

TECHNICAL MEMO



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From: David Potyondy
Re: Material Modeling Support for PFC [mmPkg9.4]
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The Material Modeling support package (**mmPkg**) supports creation of PFC2D and PFC3D materials (granular and bonded) in various material vessels followed by compression, diametral-compression, and direct-tension testing while tracking and visualizing material damage. The capability is provided in the **mmPkg9.N** package that works with PFC2D and PFC3D version 9 (where **N** is the package version number).

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1.0 INTRODUCTION

The Material Modeling support package (**mmPkg**) provides a consistent set of FISH functions to support creation of PFC2D and PFC3D materials (granular and bonded) in various material vessels followed by laboratory testing to measure mechanical properties and observe microstructural behavior while tracking and visualizing material damage. The models support practical applications via boundary-value models made from these materials and scientific inquiry via further exploration of the microstructural space provided by the PFC model.

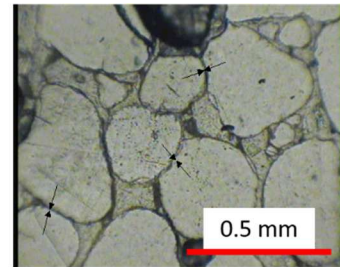
The PFC model provides a synthetic material consisting of an assembly of rigid particles that interact at contacts. This synthetic material encompasses a vast microstructural space, and only a small portion of this space has been explored. The synthetic material is a distinct-element model provided by the programs PFC2D and PFC3D (ITASCA, 2026a) that simulates the movement and interaction of rigid particles (disks/spheres, clumps [overlapping disks/spheres that behave as a rigid body], or polyhedra) and surfaces (walls) obeying Newton's laws of motion. A state-of-the-art description of bonded-particle modeling that situates it within the broader context of microstructural rock models, of which it is one example, is provided in ITASCA (2026a, PFC – Bonded-Particle Modeling).¹

Bonded materials are analogous to rock, which can be viewed as an aggregate of crystals and amorphous particles joined by varying amounts of cementing materials (see Figure 1). A rich variety of microstructures can be produced by modifying the bonded material itself. Such microstructures are obtained either by modifying the properties of the particles and cement or by modifying the packing fabric. The particle properties are size and shape. The cement properties are deformability and strength as well as evolving damage. The cement properties are embodied in the contact model, but the macroscopic material behavior is also sensitive to the ways in which new contacts form, and contacts deemed to be broken behave. The packing fabric at the time of bond installation affects the macroscopic properties of the synthetic material because bonds can be installed only at existing contacts — more bonds give increased stiffness and strength. The material modeling support package provides a well-defined and controlled procedure (pack the particles to a specified pressure and then install bonds between all particles that are within a specified distance of one another) to create BPMs.

¹ Any user of PFC should be familiar with the Section *PFC Model Essentials* in this document.

Rock is aggregate of crystals & amorphous particles
joined by varying amounts of cementing materials

Rock is modeled as
heterogeneous material comprised of cemented grains



Saint Peter sandstone

Microstructural components are at grain-scale

grain size, shape & packing
grain & cement properties (stiffness, strength, degree of cementation)

Each component influences mechanical behavior, and
may **evolve under load application**

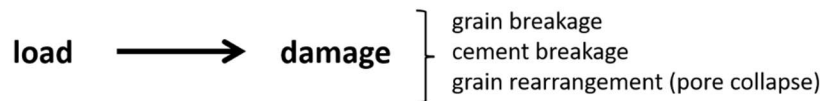


Figure 1 *Microstructural physics of rock and how it can be modeled as a bonded-particle material.*

The material modeling support package provides: a material-genesis procedure to create six types of materials; well-defined sets of microproperties to define each material; testing procedures to perform standard rock-mechanics laboratory tests upon the materials; microstructural monitoring to measure microstructural properties, visualize the microstructure, and measure and visualize material damage in the form of bond breakages; and examples of the creation and testing of each material. A concise summary of the package capabilities follows.

Material genesis of granular materials (linear and Hill²) and bonded materials (contact-bonded, parallel-bonded, soft-bonded, and flat-jointed) in polyaxial, cylindrical, and spherical physical vessels or a polyaxial periodic vessel. Material particles can be balls or clumps, and 3D flat-jointed materials of spherical, Voronoi or tetrahedral particles. Stress can be installed into the finalized periodic ensemble (after bonding), and then this ensemble can be converted into a periodic brick which is assembled into a larger geometric shape. Material tests are compression (confined, unconfined, and uniaxial strain), diametral compression, and direct tension. Microstructural monitoring includes

² A Hill material is a granular assembly in which the Hill contact model (with Hertz-Mindlin contacts) exists at all particle-particle contacts, and this material behaves like a partially saturated granular material for which capillary suction increases interparticle forces. The Hill contact model is a built-in contact model in PFC3D that will soon be documented in the manual. It is fully documented in Potyondy (2021).

computation of quantitative microstructural properties, microstructural plot sets, and crack monitoring for bonded materials.

The following information is contained in the remainder of this memo. The synthetic materials are described in Section 2.0. The microstructural-monitoring support for visualizing the material microstructures is described in Section 3.0. The material-genesis procedure that creates the material is described in Section 4.0. The testing procedures that perform standard rock-mechanics laboratory tests upon the material are described in Section 5.0. The tests are used to measure mechanical properties and observe microstructural behavior. The properties and behaviors are typically compared with those of physical material. A stress-installation procedure that initializes stress in the material for subsequent use in boundary-value modeling is described in Section 0. Examples of each synthetic material are provided in the accompanying memo "Material Modeling Support for PFC: Example Materials."

2.0 PFC MATERIALS

A PFC material consists of rigid particles that interact at contacts (see Figure 2).³ The particles of the PFC material can be either balls or clumps drawn from a general grain-size distribution. It is the type of contact model at the particle-particle contacts that defines the material as being linear, contact-bonded, parallel-bonded, soft-bonded, or flat-jointed.⁴ The linear material is a granular material, and the other materials are bonded materials. A smooth-jointed interface can be inserted into the bonded materials. A user-defined material can also be created. All materials are produced within a material vessel using a material-genesis procedure to ensure that they form a homogeneous, isotropic and well-connected particle assembly with a specified non-zero material pressure.

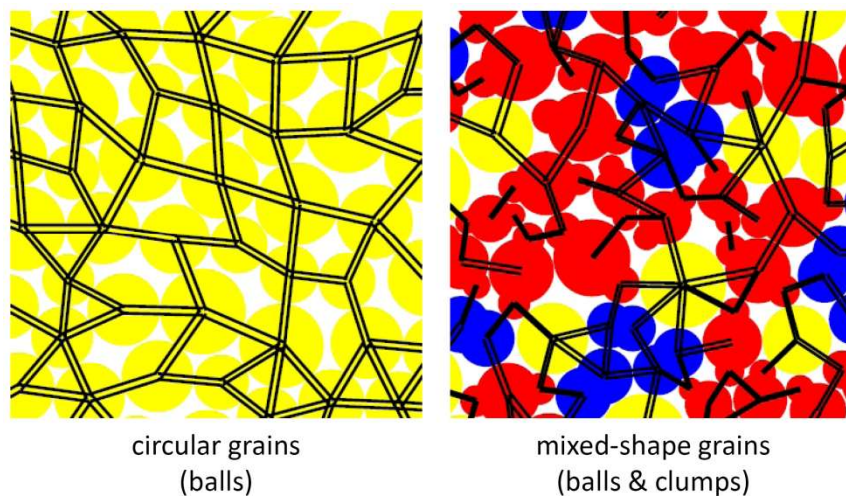


Figure 2 *Bonded material consisting of particles (with balls in yellow and clumps in blue and red) and cement (drawn as pairs of black lines).* (From Fig. 6 of Potyondy [2015])

Bonded materials are analogous to intact rock, which can be viewed as an aggregate of crystals and amorphous particles joined by varying amounts of cementing materials. The bonded materials produced by the material-genesis procedure approximate an intact compact rock with average homogeneous isotropic properties at a scale larger than the material granularity. The synthetic material is analogous to brittle cookie dough that has been solidified by baking and for

³ The physical behavior at each contact is embodied in its contact model. For the bonded-particle materials, this physical behavior mimics cement, and thus, a bonded material has been said to consist of rigid particles joined by cement at particle-particle contacts. The PFC materials include two granular materials along with the bonded materials; therefore, the present definition of a PFC material replaces "rigid particles joined by cement" with "rigid particles that interact at contacts."

⁴ The Subspring Network contact model with rigid, Breakable, Voronoi-shaped grains (SNBV model) is a type of bonded-particle model that mimics the microstructure of angular, interlocked, breakable grains with interfaces that may have an initial gap and can sustain partial damage (Potyondy et al., 2025). Support for material creation and laboratory testing (direct-tension and triaxial/biaxial in 3D/2D) is provided by the SNBV support package (**snbvPkg**, Potyondy [2026]).

which grain size corresponds with dough granularity. The granularity is quantified by means of its resolution (or number of grains across a relevant dimension).

A rich variety of microstructures can be produced by modifying the bonded material itself. Such microstructures are obtained either by modifying the properties of the particles and cement or by modifying the packing fabric. The particle properties are size and shape. The cement properties are deformability and strength as well as evolving damage. The cement properties are embodied in the contact model, but the macroscopic material behavior is also sensitive to the ways in which new contacts form, and contacts deemed to be broken behave. The packing fabric is affected by the size distribution and shapes of the particles, the material pressure applied before bonding, and the installation gap that controls where bonds will be added. Structural features at a scale larger than the material granularity can be overlaid on the base material, and such models are called grain-based models (Potyondy, 2010). These features include voids, material regions and joints (Potyondy, 2015).

The material-genesis procedure is summarized in the next subsection. Each material is defined by a set of material properties that control the material-genesis procedure, install the desired contact model at selected contacts, and assign contact-model properties. The properties common to all PFC materials are described in the second subsection, and the materials themselves are described in the remaining subsections.

2.1 Overview of Material Genesis

The material-genesis procedure is shown in Figure 3.⁵ The PFC materials are created within a material vessel by packing together a cloud of particles from a given size distribution to material pressure ($P_m > 0$) using the linear contact model. The number of contacts at the end of the packing phase is controlled by P_m such that increasing P_m increases the number of contacts. For the bonded materials, additional contacts are created to fill the gaps between particles by specifying a positive interaction gap ($g_i > 0$) as shown in Figure 4.⁶ The granular material is then transformed into a bonded material by assigning the bonded material properties to all contacts, but only those contacts with a gap less than or equal to the interaction gap are bonded. The particle connectivity is controlled by the material pressure and the interaction gap, with the interaction gap being of primary importance.

⁵ An overview of the procedure is given here. Refer to Section 4.0 for a full description of the procedure.

⁶ Contacts will exist between all particles with a gap less than or equal to the interaction gap.

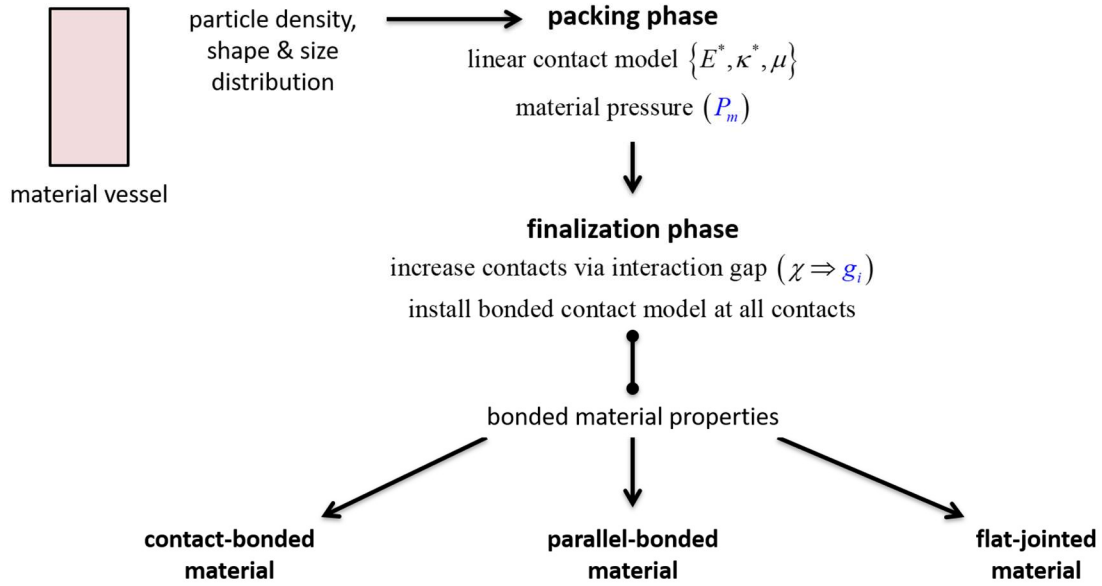


Figure 3 *Material-genesis procedure to produce a bonded material.*

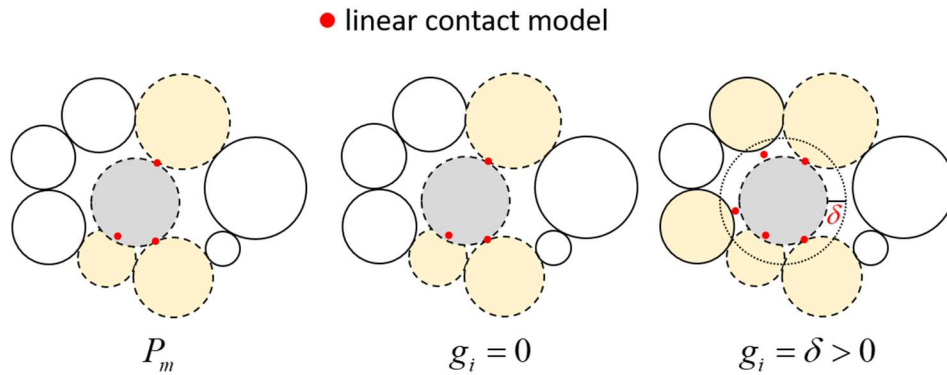


Figure 4 *Particle assembly after packing at material pressure (left), applying an interaction gap of zero (middle), or applying a positive interaction gap (right).*

The interaction gap (g_i) may be specified relative to the median particle size

$$g_i = \chi d_{50} \quad (1)$$

where χ is the interaction-gap coefficient and d_{50} is the median particle size (see Figure 5). If the interaction-gap coefficient becomes too large, then one may obtain an overly connected microstructure for which contacts exist between particles that are so far from one another that additional particles may exist between them.

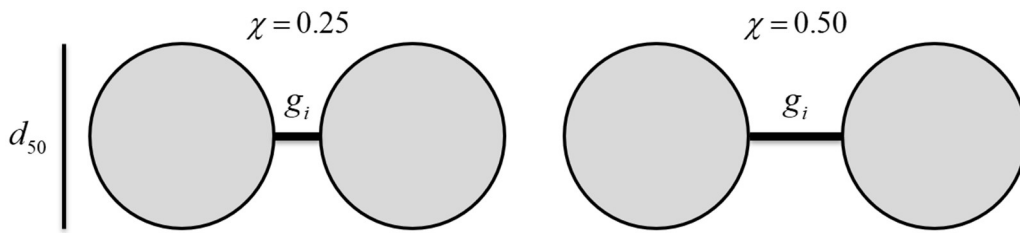


Figure 5 Interaction gap relative to median particle size for interaction-gap coefficients of 0.25 (left) and 0.50 (right).

Scholtès and Donzé (2013) study the effect of adding contacts in the gaps of a bonded-particle model by increasing the interaction range between spherical particles joined with a relatively simple contact model (see Figure 6). Increasing the interaction range increases the density of interparticle bonds, which in turn increases the degree of interlocking (see Figure 7). “The resulting medium consists in a packing where particles are not anymore described by spheres interacting through unique contact planes one with another, rather than by complex shaped equivalent particles sharing multiple contact planes all together.” They warn against obtaining an overly connected microstructure by stating that “care should be taken to avoid particles embedded in between interacting pairs” and “the initial packing density must be maximal in order to minimize the effect of collapsing pores inside the medium when a bond fails between non-contacting [particles].” Their interaction-range coefficient is related to the interaction-gap coefficient via $\lambda_{\text{int}} = \chi + 1$. They suggest limiting λ_{int} for a near uniform sphere packing with $R_{\text{max}}/R_{\text{min}} = 2$ to $\lambda_{\text{int}} \leq 1.5$ which corresponds with $\chi \leq 0.5$. As noted below, we suggest further limiting χ to $\chi \leq 0.25$ so that the flat-jointed material does not become overconnected. Scholtès and Donzé (2013) suggest that adding contacts in the gaps of their model of bonded spheres represents a way to *implicitly* account for the degree of interlocking associated with the microstructural complexity of rock. Their model allows one to obtain high ratios of compressive to tensile strength (varying the number of bonds per sphere gives ratios that range from 5 to 20) as well as nonlinear failure envelopes. These macroscopic responses are likely related to the fact that their model exhibits cohesion weakening and frictional strengthening (CWFS) as a function of rock damage. The flat-jointed material gives ratios of compressive to tensile strength up to 32 and exhibits CWFS (Potyondy, 2018).

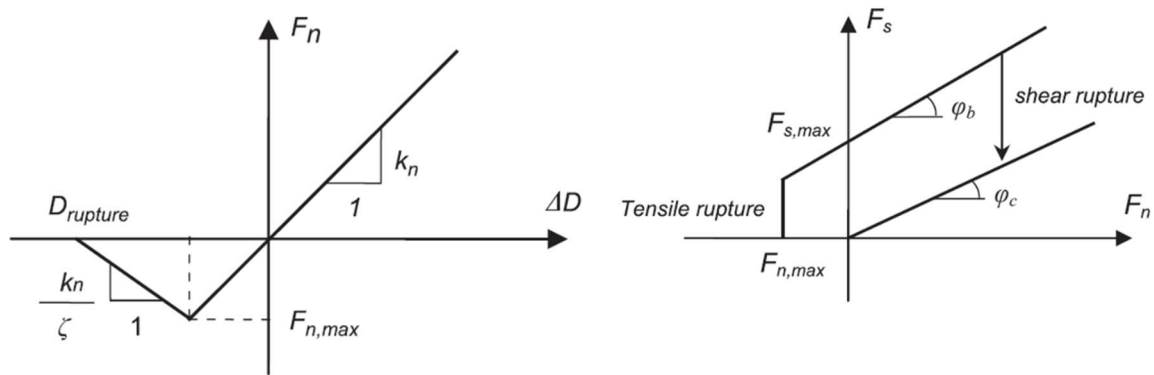


Figure 6 Force-displacement law showing normal force versus relative normal displacement (left), and shear failure envelope (right). (From Figs. 1 and 2 of Scholtès and Donzé [2013])

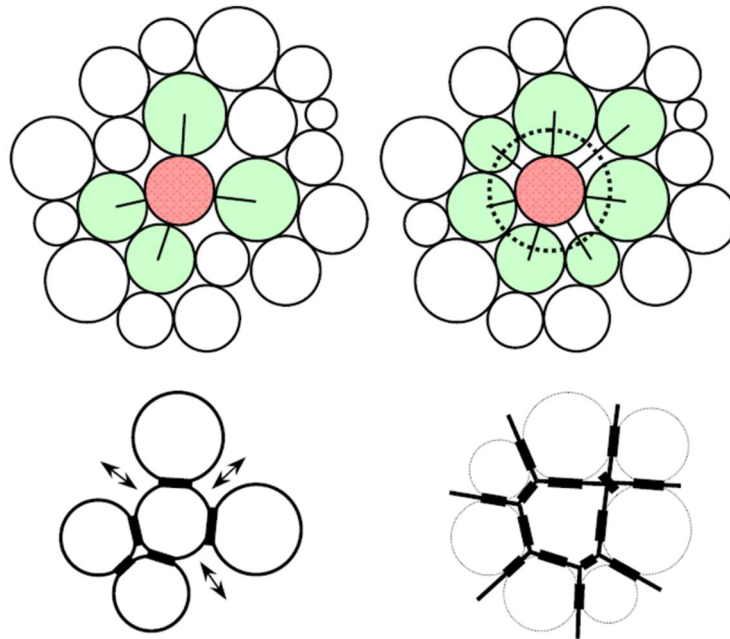


Figure 7 Effect of interaction-range coefficient (equal to one, left; greater than one, right) on contact fabric and particle interlocking. (From Fig. 3 of Scholtès and Donzé [2013])

2.2 Common Material Properties

The properties common to all PFC materials are described here and defined by the parameters listed in Table 1. The material name (N_{mt}) is used to create a model title that corresponds with the current state of the model. The material name (N_{ms}) is used to name the save states. The model title is displayed at the top of plot views. The material type may be either one of the five

supported materials or a user-defined material.⁷ Kinetic energy can be dissipated via local damping by specifying a non-zero value for the local-damping factor of each particle — quasi-static conditions are modeled by setting the local-damping factor to 0.7, and dynamic effects can be studied by choosing the local-damping factor to correspond with the seismic quality factor of the rock (Potyondy and Cundall, 2004, Eq. 3).⁸ The particle density is specified either directly or indirectly in terms of the bulk density. If the bulk density is given, then a single value of particle density is computed such that the mass of synthetic material will equal the bulk density times the vessel volume. The particle shape and size distribution are specified as follows. The particle shape must be either all balls or all clumps. If clumps are chosen, then a clump template must be provided for each clump shape. The size distribution is specified in terms of a finite number of separate size distributions, each of which is either uniform or Gaussian. The volume fraction and diameter range are given for each distribution. The size distribution can be shifted by modifying the diameter multiplier — synthetic materials that differ only in their average particle diameter can be created by varying the diameter multiplier.

Table 1 Common Parameters

Parameter	Type	Range	Default	Description
N_{mt} , cm_matName	STR	NA	PFCmat	material name (for model title)
N_{ms} , cm_matNameSAV	STR	NA	PFCmat	material name (for SAV file names)
T_m , cm_matType	INT	[0,5]	0	material-type code { 0, linear 1, contact-bonded 2, parallel-bonded 3, soft-bonded 4, flat-jointed 5, user-defined (Hill)
N_{cm} , cm_modName	STR	NA	NA	contact-model name ($T_m = 5$, also redefine ft_setMatBehavior)
C_r , cm_rblock	INT	{0,1,2}	0	rigid block code (3D only) { 0, ball or clump particles 1, Voronoi flat-jointed particles 2, tetrahedral flat-jointed particles $C_r = \{1,2\}$ requires that $T_m = 4$
ε_s , cm_rblockSizeRatMax	FLT	[0,1]	0.01	{rblock delete ratio-max}
ε_a , cm_rblockARat	FLT	(0, ∞)	6	{rblock delete size aspect-ratio}

⁷ The Hill material provides an example of a user-defined material.

⁸ Contact dashpots or Maxwell damping (ITASCA, 2026b) are more appropriate than local damping for dynamic modeling and both schemes should be considered when modeling dynamic effects. Maxwell damping is in FLAC2D, FLAC3D, and 3DEC, and it could be added to PFC2D and PFC3D.

α , cm_localDampFac	FLT	[0,0.7]	0	local-damping factor (for local damping)
C_p , cm_densityCode	INT	{0,1}	0	density code $\begin{cases} 0, & \text{particle} \\ 1, & \text{bulk} \end{cases}$
ρ_v , cm_densityVal	FLT	(0, ∞)	NA	density value (set particle density: $\rho_p = \begin{cases} \rho_v, & C_p = 0 \\ \rho_v V_v / V_p, & C_p = 1 \end{cases}$ V_v is volume of vessel, and V_p is total volume of particles)
Grain shape & size distribution group:				
S_g , cm_shape	INT	{0,1}	0	particle-shape code ($C_r = 0$) $\begin{cases} 0, & \text{all balls} \\ 1, & \text{all clumps} \end{cases}$
n_{SD} , cm_nSD	INT	$n_{SD} \geq 1$	NA	number of size distributions
T_{SD} , cm_typeSD (n_{SD})	STR	{0,1}	0	size-distribution type $\begin{cases} 0, & \text{uniform} \\ 1, & \text{gaussian} \end{cases}$
$N_{ct}^{(j)}$, cm_ctName (n_{SD})	STR	NA	NA	clump-template name ($S_g = 1$)
$D_l^{(j)}$, cm_Dlo (n_{SD})	FLT	(0, ∞)	NA	diameter range (lower)
$D_u^{(j)}$, cm_Dup (n_{SD})	FLT	$D_u^{(j)} \geq D_l^{(j)}$	NA	diameter range (upper) (clumps: volume-equiv. sphere)
$\phi^{(j)}$, cm_vfrac (n_{SD})	FLT	(0,1]	NA	volume fraction ($\sum \phi^{(j)} = 1.0$)
D_{mult} , cm_Dmult	FLT	(0, ∞)	1	diameter multiplier (shifts the size distribution)
f_s , cm_tetSFac	FLT	(0, ∞)	2	seed size spread factor ($C_r = 2$)

2.3 Linear Material

A linear material is a granular assembly in which the linear contact model exists at all particle-particle contacts. A behavior summary of the linear contact model follows in the next paragraph — refer to ITASCA (2026a)⁹ for a comprehensive description of the model.

⁹ In documentation set at PFC – Contacts and Contact Models: Contact Models – Built-in Contact Models – Linear Model.

The linear contact model provides the behavior of an infinitesimal interface that does not resist relative rotation so that the contact moment equals zero ($\mathbf{M}_c \equiv 0$). The contact force is resolved into linear and dashpot components ($\mathbf{F}_c = \mathbf{F}^l + \mathbf{F}^d$). The linear component provides linear elastic (no-tension), frictional behavior, while the dashpot component provides viscous behavior (see Figure 8). The linear force is produced by linear springs with constant normal and shear stiffnesses, k_n and k_s . The linear springs cannot sustain tension, and slip is accommodated by imposing a Coulomb limit on the shear force using the friction coefficient, μ . The dashpot force is produced by dashpots with viscosity given in terms of the normal and shear critical-damping ratios, β_n and β_s . The linear springs act in parallel with the dashpots. The linear-based models (linear, linear contact bond, linear parallel bond) support the concept of a surface gap (see Figure 9). The linear model with inactive dashpots and a reference gap of zero corresponds with the model of Cundall and Strack (1979).

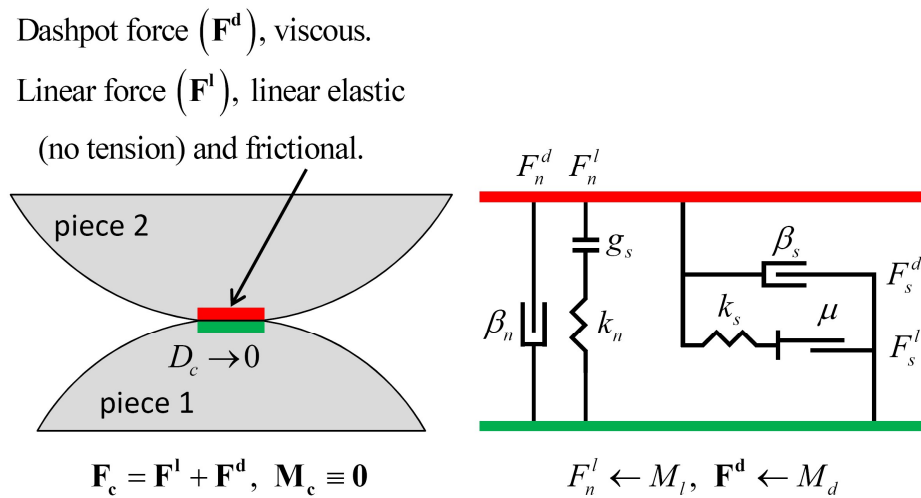


Figure 8 Behavior and rheological components of the linear contact model. (From Fig. 1 of ITASCA [2026a]¹⁰)

¹⁰ In documentation set at PFC – Contacts and Contact Models – Contact Models – Built-in Contact Models – Linear Model.

Notional surfaces (red & green) that move with the particles.

Gap between the notional surfaces is decoupled from gap between the particles.
Force-displacement law uses surface gap.

Material-modeling support creates bonded materials with notional surfaces that do not overlap
=> no forces/moments in the material.

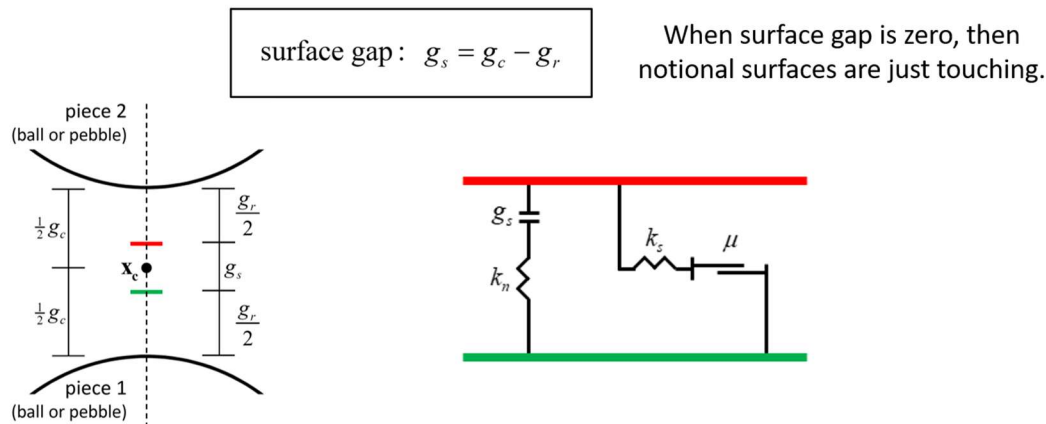


Figure 9 *Surface gap of the linear-based models.*

A linear material is defined by the primary parameters in Figure 10 and Table 2. The primary parameters (consisting of parameter names and symbols) are those that should be listed when describing a particular instance of a material — e.g., in a report or journal paper. The **particle parameters** specify the shape, density, and size distribution of the particles. The **packing parameters** specify packing pressure, local-damping factor of all particles, and deformability and strength of the linear contact model that defines the granular material during the packing phase and will be assigned to new contacts that may form during subsequent motion.

size	deformability	strength
point (zero)	$[E^*, \kappa^*] \Rightarrow [k_n, k_s]$ effective modulus stiffness ratio	μ friction coefficient

Figure 10 *Primary parameters that define a linear material.*

Table 2 Linear Material Primary Parameters

Symbol	Name
Particle (disk/sphere or clump)	
ρ	density
$\{D_l, D_u, \phi\}^{(j)}$	size distribution (min/max diameter, volume fraction)
Packing (linear model)	
α	local-damping factor (quasi-static conditions is 0.7)
P_m	material pressure (packing pressure)
$\{E^*, \kappa^*, \mu\}$	effective modulus, stiffness ratio, friction coefficient

The full parameter set, of which the primary parameters are a subset, is given in Table 3. The relevant properties of the linear model are as follows. The linear model provides linear and dashpot components. Only the linear component is active, the reference gap is zero, and the normal-force update mode is absolute. The normal and shear stiffnesses are set based on a specified contact deformability (E^* and κ^* of the **deformability** method), and the friction coefficient is set to μ .

Table 3 Linear Material Parameters

Parameter	Type	Range	Default	Description
Material microproperties are listed via <code>mpListMicroProps</code> . Common material parameters are listed in Table 1. Packing parameters are listed in Table 13.				
Linear material group				
$E^*, \text{lnm_emod}$	FLT	$[0, \infty)$	0	effective modulus
$\kappa^*, \text{lnm_krat}$	FLT	$[0, \infty)$	0	stiffness ratio
$\mu, \text{lnm_fric}$	FLT	$[0, \infty)$	0	friction coefficient

2.4 Hill Material

A Hill material is a granular assembly in which the Hill contact model (PFC3D only) exists at all particle-particle contacts. The Hill material consists of rigid particles with Hertz-Mindlin contacts. The Hertz-Mindlin contacts are provided by the Hill contact model (Potyondy, 2021) that will soon be made into a built-in contact model. The material modeling support package provides the Hill model as an example of a user-defined material (see Section 2.9). A Hill material is defined as a particle assembly in which the Hill contact model exists at all particle-particle contacts, and this

material behaves like a partially saturated granular material for which the capillary suction increases interparticle forces.

The Hill contact model employs Hertz-Mindlin springs that provide an approximation of the Hertz-Mindlin contact theory of Mindlin and Deresiewicz (1953) [see footnote 9 in Potyondy (2021)]. The theory assumes that all deformation occurs in a local region near the contact, the two surfaces in this region are characterized by their radii of curvature (R_1 and R_2), and the bodies associated with these surfaces are linear elastic isotropic (with elastic constants E_1 , ν_1 , E_2 , and ν_2). The theory considers the relative approach of the two bodies arising from local deformations associated with the compressive force that acts on the two bodies. The relative approach of the bodies is measured at large distances from the contact point. In the Hill contact model, the bodies are rigid particles, and all deformation occurs at the contact; thus, the response of a Hill material is not the same as that of elastic spherical bodies being compressed together because the deformation occurring in each body of the Hill material is only that of the local contact region. In the Hill contact model, the Hertz-Mindlin formulation is extended to include a frictional slider (μ), suction force (ψ) that mimics a liquid bridge, and dashpot (α_h)¹¹ (see Figure 11 and Table 4).

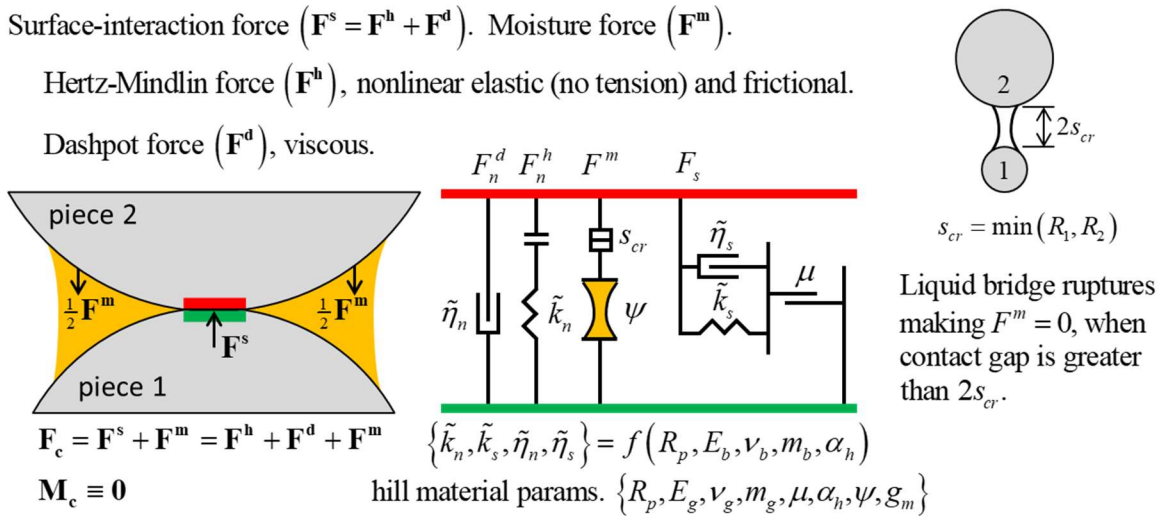


Figure 11 Behavior and rheological components of the wet Hill contact model.

¹¹ The damping constant is related directly to the coefficient of restitution in Fig. 4 of Tsuji et al. (1992), and the coefficient of restitution is independent of the body properties. The damping constant used in all of the simulations performed by Tan et al. (2014) was 0.07 (as stated in their Appendix A), which corresponds with a restitution coefficient of 0.9. The PFC3D timestep estimation procedure requires that $\alpha_h \leq 1$.

Table 4 Hill Material Parameters

Parameter	Type	Range	Default	Description
Material microproperties are listed via <code>mpListMicroProps</code> . Common material parameters are listed in Table 1. Packing parameters are listed in Table 13. Add moisture via <code>hlm_makeWet(Ψ, g_m)</code> , where Ψ is suction and g _m is moisture gap. Remove moisture via <code>hlm_makeDry</code> . Set and modify the following properties via <code>hlm_setMatBehavior</code> .				
Hill material group				
E _g , <code>hlm_youngMod</code>	FLT	[0, ∞)	0	Young's modulus of grains
ν _g , <code>hlm_poisRatio</code>	FLT	(-1, 0.5]	0	Poisson's ratio of grains
μ, <code>hlm_fricCoef</code>	FLT	[0, ∞)	0	friction coefficient
α _h , <code>hlm_dampCon</code>	FLT	[0, 1]	0	damping constant
Ψ, <code>hlm_suction</code>	FLT	[0, ∞)	0	suction

The Hill contact model can be used for particle-particle contacts where particles can be balls, clumps, or rigid blocks. The radius of curvature of each particle is obtained as shown in Figure 12. A single quantity is returned for the entire particle so that for clumps and rigid blocks, the value may not be a good measure of the surface shape near the contact.

Hill model (normal & shear force)

$$F_n^z = F_n^h + F_n^d = \begin{cases} -\tilde{k}_n \delta_o^{\frac{3}{2}} - \tilde{\eta}_n \delta_o^{\frac{1}{2}} \dot{\delta}_o, & \delta_o > 0 \\ 0, & \delta_o \leq 0 \end{cases}$$

with $\delta_o = -g_c$

$$\tilde{k}_n = \frac{4}{3} E_e \sqrt{R_e}, \quad \tilde{k}_t = 8 G_e \sqrt{R_e}; \quad R_e = \left(\frac{1}{R_1} + \frac{1}{R_2} \right)^{-1}$$

$$E_e = \left(\frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2} \right)^{-1}, \quad G_e = \left(\frac{2(1+\nu_1)(2-\nu_1)}{E_1} + \frac{2(1+\nu_2)(2-\nu_2)}{E_2} \right)^{-1}$$

A contact provides an interface between two pieces.

$$R_i = \begin{cases} R_b, & \text{piece is ball} \\ R_p, & \text{piece is pebble of clump} \\ R_{bs}, & \text{piece is rigid block} \end{cases}$$

where R_i is radius of piece (i) with $i = \{1, 2\}$;

R_b is ball radius;

R_p is pebble radius; and

R_{bs} is bounding-sphere radius.

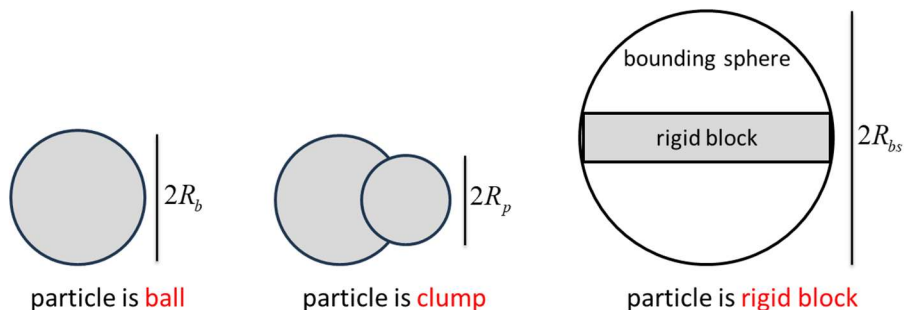


Figure 12 Surface radius used by the Hill model for balls, clumps, and rigid blocks.

2.5 Contact-Bonded Material

A contact-bonded material is a granular assembly in which the linear contact bond contact model exists at all particle-particle contacts at the end of the material-finalization phase; new particle-particle contacts that may form during subsequent motion are assigned the linear contact model. A behavior summary of the linear contact bond contact model follows in the next paragraph — refer to ITASCA (2026a)¹² for a comprehensive description of the model.

The linear contact bond model provides the behavior of an infinitesimal, linear elastic and either bonded or frictional interface that carries a force (see Figure 13). The interface does not resist relative rotation and is either bonded or unbonded. If bonded, the behavior is linear elastic until the strength limit is exceeded and the bond breaks making the interface unbonded. If unbonded, the behavior is linear elastic and frictional with slip being accommodated by imposing a Coulomb limit on the shear force. The unbonded linear contact bond model is equivalent to the linear model. The linear contact bond model with inactive dashpots and a reference gap of zero corresponds with the contact-bond model of Potyondy and Cundall (2004).

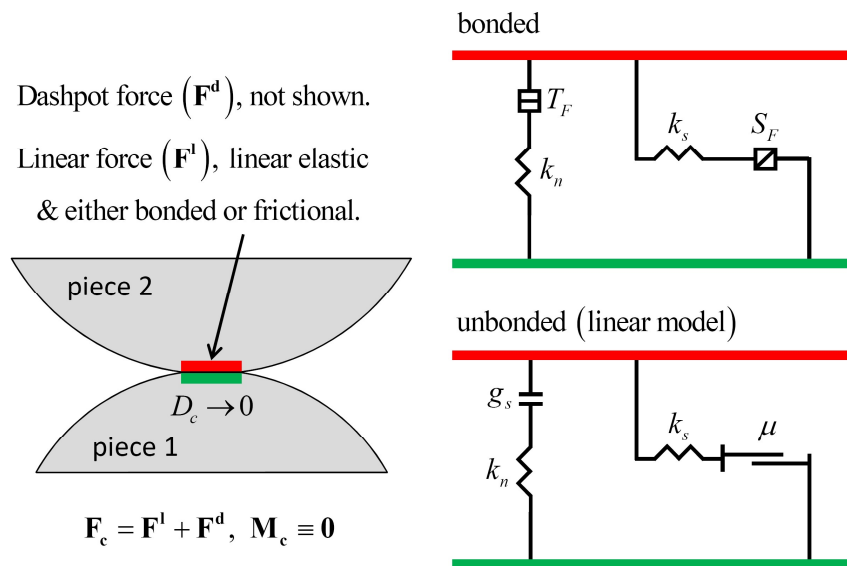


Figure 13 Behavior and rheological components of the linear contact bond model with inactive dashpots. (From Fig. 1 of ITASCA [2026a]¹³)

A contact-bonded material is defined by the primary parameters in Figure 14 and Table 5. The primary parameters (consisting of parameter names and symbols) are those that should be listed when describing a particular instance of a material — e.g., in a report or journal paper. The **particle parameters** specify the shape, density, and size distribution of the particles. The **packing**

¹² In documentation set at PFC – Contacts and Contact Models – Contact Models – Built-in Contact Models – Linear Contact Bond Model.

¹³ In documentation set at PFC – Contacts and Contact Models – Contact Models – Built-in Contact Models – Linear Contact Bond Model.

parameters specify packing pressure, local-damping factor of all particles, and deformability and strength of the linear contact model that defines the granular material during the packing phase and will be assigned to new contacts that may form during subsequent motion.

size	deformability	strength
point (zero)	$[E^*, \kappa^*] \Rightarrow [k_n, k_s]$ effective modulus stiffness ratio	$\mu, [T_\sigma, S_\sigma] \Rightarrow [T_F, S_F]$ friction coef. (unbonded) tensile & shear strengths

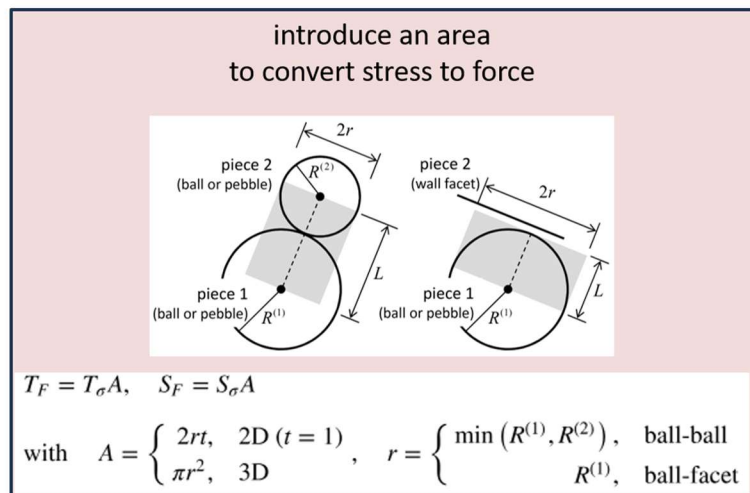


Figure 14 Primary parameters that define a contact-bonded material.

Table 5 Contact-Bonded Material Primary Parameters

Symbol	Name
Particle (disk/sphere or clump)	
ρ	density
$\{D_l, D_u, \phi\}^{(j)}$	size distribution (min/max diameter, volume fraction)
Packing (linear model)	
α	local-damping factor (quasi-static conditions is 0.7)
P_m	material pressure (packing pressure)
$\{E_n^*, \kappa_n^*, \mu_n\}$	contacts during packing & after finalization
Ensemble	
λ	interaction-gap coefficient ($g_i = \lambda d_{50}$)
Contact-bond model	
$\{E^*, \kappa^*, \mu\}$	effective modulus, stiffness ratio, friction coefficient
$(T_\sigma)_{\{m, sd\}}$	tensile-strength distribution ($T_F = T_\sigma A$, A is contact area)
γ	shear to tensile strength ratio ($S_\sigma = \gamma T_\sigma$, $S_F = S_\sigma A$)

The full parameter set of a contact-bonded material, of which the primary parameters are a subset, is given in Table 6. The properties in the contact-bonded material group are used to set the relevant properties of the linear contact bond model during material finalization, and the properties in the linear material group are assigned to particle-particle contacts during packing and that may form after material finalization.

The relevant properties of the linear contact bond model are as follows. There are linear and dashpot components. Only the linear component is active. The reference gap is zero unless a bond is installed. If a bond is installed, then the reference gap is set equal to the contact gap at the time of bond installation (thereby establishing reference surfaces that are just touching and effectively removing the overlap or extending the grain surfaces). The normal-force update mode is absolute. The normal and shear stiffnesses are set based on a specified contact deformability (E^* and κ^* of the **deformability** method), and the friction coefficient is set to μ . Bonds are installed during material finalization at the particle-particle contacts with a gap less than or equal to the installation gap (g_i). The remaining properties correspond directly with properties in the contact-bond group of the linear contact bond model.

The relevant properties of the linear model are as follows. The linear model provides linear and dashpot components. Only the linear component is active, the reference gap is zero, and the normal-force update mode is absolute. The normal and shear stiffnesses are set based on a specified contact deformability (E_n^* and κ_n^* of the **deformability** method) and the friction coefficient is set to μ_n .

Table 6 Contact-Bonded Material Parameters

Parameter	Type	Range	Default	Description
Material microproperties are listed via @mpListMicroProps . Common material parameters are listed in Table 1. Packing parameters are listed in Table 13.				
Contact-bonded material group				
Linear group				
E^* , cbm_emod	FLT	$[0, \infty)$	0	effective modulus
κ^* , cbm_krat	FLT	$[0, \infty)$	0	stiffness ratio
μ , cbm_fric	FLT	$[0, \infty)$	0	friction coefficient
Contact-bond group				
g_i , cbm_igap	FLT	$[0, \infty)$	0	installation gap (not yet settable via λ)
$(T_\sigma)_{\{msd\}}$ cbm_tens_{m,sd}	FLT	$[0, \infty)$	$\{0, 0\}$	tensile-strength dist. [stress] (mean and std. deviation)
$(S_\sigma)_{\{msd\}}$ cbm_shears_{m,sd}	FLT	$[0, \infty)$	$\{0, 0\}$	shear-strength dist. [stress] (mean and std. deviation)
γ cbm_shearsTensRatio	FLT	$[0, \infty)$	0	(At each contact, set $S_\sigma = \gamma T_\sigma$. If $\gamma = 0.0$, then $(S_\sigma)_{\{msd\}}$ is used.)
Linear material group (for particle-particle contacts during packing and that may form after material finalization)				
E_n^* , lnm_emod	FLT	$[0, \infty)$	0	effective modulus
κ_n^* , lnm_krat	FLT	$[0, \infty)$	0	stiffness ratio
μ_n , lnm_fric	FLT	$[0, \infty)$	0	friction coefficient

2.6 Parallel-Bonded Material

A parallel-bonded material is a granular assembly in which the linear parallel bond contact model exists at all particle-particle contacts at the end of the material-finalization phase; new particle-particle contacts that may form during subsequent motion are assigned the linear contact model. A behavior summary of the linear parallel bond contact model follows in the next paragraph — refer to ITASCA (2026a)¹⁴ for a comprehensive description of the model.¹⁵

The linear parallel bond model provides the behavior of two interfaces: an infinitesimal, linear elastic (no-tension) and frictional interface that carries a force, and a finite-size, linear elastic and bonded interface that carries a force and moment (see Figure 15). The first interface is equivalent to the linear model: it does not resist relative rotation, and slip is accommodated by imposing a Coulomb limit on the shear force. The second interface is called a parallel bond, because when bonded, it acts in parallel with the first interface. When the second interface is bonded, it resists relative rotation, and its behavior is linear elastic until the strength limit is exceeded and the bond breaks making it unbonded. When the second interface is unbonded, it carries no load. The unbonded linear parallel bond model is equivalent to the linear model. The linear parallel bond model with inactive dashpots and a reference gap of zero corresponds with the parallel-bond model of Potyondy and Cundall (2004).

¹⁴ In documentation set at PFC – Contacts and Contact Models – Built-in Contact Models – Contact Models – Linear Parallel Bond Model.

¹⁵ The 2D parallel bond model is used to develop a model for a very weakly cemented sandstone (Potyondy, 2025b).

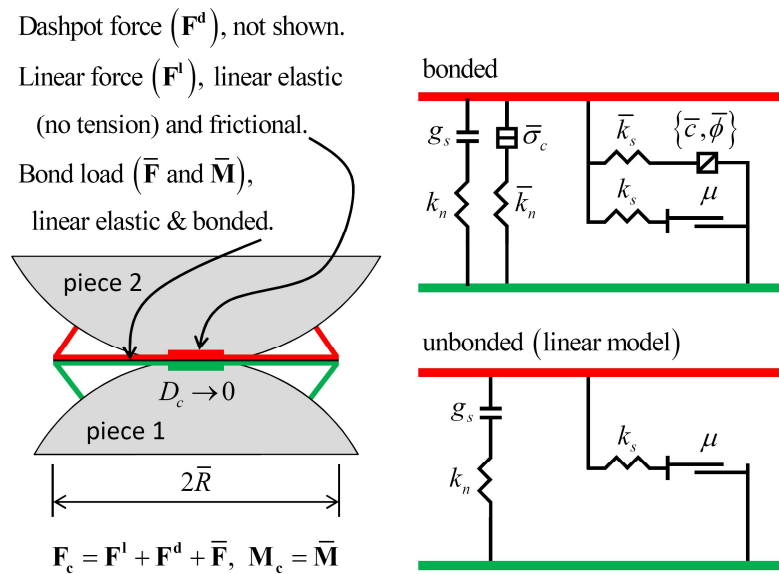


Figure 15 Behavior and rheological components of the linear parallel bond model with inactive dashpots. (From Fig. 1 of ITASCA [2026a]¹⁶)

A parallel-bonded material is defined by the primary parameters in Figure 16 and Table 7. The primary parameters (consisting of parameter names and symbols) are those that should be listed when describing a particular instance of a parallel-bonded material — e.g., in a report or journal paper. The **particle parameters** specify the shape, density, and size distribution of the particles. The **packing parameters** specify packing pressure, local-damping factor of all particles, and deformability and strength of the linear contact model that defines the granular material during the packing phase and will be assigned to new contacts that form after the bonds have been installed in the finalization phase. The **ensemble parameter** specifies a property that applies to the ensemble of packed particles: interaction-gap coefficient to create contacts in the gaps between the packed particles. The **parallel-bond model parameters** specify the deformability and strength properties that are assigned to the particle-particle interfaces.

¹⁶ In documentation set at PFC – Contacts and Contact Models – Contact Models – Built-in Contact Models – Linear Parallel Bond Model.

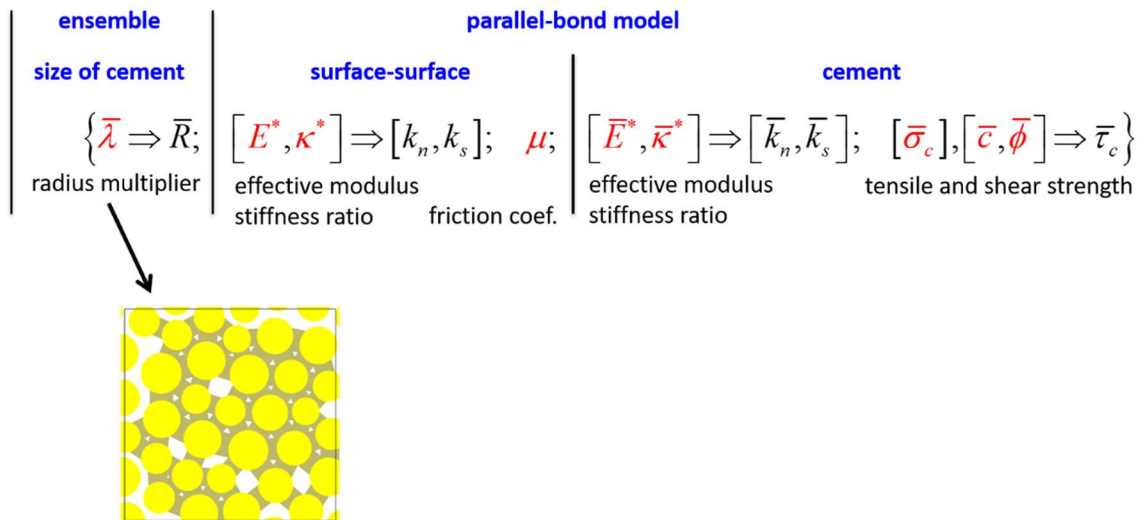


Figure 16 Primary parameters that define a parallel-bonded material.

Table 7 Parallel-Bonded Material Primary Parameters

Symbol	Name
Particle (disk/sphere or clump)	
ρ	density
$\{D_l, D_u, \phi\}^{(j)}$	size distribution (min/max diameter, volume fraction)
Packing (linear model)	
α	local-damping factor (quasi-static conditions is 0.7)
P_m	material pressure (packing pressure)
$\{E_n^*, \kappa_n^*, \mu_n\}$	contacts during packing & after finalization
Ensemble	
λ	interaction-gap coefficient ($g_i = \lambda d_{50}$)
Parallel-bond model	
$\bar{\lambda}$	radius multiplier ($\bar{R} = \bar{\lambda} \min(R^{(1)}, R^{(2)})$)
$\{E^*, \kappa^*, \mu\}$	effective modulus, stiffness ratio, friction coefficient
$\{\bar{E}^*, \bar{\kappa}^*\}$	bond effective modulus, bond stiffness ratio
$(\bar{\sigma}_c)_{\{m, sd\}}$	tensile-strength distribution
$\bar{\gamma}$	cohesion to tensile strength ratio ($\bar{c} = \bar{\gamma} \bar{\sigma}_c$)
$\bar{\phi}$	friction angle

The full parameter set of a contact-bonded material, of which the primary parameters are a subset, is given in Table 8. The properties in the parallel-bonded material group are used to set the relevant properties of the linear parallel bond model during material finalization, and the properties in the linear material group are assigned to particle-particle contacts during packing and that may form after material finalization.

The relevant properties of the linear parallel bond model are as follows. The linear parallel bond model provides the behavior of two interfaces. The first interface is equivalent to the linear model, and the second interface is called a parallel bond.

- The relevant properties of the first interface are listed in the linear group. The first interface provides linear and dashpot components. Only the linear component is active. The

reference gap is zero but may be altered when a bond is installed. If a bond is installed and the contact gap is negative, then the reference gap is set equal to the contact gap at the time of bond installation (thereby establishing reference surfaces that are just touching and effectively removing the overlap). The normal-force update mode is absolute. The normal and shear stiffnesses of the first interface are set based on a specified contact deformability (E^* and κ^* of the **deformability** method), and the friction coefficient is set to μ .

- The relevant properties of the second interface are listed in the parallel-bond group. The second interface carries load only when it is bonded. Bonds are installed during material finalization at the particle-particle contacts with a gap less than or equal to the installation gap (g_i). The normal and shear stiffnesses of the second interface are set based on a specified deformability ($\bar{E}^*$ and $\bar{\kappa}^*$ of the **pb_deformability** method). The remaining properties of the second interface correspond directly with properties in the parallel-bond group of the linear parallel bond model.

The relevant properties of the linear model are as follows. The linear model provides linear and dashpot components. Only the linear component is active, the reference gap is zero, and the normal-force update mode is absolute. The normal and shear stiffnesses are set based on a specified contact deformability (E_n^* and κ_n^* of the **deformability** method), and the friction coefficient is set to μ_n .

Table 8 Parallel-Bonded Material Parameters

Parameter	Type	Range	Default	Description
Material microproperties are listed via <code>mpListMicroProps</code> . Common material parameters are listed in Table 1. Packing parameters are listed in Table 13.				
Parallel-bonded material group				
Linear group				
E^* , <code>pbm_emod</code>	FLT	$[0, \infty)$	0	effective modulus
κ^* , <code>pbm_krat</code>	FLT	$[0, \infty)$	0	stiffness ratio
μ , <code>pbm_fric</code>	FLT	$[0, \infty)$	0	friction coefficient
Parallel-bond group				
g_i , <code>pbm_igap</code>	FLT	$[0, \infty)$	0	installation gap (not yet settable via λ)
$\bar{\lambda}$, <code>pbm_rmul</code>	FLT	$(0, \infty)$	1	radius multiplier

$\bar{E}^*$, pbm_bemod	FLT	$[0, \infty)$	0	bond effective modulus
$\bar{K}^*$, pbm_bkrat	FLT	$[0, \infty)$	1	bond stiffness ratio
$\bar{\beta}$, pbm_mcf	FLT	$[0, 1]$	0	moment-contribution factor
$(\bar{\sigma}_c)_{\{m, sd\}}$ pbm_ten_{m, sd}	FLT	$[0, \infty)$	$\{0, 0\}$	tensile-strength dist. [stress] (mean and std. deviation)
$(\bar{c})_{\{m, sd\}}$ pbm_coh_{m, sd}	FLT	$[0, \infty)$	$\{0, 0\}$	cohesion dist. [stress] (mean and std. deviation)
$\bar{\gamma}$ pbm_cohTenRatio	FLT	$[0, \infty)$	0	cohesion to tensile strength ratio (At each contact, set $\bar{c} = \bar{\gamma} \bar{\sigma}_c$. If $\bar{\gamma} = 0.0$, then $(\bar{c})_{\{m, sd\}}$ is used.)
$\bar{\phi}$, pbm_fa	FLT	$[0, 90)$	0	friction angle [degrees]
Linear material group (for particle-particle contacts during packing and that may form after material finalization):				
E_n^* , lnm_emod	FLT	$[0, \infty)$	0.0	effective modulus
κ_n^* , lnm_krat	FLT	$[0, \infty)$	0.0	stiffness ratio
μ_n , lnm_fric	FLT	$[0, \infty)$	0.0	friction coefficient

2.7 Soft-Bonded Material

A soft-bonded material¹⁷ is a granular assembly in which the soft bond contact model exists at all particle-particle contacts at the end of the material-finalization phase; new particle-particle contacts that may form during subsequent motion are assigned the linear contact model. A behavior summary of the soft bond contact model follows — refer to ITASCA (2026a)¹⁸ for a comprehensive description of the model.

The soft bond model may carry a force and moment (**F and M**) and provides two behaviors depending on its bonding state (see Figure 17). When unbonded, it provides a behavior that is linear elastic (no tension) and frictional with rolling resistance. When bonded, it provides a behavior that is linear elastic until either the shear or tensile strength limit is exceeded. If the shear strength limit is exceeded, then the bond breaks making it unbonded. If the tensile strength limit

¹⁷ The soft-bonded material should be used with caution, because the formulation is not well described in the manual. Work is underway to replace the soft bond contact model with a new and well-defined model.

¹⁸ In documentation set at PFC – Contacts and Contact Models – Contact Models – Built-in Contact Models – Soft-Bond Model.

is exceeded, then the bond may soften (see Figure 18) until it reaches a specified fraction of the tensile strength, at which point the bond breaks making it unbonded. When bonded, the soft-bond model is like the linear parallel bond model with tensile softening.

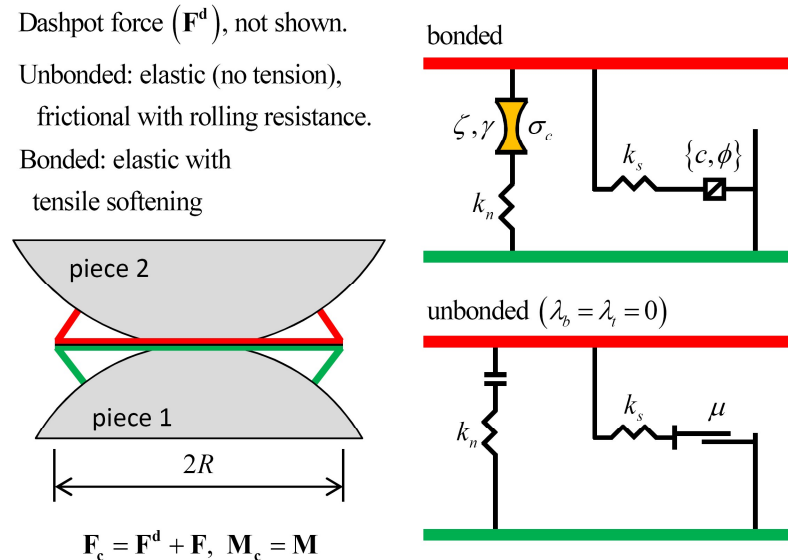
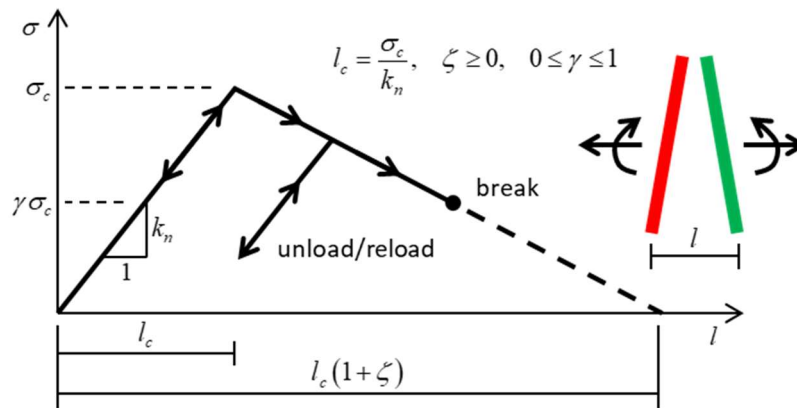


Figure 17 Behavior and rheological components of the soft bond model with friction multipliers of zero and inactive dashpots.



σ : maximum normal stress at bond periphery
 l : elongation at bond periphery ($l \geq 0$)
 l_c : critical bond elongation at peak strength

σ_c : tensile strength [stress]

k_n : normal stiffness [stress/length]

ζ : softening factor ($\zeta \geq 0$, $\zeta = 0$ is no softening)

γ : strength-reduction factor $\begin{cases} 0 \leq \gamma \leq 1 \\ \gamma = 0 \text{ is full softening} \\ \gamma = 1 \text{ is no softening} \end{cases}$

Figure 18 Softening behavior of the soft bond model.

A soft-bonded material is defined by the parameters in Table 9. The properties in the soft-bonded material group are used to set the relevant properties of the soft bond model during material finalization, and the properties in the linear material group are assigned to grain-grain contacts during packing and that may form after material finalization.

The relevant properties of the soft bond model are as follows. The dashpot component is inactive. The reference gap is zero but may be altered when a bond is installed. If a bond is installed and the contact gap is negative, then the reference gap is set equal to the contact gap at the time of bond installation (thereby establishing reference surfaces that are just touching and effectively removing the overlap). The normal-force update mode is absolute; however, it is automatically set to incremental when bonds are installed and remains incremental after they break. Bonds are installed during material finalization at the particle-particle contacts with a gap less than or equal to the installation gap (g_i). The normal and shear stiffnesses are set based on a specified deformability (E^* and κ^* of the **deformability** method). The remaining properties correspond directly with properties in the soft-bond group of the soft bond model.

The relevant properties of the linear model are as follows. The linear model provides linear and dashpot components. Only the linear component is active, the reference gap is zero, and the normal-force update mode is absolute. The normal and shear stiffnesses are set based on a

specified contact deformability (E_n^* and κ_n^* of the **deformability** method), and the friction coefficient is set to μ_n .

Table 9 Soft-Bonded Material Parameters

Parameter	Type	Range	Default	Description
Material microproperties are listed via <code>mpListMicroProps</code> . Common material parameters are listed in Table 1. Packing parameters are listed in Table 13.				
Soft-bonded material group				
g_i , sbm_igap	FLT	$[0, \infty)$	0	installation gap (not yet settable via χ)
λ , sbm_rmul	FLT	$(0, \infty)$	1	radius multiplier
E^* , sbm_emod	FLT	$[0, \infty)$	0	effective modulus
κ^* , sbm_krat	FLT	$[0, \infty)$	0	stiffness ratio
β , sbm_mcf	FLT	$[0, 1]$	0	moment-contribution factor
$(\sigma_c)_{\{m, sd\}}$ sbm_ten_{m, sd}	FLT	$[0, \infty)$	$\{0, 0\}$	tensile-strength dist. [stress] (mean and std. deviation)
$(c)_{\{m, sd\}}$ sbm_coh_{m, sd}	FLT	$[0, \infty)$	$\{0, 0\}$	cohesion dist. [stress] (mean and std. deviation)
γ sbm_cohTenRatio	FLT	$[0, \infty)$	0	(At each contact, set $c = \gamma \sigma_c$. If $\gamma = 0.0$, then $(c)_{\{m, sd\}}$ is used.)
ϕ , sbm_fa	FLT	$[0, 90)$	0	friction angle [degrees]
ζ , sbm_soft	FLT	$[0, \infty)$	0	softening factor ($\zeta = 0$ is no softening)
γ , sbm_cut	FLT	$[0, 1]$	0	strength-reduction factor ($\gamma = 0/1$ is full/no softening)
μ , sbm_fric	FLT	$[0, \infty)$	0	friction coefficient (when unbonded)
λ_b , sbm_bmul	FLT	$[0, \infty)$	0	bending-friction multiplier (when unbonded)
λ_t , sbm_tmul	FLT	$[0, \infty)$	0	twisting-friction multiplier (when unbonded)

Linear material group (for grain-grain contacts during packing and that may form after material finalization):

E_n^* , lnm_emod	FLT	$[0, \infty)$	0	effective modulus
κ_n^* , lnm_krat	FLT	$[0, \infty)$	0	stiffness ratio
μ_n , lnm_fric	FLT	$[0, \infty)$	0	friction coefficient

2.8 Flat-Jointed Material

A *flat-joint contact* and its corresponding *flat-jointed material* are shown in Figure 19. A flat-joint contact behaves like a finite-size interface between two flat surfaces (faces) that are connected rigidly with the particles. The interface is discretized into elements, each of which may be bonded or unbonded (either initially or after a bond breaks). A flat-jointed material is a particle assembly joined by flat-joint contacts. It provides a microstructure of angular, interlocked, rigid, unbreakable *faced grains* with deformable interfaces that may have an initial gap and can sustain partial damage as bonded elements break. The microstructure is like that of marble; however, the faced grains are not perfectly interlocked, because the faces do not fully enclose each grain as seen by the voids in the upper-right image of Figure 19. The breakage of each bonded element is denoted as a crack (see Figure 20).¹⁹ A faced grain remains interlocked even after the elements at all faces along its boundary have broken (see Figure 21). Damage in a flat-jointed material consists of microcracking and fragmentation (see Figure 22).

¹⁹ Cracks in the 2D flat-jointed material are depicted as colored lines lying on the interface with color denoting breakage mode and with line thickness proportional to the element gap. Cracks in the 3D flat-jointed material are depicted as colored octagons lying on the interface with color denoting breakage mode. Breakage mode is either tensile or shear. Each crack is associated with a broken element; thus, a fully broken flat-joint contact discretized into 16 elements has 16 cracks.

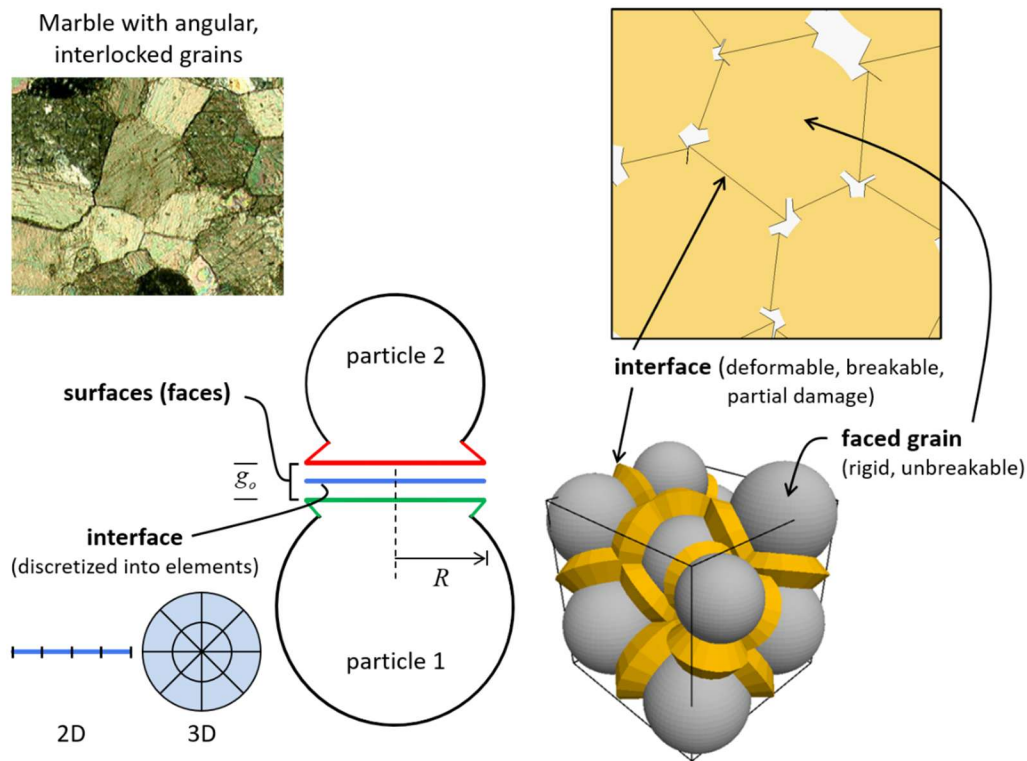


Figure 19 *Marble (upper left), flat-joint contact (middle), and flat-jointed material (right).*

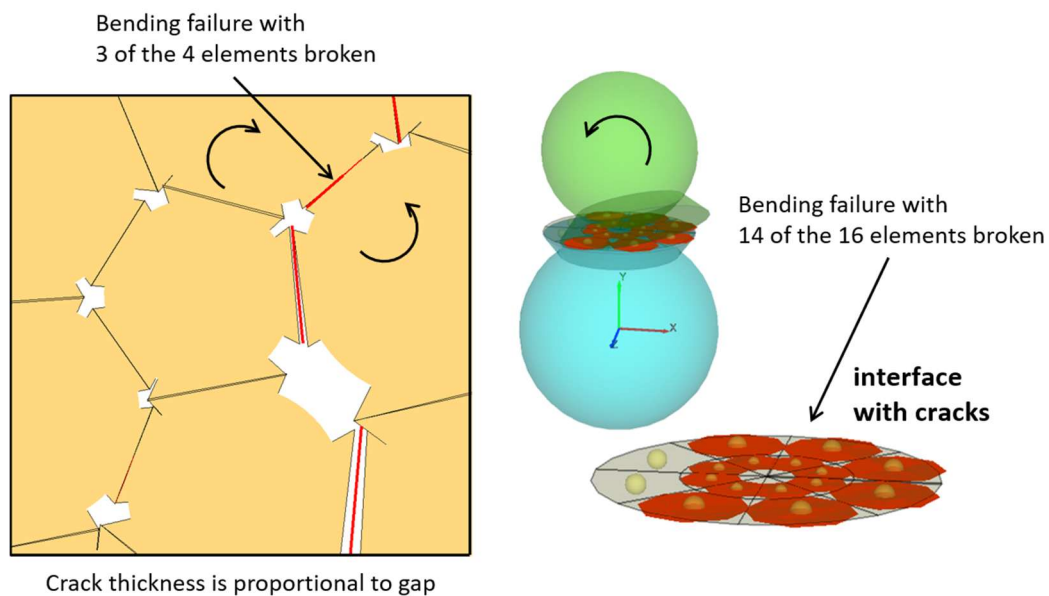


Figure 20 *Partially damaged flat-jointed material showing faced grains with cracks colored red/blue for tensile/shear failure.*

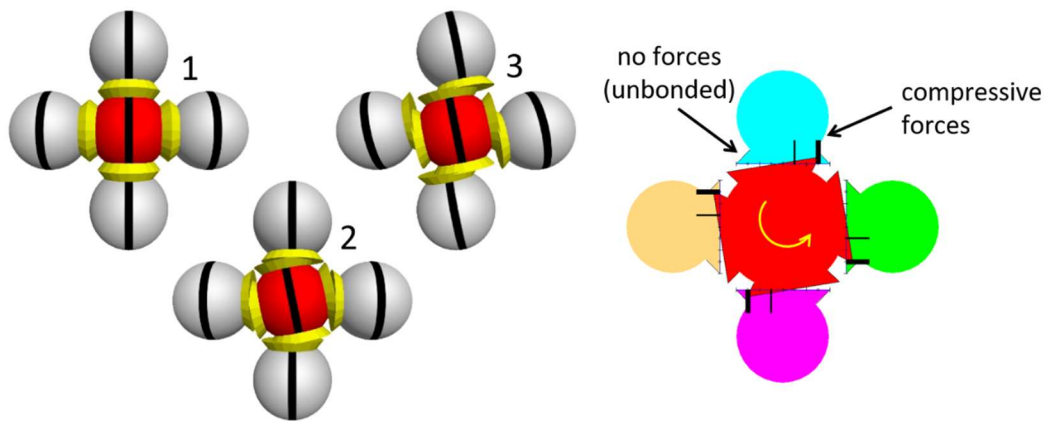


Figure 21 *Five faced grains with unbonded and frictionless interfaces before (left, 1) and after (left, 2) rotating the central faced grain. Compressive forces develop at the far end of each interface that resist the moment applied to the central faced grain (right). When the rotational restraint on the surrounding faced grains is removed, these grains rotate to relieve the compressive forces (left, 3).*

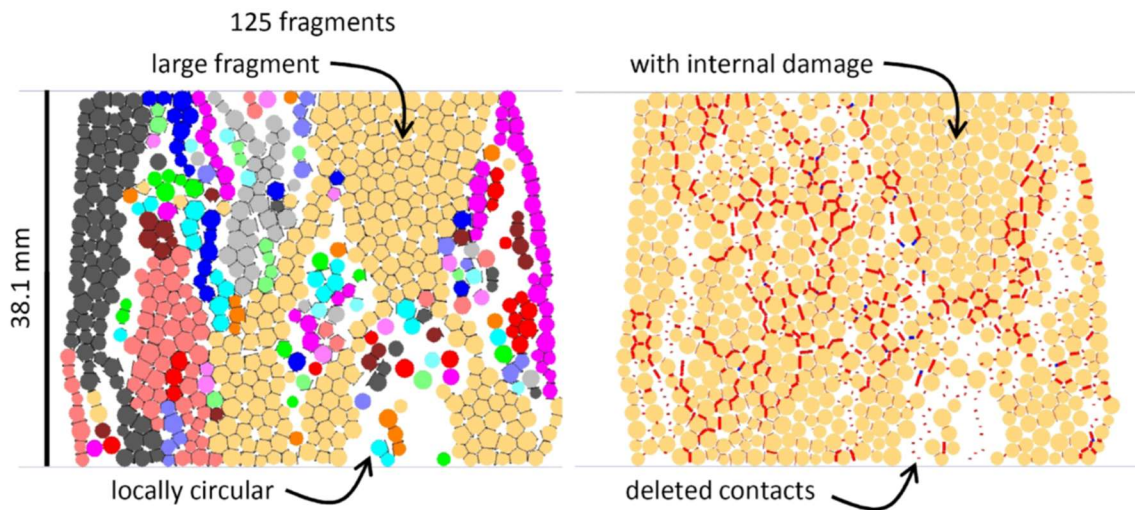


Figure 22 *Fragmentation of a PFC2D flat-jointed material in the post-peak portion of a UCS test when the axial load has dropped to zero: particles drawn as faced grains and colored by fragment (left); particles drawn as disks and cracks colored red/blue for tensile/shear failure with thickness proportional to gap (right). (from Fig. 4 of Potyondy [2017]).*

A flat-joint contact behaves like a finite-size interface (defined by radius multiplier, λ) between two faces that are connected rigidly with the particles (see Figure 23). The radius is assigned as $R = \lambda \min\{R^{(1)}, R^{(2)}\}$, where $R^{(i)}$ is the radius of ball i . The interface is a rectangle of width $2R$ and unit-thickness in 2D and a disk of diameter $2R$ in 3D. The faces need not lie on the particle surfaces and are created when the flat-joint contact model is installed with a specified gap (defined by initial surface gap, g_o) at an existing contact of a packed particle assembly (see Figure 24). If all

contacts of a particle are flat-joint contacts, then the particle behaves like a faced grain that is depicted as a circular or spherical core with skirted faces. The interstitial fabric (see below) of the flat-jointed microstructure is independent of the gaps and overlaps of the packed particle assembly.

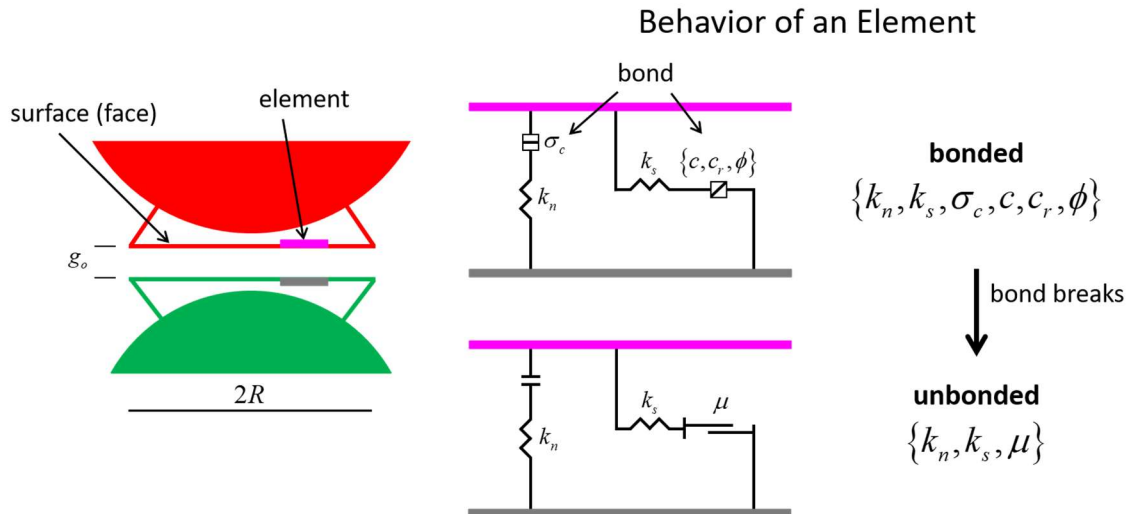


Figure 23 Geometric and rheological components of the flat-joint contact model.

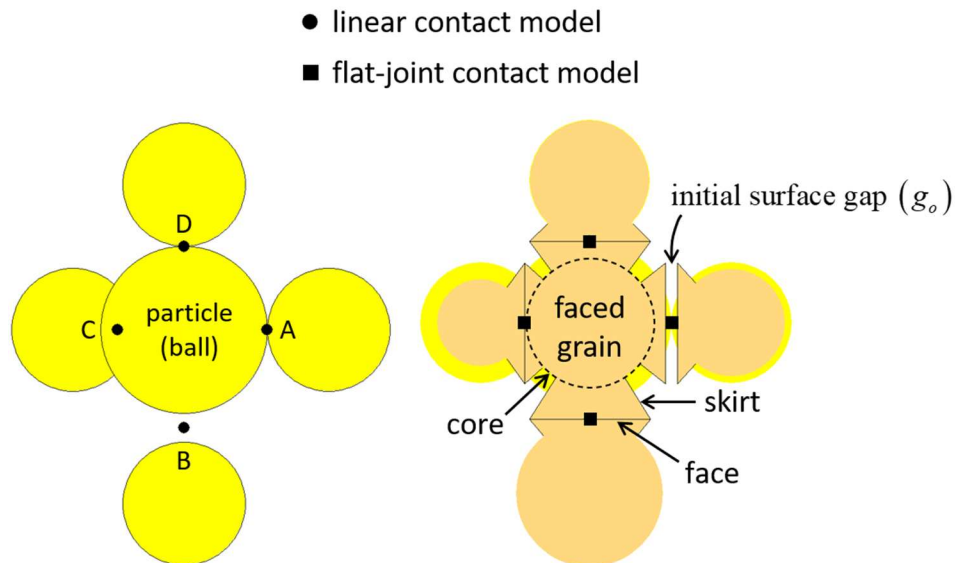


Figure 24 Particle assembly at end of packing phase (left) and corresponding faced-grain assembly (right) that is created when a flat-joint contact model is installed at each contact. The initial surface gap is nonzero at contact A and zero at contacts B–D. The gaps between the faced grains are decoupled from the gaps between the particle assembly.

A flat-joint contact behaves like a finite-size interface that is discretized into elements, each of which carries a force²⁰ that obeys the following force-displacement law. The element may be bonded or unbonded. The behavior of a bonded element is linear elastic until the strength limit is exceeded and the bond breaks, making the element unbonded; the behavior of an unbonded element is linear elastic and frictional, with slip accommodated by imposing a Coulomb limit on the shear force. The force-displacement and moment-rotation response of the flat-joint contact is emergent and includes evolving from a fully bonded state to a fully unbonded and frictional state. If the particles joined by a flat-joint contact move far apart, then the contact may be deleted and the faces associated with that contact will be removed.

The interaction gap may be specified relative to the median particle size via the interaction-gap coefficient as discussed above in Section 2.1. The faced grains are not perfectly interlocked, because the faces do not fully enclose each grain. The size of each face is defined by its radius multiplier. The radius multipliers may be specified to control whether the faces overlap one another. The concept of whether faces overlap one another is called physical realizability and is discussed in the first subsection. The microstructural connectivity is related to both the interaction-gap coefficient and the physical realizability and is discussed in the second subsection. The interstitial fabric of a flat-jointed material describes the initial state of the interfaces as being bonded, gapped, or slit and is discussed in the third subsection. The material parameters that define a flat-jointed material are defined in the fourth subsection. The final subsection describes ways in which the microstructural properties of the flat-jointed material can be quantified.

2.8.1 Physical Realizability

Physical realizability describes whether the faces of a faced-grain overlap one another. A flat-jointed material has a physically realizable microstructure if and only if the boundaries of the faces of each faced grain can be connected to the grain center with no overlap (see Figure 25). A physical replica of a physically realizable (PR) microstructure could be constructed. A physically unrealizable (non-PR) microstructure may produce useful behavior, and as such, its use can be justified. Parallel-bonded materials with radius multipliers of one have non-PR microstructures; nonetheless, such models have been used for both research and application (Potyondy, 2015). The error introduced for a non-PR material is discussed at the end of this subsection.

²⁰ The elements of the 2D flat-joint contact model also carry a moment.

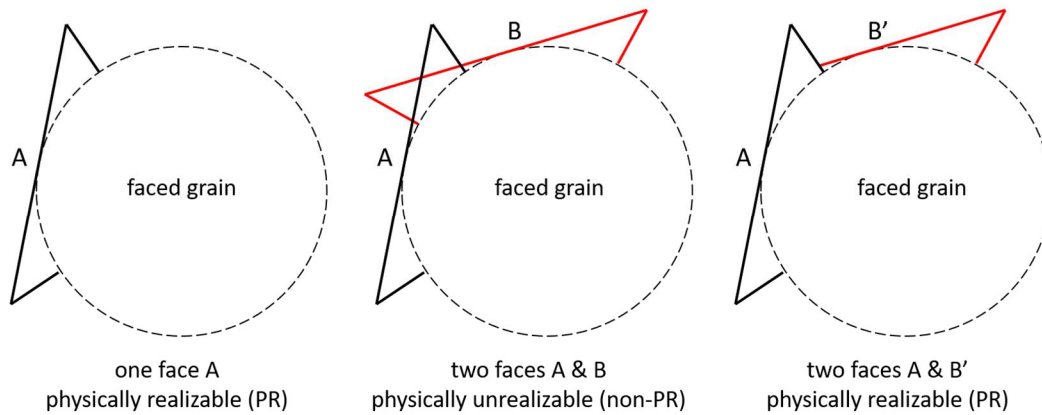
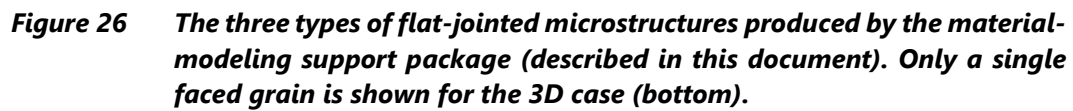


Figure 25 *Physical-realizability concept. Cutting face B makes the faced grain physically realizable.*

The physical realizability of flat-jointed materials can be controlled (with parameters $C_\lambda = \{0, 1, 2\}$ and λ_v) as follows (see Figure 26). If $C_\lambda = 0$, then all radius multipliers are set equal to λ_v and no PR check²¹ is performed — the microstructure may be PR or non-PR. Physically realizable material can be created by setting all radius multipliers equal to λ_v , and then reducing them either uniformly ($C_\lambda = 1$) or non-uniformly ($C_\lambda = 2$) until all faced grains are PR. The non-uniform reduction algorithm visits the flat-jointed contacts of each ball in the model. The flat-jointed contacts of a given ball are compared with one another, and those with overlapping facets have their flat-joint radii reduced uniformly until they no longer overlap.

²¹ The PR check uses the equations in Figure 27.



We now explore the error introduced for a non-PR material by addressing the question: Is there physical meaning to having two flat-joint interfaces of the same ball overlap? The argument refers to the model sketched in Figure 28. Each interface should behave like a crack that is glued together when fully bonded and frictional when fully broken. While bonded, the interface transfers stress. When broken, the interface transfers stress only while in compression. If tension occurs to a fully broken interface, then it should shield its neighbor from receiving this load along its full length. Consider that interface **A** is fully broken, interface **B** is fully bonded, and the ball is moved to the right while the two adjoining balls are fixed. The proper behavior is that no load is transferred across **A**, and thus, no load acts on the **bc**-portion of **B**. The flat-jointed material behavior is that the load acts over all of **B**. The error is that tensile load transfer across the fully broken interfaces is too large. Is the tensile load transfer error acceptable? The error should have a negligible effect on the macroscopic response of the material. The error will become important when examining the local behavior of the material; thus, the error may limit the scale at which one can interrogate the model. In most cases, the microstructure is a surrogate for a physical material. If one wishes to replicate a physical material, such as cemented spherical quartz grains of a sandstone, then the material should be made physically realizable. For borehole models used to study spalling, the extent of damage should be well modeled, but the detailed mechanisms of grain rotation leading to dilation and the formation of notch slabs may not be modeled accurately.

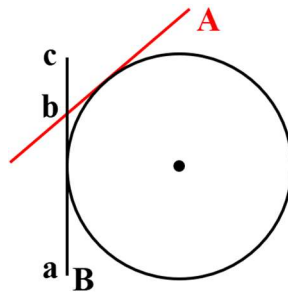


Figure 28 *A ball with two overlapping flat-joint interfaces. The two adjoining balls are not shown.*

2.8.2 Microstructural Connectivity

Microstructural connectivity relates to both the interaction gap and the size of the faces and controls material response. For example, increasing the interaction gap and/or increasing the size of the faces increases the material modulus and strength. However, there are limits to how much these quantities can be increased. If the interaction gap becomes too large, then one obtains an overly connected microstructure for which the faces between connected grains overlap one another. If the size of the faces becomes too large, then one obtains a non-PR material. We define minimally and maximally connected materials as those with $\chi = 0$ and $\chi = 0.25$, respectively, and

materials with $\chi > 0.25$ as being overly connected (see Figure 29). The physical realizability is related to the connectivity in Figure 30.²²

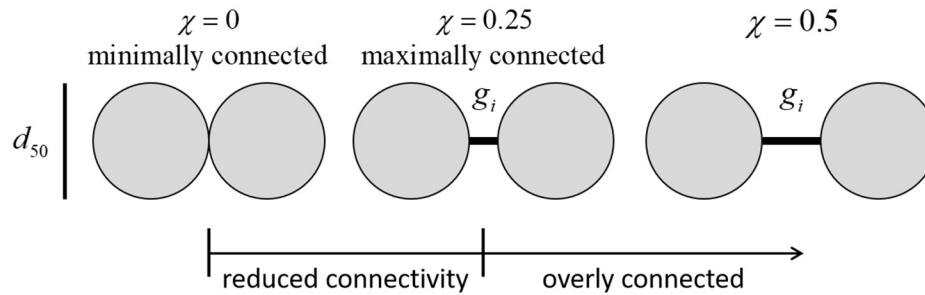


Figure 29 Quantification of connectivity via interaction-gap coefficient.

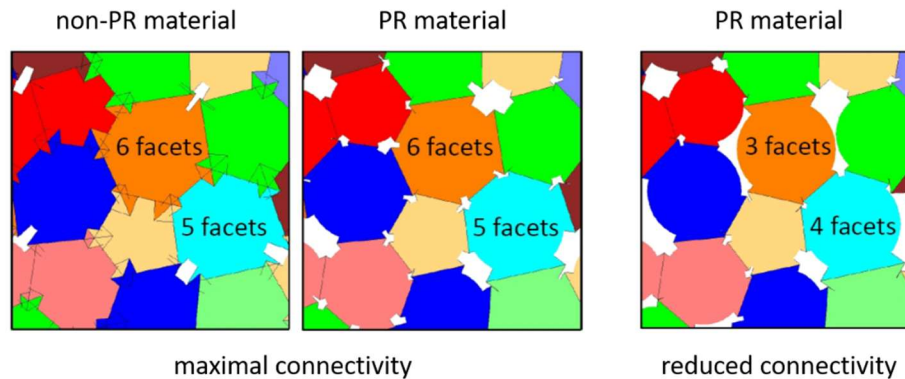


Figure 30 Materials with maximal and reduced grain connectivities.

Potyondy (2019) studied the effects of microstructural connectivity on material behavior by creating flat-jointed materials that are either PR or non-PR and have minimal grain connectivity ($\chi=0$), near maximal grain connectivity ($\chi=0.21$), or are overly connected ($\chi=0.5$). The microstructures with near maximal grain connectivity and those that are overconnected are called compact microstructures and are shown in Figures 31–34. PR and non-PR materials that match most of the properties of Äspö diorite were created and are shown in Figure 35. The models were subsequently used to study spalling in boreholes. The PR 2D material with near maximal grain connectivity (upper-left image in Figure 35) was selected for the borehole models because it is compact and physically realizable. The non-PR 3D material with near maximal grain connectivity (lower-right image in Figure 35) was selected for the borehole models. The PR 3D material (lower-left image in Figure 35) was deemed to be unrealistic — having a very small amount of cement with excessively long cement bridges that overlap between connected grains (making it overconnected) and microproperties approximately 3.5 times larger than their corresponding macroproperties to compensate for the fact that the interfaces do not fully cover the grain

²² The following question merits further study. How are these concepts related to the response of the synthetic material and to the physical rock microstructures?

surfaces. See the discussion in Potyondy (2019, Section 2.4.1) that is summarized in the next two paragraphs.

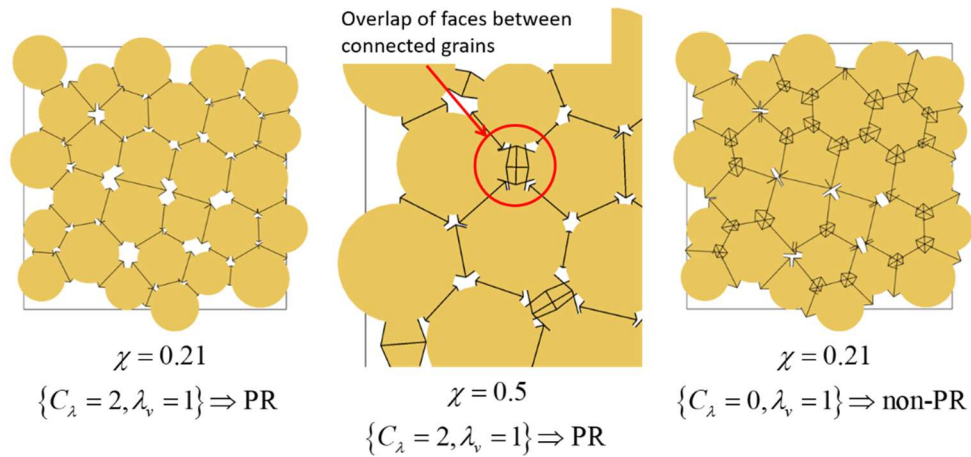


Figure 31 Compact microstructures of 2D flat-jointed material: PR with near maximal grain connectivity (left); PR and overly connected (center); and non-PR with near maximal grain connectivity (right).

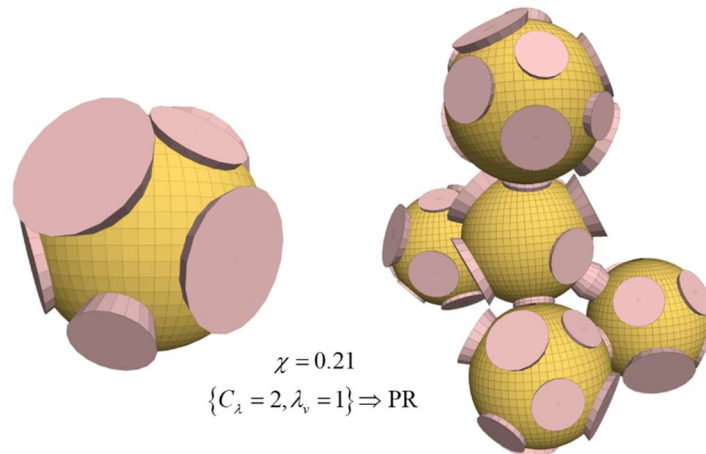


Figure 32 Compact microstructure of 3D flat-jointed material: PR with near maximal grain connectivity.

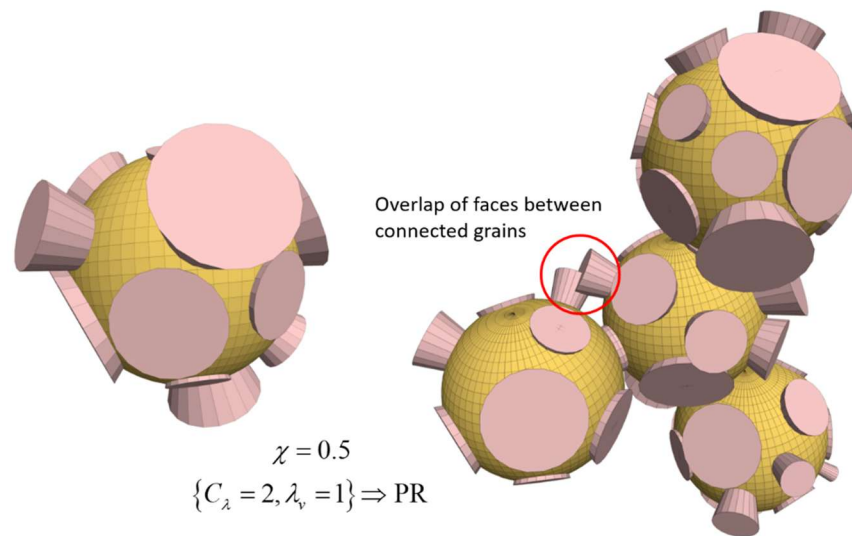


Figure 33 Compact microstructure of 3D flat-jointed material: PR and overly connected.

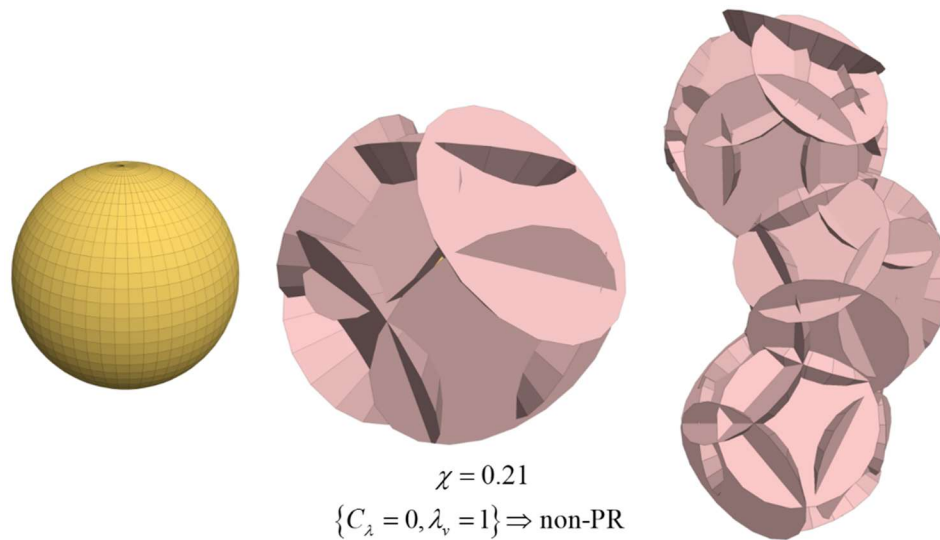


Figure 34 Compact microstructure of 3D flat-jointed material: non-PR with near maximal grain connectivity.

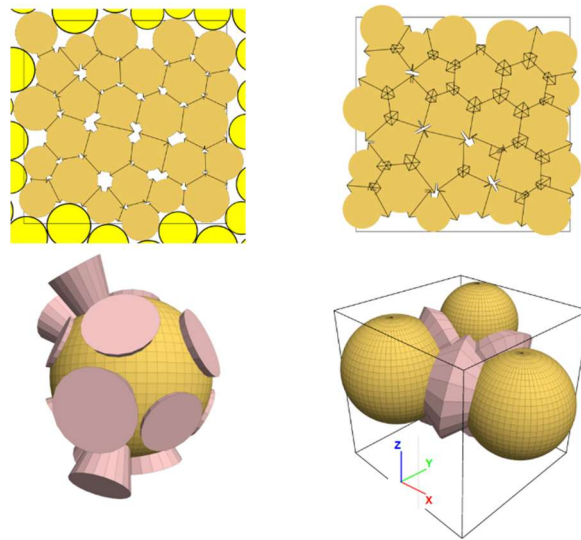


Figure 35 *Microstructures of four materials (physically realizable, left; physically unrealizable, right) that match most of the properties of Äspö diorite.*

The microstructures of the 3D materials that match most of the properties of Äspö diorite are shown in Figures 36 and 37. The grain connectivity is quantified by the average face coordination number ($\bar{Z}$), which is the average number of faces per grain, and the cover ratio ($\bar{C}_r$), which is the ratio of total area of the faces of a grain over the surface area of its circular or spherical core. The average cover ratio over all grains is denoted by $\bar{C}_r$. The non-PR material has a near maximal grain connectivity, while the PR material is overly connected. To obtain the PR material, $\bar{Z}$ increased from 10.2 to 14.6 (more faces per grain), and $\bar{C}_r$ decreased from 2.3 to 0.57 (less coverage of grain surface). The non-PR material has extensive face overlap ($\bar{C}_r \gg 1$), while the faces of the PR material do not fully cover the grain surfaces ($\bar{C}_r < 1$). The PR material does match the properties of Äspö diorite; however, this is achieved by increasing the interaction-gap coefficient to 0.5 to give a microstructure in which there is overlap of faces between connected grains (see Figure 33). The modulus and strength microproperties of the non-PR material are approximately equal to the corresponding rock macroproperties, but these microproperties of the PR material had to be increased by a factor of 3.5 to compensate for the fact that the faces do not fully cover the grain surfaces (e.g., the micro tensile strength of the non-PR material is 10 MPa, while that of the PR material is 35 MPa). The non-PR material was selected for the borehole models, because the PR material had excessively long cement bridges (overlap of faces between connected grains) and unrealistically large modulus and strength microproperties.

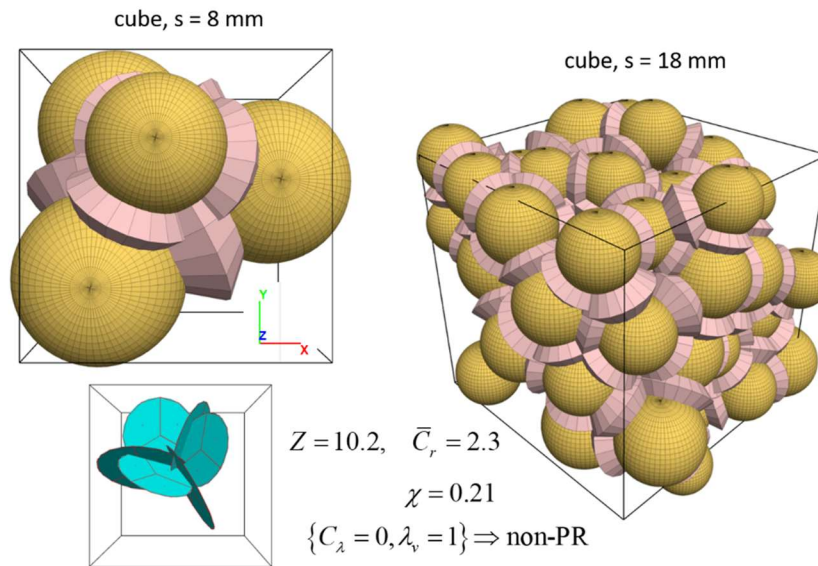


Figure 36 *Microstructure of non-PR material that matches most of the properties of Äspö diorite.* (From Fig. 27 of Potyondy [2019])

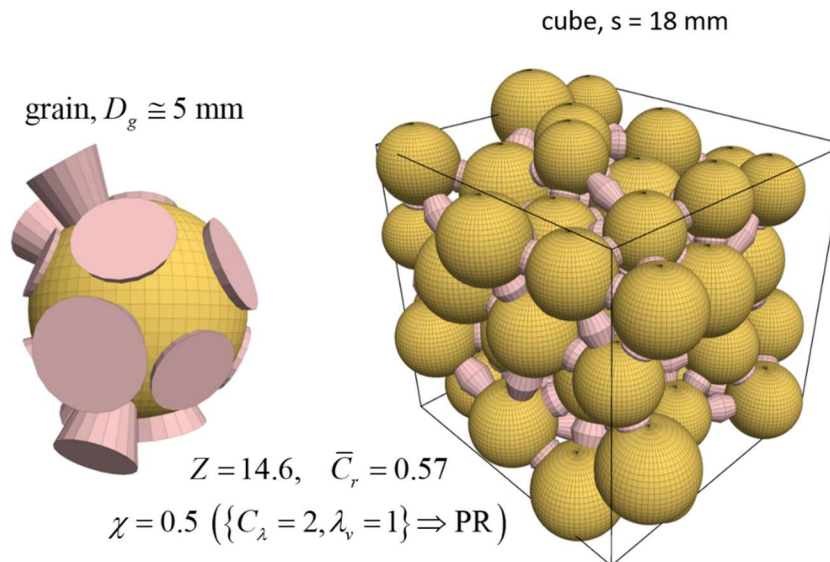


Figure 37 *Microstructure of PR material that matches most of the properties of Äspö diorite.* (From Fig. 28 of Potyondy [2019])

It is interesting to note that a physically realizable 2D material with a reasonable microstructure and realistic microproperties could be constructed, but it was not possible to do so for the 3D material. This suggests that the 3D flat-jointed material may not be well-suited to model a compact rock like granite and may be better suited to model a porous rock like sandstone.²³ The

²³ The brittle mechanical properties of intact rock are controlled by the nature of its pore space; therefore, we classify intact rock as either *compact* or *porous*. Compact rock has very small porosity, less than a few

3D Subspring Network contact model with rigid, Breakable, Voronoi-shaped grains (SNBV model of Potyondy et al. [2025]) may be better suited to model a compact rock like granite (see Figure 38).

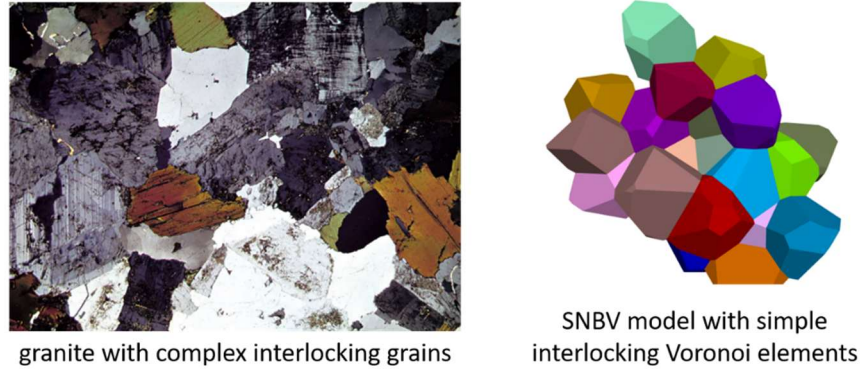


Figure 38 Granite thin section (left) and SNBV model (right). (From Fig. 10 of Potyondy et al. [2025])

2.8.3 Interstitial Fabric

The interstitial fabric of a flat-jointed material describes the initial state of the interfaces with respect to their bond state and the proximity of their adjoining surfaces. Each flat-joint contact is either bonded, gapped, or slit based on the number fractions of the bonded and gapped types (see Figure 39). The number fractions are defined as

$$\begin{aligned} \varphi_B &= n_B / n_c, \quad \varphi_G = n_G / n_c, \quad \varphi_S = n_S / n_c \\ n_c &= n_B + n_G + n_S, \quad \varphi_B + \varphi_G + \varphi_S = 1 \end{aligned} \quad (2)$$

where φ_B , φ_G , and φ_S are bonded, gapped, and slit number fractions, respectively; n_B , n_G , and n_S are the number of bonded, gapped, and slit contacts, respectively; and n_c is the total number of flat-joint contacts.

When the flat-jointed material is created, each flat-joint contact is assigned a fabric type of B, G, or S based on the specified values of φ_B and φ_G . The fabric types are assigned randomly to obtain the specified number fractions. The slit and bonded contacts are assigned an initial surface gap of zero. The gapped contacts are assigned initial surface gaps that satisfy a normal distribution with mean $(g_o)_m$ and standard deviation $(g_o)_{sd}$. The fabric type is stored in the flat joint contact model property **fj_mtype**. The interstitial-fabric information is listed by

percent, while porous rock has a substantial amount of pore space, especially as intergranular space. Compact rock has a crack-like pore space, while porous rock has a more open pore space. Compact rock includes igneous, low-porosity sedimentary and high-grade metamorphic types, while porous rock includes high-porosity sedimentary and low-grade metamorphic types.

mpListMicroStrucProps which returns the number of flat-joint contacts initially bonded (**mp_nFJiB**), gapped (**mp_nFJiG**), slit (**mp_nFJiS**), or undefined (**mp_nFJiU**).



Figure 39 *Interstitial fabric consisting of bonded, gapped, and slit flat-joint contacts. The bonded and slit contacts have coincident surfaces, while the gapped contacts have a uniform, non-zero gap between the surfaces.*

2.8.4 Material Parameters

A flat-jointed material is defined by the primary parameters in Figure 40 and Table 10. The primary parameters (consisting of parameter names and symbols) are those that should be listed when describing a particular instance of a flat-jointed material — e.g., in a report or journal paper. The **particle parameters** specify the density and size distribution of the particles. The **packing parameters** specify packing pressure, local-damping factor of all particles, and deformability and strength of the linear contact model that defines the granular material during the packing phase and will be assigned to new contacts that form after the bonds have been installed in the finalization phase. The **ensemble parameters** specify properties that apply to the ensemble of packed particles: interaction-gap coefficient to create contacts in the gaps between the packed particles, face-size control properties to control the assignment of radius multipliers to all contacts (thereby defining the shape of the faced grains and the size of the grain-grain interfaces), and interstitial fabric. The **flat-joint model parameters** specify the deformability and strength properties that are assigned to the grain-grain interfaces.

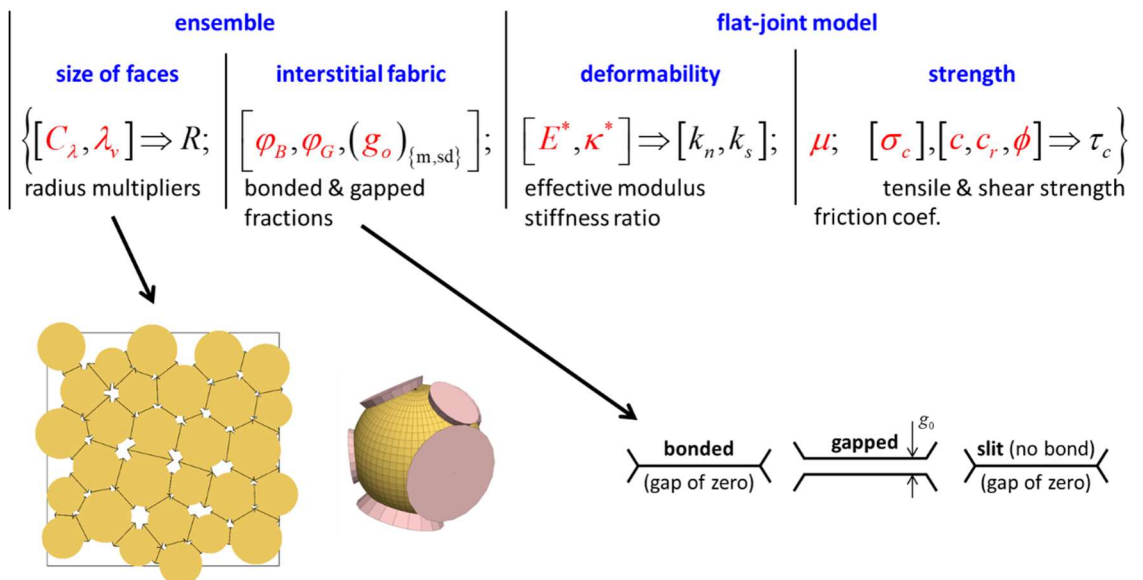


Figure 40 *Primary parameters that define a flat-jointed material.*

Table 10 Flat-Jointed Material Primary Parameters

Symbol	Name
Particle (disk/sphere)	
ρ	density
$\{D_l, D_u, \phi\}^{(j)}$	size distribution (min/max diameter, volume fraction)
Packing (linear model)	
α	local-damping factor (quasi-static conditions is 0.7)
P_m	material pressure (packing pressure)
$\{E_n^*, \kappa_n^*, \mu_n\}$	contacts during packing & after finalization
Ensemble	
χ	interaction-gap coefficient ($g_i = \chi d_{50}$)
$\{C_\lambda, \lambda_v\}$	face-sizes control
$\{\varphi_B, \varphi_G, (g_o)_{\{m, sd\}}\}$	interstitial fabric
Flat-joint model	
$\{E^*, \kappa^*, \mu\}$	effective modulus, stiffness ratio, friction coefficient
$(\sigma_c)_{\{m, sd\}}$	tensile-strength distribution
γ	cohesion to tensile strength ratio ($c = \gamma \sigma_c$)
c_r	residual cohesion
ϕ	friction angle

The full parameter set, of which the primary parameters are a subset, is given in Table 11. The properties in the flat-jointed material group are used to set the properties of the flat-joint contact model during material finalization. The properties in the linear material group are assigned to particle-particle contacts during the packing phase and to those that may form after material finalization.

The properties of the flat-jointed material group are as follows. The microstructure-tracking flag (C_{MS}) must be true to visualize the flat-jointed microstructure with the faced grain plot set. The discretization of the flat-jointed interfaces is controlled by the property set $\{N_r, N_\alpha\}$. The flat-joint contact model is installed after the packing phase at all particle-particle contacts with a contact

gap less than or equal to the interaction gap (g_i). The radius multipliers are specified such that the physical realizability of the microstructure can be controlled by the property set $\{\lambda_v, C_\lambda\}$. The interstitial fabric is defined by the property set $\{\varphi_B, \varphi_G, (g_o)_{\{m, sd\}}\}$. The normal and shear stiffnesses are set based on the deformability properties (E^* and κ^* of the **deformability** method). The remaining properties correspond directly with properties of the flat-joint contact model (ITASCA, 2026a, PFC – Contacts and Contact Models – Contact Models – Built-in Contact Models – Flat-Joint Model).

The properties of the linear material group are as follows. The linear model provides linear and dashpot components. Only the linear component is active, the reference gap is zero, and the normal-force update mode is absolute. The normal and shear stiffnesses are set based on a specified contact deformability (E_n^* and κ_n^* of the **deformability** method) and the friction coefficient is set to μ_n .

Table 11 Flat-Jointed Material Parameters

Parameter	Type	Range	Default	Description
Material microproperties are listed via <code>mpListMicroProps</code> . Common material parameters are listed in Table 1 of Potyondy (2025). Packing parameters are listed Table 9 of Potyondy (2025).				
Flat-jointed material group				
$C_{MS}, \mathbf{fjm_trackMS}$	BOOL	$\{\text{true}, \text{false}\}$	false	microstructure-tracking flag (draw microstructure with the faced grain plot set)
$N_r, \mathbf{fjm_Nr}$	INT	$[1, \infty)$	2	elements in radial direc. (2D model: total elements)
$N_\alpha, \mathbf{fjm_Na1}$	INT	$[3, \infty)$	4	elements in circumf. direc. (3D model only)
$g_i, \mathbf{fjm_igap}$	FLT	$[0, \infty)$	0	installation gap (not yet settable via λ)
$C_\lambda, \mathbf{fjm_rmulCode}$	INT	$\{0, 1, 2\}$	0	radius-multiplier code $\begin{cases} 0, \lambda \text{ constant (no PR check)} \\ 1, \lambda \text{ non-uniform reduce} \Rightarrow \text{PR} \\ 2, \lambda \text{ uniform reduce} \Rightarrow \text{PR} \end{cases}$
$\lambda_v, \mathbf{fjm_rmulVal}$	FLT	$(0, \infty)$	1.0	initial radius multiplier
$\{\varphi_B, \varphi_G\}, \mathbf{fjm_}\{\mathbf{B}, \mathbf{G}\}_\mathbf{frac}$	FLT	$[0, 1]$	NA	Bonded & gapped fractions, slit fraction $\varphi_S = 1 - \varphi_B - \varphi_G$
$(g_o)_{\{m, sd\}}, \mathbf{fjm_G_}\{\mathbf{m}, \mathbf{sd}\}$	FLT	$[0, \infty)$	$\{0, 0\}$	initial surface gap distribution

				(mean and std. deviation)
E^* , fjm_emod	FLT	$[0, \infty)$	0.0	effective modulus
κ^* , fjm_krat	FLT	$[0, \infty)$	0.0	stiffness ratio
μ , fjm_fric	FLT	$[0, \infty)$	0.0	friction coefficient
$(\sigma_c)_{\{msd\}}$	FLT	$[0, \infty)$	$\{0, 0\}$	tensile-strength dist. [stress]
fjm_ten_{m, sd}				(mean and std. deviation)
$(c)_{\{msd\}}$	FLT	$[0, \infty)$	$\{0, 0\}$	cohesion dist. [stress]
fjm_coh_{m, sd}				(mean and std. deviation)
γ				cohesion to tensile strength ratio
fjm_cohTenRatio	FLT	$[0, \infty)$	0.0	(At each contact, set $c = \gamma \sigma_c$. If $\gamma = 0.0$, then $(c)_{\{m, sd\}}$ is used.)
c_r				
fjm_cohres	FLT	$[0, \infty)$	0.0	residual cohesion [stress]
M_r , fjm_resmode	INT	$\{0, 1\}$	0	shear-drop residual mode
ϕ , fjm_fa	FLT	$[0.0, 90.0)$	0.0	friction angle [degrees]
Linear material group (for particle-particle contacts during packing that are not flat-jointed and may form after material finalization)				
E_n^* , lnm_emod	FLT	$[0.0, \infty)$	0.0	effective modulus
κ_n^* , lnm_krat	FLT	$[0.0, \infty)$	0.0	stiffness ratio
μ_n , lnm_fric	FLT	$[0.0, \infty)$	0.0	friction coefficient

+ Slit fraction: $\varphi_s = 1 - \varphi_B - \varphi_G$ ($0 \leq \varphi_s \leq 1$).

2.8.5 Microstructural Properties

A rich variety of microstructures can be produced with flat-jointed materials. The microstructural properties encompass particle shape and size distribution, faced-grain shape, and material connectivity. Such information can be compared with petrophysical properties²⁴ of the physical rock, and construction of a flat-jointed material should be informed by these properties.²⁵ Each faced-grain can be physically realizable (PR) or physically unrealizable (non-PR) as shown in Figure

²⁴ Petrology is the branch of geology that studies rocks, their mineralogy, composition, texture, structure and the conditions under which they form ("Petrology," 2026). Lithology was once approximately synonymous with petrography, but in current usage, lithology focuses on macroscopic hand-sample or outcrop-scale description of rocks while petrography is the specialty that deals with microscopic details.

²⁵ Rock microstructure is described by Vernon (2018) who focuses on interpreting microscopic thin sections of rocks. The book contains hundreds of excellent thin-section images at length scales ranging from 1 to 10 mm.

25, and if all faced-grains have the same realizability, then the material is said to be PR or non-PR as shown in Figure 26. The material can be minimally, maximally, or overly connected (see Figures 29 and 31). The microstructural properties are described by the following properties (average face coordination number; average cover ratio; and total, bonded, and frictional specific surface areas) that are measured for all faced grains whose centroids lie within a microstructural box (defined as a parallelepiped-shaped region).

The **average face coordination number** (average number of faces per grain) is

$$Z = \frac{\sum_{g=1}^{N_g} n_f^{(g)}}{N_g} \quad (3)$$

where N_g is the number of grains whose centroids lie within the microstructural box, and $n_f^{(g)}$ is the number of faces of grain g . The average face coordination number describes the tightness of the grain packing with larger Z corresponding with tighter packing, and thus larger macroscopic modulus and strength. The average coordination number defined in terms of average number of contacts per particle is used to understand the macroscopic behavior of granular materials (Wang et al., 2026). It is expected that the average face coordination number will help us to better understand the macroscopic behavior of flat-jointed materials.

The cover ratio (surface area of faces over surface area of core) of a single grain is

$$C_r = \frac{\sum_{f=1}^{n_f} A^{(f)}}{A_c}, \quad A_c = \begin{cases} 2\pi r, & 2D \\ 4\pi r^2, & 3D \end{cases}, \quad r : \text{core radius} \quad (4)$$

where N_g is the number of grains whose centroids lie within the microstructural box, and $C_r^{(g)}$ is the cover ratio of grain g . The **average cover ratio** describes how well the faces cover the grain surfaces. The relation between $\bar{C}_r$ and macroscopic properties remains to be explored.

The flat-jointed material consists of rigid grains with all deformation and damage occurring at the grain-grain interfaces, each of which has two opposing faces that are discretized into elements. Damage consists of bond breakage and frictional sliding at unbonded (either initially or after a bond breaks) elements. The interface area per unit volume is called the specific surface area (SSA). The **total specific surface area** (S) is the sum of the **bonded specific surface area** (S_b) and the **frictional specific surface area** (S_f) via

$$S = \frac{\sum_{g=1}^{N_g} \sum_{f=1}^{n_f^{(g)}} A^{(f,g)}}{V}, \quad S_b = \frac{\sum_{g=1}^{N_g} \sum_{f=1}^{n_f^{(g)}} A_b^{(f,g)}}{V}, \quad S_f = S - S_b \quad (5)$$

where V is the volume of the microstructural box, N_g is the number of grains whose centroids lie within the microstructural box, $n_f^{(g)}$ is the number of faces of grain g , $A^{(f,g)}$ is the total area of face f of grain g , and $A_b^{(f,g)}$ is the bonded area of face f of grain g . These properties characterize the initial microstructure (solid material) and the damage evolution whereby S_b decreases and S_f increases until all bonds have broken to obtain a granular material. The relation between the SSA property set $\{S, S_b, S_f\}$ and macroscopic properties remains to be explored.

The microstructural properties of the flat-jointed material that are described in this subsection have not yet been implemented in the material-modeling support package.

2.9 User-Defined Material

A user-defined material is a granular assembly in which a user-defined contact model exists at all grain-grain contacts. The user-defined contact model is referred to in commands and FISH by the contact-model name (N_{cm} in Table 1) and is provided as a dynamic link library (DLL) file that is loaded into PFC at runtime. The user-defined material example creates a 3D Hill material (Potyondy, 2021; Potyondy et al., 2016; Siekmeier et al., 2016) that uses the Hill contact model by specifying the contact-model name as **hill**. The user-defined material is defined by a set of parameters that are used to set the relevant properties of the contact model during material genesis and subsequent modeling — the properties are specified in the redefinition of the **ft_setMatBehavior** FISH function. The following additional FISH functions must also be provided for a user-defined material: **udm_checkParams**, **udm_listProps**, **udm_computeMicroStrucProps**, and **udm_listMicroStrucProps**. Refer to the user-defined material example for more information about how to create a user-defined material.

2.10 Smooth-Jointed Interface

A smooth-jointed interface can be inserted into the bonded materials by identifying the contacts near the interface and replacing their contact models with the smooth-joint contact model. New grain-grain contacts that may form during subsequent motion are assigned the linear contact model, except for the new contacts associated with the interface, which are assigned the smooth-joint contact model and aligned with the interface direction. This capability is not provided in the material-modeling support package, but it is relatively straightforward to perform this operation as described in ITASCA (2026a).²⁶ This capability has been used to create grain-based models (Potyondy, 2010; Zhou et al., 2019).

²⁶ In documentation set at PFC – Examples – Tutorials – Slip on a Fault.

3.0 MICROSTRUCTURAL MONITORING

The macroscopic behavior of the synthetic material arises from the evolution of the microstructural features. Microstructural monitoring includes computation of quantitative microstructural properties, microstructural plot sets, and crack monitoring for bonded materials. These items are described in the following three subsections.

3.1 Microstructural Properties

The microstructural properties of the material are computed and listed by `mpListMicroStrucProps` and include the following items.²⁷

- **Grain Size and Packing Information.** Number of grains in the model, grain-size distribution (discussed below), average and median grain diameters, vessel resolutions wrt the average and median grain diameters,²⁸ measurement-based porosity (defined in Section 5.1), and overlap ratios.²⁹
- **Contact Information.** The number of active linear-based contacts along with the number of such contacts that are grain-grain and grain-wall.
- **Bonded-Material Information.** The bonded materials provide this information. Bond coordination number (c_b).³⁰ Number of contact-bonded bonds, parallel-bonded bonds, soft-bonded bonds, flat-jointed contacts, flat-jointed elements, and flat-jointed bonds. The initial microstructural types of the flat-jointed material (defined in Section **Error! Reference source not found.**).
- **User-Defined Material Information.** A user-defined material may provide this information via `udm_{compute,list}MicroStrucProps`.

3.2 Microstructural Plot Sets

Microstructural plot sets are provided for the bonded materials to display the material microstructure and thereby reveal how the evolution of the microstructure influences the macroscopic behavior. The microstructural plot sets include depictions of the grains and the grain-grain interfaces, and when used with the crack-monitoring package, include the interface damage in the form of bond breakages.

²⁷ Additional microstructural properties of the flat-jointed material are described in Section 2.8.5.

²⁸ Vessel resolution is defined as the number of grains across the minimum vessel dimension.

²⁹ The overlap ratios (ORs) of all active contacts are computed, and the maximum, minimum and average values are returned. The OR is the overlap divided by the piece diameter. For grain-grain contacts, there are two ORs, while for grain-wall contacts, there is one OR.

³⁰ The bond coordination number is defined for the bonded materials as the average number of intact bonds per grain.

A plot set is defined as a plot in which the plot information is stored as a geometry set and displayed by the geometry set plot item by specifying: {ColorBy: Set}, and {Sets: <geometry set name>}. The microstructural plot set capability is activated via **msOn**, the plot sets are regenerated at a specified rate (**msUpdateRate**) during cycling, and the regeneration can be forced to occur via **msForceUpdate**. An axis-aligned microstructural box (defined by **msBoxDefine**) is associated with the microstructural plot sets. The box is displayed by the geometry set plot item by specifying: {ColorBy: Set}, and {Sets: msBox}. The grains with centers inside the box can be displayed with either: (a) the ball and clump plot items by specifying: {Color By: Text Val: msBox}, or (b) the grain and faced grain plot sets. The contact-based plot sets display only the entities joining the grains in the box. The faced grain plot set displays only the faces joining grains with centers inside the box. The following microstructural plot sets are available: grains, contact bonds, pbond interfaces, pbond cement, FJ interfaces, faced grains and cracks (see Figures 41 to 44).

Grains. The bonded materials mimic the microstructure of rigid ball- or clump-shaped grains cemented with either spot welds (contact-bonded material) or epoxy (parallel- and soft-bonded materials). The grain plot set (geometry set name: **"grains"**) displays each grain as a sphere — only ball-shaped grains are displayed, clump-shaped grains are not supported. The sphere is centered at the ball location and has radius equal to the scale factor (**msGN_sfRad**) times the ball radius. For the 2D model, the grains are displayed as circles.

Contact bonds. A contact-bonded material mimics the microstructure of rigid grains cemented with spot welds. The contact bond plot set (geometry set name: **"contact bonds"**) displays each intact grain-grain contact bond as a line. The line is centered at the contact location and has length equal to the scale factor (**msCB_sfLen**) times the distance between the centers of the two contacting pieces.

Parallel bonds. A parallel-bonded material mimics the microstructure of rigid grains cemented with epoxy. There are two plots sets. The first plot set depicts the parallel bond as an interface, while the second plot set depicts the parallel bond as cement.

The parallel-bond interfaces plot set (geometry set name: **"pbond interfaces"**) displays each intact grain-grain parallel bond as a disk with radius equal to the scale factor (α , **msPBi_sfRad**) times the parallel-bond radius ($\bar{R}$). The disk is centered at the contact location and lies on the contact plane. For the 2D model, the parallel-bond interfaces are displayed as lines (of length $2\alpha\bar{R}$, and unit-thickness depth).

The parallel-bond cement plot set (geometry set name: **"pbond cement"**) displays each intact grain-grain parallel bond as a cylinder with radius equal to the scale factor (α , **msPBc_sfRad**) times the parallel-bond radius ($\bar{R}$). The cylinder is centered at the contact location and has a length (L) equal to the scale factor (**msPBc_sfLen**) times the distance between the centers of the two contacting pieces. For the 2D model, the

parallel-bond cement is displayed as a thick line (of length L , thickness $2\alpha \bar{R}$, and unit-thickness depth).

Soft bonds. A soft-bonded material mimics the microstructure of rigid grains cemented with epoxy that may soften after reaching its tensile strength. There is one plot set that depicts the soft bond as an interface.

The soft-bond interfaces plot set (geometry set name: **"sbond interfaces"**) displays each grain-grain soft bond as a disk with radius equal to the scale factor (α , **msSBi_sfRad**) times the soft-bond radius (R). The disk is centered at the contact location and lies on the contact plane. For the 2D model, the interfaces are displayed as lines (of length $2\alpha R$, and unit-thickness depth). The state of the interface is based on the value of the soft-bond property **sb_state** and can be displayed by the geometry plot item by specifying {Label: Group} and {Model Sets: sbond interfaces}, with {Color-List:} used to turn each type of interface on/off and specify its color.

Flat-Jointed Material. A flat-jointed material mimics the microstructure of rigid faced grains with bonded and frictional interfaces. There are two plots sets. The first plot set depicts the interfaces, while the second plot set depicts the faced grains.

The flat-joint interfaces plot set (geometry set name: **"FJ interfaces"**) displays the interface of each grain-grain flat-jointed contact. The interface, coordinate systems and discretization can be displayed by the geometry set plot item by specifying {Label: Group} and {Model Sets: FJ interfaces}, with {Color-List:} used to turn each entity on/off and specify its color. The visualization scheme for each entity is as follows.

- a. **Interface** (group 'interface'). The interface is drawn as a disk with radius equal to the scale factor (α , **msFJi_sfRad**) times the flat-joint radius (R). The disk is centered at the contact location and lies on the contact plane. For the 2D model, the flat-joint interfaces are displayed as lines (of length $2\alpha R$, and unit-thickness depth).
- b. **Coordinate systems** (groups 's-tSys' and 'xi-etaSys'). The two coordinate systems associated with the interface (nst) and ($n\xi\eta$) are drawn as lines from interface center extending just beyond the interface edge, with the lines in the s and ξ directions being shorter than the lines in the t and S directions. For the 2D model, the group is 'n-tSys', and only the n and t directions of the nst coordinate system are drawn.
- c. **Discretization** (group 'elements'). The interface discretization shows elements and centroid locations. The outline of each element is drawn as a set of edges, and there is a short line (aligned with the s direction) at each element centroid. For the

2D model, each element is outlined by edges oriented perpendicular to the interface, with a shorter perpendicular line at each element centroid.

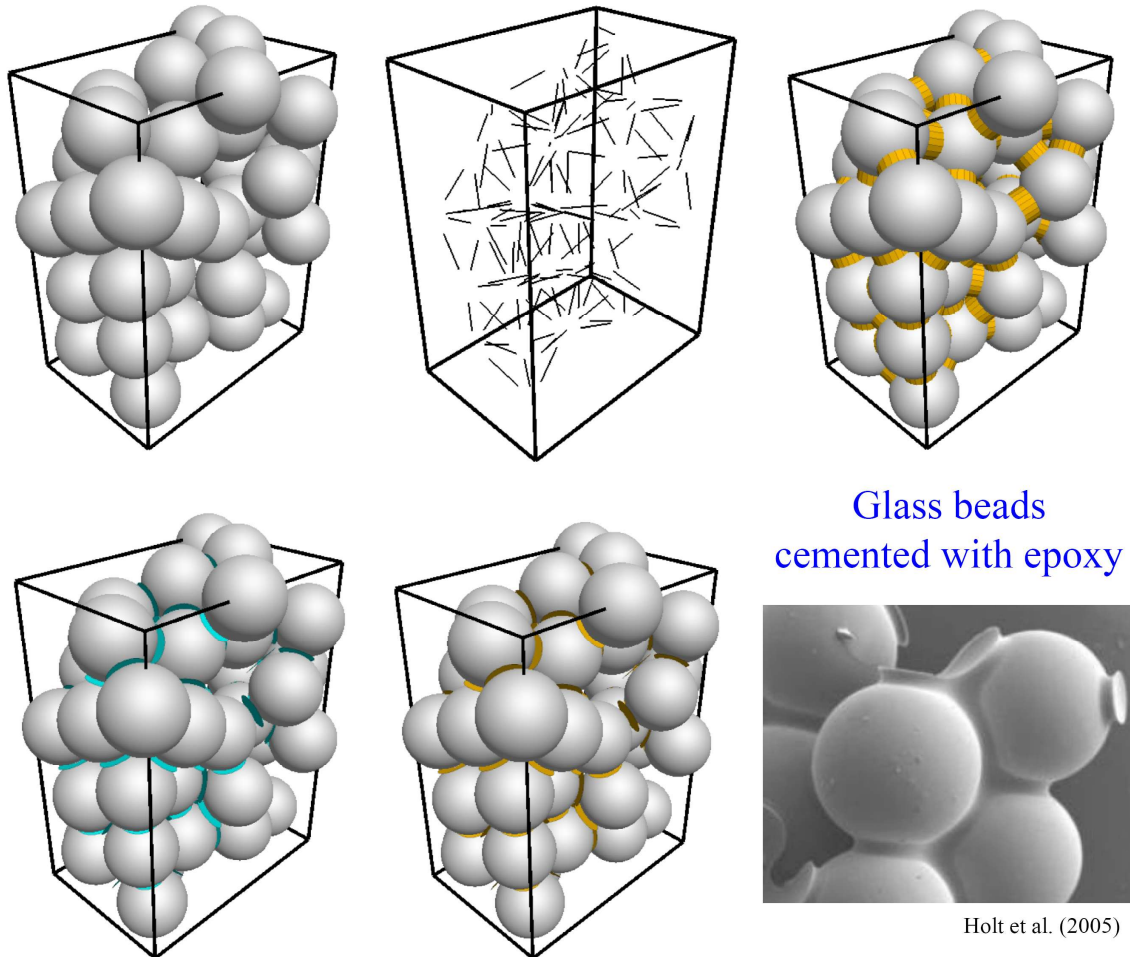


Figure 41 *Microstructural plot sets for bonded materials with the same initial packing showing (clockwise from upper left): microstructural box and grains in the box (grey); contact-bonded material with contact bonds in the box; parallel-bonded material with parallel-bond cement (gold, 50% size) and parallel-bond interfaces (gold, 50% size); and flat-jointed material with flat-jointed interfaces (blue, 50% size).*

The faced grain plot set (geometry set name: **“faced grains”**) displays each grain of a flat-jointed material as a faced grain — only ball-shaped grains are displayed, clump-shaped grains are not supported (see Figure 42). To draw faced grains, the microstructure-tracking flag (C_{MS} in **Error! Reference source not found.**) must be set to true. The faced grains are created when the flat-joint model is installed at the ball-ball contacts of a packed ball assembly such that each face remains rigidly connected to its corresponding grain during subsequent motion. The faced grain is drawn as a spherical core with a skirted face at the associated notional surface of each flat-jointed contact. The core and skirted faces of each

grain can be displayed by the geometry set plot item by specifying {Label: Group}, {Slot: 1} and {Model Sets: faced grains}, with {Color-List:} used to turn each entity on/off and specify its color. For the 2D model, two geometry set plot items should be used. The first geometry set plot item turns on the entities 'core' and 'grain in skirt', with {Edges: Off}, {Polygons: checked} and {Polygons: Polygons: Outline: unchecked}. The second geometry set plot item turns on the entity 'skirted face', with {Edges: On} and {Polygons: unchecked}. The visualization scheme for each entity is as follows.

- a. **Core** (group 'core'). The core is drawn as a sphere with radius equal to the minimum of all facet radial distances. For the 2D model, the core is drawn as a circle.
- b. **Skirted Face** (group 'skirted face', also 'grain in skirt' for the 2D model). The skirted face is drawn as a disk (line for the 2D model) surrounded by a skirt that extends toward the core center until it intersects the core surface.

The faced grain plot set displays only the faces joining grains with centers inside the microstructural box. This behavior can be modified by specifying the ID number of a seed grain (via **msFG_seedID**), and the number of grains connected directly to the seed grain (via **msFG_seedNum**) that should also be drawn.

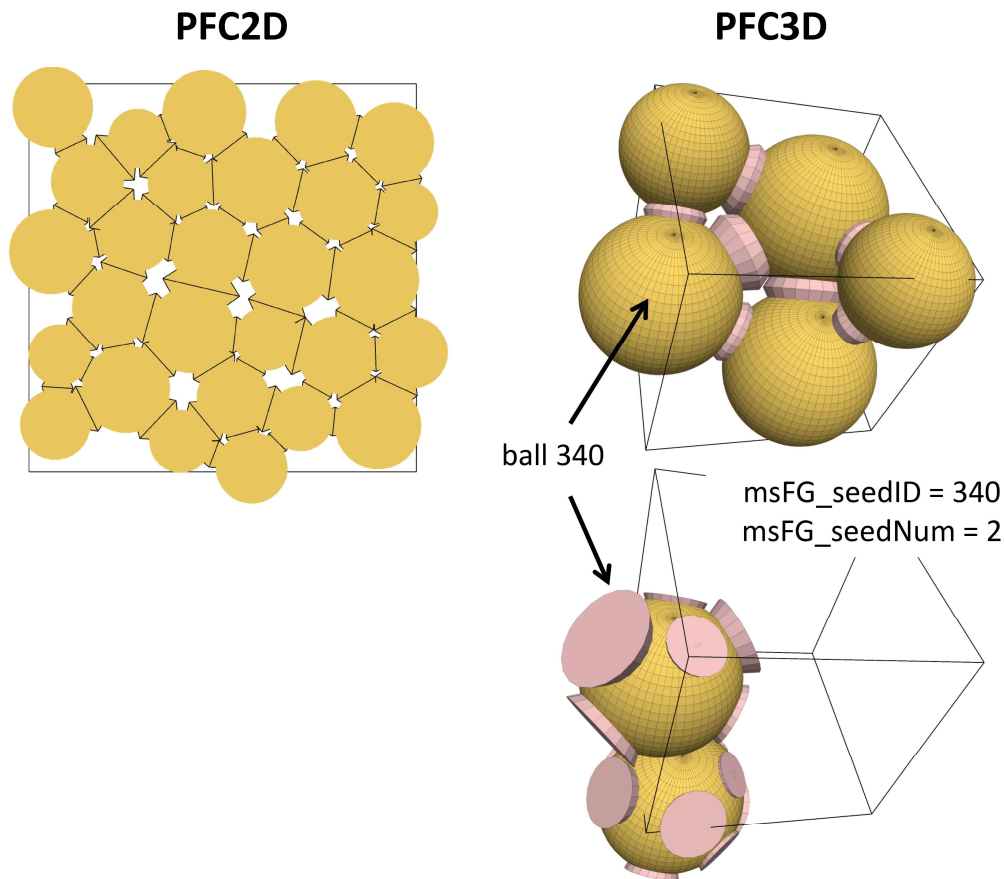


Figure 42 *Faced grain plot set showing faced grains in the microstructural box (top) and connected to a seed grain (bottom).*

Cracks. Damage in the bonded materials consists of bond breakages which we denote as cracks. Cracks are stored and visualized by the crack-monitoring package (see Section 3.3). The crack plot set (geometry set name: “**cracks**”) displays the cracks with thickness proportional to gap. The cracks and gap are taken from the crack-monitoring package. Cracks are drawn as thick disks for the 3D model, and thick lines of unit-thickness depth for the 2D model. The crack size is taken as the scale factor (**msCK_sfacSize**) times the size returned by the crack-monitoring package. The cracks can be displayed by the geometry set plot item by specifying {Label: Group}, {Model Sets: cracks}, and {Polygons: checked}, with {Color-List:} used to turn each entity (crack type and failure mode) on/off and specify its color. Filtered cracks can be displayed by setting **msCK_ckFilter** to true. Ghost cracks, defined as the cracks for which the originating contact no longer exists, are not displayed. Only grain-grain cracks with both parent grains inside of the microstructural box are drawn.

Crack thickness is equal to the true gap, with the restriction that the thickness lies in the range $[t_{\min}, t_{\max}]$ where $t_{\min} = \alpha_1 \tilde{s}$, $t_{\max} = \alpha_2 \tilde{s}$; α_1 and α_2 (**msCK_sfacMinThick** and

msCK_sf and **msCK_sfacMaxThick** are scale factors, and $\bar{s}$ is the average size of all displayed cracks. To draw all cracks with thickness equal to the positive gap (and minimum thickness for cracks with negative gap), set **sCK_sf** = **1e20** (the default value). Examples of the 2D and 3D crack plot sets are shown in Figures 43 and 44.

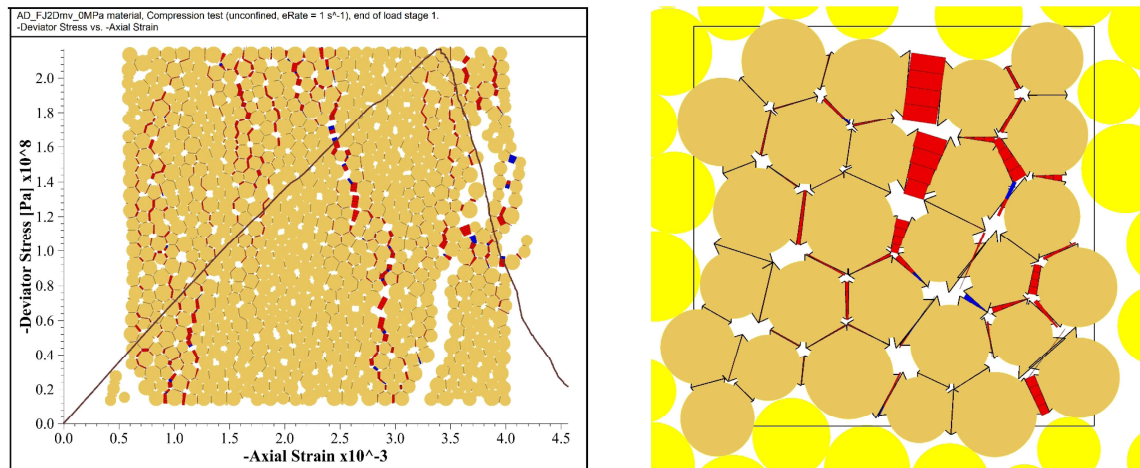


Figure 43 Crack and faced grain plot sets in 2D showing cracks, with crack thickness equal to gap, and cracks colored red/blue for tensile/shear failure. 2D flat-jointed material at end of UCS test as the specimen exhibits axial splitting.

The right-most grain was moved to the right until all 16 flat-joint elements broke in tension. Then the inner grain was rotated causing the unbroken faces to break in shear.

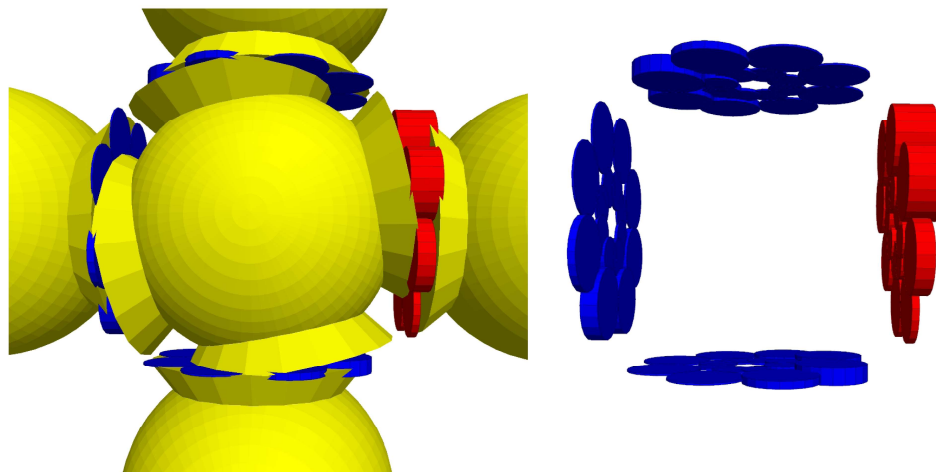


Figure 44 Crack and faced grain plot sets in 3D showing cracks, with crack thickness equal to gap, and cracks colored red/blue for tensile/shear failure.

3.3 Crack Monitoring

Damage in the bonded materials consists of bond breakages, which we denote as cracks. Each crack has: type (contact bonded, parallel bonded, soft bonded,³¹ flat jointed or smooth jointed); failure mode (tensile or shear); geometric information (size, position, normal direction and gap); step number at which it formed; and orphan indicator. The numbers of all cracks (partitioned by type and failure mode) are returned by the **ck_nX** functions. Crack data is stored as a Discrete Fracture Network (DFN). The Fracture plot item supports visualization of the cracks.³² Crack filtering occurs by calling the FISH function **ckFilter(g)**, which selects cracks with a gap less or greater than *g* (based on the value of **ckFilterOpen**). The **ckFilter** function can be redefined to provide a user-defined filtering criterion. The Fracture plot item displays cracks by specifying: {Shape: Fracture}, {Color By: Text Val: group (slot 1 or 2, for all or filtered cracks, respectively)}, and {Color Opt: Color-List: select on/off and color for each type and failure mode}. The size of the displayed cracks is scaled by the shrink factor in the Shape attribute of the Fracture plot item: {Shape: Shrink Factor}.

Geometric Information:

A crack is a disk for the 3D model and a linear segment of unit-thickness depth for the 2D model. A crack has a size (diameter for the 3D model and length for the 2D model), position, normal direction and gap.

- The size is set at creation and then frozen. The size for each type of crack is:
 - contact-bonded crack: two times the radius of the deformability method.
 - parallel-bonded crack: two times the parallel-bond radius.
 - soft-bonded crack: two times the soft-bond radius
 - flat-jointed crack: two times the element radius (which is the radius giving the same area as the element), or the element length (for the 2D model).
 - smooth-jointed crack: two times the smooth-joint radius.
- The position, normal direction and gap are updated to correspond with material motion after bond breakage (see **ckForceUpdate**). If the originating contact exists, then these quantities are obtained from the contact and its associated contact model as described below. If the originating contact no longer exists, then these quantities are set equal to the contact-plane location, contact-plane normal direction and contact gap, respectively, that would be assigned to a contact between the two parent pieces.³³ However, if at least one

³¹ Only soft bonds that have broken (**sb_state** = 1 or 2) are defined as cracks. Use the microstructural plot set {**sbond interfaces**} to display all grain-grain soft-bonded contacts as interfaces that can be turned on/off and colored by the value of **sb_state**.

³² The cracks displayed by the Fracture plot item have zero thickness. The microstructural plot set "cracks" displays cracks with thickness proportional to gap.

³³ The three geometric quantities are given by Eq. (2) in ITASCA (2026a, PFC – Contacts and Contact Models – Contact Resolution).

of the parent pieces no longer exists, then these quantities are frozen at their last updated values, and such cracks are called orphans. The crack position is given by

$$\mathbf{x} = \begin{cases} \mathbf{x}^{(e)}, & \text{flat-jointed crack} \\ \mathbf{x}_c, & \text{otherwise} \end{cases} \quad (6)$$

where $\mathbf{x}^{(e)}$ is the centroid location of element (e) , and $\mathbf{x}_c$ is the contact-plane location. The crack normal direction is given by

$$\hat{\mathbf{n}} = \begin{cases} \hat{\mathbf{n}}_j, & \text{smooth-jointed crack} \\ \hat{\mathbf{n}}_c, & \text{otherwise} \end{cases} \quad (7)$$

where $\hat{\mathbf{n}}_j$ is the joint normal direction, and $\hat{\mathbf{n}}_c$ is the contact-plane normal direction. The crack gap is given by

$$g = \begin{cases} g_s = g_c - g_r, & \text{contact-, parallel- or soft-bonded crack} \\ g^{(e)}, & \text{flat-jointed crack} \\ g_j, & \text{smooth-jointed crack} \end{cases} \quad (8)$$

where g_s is the surface gap, g_c is the contact gap, g_r is the reference gap, $g^{(e)}$ is the gap at the centroid of element (e) , and g_j is the joint gap.

Global Functions:

- **ckInit**, **ckOn**, **ckOff**, **ckForceUpdate**, **ckListData**, **ck_nOrphans**, **ck_nFiltered**. The crack-monitoring package is initialized and turned on by calling **ckInit**. If the package is reinitialized, then crack data is reset. The package is activated by **ckOn**, and deactivated by **ckOff**. Cracks are only monitored when the package is on. The crack data can be listed to the screen by **ckListData**.

Global Variables:

- **ck_nAll**, **ck_n{CB,PB,SB,FJ,SJ}{t,s}** : crack counts (used with history logic to monitor cracking during a simulation)
- **ckUpdateRate** : crack geometry update rate (number of cycles)
- **ckFilterGap** : display cracks with gap less (**ckFilterOpen** = 0) or greater (**ckFilterOpen** # 0) than this value (used by **ckFilter**)
- **ckFilterOpen** : see **ckFilterGap**

Crack Data (stored for each crack, which is a DFN fracture):

- The size, position and normal direction are stored as DFN data.

- **group (slot 1)** : name indicating type & failure mode (**{CB,PB,SB,FJ,SJ}** - **{ten,shear}Fail**) of all cracks
group (slot 2) : name indicating type, failure mode and gap-based filtering criterion (**{CB,PB,SB,FJ,SJ}** - **{ten,shear}Fail (gap < [ckFilterGap])**) of filtered cracks
- **extra 1** : originating contact
extra 2 : originating element (for flat-jointed cracks only)
extra 3 : parent piece-1 (ball or pebble)
extra 4 : parent piece-2 (ball, pebble or facet)
extra 5 : gap
extra 6 : step number at which the crack formed
extra 7 : orphan indicator (1: orphaned crack, 0: not an orphaned crack)

4.0 MATERIAL GENESIS

Material behavior is embodied in the contact model at the grain-grain contacts. The material-genesis procedure creates granular (linear and Hill) and bonded (contact-bonded, parallel-bonded, soft-bonded, and flat-jointed) materials. The materials consist of a homogeneous, isotropic and well-connected grain assembly with a specified non-zero material pressure.³⁴ Material genesis occurs within a material vessel that may be either a physical vessel or a periodic space. Materials formed in a physical vessel may be removed from the vessel for subsequent boundary-value modeling, while materials formed in periodic space may also have an installed stress state and are converted into a periodic brick, and then assembled into a specimen for subsequent boundary-value modeling.³⁵ The boundary-value modeling may involve trimming the material into a desired shape and applying boundary conditions. The material vessels are described in the first subsection. The material-genesis procedure is described in the second subsection.

4.1 Material Vessels

Material genesis occurs within a material vessel that may be either a physical vessel or a periodic space. The physical vessels include polyaxial, cylindrical and spherical cells (see Figure 45). A polyaxial cell consists of planar walls that form a rectangular cuboid (for which each pair of adjacent faces meets in a right angle). A cylindrical cell consists of two planar walls and a cylinder wall. A spherical cell consists of a sphere wall. Walls of the physical vessels are expanded to prevent grains from escaping if the walls are moved outwards during subsequent compression testing — the wall-wall overlap is ignored, because walls interact only with grains. For materials formed in periodic space, the periodic cell is a rectangular cuboid (see Figure 46). A stress state that has no shear components and does not vary with position can be installed into the finalized periodic assembly (after bonding) by deforming the periodic space ($C_s=1$) using a subset of the more general scheme of ITASCA (2008a&b, Section 3.9 Stress-Installation Procedure, in the *FISH in PFC3D/2D* volumes).³⁶ Three spherical measurement regions are placed symmetrically along the axis of the largest vessel dimension (with a spanning length of α_l times the largest vessel dimension, and with a diameter of α_d times the smallest vessel dimension). For materials formed in a physical vessel, the linear contact model is installed at the grain-wall contacts. The walls are frictionless, and grain-wall contact stiffness is set based on a specified contact deformability (E^* of the **deformability** method of the linear model). The material vessel parameters are listed in Table 12.

³⁴ A packing procedure that mimics the physical packing process of air pluviation to produce a particle assembly with a gravity-induced density gradient is implemented in Potyondy (2025a, 2025b).

³⁵ The brick is assembled into a specimen by calling **Assemble.p{2,3}dvr** from the **MatGen** project.

³⁶ The deformation occurs such that the difference between the current and target stresses is reduced by approximately one half during each step.

Table 12 Material-Vessel Parameters

Parameter, FISH	Type	Range	Default	Description
Material-vessel properties (including current vessel dimensions) are listed via <code>@mvListProps</code> .				
$T_v, \text{mv_type}$	INT	$\{0,1\}$	0	vessel-type code $\begin{cases} 0, \text{ physical} \\ 1, \text{ periodic} \end{cases}$
$S_v, \text{mv_shape}$	INT	$\{0,1,2\}$	0	vessel-shape code $\begin{cases} 0, \text{ rectangular cuboid} \\ 1, \text{ cylinder} \\ 2, \text{ sphere} \end{cases}$ (2D model: $S_v \equiv 0$)
$\{H,W,D\}, \text{mv}_{\{H,W,D\}}$	FLT	$(0.0,\infty)$	NA	height, width and depth (sphere diameter is H ; 2D model: $D \equiv 1$, see Figure 45)
$C_s, \text{mv_Sinstall}$	INT	$\{0,1\}$	0	stress-installation code $\begin{cases} 0, \text{ do not install stress} \\ 1, \text{ install stress} \end{cases}$
$\{\sigma_{xx}, \sigma_{yy}, \sigma_{zz}\}, \text{mv_S}\{x,y,z\}$	FLT	$(-\infty,\infty)$	NA	installation stresses ($T_v = 1$ and $C_s = 1$)
$\varepsilon_s, \text{mv_Stol}$	FLT	$(0.0,\infty)$	1×10^{-2}	stress tolerance $\left(\left \frac{\sigma_{ii} - \sigma_{ii}^t}{\sigma_{ii}^t} \right \leq \varepsilon_s \right), i=1,2,3$
$E, \text{mv_Semod}$	FLT	$(0.0,\infty)$	NA	where σ_{ii} is current stress ensemble modulus $\left(\dot{\varepsilon}_{ii} = \frac{1}{2E\Delta t} (\sigma_{ii} - \sigma_{ii}^t) \right)$
$\varepsilon_{\text{lim}}, \text{mv_SARatLimit}$	FLT	$(0.0,\infty)$	1×10^{-5}	equilibrium-ratio limit (parameter of <code>ft_eq</code>)
$\alpha, \text{mv_expandFac}$	FLT	$[1.0,\infty)$	1.2	expansion factor of physical vessel
$\{\alpha_l, \alpha_d\}, \text{mv_inset}\{L,D\}\text{Fac}$	FLT	$(0.0,1.0]$	$\{0.8, 0.8\}$	inset factors of measurement regions
$E_v^*, \text{mv_emod}$	FLT	$(0.0,\infty)$	NA	effective modulus of physical vessel

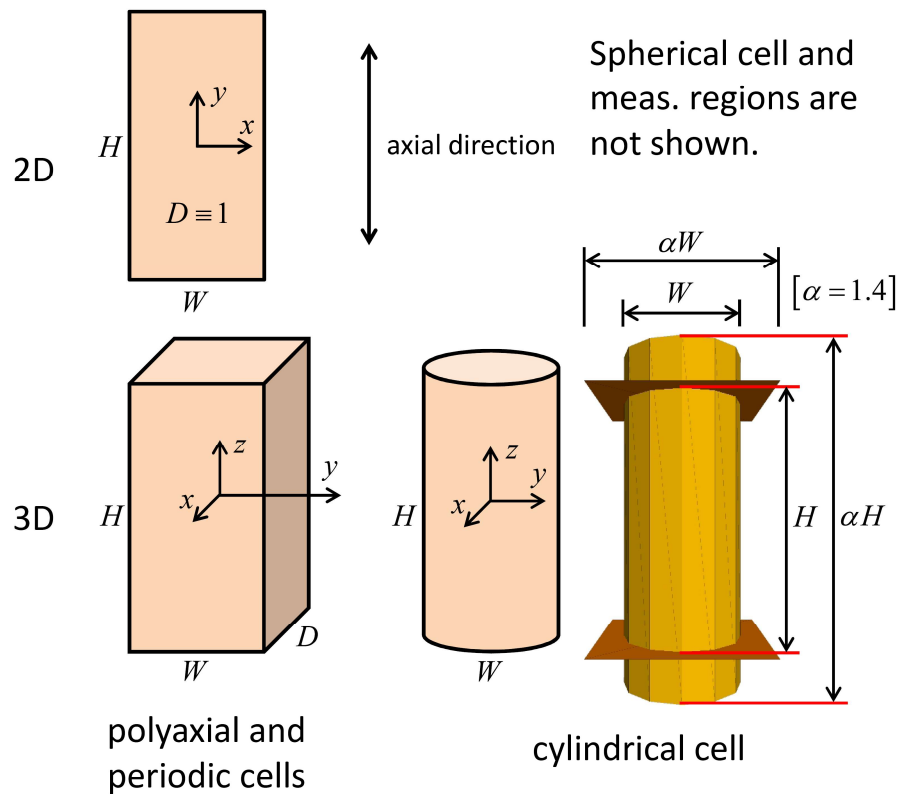


Figure 45 *Material vessels with global coordinate system centered in each cell and associated axial direction.*

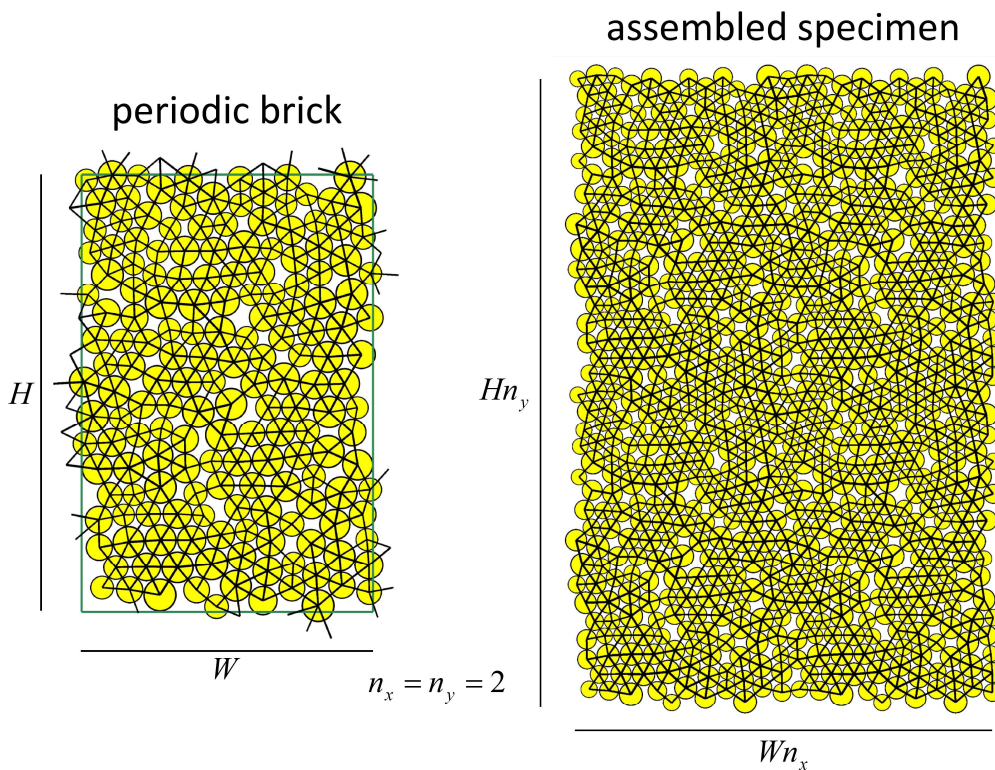


Figure 46 *Packed particle ensemble in periodic material vessel (left) and assembled into a larger geometric shape (right), with contacts shown as black lines.*

4.2 Material-Genesis Procedure

The material-genesis procedure occurs within the material vessel and produces a specimen consisting of a homogeneous, isotropic and well-connected grain assembly with a specified non-zero material pressure. The material-genesis procedure consists of a packing phase followed by a finalization phase. During the packing phase, the grain assembly is subjected to a specified packing procedure. During the finalization phase, the final material properties are assigned to the grain-grain contacts, and additional material properties are specified that will be assigned to new contacts that may form during subsequent motion. The two phases are described in the following two subsections.

4.2.1 Packing Phase

During the packing phase, the grain assembly is subjected to a specified packing procedure during which the effective behavior at all grain-grain contacts is that of either the linear contact model or a user-defined contact model. For the linear model, the properties are deformability (`lnm_emod` and `lnm_krat`); for the user-defined model, the properties are specified in the redefined `ft_setMatBehavior` FISH function. The friction coefficient is a packing parameter (either zero or μ_{CA} in Table 13).

The packing procedures include boundary contraction and grain scaling. Boundary contraction is available only for the physical material vessel, while grain scaling is available for both the physical and periodic material vessels. The boundary-contraction procedure produces a dense or loose packing of a granular material, while the grain-scaling procedure produces a dense packing of a granular material that will subsequently become a bonded material during the material-finalization phase. Both procedures generate a cloud of grains and allow them to rearrange into a packed state under conditions of zero friction. The desired material pressure is obtained differently for each procedure. For the boundary-contraction procedure, confinement is applied by moving the vessel walls under control of the servomechanism described in Section 5.3, whereas for the grain-scaling procedure, the grain sizes are scaled iteratively to modify the mean stress of the assembly. For the boundary-contraction procedure, the material friction coefficient is chosen during confinement application to achieve a dense or loose packing, whereas for the grain-scaling procedure, the material friction coefficient remains equal to zero throughout the entire packing process to achieve a dense packing. The packing parameters are listed in Table 13. A series of material instances can be created with the same statistical properties but different packing arrangements by varying the seed of the random-number generator.

Table 13 Packing Parameters

Parameter	Type	Range	Default	Description
S_{RN} , pk_seed	INT	$S_{RN} \geq 10,000$	10,000	seed of random-number generator (affects packing)
P_m , pk_Pm	FLT	$(0.0, \infty)$	NA	material pressure
ε_p , pk_PTo1	FLT	$(0.0, \infty)$	1×10^{-2}	pressure tolerance $\left(\frac{ P - P_m }{P_m} \leq \varepsilon_p \right)$ where P is current pressure
ε_{lim} , pk_ARatLimit	FLT	$(0.0, \infty)$	8×10^{-3}	equilibrium-ratio limit (parameter of ft_eq)
n_{lim} , pk_stepLimit	INT	$[1, \infty)$	2×10^6	step limit (parameter of ft_eq)
C_p , pk_procCode	INT	$\{0, 1\}$	0	packing-procedure code $\begin{cases} 0, & \text{boundary contraction} \\ 1, & \text{grain scaling} \end{cases}$
η_t , pk_nc	FLT	$(0.0, 1.0)$	$\begin{cases} \begin{cases} 0.58, & 3D \\ 0.25, & 2D \end{cases}, & C_p = 0 \\ \begin{cases} 0.35, & 3D \\ 0.08, & 2D \end{cases}, & C_p = 1 \end{cases}$	grain-cloud porosity
Boundary-contraction group ($C_p = 0$):				

μ_{CA} , pk_fricCA	FLT	$[0.0, \infty)$	0.0	material friction coefficient during confinement application
v_{lim} , pk_vLimit	FLT	$(0.0, \infty)$	NA	servo velocity limit (see Table 15)

Static-equilibrium is determined by successful return from the **ft_eq** FISH function.

- **ft_eq**(ε_{lim} , n_{lim}) cycles the model until a state of static equilibrium is obtained. Cycling continues until the mechanical ratio-average (ε_{arat}) falls below the equilibrium-ratio limit (ε_{lim}):

$$\varepsilon_{arat} \leq \varepsilon_{lim} \quad [\text{command: model solve ratio-average } \varepsilon_{lim}]$$

or the number of steps (n_s) exceeds the step limit (n_{lim}):

$$n_s > n_{lim} \quad [\text{command: model solve cycles } n_{lim}]$$

The ratio-average is defined via Eq. **Error! Reference source not found..**

The boundary-contraction procedure is adapted from McDowell et al. (2006) and consists of the following three steps (see Figure 47).

1. Generate a cloud of grains with porosity of n_c . This porosity does not account for overlaps: $n_c = (V_v - V_g)/V_g$, where V_v is the volume of the material vessel and V_g is the total volume of grains. The grains are drawn from the specified size distribution, and then placed at arbitrarily chosen positions that lie fully within the material vessel such that there may be large grain-grain overlaps. Typically, n_c is chosen equal to n_l , where n_l corresponds with the loose state for which grains are just in contact at zero mean stress. For a linear material of equal-sized spheres, $n_l = 0.58$. For a linear material of equal-sized disks, $n_l = 0.25$.
2. Set the material friction coefficient to zero, and then allow the grains to rearrange until either the mean stress is near zero (within 0.1% of P_m) or static-equilibrium is obtained.³⁷ This step eliminates the large overlaps and should provide an isotropic state.

³⁷ During the first set of cycles, the model is calmed (by setting all grain translational and rotational velocities to zero) every five steps, and the calming continues until the maximum overlap ratio (defined at the active contacts as the contact gap divided by the piece diameter) is small (less than **_pkORmaxLimit**, which defaults to 0.25). The calming process prevents most grains from passing through the walls of the material vessel; those grains with centers lying outside of the material vessel at the end of step 2 are deleted, and for clumped materials, those pebbles with centers lying outside of the material vessel are also deleted.

- Set the material friction coefficient to μ_{C4} , and then apply confinement of P_m . The confinement is applied by moving the vessel walls under control of the servomechanism until the wall pressures are within the specified pressure tolerance of the material pressure and static-equilibrium has been obtained. Setting $\mu_{C4}=0$ gives the densest packing, and progressively looser packings are obtained by increasing μ_{C4} .

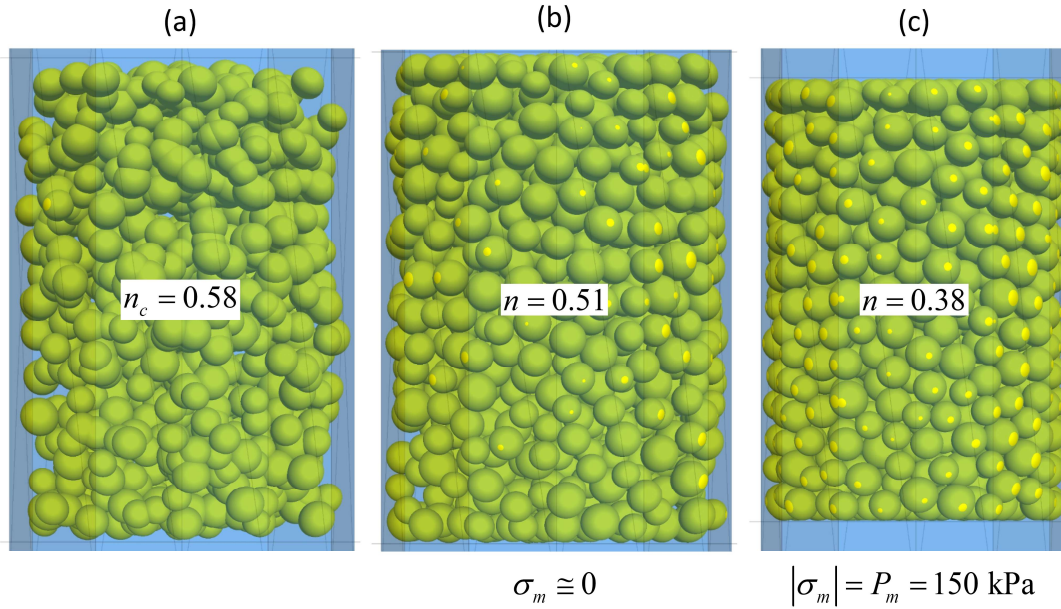


Figure 47 *Boundary-contraction packing procedure: (a) initial grain cloud at end of step 1, (b) relaxed grain cloud at end of step 2, and (c) compacted granular assembly at end of step 3. The images show the AG_Linear material of the linear material example.*

The grain-scaling procedure is similar to what is referred to as the material-genesis procedure in Potyondy and Cundall (2004) and ITASCA (2008a&b, Section 3.6.2 Material-Genesis Procedure, in *FISH* in *PFC3D/PFC2D* volumes) and consists of the following three steps (see Figure 48).

- Generate a cloud of grains with porosity of n_c . This porosity does not account for overlaps: $n_c = (V_v - V_g)/V_g$, where V_v is the volume of the material vessel and V_g is the total volume of grains. The grains are drawn from the specified size distribution, and then placed at arbitrarily chosen positions that lie fully within the material vessel such that there may be large grain-grain overlaps. Typically, n_c is chosen equal to n_d , where n_d corresponds with the dense state for which grains are well packed and in good contact with one another at a large mean stress but with relatively small overlaps. For a linear material of equal-sized spheres, $n_d = 0.35$. For a linear material of equal-sized disks, $n_d = 0.08$.

2. Set the material friction coefficient to zero, and then allow the grains to rearrange until either the mean stress is near zero (within 0.1% of P_m) or static-equilibrium is obtained (see footnote 37). This step eliminates the large overlaps and should provide an isotropic and close-packed state.
3. Scale the grain size iteratively to modify the mean stress of the assembly until the mean stress is within the specified pressure tolerance of the material pressure and static-equilibrium has been obtained. The grain-scaling procedure is described in ITASCA (2008a&b, Section 3.10.3 Isotropic Stress Installation Procedure, in *FISH* in *PFC3D/PFC2D* volumes). For a bonded material, the material pressure is typically set to a low value relative to the material strength.

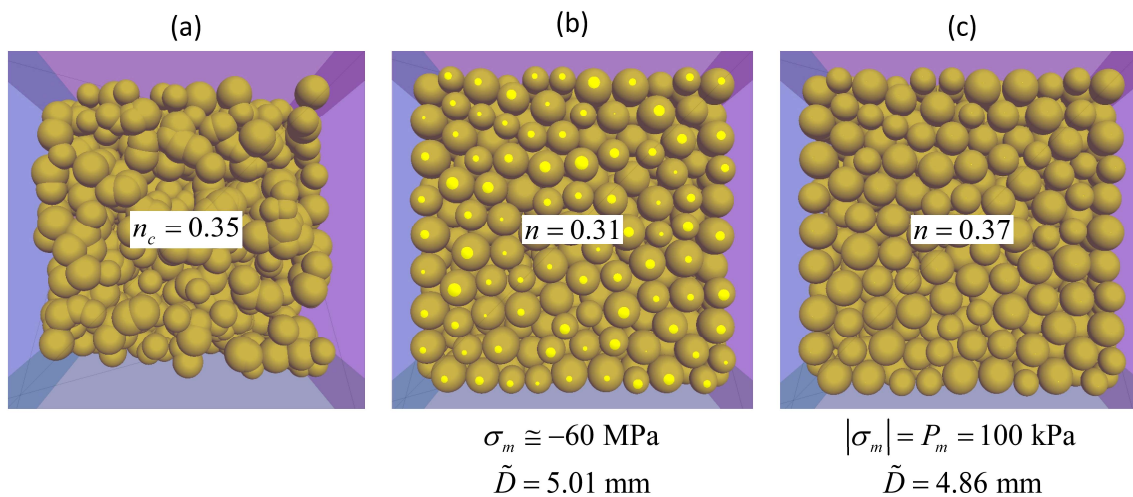


Figure 48 *Grain-scaling packing procedure: (a) initial grain cloud at end of step 1, (b) relaxed grain cloud at end of step 2, and (c) compacted granular assembly at end of step 3. The images show the SS_ContactBonded material of the contact-bonded material example.*

4.2.2 Finalization Phase

During the finalization phase, the final material properties are assigned to the grain-grain contacts, and additional material properties are specified that will be assigned to new contacts that may form during subsequent motion. The first step of the finalization phase occurs only for the bonded materials. We ensure the existence of contacts between all grains with a gap less than or equal to the installation gap by specifying the installation gap as the proximity in the Contact Model Assignment Table and executing the CLEAN command; this operation may create new grain-grain contacts in the grain assembly. The grain connectivity is controlled by the material pressure and the installation gap, with the installation gap being of primary importance (see Figure 49). The next step of the material-finalization phase differs for each material as follows.

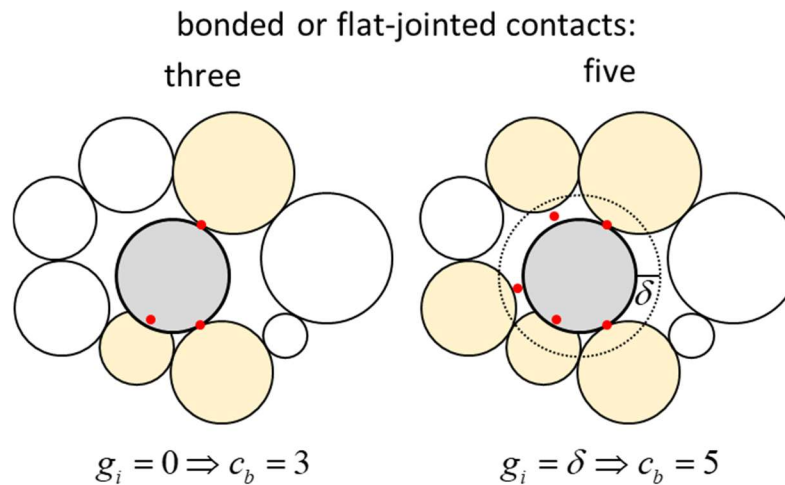


Figure 49 Grain assembly at end of packing phase with the bonded or flat-jointed contacts of a typical grain when the installation gap is zero (left) and greater than zero (right). Increasing the installation gap increases the bond coordination number.

- For a **linear material**, the linear material properties (from Table 3) are assigned to all grain-grain contacts. New grain-grain contacts that may form during subsequent motion are assigned the linear model with properties derived from the linear material properties.
- For a **contact-bonded material**, the contact-bonded material properties (from Table 6) are assigned to all grain-grain contacts, but only those grain-grain contacts with a gap less than or equal to the installation gap are bonded. New grain-grain contacts that may form during subsequent motion are assigned the linear contact bond model with properties derived from the linear material group of the contact-bonded material properties, and the new contacts are unbonded.
- For a **parallel-bonded material**, the parallel-bonded material properties (from Table 8) are assigned to all grain-grain contacts, but only those grain-grain contacts with a gap less than or equal to the installation gap are bonded. New grain-grain contacts that may form during subsequent motion are assigned the linear parallel bond model with properties derived from the linear material group of the parallel-bonded material properties, and the new contacts are unbonded.
- For a **soft-bonded material**, the soft-bonded material properties (from Table 9) are assigned to all grain-grain contacts, but only those grain-grain contacts with a gap less than or equal to the installation gap are bonded. New grain-grain contacts that may form during subsequent motion are assigned the linear model with properties derived from the linear material group of the soft-bonded material properties.

- For a **flat-jointed material**, the flat-joint contact model is installed at all grain-grain contacts with a gap less than or equal to the installation gap, and the flat-jointed material properties (from **Error! Reference source not found.**) are assigned to these flat-jointed contacts. The remaining grain-grain contacts as well as new grain-grain contacts that may form during subsequent motion are assigned the linear model with properties derived from the linear material group of the flat-jointed material properties.
- For a **user-defined material**, the user-defined material properties are assigned to all grain-grain contacts. New grain-grain contacts that may form during subsequent motion are assigned the user-defined model with properties derived from the user-defined material properties.

For the bonded materials, the final material properties are set to establish reference surfaces that do not overlap (see Figure 50); therefore, there are no forces or moments in the bonded material. For the bonded materials, the grain-vessel interface is smoothed (see Figure 51). The smoothing operation consists of setting the reference gap equal to the contact gap for all grain-wall contacts with a negative contact gap (thereby establishing reference surfaces that are just touching and effectively removing the overlap). After the smoothing operation and the assignment of the final material properties, there are no forces at the grain-wall interface and no forces or moments in the bonded material. Subsequent compression testing will proceed as expected, because the specimen will become loaded during the seating phase as the vessel walls move inward. New grain-wall contacts will be created naturally, because only the grain-wall contacts protruding from the vessel at the time of smoothing were affected by the smoothing operation.

The system is brought to static equilibrium while keeping the walls fixed. The specimen remains within the material vessel, and the model state is saved. This model state can be restored for subsequent materials testing. If a bonded material is being created, then the specimen is removed from the material vessel and brought to static equilibrium, and the model state is saved. This model state can be restored for subsequent boundary-value simulation.

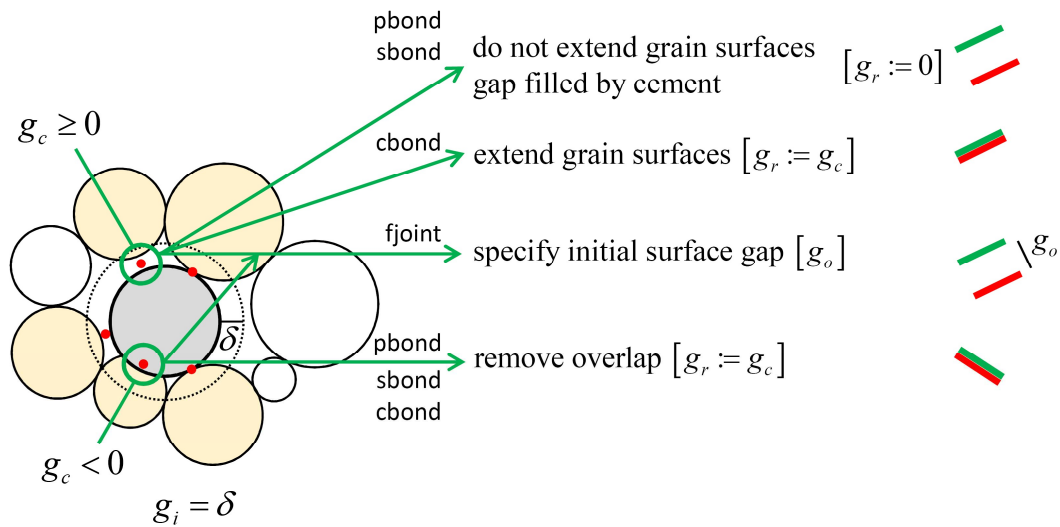


Figure 50 *Setting final material properties of bonded materials to establish reference surfaces that do not overlap (contact-bonded, parallel-bonded, soft-bonded and flat-jointed materials denoted by cbond, pbond, sbond and fjoint, respectively).*

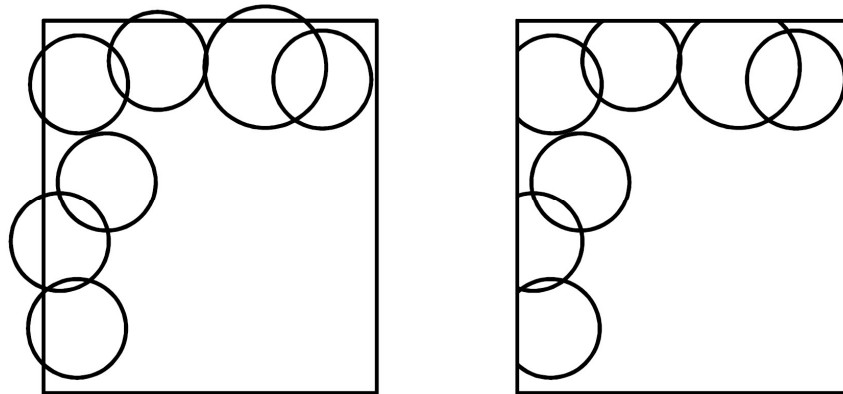


Figure 51 *The effective grain-vessel interface before (left) and after (right) the smoothing operation, which effectively cuts off the part of each ball or pebble that protrudes from the material vessel.*

5.0 LABORATORY-TESTING PROCEDURES

The following standard rock-mechanics laboratory tests are supported: compression (confined, unconfined and uniaxial strain), diametral-compression, direct tension and fracture toughness (see Figure 52). The tests are performed upon materials that were created within the physical material vessel; however, the diametral-compression test can be performed upon any specimen that is centered at the origin. The loading axis corresponds with the axial direction shown in Figure 45. The specimen is loaded by walls in the compression and diametral-compression tests, and by surface grains in the direct-tension and fracture-toughness tests (after having been removed from the material vessel and allowed to relax). In the compression tests, the specimen is loaded in either a polyaxial or cylindrical cell in which the axial walls act as loading platens. For the confined test, the velocities of the radial walls are controlled by a servomechanism to maintain a constant confining pressure (P_c); for the unconfined test, the radial walls do not contact the specimen; and for the uniaxial-strain test, the radial walls are kept motionless. In the diametral-compression test, the specimen (typically of a cylindrical or spherical shape) is loaded by the axial walls. In the direct-tension and fracture-toughness tests, the velocities of selected surface grains are fixed in the axial direction, thereby pulling apart the opposing specimen surfaces.

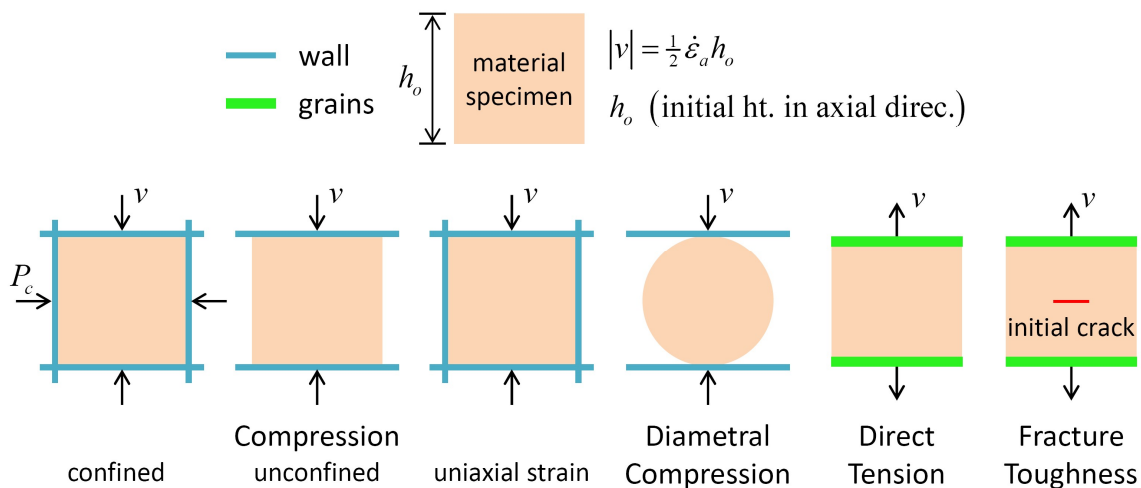


Figure 52 Loading conditions of laboratory-testing procedures.

The techniques used to measure stress, strain and porosity of the specimen within the material vessel are described in the first subsection. The measurement of material deformability is discussed in the second subsection. The servomechanism that controls wall velocities of the polyaxial, cylindrical and spherical cells is described in the third subsection. A discussion of how loading rate affects material response is given in the fourth subsection. The laboratory-test procedures are described in the remaining subsections.

5.1 Stress, Strain and Porosity in the Material

Stress and strain of the specimen within the material vessel is measured in three different ways via measurement regions, walls and gauge grains. The measurement-based quantities are taken

as the average values from three spherical measurement regions that are placed symmetrically along the axis of the largest vessel dimension. The measurement logic is described in ITASCA (2026a)³⁸. The wall-based quantities provide stress as wall force divided by cross-sectional area of specimen side (using either the current or initial vessel dimensions), and strain based on the change of distance between opposing walls. The gauge-based quantities are obtained from gauge grains that mimic LVDTs touching the specimen surface. Each gauge grain is the ball or clump that lies closest to the center of the corresponding specimen surface. The gauge-based quantities provide strain based on the change of distance between opposing gauge grains. Damage formation in a bonded material may perturb the gauge grains, and thus, wall-based quantities provide a more uniform average response over the entire specimen surface.

Porosity of the specimen within the material vessel is measured in two different ways via the above measurement regions and walls. The measurement-based porosity (n) accounts for grain-grain overlap via the procedure described in ITASCA (2026a)³⁹. The wall-based porosity (n_w) does not account for overlaps: $n_w = (V_v - V_g) / V_g$, where V_v is the current volume of the material vessel and V_g is the total volume of grains.

We denote stress and strain by

$$\begin{aligned} \text{stress: } & \{ \sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz} \} \\ \text{strain: } & \{ \epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}, \epsilon_{xy}, \epsilon_{xz}, \epsilon_{yz} \} \end{aligned} \quad (9)$$

where $\sigma_{ii} > 0$ is tension and $\epsilon_{ii} > 0$ is extension. For the 2D model, the out-of-plane stress and strain components are equal to zero so that stress is $\{ \sigma_{xx}, \sigma_{yy}, \sigma_{xy} \}$ and strain is $\{ \epsilon_{xx}, \epsilon_{yy}, \epsilon_{xy} \}$. An axial direction is associated with each material vessel: the axial direction of the polyaxial and cylindrical cells for the 3D model corresponds with the z-direction, while the axial direction of the polyaxial cell for the 2D model corresponds with the y-direction (see Figure 45). The radial direction is perpendicular to the axial direction. We define the following stress and strain quantities.

- Axial and radial stress and strain (3D model):

$$\begin{aligned} \sigma_a &= \sigma_{zz}, \quad \sigma_r = \frac{1}{2}(\sigma_{xx} + \sigma_{yy}) \\ \epsilon_a &= \epsilon_{zz}, \quad \epsilon_r = \frac{1}{2}(\epsilon_{xx} + \epsilon_{yy}) \end{aligned} \quad (10)$$

³⁸ In documentation set at PFC – Additional Features – Measure.

³⁹ In documentation set at PFC – Additional Features – Measure – Measured Quantities – Porosity.

- Axial and radial stress and strain (2D model, $\varepsilon_{zz} \equiv \sigma_{zz} \equiv 0$):

$$\begin{aligned}\sigma_a &= \sigma_{yy}, & \sigma_r &= \sigma_{xx} \\ \varepsilon_a &= \varepsilon_{yy}, & \varepsilon_r &= \varepsilon_{xx}\end{aligned}\quad (11)$$

- Deviator stress and strain:⁴⁰

$$\sigma_d = \sigma_a - \sigma_r, \quad \varepsilon_d = \varepsilon_a - \varepsilon_r \quad (12)$$

- Mean stress and volumetric strain (3D model):

$$\sigma_m = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) = \frac{1}{3}(\sigma_a + 2\sigma_r), \quad \varepsilon_v = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = \varepsilon_a + 2\varepsilon_r \quad (13)$$

- Mean stress⁴¹ and volumetric strain (2D model, $\varepsilon_{zz} \equiv 0$):

$$\sigma_m = \frac{1}{2}(\sigma_{xx} + \sigma_{yy}) = \frac{1}{2}(\sigma_a + \sigma_r), \quad \varepsilon_v = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = \varepsilon_a + \varepsilon_r \quad (14)$$

The material-vessel stress, strain and porosity quantities are listed in Table 14. The FISH variables for the measurement-based quantities are denoted by **mv_mX**, while the wall- and gauge-based quantities are denoted by **mv_wX** and **mv_gX**, respectively.

Table 14 Material-Vessel Stress, Strain and Porosity Quantities

Quantity, FISH	Description
$\{\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz}\},$ mv_ms {xx, yy, zz, xy, xz, yz}	material stress (2D model: $\sigma_{zz} \equiv \sigma_{xz} \equiv \sigma_{yz} \equiv 0$)
$\{\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{xy}, \varepsilon_{xz}, \varepsilon_{yz}\},$ mv_me {xx, yy, zz, xy, xz, yz}	material strain (2D model: $\varepsilon_{zz} \equiv \varepsilon_{xz} \equiv \varepsilon_{yz} \equiv 0$)
$\{\sigma_a, \sigma_r\},$ mv_ms {a, r}	axial & radial stress
$\{\varepsilon_a, \varepsilon_r\},$ mv_me {a, r}	axial & radial strain
$\sigma_d,$ mv_msd	deviator stress
$\sigma_m,$ mv_msm	mean stress
$\varepsilon_d,$ mv_med	deviator strain

⁴⁰ The deviator stress should not be confused with the deviatoric stress (Engelder, 1994). The amount by which the axial stress component departs from the confining pressure in a triaxial test is commonly called the differential stress in the rock mechanics and geological literature, and is used by Paterson and Wong (2005, p. 6) in the direct reporting of triaxial test results.

⁴¹ The mean stress for the 2D model is defined as the average of the in-plane stresses. It is not obtained by setting $\sigma_{zz} \equiv 0$ in the expression for mean stress of the 3D model.

$\varepsilon_v, \mathbf{mv_mev}$	volumetric strain
$n, \mathbf{mv_mn}$	measurement-based porosity
$n_w, \mathbf{mv_wn}$	wall-based porosity

The three measurement techniques measure the following quantities:

$$\begin{aligned}
 \sigma_{ij}^m \quad \varepsilon_{ij}^m & \text{ measurement-based (6 terms each, symmetric)} \\
 \sigma_k^w \quad \varepsilon_k^w & \text{ wall-based (3 terms each)} \\
 \underbrace{\varepsilon_k^g}_{\substack{i,j=\{x,y,z\} \\ k=\{x,y,z,r\}}} & \text{ gauge-based (3 terms)}
 \end{aligned} \tag{15}$$

For the 2D model, the above equation satisfies the condition: $i, j, k = \{x, y\}$. The wall- and gauge-based techniques measure only the direct stress and strain components, which we denote by a single subscript (e.g., σ_{xx} is denoted by σ_x). The cylindrical and spherical cells measure the radial components (σ_r and ε_r).

The wall-based stress quantities are the average force on opposing walls divided by the corresponding cross-sectional area:

$$\sigma_k^w = \frac{\frac{1}{2} \left((F_k^w)^- - (F_k^w)^+ \right)}{A_k}, \quad k = \{x, y, z\} \quad (2D \text{ model: } k = \{x, y\}) \tag{16}$$

where $(F_k^w)^-$ and $(F_k^w)^+$ are the total force on the walls in the negative and positive k directions, respectively, and A_k is the specimen cross-sectional area perpendicular to direction k . For the cylindrical and spherical cells, the radial stress acting on the corresponding wall is

$$\sigma_r^w = \frac{-\sum F_r^w}{A_r} \quad (\text{cylindrical and spherical cells}) \tag{17}$$

where the numerator is the sum of the radial components of the forces on the wall, and A_r is the surface area of the wall. The surface areas are determined (by **mv_wAreaMode**, M_a) using either the current ($M_a=0$) or initial ($M_a=1$) vessel dimensions, and expressed in terms of the distances between opposing walls (d_k^w). For the polyaxial cell: $A_x = d_y^w d_z^w$, $A_y = d_x^w d_z^w$ and $A_z = d_x^w d_y^w$; for the cylindrical cell: $A_z = \pi (d_r^w)^2 / 4$ and $A_r = \pi d_r^w d_z^w$; and for the spherical cell $A_r = \pi (d_r^w)^2$. For the polyaxial cell of the 2D model: $A_x = d_y^w t (t=1)$ and $A_y = d_x^w t (t=1)$.

The wall-based strain quantities are based on the change of distance between opposing walls:

$$\varepsilon_k^w = \frac{d_k^w - (d_k^w)_o}{(d_k^w)_o}, \quad k = \{x, y, z, r\} \quad (2D \text{ model: } k = \{x, y\}) \quad (18)$$

where d_k^w is the distance between opposing walls in direction k , and $(d_k^w)_o$ is the initial distance between these walls. The gauge-based strain quantities are based on the change of distance between opposing gauge grains:

$$\varepsilon_k^g = \frac{d_k^g - (d_k^g)_o}{(d_k^g)_o}, \quad k = \{x, y, z, r\} \quad (2D \text{ model: } k = \{x, y\}) \quad (19)$$

where d_k^g is the distance between opposing gauge grains in direction k , and $(d_k^g)_o$ is the initial distance between these grains. The initial distances provide a reference for the strain measurement and can be reset by the FISH functions `mv_{w,g}StrainZero`.

5.2 Material Deformability

The deformability of a bonded material can be quantified by the elastic constants, and the deformability of a granular material can be quantified by the resilient modulus. The discussion begins by considering the stiffness tensor of PFC material. Then the definition and measurement of the elastic constants and resilient modulus are presented.

The stiffness tensor relates stresses to strains. The two fundamental assumptions of linear elastic theory (that treats the material as a continuum) are that (a) stress-strain relations are linear, and (b) deformations are reversible. The first assumption is expressed by Hooke's law, giving 36 independent elastic constants. The existence of a unique strain-energy potential (from assumption b) reduces the number of independent elastic constants to 21. By assuming different levels of material symmetry, the number of independent elastic constants can be reduced significantly. For example, an *isotropic* system has the property that all directions are elastically equivalent and principal, which reduces the number of independent elastic constants to two. Therefore, a linear elastic isotropic material model has two independent elastic constants. A hexagonal system has a plane of elastic isotropy at each point, and these planes are parallel at all points. Such a body is said to be *transversely isotropic*, and there are five independent elastic constants. The stiffness tensor of the PFC material is affected by stress and damage so that, in general, the material response does not correspond with that of a linear elastic isotropic material model — e.g., the material response may become transversely isotropic as a result of cracking (Potyondy and Hazzard, 2008). In the general case, the response of the damaged material may become fully anisotropic. Potyondy and Hazzard (2004) describe a scheme to measure all 21 independent elastic constants using either wave-velocity or stiffness probes.

One can characterize the stiffness of a PFC material by assuming that it is behaving like a linear elastic isotropic material for which the elastic constants are Young's modulus (E) and Poisson's ratio (ν). The 3D model is an assembly of rigid three-dimensional particles with soft contacts for which the elastic constants are computed via Eqs. (30) and (33). The 2D model is an assembly of rigid unit-thickness particles with soft contacts that cannot be loaded in the out-of-plane direction and does not deform in the out-of-plane direction making it unclear how to define the elastic constants.⁴² By performing a biaxial test on the 2D material, one can *interpret* the macroscopic force-displacement response to obtain effective elastic constants (E' and ν') via Eqs. (39) and (42). The process involves the following considerations.

The rigid unit-thickness particles do not expand in the out-of-plane direction. A continuum material subjected to plane-strain conditions (no deformation in the out of plane direction) will be stiffer in its plane of loading than the same material subjected to plane-stress conditions (no stress in the out of plane direction). But note that neither of these conditions can be imposed on the 2D model because the out-of-plane forces and displacements do not enter into the force-displacement law at the contact level — there is no stress-strain law enforced, rather, the stress-strain response is emergent. The best that one can do is to define effective Young's modulus and effective Poisson's ratio by assuming constitutive relations for a 2D DEM linear elastic isotropic material (see Eq. (34)).

The resilient modulus (M_R) is defined as the ratio of applied deviator stress to recoverable or "resilient" strain (see Figure 53). It is a granular material characterization parameter that is stress dependent. The resilient modulus is used to perform layered elastic analysis (LEA). LEA is utilized extensively for pavement system evaluation and is a means of calculating pavement response under loading. Each pavement layer is defined by its resilient modulus and Poisson's ratio, even though granular bases exhibit nonlinear elastoplastic behavior in laboratory and field applications. LEA is used because it is a relatively simple analysis procedure and, more importantly, pavement loading is generally of low enough magnitude that a linear-elastic approximation of pavement material behavior is deemed suitable (Potyondy et al., 2018). According to Han and Vanapalli (2016), the resilient modulus is "...the key soil property in the mechanistic pavement design methods to rationally characterize the resilient behavior of the pavement materials, analyze the fatigue failure of the surface layer, and dimension the multi-layer system of the pavement structure." We obtain an effective resilient modulus (M'_R) for the 2D material (see preceding paragraph).

⁴² I have never seen this discussed in the DEM literature. If the reader is aware of any such discussion, please inform David Potyondy.

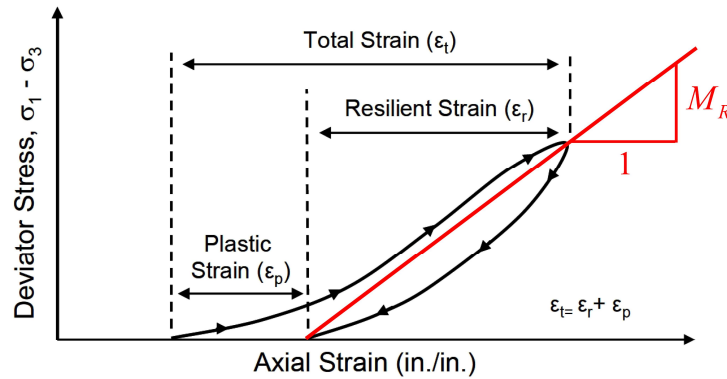


Figure 53 *Response of granular material subjected to triaxial loading, and measurement of resilient modulus.* (From Fig. 1 of Buchanan [2007])

5.3 Servomechanism

The velocities of the walls of the polyaxial and cylindrical cells are controlled by a servomechanism. The servo-control procedure is described in ITASCA (2008a&b, Section 3.10.5 Controlling Wall Velocity to Maintain Specified Stress, in *FISH* in *PFC3D/PFC2D* volumes). The servomechanism parameters are listed in

Table 15. The polyaxial cell consists of three pairs of opposing walls for the 3D model and two pairs of opposing walls for the 2D model. The cylindrical cell consists of a pair of opposing axial walls and a cylinder wall. The spherical cell consists of a sphere wall. The boundary condition for each pair of walls as well as the cylinder and sphere walls can be either velocity or pressure. A velocity boundary condition sets the velocity of the wall pair to be equal and opposite and the velocity of the cylinder- and sphere-wall vertices to be radial (with a positive or negative value indicating opening or closing motion, respectively). A pressure boundary condition activates a servomechanism that controls the velocities to maintain the specified pressure. The pressure acting on the opposing walls in the k direction is given by

$$P_k^w = -\sigma_k^w, \quad (P_k^w > 0 \text{ is compression})$$

$$\text{with } k = \begin{cases} \{x, y, z\}, & \text{polyaxial cell (2D model: } k = \{x, y\}) \\ \{z, r\}, & \text{cylindrical cell} \\ \{r\}, & \text{spherical cell.} \end{cases} \quad (20)$$

The servomechanism is turned on and off by `mvs_on` and `mvs_off`, respectively. When the servomechanism is on, the boundary conditions (set by `mvs_setBCs`) are enforced during subsequent cycling. Application of the specified pressures is determined by successful return from the `mvs_eqP` FISH function:

- **mvs_eqP**(ε_p , n_{lim}) cycles the model until either the pressures of all servo-controlled walls (P_k^w) are within the equilibrium-pressure tolerance (ε_p) of the target values (P_k^t):

$$\left(\frac{|P_k^w - P_k^t|}{P_k^t} \leq \varepsilon_p \right), \quad k = \{x, y, z, r\} \quad (2D \text{ model: } k = \{x, y\})$$

or the number of steps (n_s) exceeds the step limit (n_{lim}):

$$n_s > n_{lim} \quad [\text{command: solve max_cycles } n_{lim}]$$

Table 15 Servomechanism Parameters

Parameter	Type	Range	Def.	Description
$(B_c)_k$, mvs_BC { x , y , z , r }	INT	{0,1}	NA	boundary-condition code $\begin{cases} 0, & \text{velocity} \\ 1, & \text{pressure} \end{cases}, \quad k = \{x, y, z\} \text{ or } \{z, r\}$ (2D model: $k = \{x, y\}$)
$(B_v)_k$, mvs_BC { x , y , z , r } Val	FLT	{0,1}	NA	boundary-condition value $\begin{cases} v_k, & \text{velocity } ((B_c)_k = 0) \\ P_k^t, & \text{pressure } ((B_c)_k = 1) \end{cases}, \quad k = \{x, y, z\} \text{ or } \{z, r\}$ (2D model: $k = \{x, y\}$)
n_{gain} , mvs_gainUpdateRate	FLT	[1,∞)	25	servo gain update rate
v_{lim} , mvs_vLimit	FLT	(0.0,∞)	NA	velocity limit ($ v_k \leq v_{lim}, v_{lim} > 0$)

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.

When calibrating a DEM model, we might compare the quasi-static response with the quasi-static response obtained for the real material (from a test that may have been performed at a different strain rate). This allows us to compare the results of the DEM model and the real material. If dynamic effects are also affecting the real system response, then these effects would also need to be included in the DEM model, which involves a more complex calibration process, whereby we match the dissipative mechanisms occurring in the real material. If we only compare quasi-static responses, then the dissipative mechanisms need not be replicated in the DEM model (e.g., the DEM model can be heavily damped by using local damping with a default damping coefficient of 0.7 to approximate quasi-static conditions).

The loading rate for the compression, diametral-compression, and direct-tension tests is the axial strain rate ($\dot{\epsilon}_a$). The axial strain rate is related to the platen velocity as shown in Figure 54. The axial strain rate should be chosen based on the previous considerations. Note that an axial strain rate that is sufficient to produce quasi-static loading on a specimen of a given length will most likely not produce quasi-static loading on a specimen of a different length. A reasonable estimate of the strain rate needed for the different-length specimen is found by equating the loading velocities for the two cases.

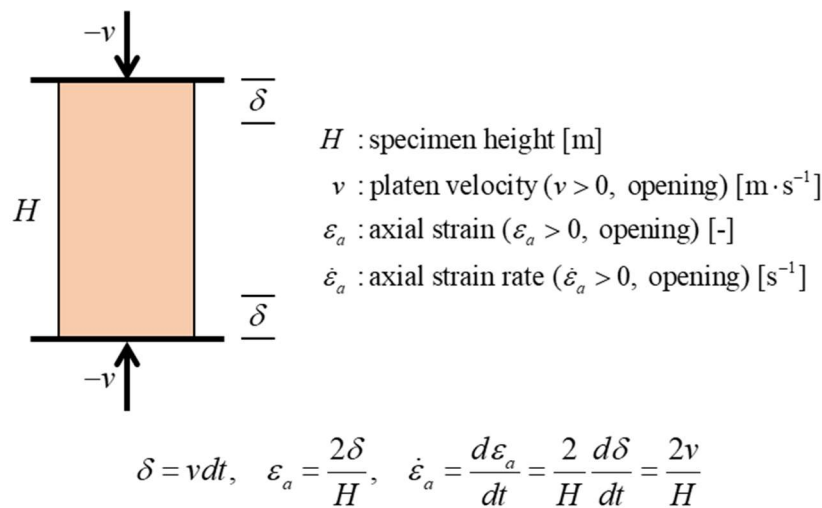


Figure 54 Definitions of axial strain, axial strain rate, and platen velocity.

5.5 Compression Test

Compression tests (confined, unconfined and uniaxial strain) are performed upon specimens that are centered wrt the origin. The specimens may have been created either in the physical material vessel or in the periodic material vessel and assembled into a block of material. If the specimen has been created in the physical material vessel, then the vessel walls are used to perform the test; otherwise, the specimen is carved out of the block of material and walls are created. Carving is available only for 3D models. The walls provide a polyaxial or cylindrical cell. The polyaxial cell provides a polyaxial loading condition while the cylindrical cell provides a triaxial loading condition. The loading axis corresponds with the axial direction shown in Figure 45, and the

loading conditions for the three test types are shown in Figure 52. The axial walls act as loading platens. For a confined test, the velocities of the radial walls are controlled by a servomechanism to maintain a constant confining pressure. For an unconfined test, the radial walls are moved away from the specimen and kept motionless.⁴³ For a uniaxial-strain test, the radial walls are kept motionless. The compression-test parameters are listed in Table 16. Compression testing is provided by the **CompTest** project, which is a subdirectory of each **mg_X** directory.

Table 16 Compression-Test Parameters

Parameter	Type	Range	Default	Description
Material-vessel parameters are listed in Table 12.				
B_c , sp_carve	INT	{0,1}	0	carve flag $\begin{cases} 0, & \text{do not carve} \\ 1, & \text{carve} \end{cases}$ If $B_c = 1$, then specify: shape, {H, W, D} and wall eff. modulus (see sp.p3fis).
T_t , ct_testType	INT	{0,1,2}	0	compression test type code $\begin{cases} 0, & \text{confined} \\ 1, & \text{unconfined} \\ 2, & \text{uniaxial strain} \end{cases}$
P_c , ct_Pc	FLT	(0.0, ∞)	NA	confining pressure ($P_c > 0$ is compression)
$\dot{\epsilon}_a$, ct_eRate	FLT	(0.0, ∞)	NA	axial strain rate ($ v = \frac{1}{2} \dot{\epsilon}_a h_o$, $\dot{\epsilon}_a > 0$, see Figure 52 and Section 5.4)
C_l , ct_loadCode	INT	{0,1}	0	loading-phase code $\begin{cases} 0, & \text{single stage} \\ 1, & \text{multiple stages} \end{cases}$
α , ct_loadFac	FLT	(0.0,1.0)	0.8	load-termination factor ($C_l = 0$) for termination criterion: $ \sigma_d^w \leq \alpha \sigma_d^w _{\max}$
Servo-control group:				
ϵ_p , ct_PTo1	FLT	(0.0, ∞)	pk_PTo1	pressure tolerance $\left(\frac{ P - P_c }{P_c} \leq \epsilon_p \right)$ where p is current pressure

⁴³ The wall-based axial stress is computed using the axial cross-sectional area of the initial vessel. The wall-based radial stress, radial strain and volumetric strain are zero; the corresponding measurement-based quantities remain valid and are used by the hidden views **p1-mer_wea** and **p1-mev_wea**. The radial walls can be removed from model views by adding these walls to the filter of the wall plot item.

ε_{lim} , ct_ARatLimit	FLT	$(0.0, \infty)$	1×10^{-5}	equilibrium-ratio limit (parameter of ft_eq)
n_{lim} , ct_stepLimit	INT	$[1, \infty)$	pk_stepLimit	step limit (parameter of ft_eq)
v_{lim} , ct_vLimit	FLT	$(0.0, \infty)$	$10H\dot{\varepsilon}_a$	servo velocity limit (see Table 15)

The compression test consists of a seating phase followed by a loading phase. During the seating phase, the strains are reset to zero. For a confined test, confining pressure is applied by activating the servomechanism with a pressure boundary condition in all directions. For an unconfined test, the radial walls are first moved away from the specimen, whereas for a uniaxial-strain test, the radial walls are kept in their initial position. Then for both unconfined and uniaxial-strain tests, an axial pressure (equal to P_c) is applied by activating the servomechanism with a pressure boundary condition in the axial direction and a velocity boundary condition of zero in the radial direction. Seating is successful if both **mvs_eqP()** and **ft_eq()** indicate that static-equilibrium has been obtained. The model state is saved at the end of the seating phase.

Grain displacements are reset to zero after the seating phase. At the start of the loading phase, strains are reset to zero. Then axial strain is applied by moving the axial walls at the specified strain rate while keeping the confining pressure constant for a confined test or keeping the radial walls motionless for either an unconfined or uniaxial-strain test. The loading phase may consist either of a single stage that ends when the applied deviator stress falls below a specified fraction of its peak value or multiple stages during which the axial-strain increments ($\Delta\varepsilon_a$, $\Delta\varepsilon_a > 0$ is opening) are specified in the function **ctPerformStages**. At the end of each stage, the axial wall velocities are set to zero and the model state is saved.

During the compression test, the crack-monitoring package is on (for bonded materials), and the specimen behavior is monitored using the history mechanism to sample and store relevant quantities. The monitored quantities include average stress and strain within the specimen and numbers of cracks (for bonded materials).

5.6 Diametral-Compression Test

Diametral-compression tests are performed upon specimens that are centered wrt the origin. Axial walls that act as loading platens are created and centered wrt the origin such that the loading axis corresponds with the y-direction (see Figure 55). The platens are frictionless, and the grain-wall contact stiffness is set based on a specified effective modulus. The diametral-compression test parameters are listed in Table 17. Diametral-compression testing is provided by the **DiamCompTest** project, which is a subdirectory of each **mg_X** directory.

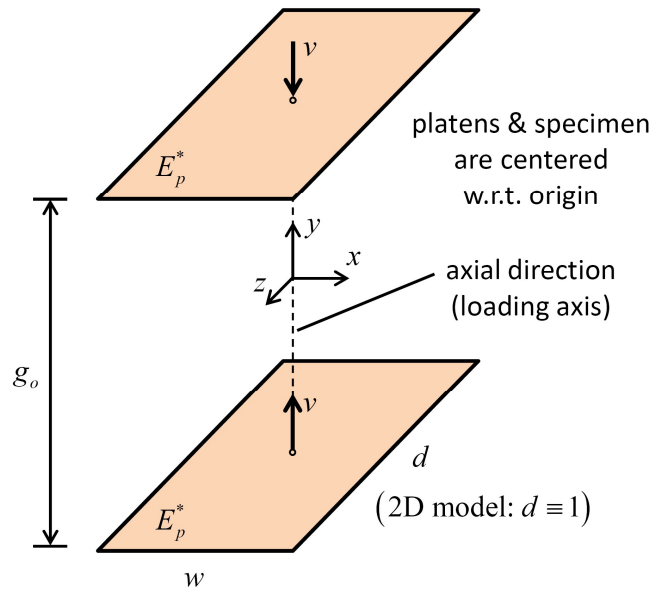


Figure 55 Loading configuration of diametral-compression test.

Table 17 Diametral-Compression Test Parameters

Parameter	Type	Range	Default	Description
$\{w, d\}, \mathbf{dc_}\{w, d\}$	FLT	$(0.0, \infty)$	NA	platen width and depth (2D model: $d \equiv 1$)
$g_o, \mathbf{dc_}g0$	FLT	$(0.0, \infty)$	NA	initial platen gap
$E_p^*, \mathbf{dc_}emod$	FLT	$(0.0, \infty)$	$\mathbf{mv_}emod$ or NA	platen effective modulus (used by linear contact model)
$\dot{\epsilon}_a, \mathbf{dc_}eRate$	FLT	$(0.0, \infty)$	NA	axial strain rate ($ v = \frac{1}{2} \dot{\epsilon}_a g_o$, $\dot{\epsilon}_a > 0$, see Figure 55 and Section 5.4)
$C_l, \mathbf{dc_}loadCode$	INT	$\{0, 1\}$	0	loading-phase code $\left\{ \begin{array}{l} 0, \text{ single stage} \\ 1, \text{ multiple stages} \end{array} \right.$
$\alpha, \mathbf{dc_}loadFac$	FLT	$(0.0, 1.0)$	0.8	load-termination factor ($C_l = 0$) for termination criterion: $ F_a \leq \alpha F_a _{\max}$
Static-equilibrium group:				
$\epsilon_{lim}, \mathbf{dc_}ARatLimit$	FLT	$(0.0, \infty)$	1×10^{-5}	equilibrium-ratio limit (parameter of ft_eq)
$\alpha, \mathbf{dc_}stepLimit$	INT	$[1.0, \infty)$	pk_stepLimit or 2×10^6	step limit (parameter of ft_eq)

The diametral-compression test consists of a set-up phase followed by a loading phase. During the set-up phase, the walls are created, and the system is brought to static equilibrium (via the `ft_eq` FISH function). The model state is saved at the end of the set-up phase.

Grain displacements are reset to zero after the set-up phase. During the loading phase, axial strain is applied by moving the axial walls at the specified strain rate ($\dot{\epsilon}_a$). The loading phase may consist of either a single stage that ends when the axial-force magnitude falls below a specified fraction of its peak value, or multiple stages during which the axial-strain increments ($\Delta\epsilon_a, \Delta\epsilon_a > 0$ is opening) are specified in the function `dcPerformStages`. At the end of each stage, the wall velocities are set to zero and the model state is saved.

During the diametral-compression test, the crack-monitoring package is on, and the specimen behavior is monitored using the history mechanism to sample and store relevant quantities. The monitored quantities include axial force and axial strain. The axial force is the average force on the opposing walls:

$$F_a = \frac{1}{2} \left((F_y)^- - (F_y)^+ \right), \quad (F_a > 0 \text{ is tension}) \quad (21)$$

where $(F_y)^-$ and $(F_y)^+$ are the total force on the bottom and top walls, respectively. The axial strain is based on the change of distance between the opposing walls:

$$\epsilon_a = \frac{g - g_o}{g_o}, \quad (\epsilon_a > 0 \text{ is extension}) \quad (22)$$

where g is the wall gap, and g_o is the initial wall gap.

When the diametral-compression test is performed upon a cylindrical specimen oriented such that the loading axis coincides with the cylinder radial direction, then the Brazilian tensile strength is given by

$$\sigma_B = \frac{|F_a|_{\max}}{\pi R t}, \quad (2D \text{ model: } t \equiv 1) \quad (23)$$

where $|F_a|_{\max}$ is the peak axial force, and R and t are the radius and thickness, respectively, of the Brazilian disk (Goodman, 1980).

5.7 Direct-Tension Test

Direct-tension tests are performed upon specimens that are centered wrt the origin. The specimens may have been created either in the physical material vessel or in the periodic material vessel and assembled into a block of material, in which case they are carved out of the block of

material. Carving is available only for 3D models. The loading axis corresponds with the axial direction shown in Figure 45. During the direct-tension test, the specimen is gripped at its ends and pulled apart slowly while monitoring the axial stress and strain (using the measurement-based quantities of σ_a^m and ϵ_a^m listed in Table 14). The direct-tension test parameters are listed in Table 18. Direct-tension testing is provided by the **TenTest** project, which is a subdirectory of each **mg_X** directory.

The specimen is gripped by identifying a thin layer of surface grains that will be used to load the specimen. The surface grains are referred to as grip grains and identified based on the specified grip thickness (t_g). The velocities of the grip grains are fixed in the axial direction, thereby pulling apart the opposing specimen surfaces. The grip grains are not allowed to translate or spin during the test, which is equivalent to the opposing surfaces being glued to flat and rigid platens. The velocity of the grip grains is specified via the axial strain rate ($\dot{\epsilon}_a$).

Table 18 Direct-Tension Test Parameters

Parameter	Type	Range	Default	Description
Material-vessel parameters are listed in Table 12.				
B_c , sp_carve	INT	{0,1}	0	carve flag $\begin{cases} 0, & \text{do not carve} \\ 1, & \text{carve} \end{cases}$ If $B_c = 1$, then specify: shape and {H, W, D} (see sp.p3fis).
t_g , tt_tg	FLT	(0.0, ∞)	$\tilde{D}$	grip thickness
$\dot{\epsilon}_a$, tt_eRate	FLT	(0.0, ∞)	NA	axial strain rate ($ v = \frac{1}{2} \dot{\epsilon}_a h_o$, $\dot{\epsilon}_a > 0$, see Figure 52 and Section 5.4)
C_l , tt_loadCode	INT	{0,1}	0	loading-phase code $\begin{cases} 0, & \text{single stage} \\ 1, & \text{multiple stages} \end{cases}$
α , tt_loadFac	FLT	(0.0, 1.0)	0.8	load-termination factor ($C_l = 0$) for termination criterion: $ \sigma_a^m \leq \alpha \sigma_a^m _{\max}$

The direct-tension test consists of a set-up phase followed by a loading phase. During the set-up phase, the grip grains are identified (by assigning the names **ttGripTop** and **ttGripBottom** to the first slot of the group data for these grains), the motion of these grains is specified and the strains are reset to zero. The model state is saved at the end of the set-up phase.

Grain displacements are reset to zero after the set-up phase. During the loading phase, axial strain is applied by moving the grip grains at the specified strain rate. The loading phase may consist either of a single stage that ends when the axial stress falls below a specified fraction of its peak value or multiple stages during which the axial-strain increments ($\Delta\epsilon_a, \Delta\epsilon_a > 0$ is opening) are specified in the function **ttPerformStages**. At the end of each stage, the grip-grain velocities are set to zero and the model state is saved.

During the direct-tension test, the crack-monitoring package is on, and the specimen behavior is monitored using the history mechanism to sample and store relevant quantities. The monitored quantities include axial stress and axial strain within the specimen and numbers of cracks.

5.8 Fracture-Toughness Test

A fracture-toughness test is not provided in the material-modeling support package. It could be performed as illustrated in Figure 52, and described in Potyondy and Emam (2014a&b, Sections 16.0&12.0 Fracture Toughness (KIC) Measurement). Work is underway to provide this test.

6.0 STRESS-INSTALLATION PROCEDURE

Stresses can be installed in the material that is formed in the periodic material vessel, and these stresses provide the initial stress state when the model is converted into a periodic brick and then assembled into a specimen for subsequent boundary-value modeling. The stress state has no shear components and does not vary with position. It would be relatively straightforward to enhance the procedure to support a general uniform stress state (with shear components) by following the procedure described in ITASCA (2008a&b, Section 3.9 Stress-Installation Procedure, in the *FISH in PFC3D/2D* volumes). That procedure describes how to install a stress field that may vary linearly in space within an arbitrarily shaped particle ensemble by imposing a deformation field on the particles.⁴⁴

⁴⁴ The general stress-installation procedure has not been implemented in the current material modeling support package; however, it was implemented in the package that was provided with PFC version 4, and thus, could be implemented for PFC version 9 (either by a user or Itasca).

7.0 APPENDIX

7.1 Measuring Elastic Constants

Expressions for the elastic constants measured during triaxial (in 3D) and biaxial (in 2D) tests are derived in this appendix.

7.1.1 Triaxial Test

The constitutive relations for a linear elastic isotropic material are

$$\begin{aligned}\varepsilon_x &= \frac{1}{E} [\sigma_x - \nu(\sigma_y + \sigma_z)] & \gamma_{xy} &= \tau_{xy}/G \\ \varepsilon_y &= \frac{1}{E} [\sigma_y - \nu(\sigma_x + \sigma_z)] & \gamma_{xz} &= \tau_{xz}/G, \quad G = \frac{E}{2(1+\nu)} \\ \varepsilon_z &= \frac{1}{E} [\sigma_z - \nu(\sigma_x + \sigma_y)] & \gamma_{yz} &= \tau_{yz}/G\end{aligned}\quad (24)$$

where the elastic constants are Young's modulus (E) and Poisson's ratio (ν). The elastic constants of a material can be measured by performing a triaxial test as shown in Figure 56. The loading conditions are as follows

$$\begin{aligned}\text{initial conditions: } & \sigma_x = \sigma_y = \sigma_z = P_c \\ \text{during test: } & \begin{cases} \sigma_x = \sigma_y = P_c \text{ (constant)} \\ \sigma_z \text{ varies} \end{cases}\end{aligned}\quad (25)$$

where P_c is the confining pressure. We obtain expressions for the elastic constants by substituting the increments of stress and strain that occur during the test after confinement application into the incremental form of Eq. (24):

$$\begin{aligned}\Delta\sigma_x = \Delta\sigma_y = \Delta\gamma_{xy} = \Delta\gamma_{xz} = \Delta\gamma_{yz} &= 0 \\ \Delta\sigma_z &\neq 0\end{aligned}\quad (26)$$

$$\Delta\varepsilon_x = \frac{-\nu}{E} \Delta\sigma_z \quad (27)$$

$$\Delta\varepsilon_y = \frac{-\nu}{E} \Delta\sigma_z \quad (28)$$

$$\Delta\varepsilon_z = \frac{1}{E} \Delta\sigma_z \quad (29)$$

The Young's modulus is obtained from Eq. (29) as

$$E = \frac{\Delta \sigma_z}{\Delta \varepsilon_z} \quad (30)$$

The Poisson's ratio is obtained by substituting Eq. (30) into Eq. (28), and solving for ν :

$$\nu = -\frac{\Delta \varepsilon_y}{\Delta \varepsilon_z} \quad (31)$$

We define the radial strain

$$\varepsilon_r = \varepsilon_x = \varepsilon_y \quad (32)$$

such that the expression for the Poisson's ratio becomes

$$\nu = -\frac{\Delta \varepsilon_r}{\Delta \varepsilon_z} \quad (33)$$

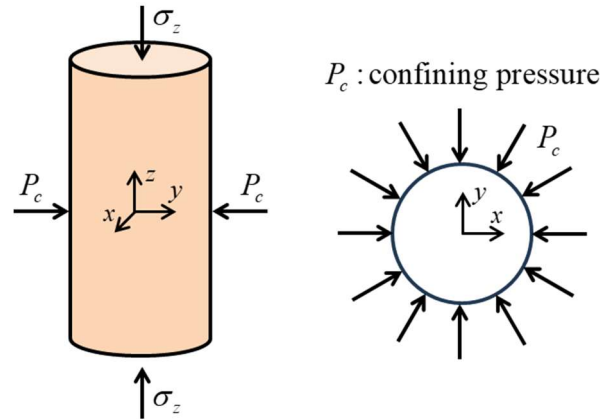


Figure 56 Cylindrical specimen used in a triaxial test showing loading conditions and coordinate system.

7.1.2 Biaxial Test

The constitutive relations for a linear elastic isotropic material are given by Eq. (24) where the elastic constants are Young's modulus (E) and Poisson's ratio (ν). The constitutive relations for a 2D DEM linear elastic isotropic material (consisting of rigid unit-thickness particles):

$$\begin{aligned} \varepsilon_x &= \frac{1}{E'} [\sigma_x - \nu' \sigma_y] \\ \varepsilon_y &= \frac{1}{E'} [\sigma_y - \nu' \sigma_x] \end{aligned} \quad \gamma_{xy} = \tau_{xy} / G', \quad G' = \frac{E'}{2(1 + \nu')} \quad (34)$$

where E' and ν' are the effective Young's modulus and effective Poisson's ratio, respectively. The relations in this equation are obtained by noting that there is no stress or strain in the out-

of-plane direction (the unit-thickness particles are rigid and do not expand or contract), and thus, we remove σ_z and ε_z from the 3D constitutive relations of Eq. (24), and disregard the third equation for ε_z . This is the constitutive relation for a linear elastic isotropic material subjected to plane-stress boundary conditions ($\sigma_z = \tau_{xz} = \tau_{yz} = 0$). It would be interesting to determine whether or not a 2D bonded material, perhaps of a thin plate with a circular hole loaded in uniaxial tension with plane-stress boundary conditions, would match the analytical solution.

The values of E' and ν' can be measured by performing a biaxial test as shown in Figure 57. The loading conditions are as follows

$$\begin{aligned} \text{initial conditions: } & \sigma_x = \sigma_y = P_c \\ \text{during test: } & \begin{cases} \sigma_x = P_c \text{ (constant)} \\ \sigma_y \text{ varies} \end{cases} \end{aligned} \quad (35)$$

where P_c is the confining pressure. We obtain expressions for the effective elastic constants by substituting the increments of stress and strain that occur during the test after confinement application into the incremental form of Eq. (34):

$$\begin{aligned} \Delta\sigma_x &= \Delta\gamma_{xy} = 0 \\ \Delta\sigma_y &\neq 0 \end{aligned} \quad (36)$$

$$\Delta\varepsilon_x = \frac{-\nu'}{E'} \Delta\sigma_y \quad (37)$$

$$\Delta\varepsilon_y = \frac{1}{E'} \Delta\sigma_y \quad (38)$$

The effective Young's modulus is obtained from Eq. (38) as

$$E' = \frac{\Delta\sigma_y}{\Delta\varepsilon_y} \quad (39)$$

The effective Poisson's ratio is obtained by substituting Eq. (39) into Eq. (37), and solving for ν' :

$$\nu' = -\frac{\Delta\varepsilon_x}{\Delta\varepsilon_y} \quad (40)$$

We define the radial strain

$$\varepsilon_r = \varepsilon_x \quad (41)$$

such that the expression for effective Poisson's ratio becomes

$$\nu' = -\frac{\Delta \varepsilon_r}{\Delta \varepsilon_y} \quad (42)$$

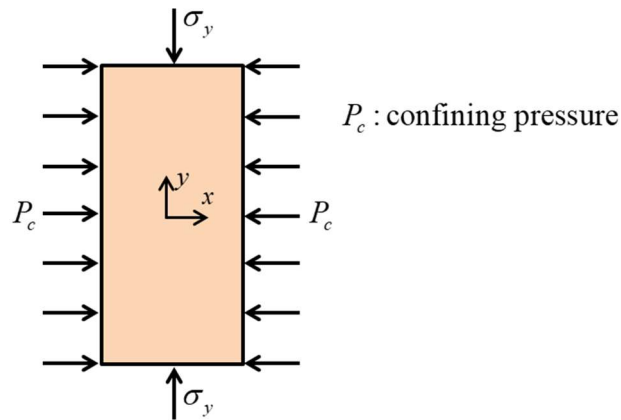


Figure 57 Rectangular specimen used in a biaxial test showing loading conditions and coordinate system.

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