip will deform in both vertical and horizontal directions. But the volume is constant. I need to use parallel bond contact model, how to generate the rubber sample to obtain a 0.5 Poisson ratio? We can assume the size of the rubber strip sample is 20mm(Length)x10mm(width)x100mm(height). Thanks.

A: You wish to construct a bonded material that exhibits a 0.5 Poisson ratio. It is not clear to me how this would be done, and I am not aware of anyone who has done this. If a reader of this document is aware of this, please contact me and I will pass along the information to the person who asked this question. The Poisson's ratio of a bonded material is related to the packing arrangement as well as the ratio of normal to shear stiffness. It should be possible to create a material with a 0.5 Poisson ratio by controlling these parameters.

QUESTION 12

<u>Brazilian test:</u>

In the Brazilian loading frame (ISRM suggested method for Brazilian test) the initial contact between the frame and the sample is a line contact. However, in *PFC*, it is surface contact (near the platen few particles are not deleted because their center lies within the circle).

In *PFC* the cracks start near the platen instead of the center of the Brazilian disk. The formula for the Brazilian strength (from the elastic solution, =2P/pi/D/t) is for the center point of the Brazilian disk. So, is it wrong applying the formula and is the test more like a compression test in *PFC*?

A: The Brazilian test performed by the material-modeling support package is a valid test for the synthetic material comprised of unbreakable grains --- i.e., you cannot cut through a grain to make a smooth platen-specimen boundary. If the damage is originating from the boundary, and if this damage occurs at the time of peak force, then this is not considered to be a valid Brazilian test, meaning that the formula you cite does not apply as it gives the tensile stress near the specimen center. It is up to you to determine whether or not the *PFC* test can be interpreted as a valid Brazilian test. In my work, I have obtained 2D results for which the damage begins in the center. My results are summarized on the following three slides, which are taken from a confidential report. The TB material is a parallel-bonded material created with the material-modeling support package.

The behavior of the TB material during Brazilian tests is summarized in Figure 15. The damage process is similar for all specimen sizes. The Brazilian strengths (σ_B as defined by Eq. (20) in Potyondy [2015a]) decrease slightly with increasing specimen size. Very little cracking occurs until just before the peak axial force is reached. Peak axial force coincides with the formation of a tensile fracture aligned parallel to the loading axis. This fracture consists of tensile cracks that originate near the center of the specimen and propagate along the loading axis as shown in Figure 16. This behavior coincides with the observation by Richard (undated report) that during a Brazilian test on Torrey Buff sandstone a "single split-crack originates in the center of the sample and propagates outwards." Formation of the tensile fracture produces a brittle stress-strain curve with no residual strength.
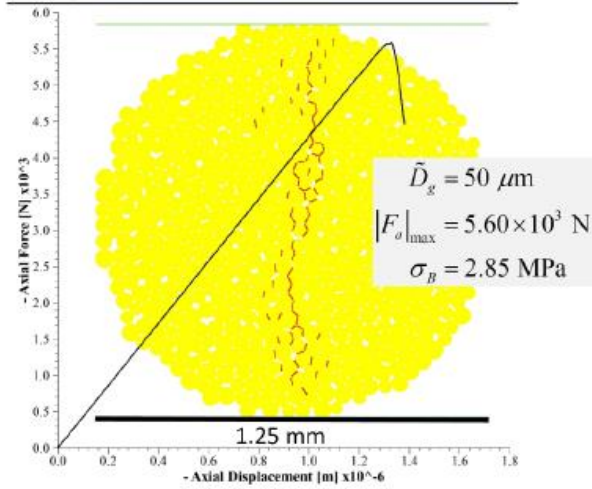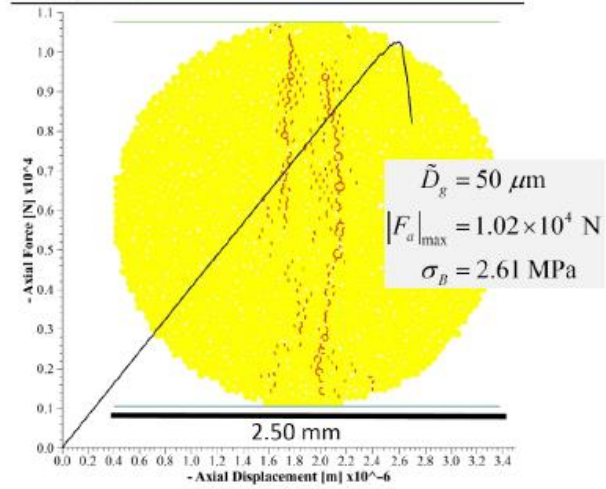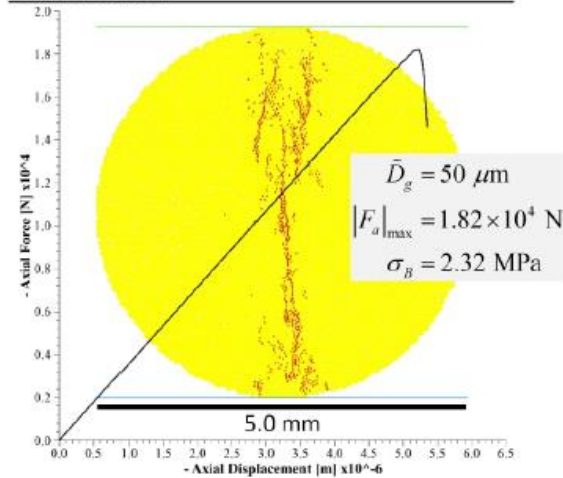
Figure 15   Brazilian test behavior of TB material ($\tilde{D}_g = 50$ μm) showing damaged microstructure (cracks at 50% size; red/blue denotes tensile/shear failure) and overlay of axial force versus axial displacement curves.
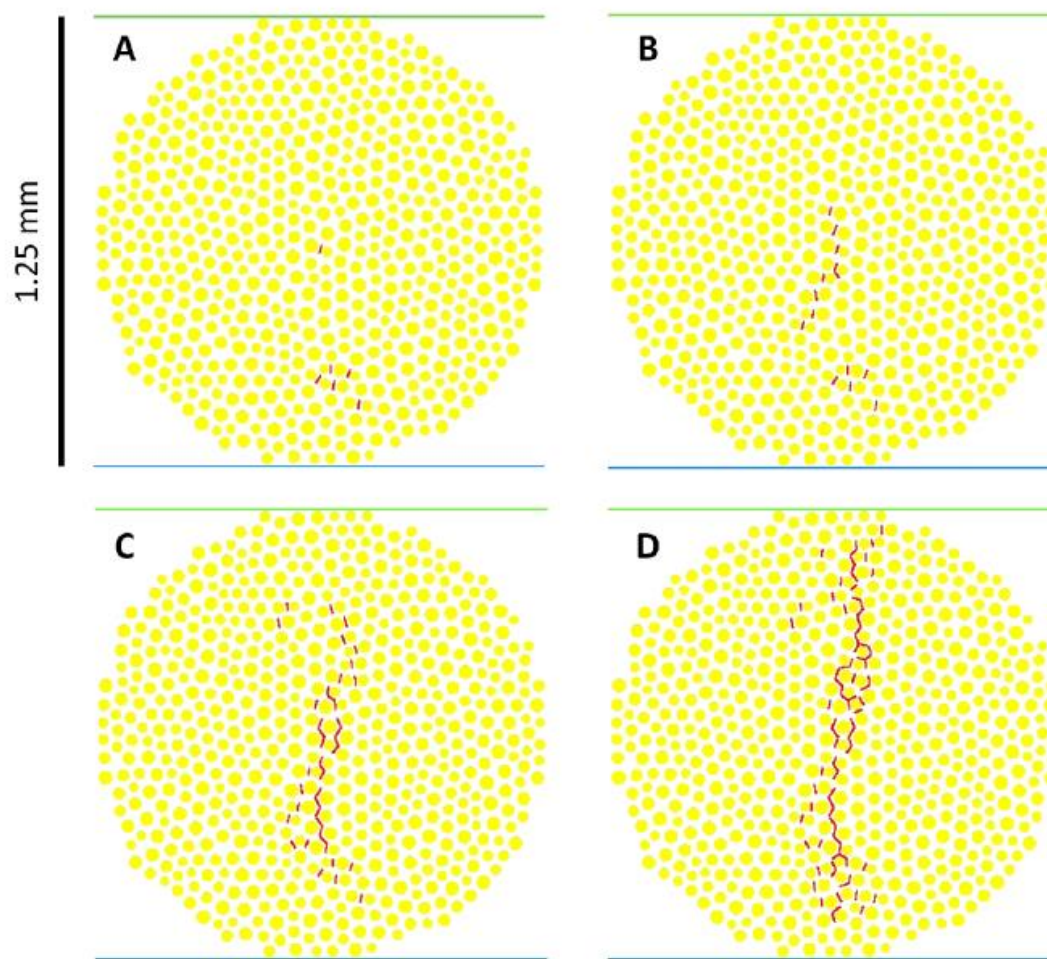
Figure 16 *Damage evolution during Brazilian test on the TB material ($\tilde{D}_g = 50 \ \mu m$) showing grains (80% size) and cracks (50% size). Image B corresponds with the peak axial force.*

QUESTION 14

Triaxial test:
Do the boundary particles at some (critical) locations get higher confinement even before the peak due to the rigid boundary, especially, at high confinement?

A: The boundary particles do not get higher confinement. The force acting on any boundary particle is proportional to its overlap with the confining wall. The boundary is not rigid; instead, the particles and the wall do not deform, but all deformation occurs at the contact at which an overlap is allowed to develop. This is the soft-contact approach discussed on slide X of the webinar.

One issue to consider is the inhibition of bulging, which is discussed in the excerpt on the next slide from Appendix A.7 of Potyondy and Cundall (2004).

REFERENCE

Potyondy, D.O., and P.A. Cundall (2004) "A Bonded-Particle Model for Rock," *Int. J. Rock Mech. & Min. Sci.*, **41**(8), 1329–1364 (2004).

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A.7. Biaxial, triaxial and Brazilian testing procedures

The macroscopic properties of the model material are obtained by performing biaxial, triaxial and Brazilian tests, in which each specimen is confined and loaded by pairs of opposing frictionless walls. These are the walls of the material vessel used during material genesis. For the biaxial and triaxial tests, the top and bottom walls act as loading platens, and the velocities of the lateral walls are controlled by a servo-mechanism that maintains a specified confining stress. Strictly speaking, the biaxial and triaxial tests simulate a polyaxial loading test—not a triaxial test, in which a specimen is encased in a membrane and confined by fluid pressure. Such a triaxial test could be simulated by replacing the side walls with a sheet of particles joined by parallel bonds to mimic the elastic membrane. The current biaxial and triaxial tests inhibit specimen bulging, whereby the specimen sides deform into a barrel shape, because the side walls remain straight. Such bulging should be minimal for granite, but may be important for softer rocks or cohesive soils.
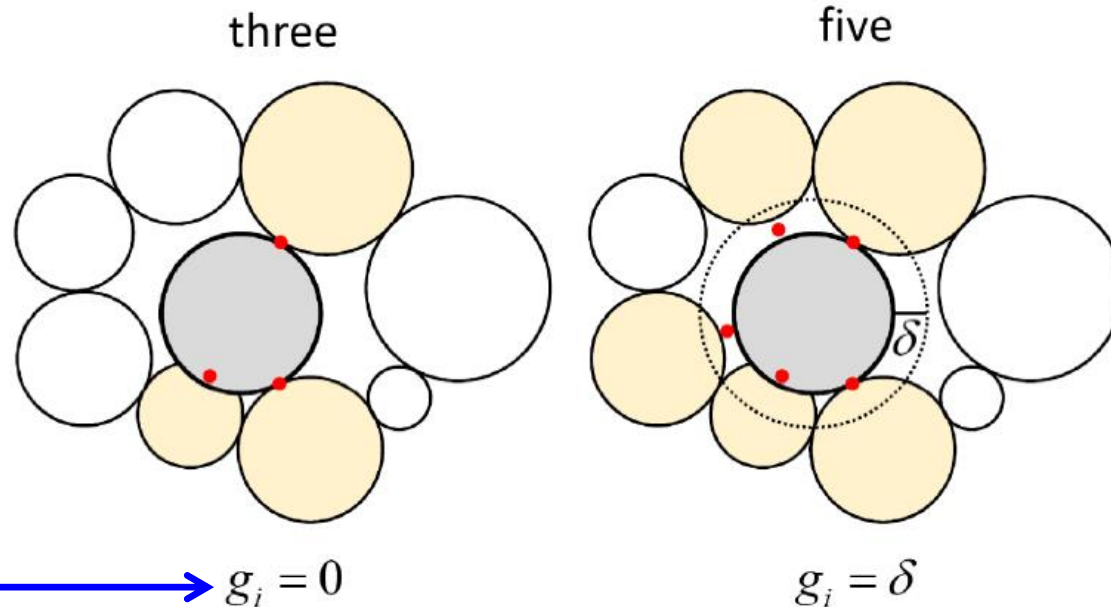
QUESTION 15

I recently attended the webinar on *PFC* by Potyondy. In that it was mentioned that the increase in bond gap increases the modulus and the strength of the specimen. Can you please suggest how to choose the bond gap? For example, the ball size is about 1.5mm to 2.5mm, what can be the range of bond gap that can be sued?

A: I believe that you are referring to the installation gap, as shown on the next slide. I would suggest keeping this gap small enough such that contacts do not form between a ball and another ball that is not in near-contact with the first ball --- i.e., do not allow contacts to form that join balls such that there is another ball in between them, as this is not physically reproducible. I believe that a microstructural model should satisfy the condition that one could construct a physical replica of the model. If this is not possible, then the model becomes a mathematical abstraction, and should not be considered microstructural as there is no longer a mapping between model components and physical entities (e.g., balls and grains, contacts and cement, etc.).

In my work thus far, I have kept the installation gap small enough such that the ratio of installation gap to smallest particle radius is less than or equal to one. This gives a dotted ring as shown in the right-most image on the next slide that extends out from the smallest particle by a distance equal to its radius --- in that image, delta is equal to the radius of the marked ball.

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Material-Genesis Procedure (finalization phase)

For the bonded materials, the installation gap controls the grain connectivity --- key parameter!

three

five

installation gap $\longrightarrow$ $g_i = 0$

$g_i = \delta$

Increasing the installation gap, increases the grain connectivity,

which increases the material modulus and strength.

This is the last slide of the question and answer document. I plan to present another webinar in Spring 2018, in which I will discuss how to calibrate a bonded-particle model to match the response of a particular rock. Be aware that I do not have all of the answers to this question, but I will share with you what I have learned about this process during my years of developing and applying the BPM methodology.

---David Potyondy, Jan12_2018