Material-Modeling Support for PFC

David Potyondy

Originally: Itasca Webinar (December 14, 2017)
Updated for fistPkg26, fistPkg6.6, fistPkg{7.1, 7.2}
June 24, 2021
Preamble

• **BPM methodology** is described in Potyondy (2015), it will be *briefly* described in this webinar.

Preamble

- Material-Modeling Support package is described in Potyondy (2017), and is the focus of this webinar.


*Operates within PFC, see Material Modeling Support link: www.itascacg.com/material-modelling-support.

fistPkg for PFC version 7 is fistPkg7.N, where N is package version number

Preamble

- **Future webinars** will introduce the BPM methodology, and discuss how to calibrate a BPM to match behavior of a particular rock.

For now, calibration notes:

Questions?

• The large number of webinar attendees makes it impossible for me to reply to questions on-the-fly.

• However, you can submit your questions during the webinar using the chat-tool, or send them to Judy Zetterlund <jzetterlund@itascacg.com>.

• All questions will be answered, and the answers will be posted to the Itasca website within two weeks. This webinar will also be posted to the Itasca website. A link to the materials will be sent to all registrants.
Overview

Bonded-Particle Modeling (Essential Features)

Material-Modeling Support Package (Walk-Through, lecture)

Material-Modeling Support Package (Hands-On, usage)
Bonded-Particle Modeling (Essential Features)

From Martin Schöpfer

Structural-geology application
Bonded-Particle Modeling (Essential Features)

Increasing horizontal extension

From Martin Schöpfer: animation
Evolution of layer-bound fault systems

Fault systems occur on a wide range of scales (km to mm) and exhibit a wide range of geometries, ranging from symmetric (i.e., equal proportions of 'right' and 'left' dipping faults) to asymmetric (all faults dip in one direction). Asymmetric fault systems are often interpreted to form due to layer parallel shearing (e.g., domino or bookshelf-type faulting). 2D DEM models of fault systems under co-axial strain boundary conditions reveal that this interpretation may sometimes be incorrect.

Symmetric fault system

Photo: B. Grassmann
Quartzitic Marble, Serifos, Greece

Asymmetric fault system

Shear?

Photo: B. Grassmann
Pegmatitic dyke in marble, Naxos, Greece

2D DEM model boundary conditions

\[ \sigma_{yy} = \sigma_1 = \text{constant} \]

\[ v_x = \text{constant} \]

Six realisations at 10% extension
Passive markers obtained by intersecting triangulation of particle centres with initially horizontal lines
Essential Features of a BPM

Damage consists of bond breakages.
Essential Features of a BPM

BPM consists of a base material (intact rock) to which larger-scale joints can be added.

- base material: bonded rigid grains
- joints: interfaces

Damage consists of bond breakages.
Bonded-Particle Modeling Methodology (PFC model)

PFC programs (PFC2D & PFC3D) provide a general-purpose, distinct-element modeling framework that includes a computational engine and a graphical user interface.

Simulate movement & interaction of many finite-sized particles via distinct-element method, which provides an explicit dynamic solution to Newton’s laws of motion.

Contact forces are equal & opposite
**Bonded-Particle Modeling Methodology (PFC model)**

Particles are rigid bodies with finite mass that move independently of one another and can both translate and rotate. Particles interact at pair-wise contacts by means of internal force and moment.

Contact mechanics is embodied in particle-interaction laws that employ a soft-contact approach for which all deformation occurs at the contacts between the rigid bodies. The particle-interaction law (contact model) updates the internal force and moment.

Contact forces are equal & opposite
soft-contact approach

Consider the system of me standing on two baseballs, pressed between steel plates. Top plate moves down by $\Delta$.

Initial system

$\Delta$ 

Loaded system

$W = mg$

Baseballs contract and expand.
soft-contact approach

Consider the system of me standing on two baseballs, pressed between steel plates. Top plate moves down by \( \Delta \).

DEM model employs a “soft contact” approach: all deformation occurs at the contacts between the rigid bodies.

The stiffnesses can be related to the effective modulus of an equivalent continuum. . .
soft-contact approach

Consider the system of me standing on two baseballs, pressed between steel plates. Top plate moves down by $\Delta$.

\[ W = mg \]

\[ k_{bw} = \frac{AE^*}{R} = \pi RE^* \]

\[ k_{bb} = \frac{AE^*}{2R} = \frac{1}{2} k_{bw} \]

The DEM model contracts but does not expand.
Bonded-Particle Modeling Methodology (PFC model)

PFC model provides three basic entities:

balls and clumps
- obey laws of motion
- interact with one another and with walls

walls
- do not obey laws of motion
- used to apply velocity boundary conditions
- interact only with balls and clumps
- made of facets

These entities interact at contacts.
Each contact stores force & moment that act on the two contacting entities.
Bonded-Particle Modeling Methodology (PFC model, 2D)

PFC2D model: unit-thickness disks and linear segments
PFC model provides a synthetic material: rigid grains that interact at contacts, which encompasses a vast microstructural space --- only a small portion of this space has been explored.

PFC model includes both granular and bonded materials as well as an interface that can be inserted into the bonded materials.

The most up-to-date incarnation of the PFC model is provided in the form of the linear, contact-bonded, parallel-bonded, and flat-jointed materials to support:

- **practical applications** (via boundary-value models made from them)
- **scientific inquiry** (via further exploration of microstructural space)
Microstructural Models Provided by BPM

Base material itself can serve as model of intact rock

- rigid **grains** joined by deformable & breakable **cement**

**grains** can be balls or clumps

**cement** can be

- contact-, parallel- or soft-bonded contact
- flat-jointed contact

When bond breaks, behaves as **linear** contact.
cement can be
• contact-, parallel- or soft-bonded contact
• flat-jointed contact
When bond breaks, behaves as linear contact.

It is the type of contact model at the grain-grain contacts that defines the PFC material as being linear, contact-bonded, parallel-bonded or flat-jointed.

Each material is defined by a set of material properties. These properties control the material-genesis procedure, install the desired contact model at selected contacts and assign contact-model properties.

Let’s examine each contact model:
• Linear Model
• Linear Contact Bond Model
• Linear Parallel Bond Model
• Flat-Joint Model

No time, future webinar!
Let’s begin. . .
Introduction

The PFC model provides a synthetic material consisting of an assembly of rigid grains that interact at contacts. This synthetic material encompasses a vast microstructural space, and only a small portion of this space has been explored.

The PFC model includes both granular and bonded materials. The bonded materials are also called Bonded-Particle Models (or BPMs).

The support for material modeling provided by PFC 5.0 consists of a consistent set of FISH functions, which we call the PFC 5.0 FISHTank (or fistPkg).

fistPkg for PFC version 7 is fistPkg7.N, where N is package version number
Overview of fistPkg

- Material Vessels & Material-Genesis Procedure
  - packing phase, then finalization phase
- Materials
  - common material properties
  - specific material properties (for each material type)
- Microstructural Monitoring
- Laboratory-Testing Procedures
  - measuring stress-strain-porosity
  - compression, diametral compression & direct tension
- Example Materials
Material Vessels

All materials are produced within a material vessel such that they form a homogeneous, isotropic and well-connected grain assembly with a specified non-zero material pressure.

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 (effective modulus).
Material Vessels

All materials are produced within a material vessel such that they form a homogeneous, isotropic and well-connected grain assembly with a specified non-zero material pressure.

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 (effective modulus).

Should be greater than or equal to modulus of the material.
Material Vessels

2D

polyaxial and periodic cells

3D

cylindrical cell
Material Vessels (*periodic vessel*)

Bricks are assembled into a perfectly packed ensemble, may have installed stress.
Material Vessels (periodic vessel)

Installed stress: $S_{xx} = -78 \text{ MPa}$, $S_{yy} = -19.5 \text{ MPa}$

Force chains in bonded ensemble
# Material Vessels

## Table 6 Material-Vessel Parameters

<table>
<thead>
<tr>
<th>Parameter, FISH</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
</table>
| \(T_v, \text{mv\_type}\) | INT | \{0,1\} | 0 | vessel-type code  
| | | | | \{0. physical  
| | | | | 1. periodic  
| \(S_v, \text{mv\_shape}\) | INT | \{0,1,2\} | 0 | vessel-shape code  
| | | | | \{0. rectangular cuboid  
| | | | | 1. cylinder  
| | | | | 2. sphere  
| \(\{H,W,D\}, \text{mv\_\{H,W,D\}}\) | FLT | \((0.0,\infty)\) | NA | height, width and depth (sphere diameter is \(H\) ; 2D model: \(D=1\)  
| \(\alpha, \text{mv\_expandFac}\) | FLT | \([1.0,\infty)\) | 1.2 | expansion factor of physical vessel  
| \(\{\alpha_i, \alpha_d\}, \text{mv\_inset\{L,D\}Fac}\) | 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  

Material-vessel properties (including current vessel dimensions) are listed via @mvListProps.
Material Vessels

```python
Edit mvParams.p3dat

; fname: mvParams.p3dat

def mvSetParams
; Set Material-Vessel Parameters.
; ** Cylindrical vessel (of 240-mm height and 170-mm diameter,
; ** with a 500 MPa effective modulus).
    mv_type = 0
    mv_shape = 1
    mv_H = 240e-3
    mv_W = 170e-3
    mv_emod = 500e6
end
@mvSetParams
@_mvCheckParams
@mvListProps

@msBoxDefine( [vector(0.0, 0.0, 0.0)], [vector(50e-3, 50e-3, 50e-3)] )

return
; EOF: mvParams.p3dat
```

pfc3d>@mvListProps
## Material-Vessel Properties:
- **mv_type**: 0 (physical)
- **mv_shape**: 1 (cylinder, \_mvCylRes: 0.55)
- \(mv_H, _mwz\) (height (initial, current), aligned with z-axis): (0.24, 0.220127)
- \(mv_W, _wdr\) (diameter (initial, current), lies in xy-plane): (0.17, 0.152297)
- **mv_expandFac**: 1.2
- **mv_emod** (effective modulus): 5e08
- **mv_insetLFac** (measurement region spanning-length factor): 0.8
- **mv_insetDFac** (measurement region diameter factor): 0.8
Material Vessels

Material-Vessel Properties:

```
## Material-Vessel Properties:
  mv_type: 0 (physical)
  mv_shape: 1 (cylinder, _mvCylRes: 0.55)
  (mv_H, _wz) (height (initial, current), aligned with z-axis): (0.24, 0.220127)
  (mv_O, _wdr) (diameter (initial, current), lies in xy-plane): (0.17, 0.152297)
  mv-expandFac: 1.2
  mv_emod (effective modulus): 5e+08
  mv_insetIFac (measurement region spanning-length factor): 0.8
  mv_insetDFac (measurement region diameter factor): 0.8
```
Material Vessels

```python
# mvSetParams
; Set Material-Vessel Parameters.
; ** Cylindrical vessel (of 240-mm height and 170-mm diameter,
; with a 500 MPa effective modulus).
  mv_type = 0
  mv_shape = 1
  mv_H = 240e-3
  mv_W = 170e-3
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@mvSetParams
@mvCheckParams
@mvListProps

@msBoxDefine( [vector(0.0, 0.0, 0.0)], [vector(50e-3, 50e-3, 50e-3)] )

return
:EOF: mvParams.p3dat
```

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## Material-Vessel Properties:
- mv_type: 0 (physical)
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- mv_insetLFac (measurement region spanning-length factor): 0.8
- mv_insetDFac (measurement region diameter factor): 0.8

SI units, for legends of plots

microstructural box
Materials

Material consist of circular/spherical, Voronoi and tetrahedral grains joined by contact, parallel or flat-joint bonds. Current implementation of Voronoi and tetrahedral grains is limited to 3D flat-joint contacts. The spherical, Voronoi and tetrahedral grains are shown here and will not be discussed further in this slide set. Refer to Potyondy et al. (2020) for a material description.

Figure 7  The three flat-jointed materials with spherical, Voronoi and tetrahedral grains at specimen resolutions of 10. (From Fig. 9 of Potyondy et al. [2020])
Material-Genesis Procedure (packing phase)

Generate cloud of grains drawn from specified size distribution at specified grain-cloud porosity. Allow them to rearrange into a packed state under conditions of zero friction. Then, obtain specified material pressure via:

**boundary contraction:**
move vessel walls under control of servomechanism
[set $\mu = \mu_{CA}$, choose $\mu_{CA}$ to obtain dense or loose packing]

**grain scaling:**
grain sizes are scaled iteratively
[ $\mu = 0$ to obtain dense packing]
Material-Genesis Procedure (packing phase)

Generate cloud of grains drawn from specified size distribution at specified grain-cloud porosity. Allow them to rearrange into a packed state under conditions of zero friction. Then, obtain specified material pressure via:

**boundary contraction:**
move vessel walls under control of servomechanism
[set $\mu = \mu_{CA}$, choose $\mu_{CA}$ to obtain dense or loose packing]

**grain scaling:**
grain sizes are scaled iteratively
[$\mu \equiv 0$ to obtain dense packing]

\[\mu_{CA} = 0 \text{ (dense)}\]
\[\mu_{CA} = \mu_m \text{ (loose)}\]
# Material-Genesis Procedure (packing phase)

## Table 7 Packing Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S_{\text{gen}} ), ( \text{pk}_\text{seed} )</td>
<td>INT</td>
<td>( S_{\text{gen}} \geq 10,000 )</td>
<td>10,000</td>
<td>seed of random-number generator (affects packing)</td>
</tr>
<tr>
<td>( p_m ), ( \text{pk}_\text{Pm} )</td>
<td>FLT</td>
<td>( 0.0, \infty )</td>
<td>NA</td>
<td>material pressure</td>
</tr>
<tr>
<td>( \varepsilon_p ), ( \text{pk}_\text{PTol} )</td>
<td>FLT</td>
<td>( 0.0, \infty )</td>
<td>( 1 \times 10^{-2} )</td>
<td>pressure tolerance ( \left( \frac{P - P_m}{P_m} \leq \varepsilon_p \right) )</td>
</tr>
<tr>
<td>( \varepsilon_{\text{im}} ), ( \text{pk}_\text{ARatLimit} )</td>
<td>FLT</td>
<td>( 0.0, \infty )</td>
<td>( 8 \times 10^{-3} )</td>
<td>where ( P ) is current pressure equilibrium-ratio limit (parameter of ( \text{ft}_\text{eq} ))</td>
</tr>
<tr>
<td>( n_{\text{im}} ), ( \text{pk}_\text{stepLimit} )</td>
<td>INT</td>
<td>( [1, \infty) )</td>
<td>25000</td>
<td>step limit (parameter of ( \text{ft}_\text{eq} )) packing-procedure code</td>
</tr>
<tr>
<td>( C_p ), ( \text{pk}_\text{procCode} )</td>
<td>INT</td>
<td>{0,1}</td>
<td>0</td>
<td>{0, boundary contraction } {1, grain scaling}</td>
</tr>
<tr>
<td>( n_c ), ( \text{pk}_\text{nc} )</td>
<td>FLT</td>
<td>( 0.0,1.0 )</td>
<td></td>
<td>grain-cloud porosity</td>
</tr>
</tbody>
</table>

### Boundary-contraction group (\( C_p = 0 \)):

- \( \mu_{\text{nl}} \), \( \text{pk}_\text{fricCA} \) | FLT  | \( 0.0, \infty \) | 0.0 | material friction coefficient during confinement application |
- \( v_{\text{lim}} \), \( \text{pk}_\text{vLimit} \) | FLT  | \( 0.0, \infty \) | NA  | servo velocity limit (see Table 9) |
Material-Genesis Procedure *(packing phase)*

---

**Table 7 Packing Parameters**

<table>
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<th>Description</th>
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<tbody>
<tr>
<td>(S_{PK} ), (pk_seed)</td>
<td>INT</td>
<td>(S_{PK} \geq 10,000)</td>
<td>10,000</td>
<td>seed of random-number generator (affects packing)</td>
</tr>
<tr>
<td>(P_m ), (pk_Pm)</td>
<td>FLT</td>
<td>(0.0, (\infty))</td>
<td>NA</td>
<td>material pressure</td>
</tr>
<tr>
<td>(\varepsilon_p ), (pk_PTol)</td>
<td>FLT</td>
<td>(0.0, (\infty))</td>
<td>(1 \times 10^{-2})</td>
<td>pressure tolerance (\frac{</td>
</tr>
<tr>
<td>(\varepsilon_{im} ), (pk_ARatLimit)</td>
<td>FLT</td>
<td>(0.0, (\infty))</td>
<td>(8 \times 10^{-3})</td>
<td>step limit (parameter of (ft_eq)) packing-procedure code ({) 0, boundary contraction (}) grain scaling</td>
</tr>
<tr>
<td>(n_{im} ), (pk_stepLimit)</td>
<td>INT</td>
<td>([1, \infty))</td>
<td>25000</td>
<td></td>
</tr>
<tr>
<td>(C_p ), (pk_procCode)</td>
<td>INT</td>
<td>{0, 1}</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>(n_c ), (pk_nc)</td>
<td>FLT</td>
<td>(0.0, 1.0)</td>
<td>(0.58, 3D) (0.25, 2D) (0.35, 3D) (0.08, 2D)</td>
<td>grain-cloud porosity</td>
</tr>
</tbody>
</table>

---

**Boundary-contraction group \((C_p = 0)\):**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\mu_{CA} ), (pk_fricCA)</td>
<td>FLT</td>
<td>(0.0, (\infty))</td>
<td>0.0</td>
<td>material friction coefficient during confinement application</td>
</tr>
<tr>
<td>(v_{lim} ), (pk_vLimit)</td>
<td>FLT</td>
<td>(0.0, (\infty))</td>
<td>NA</td>
<td>servo velocity limit (see Table 9)</td>
</tr>
</tbody>
</table>

---

*pk\_seed*: affects particle arrangement
Material-Genesis Procedure (packing phase)

```python
def mpSetPackingParams
    ; Set packing parameters.
    pk_Pm = 150.0e3
    pk_procCode = 0
    pk_nc = 0.58
    ; Boundary-contraction group:
    pk_fricCA = 0.0
    pk_vLimit = 1.0
end
@mpSetPackingParams
```

```
pfc3d>@mpListMicroProps
# Material Microproperties: ....
Packing group:
    pk_seed (seed of random-number generator): 10000
    pk_Pm (material pressure): 150000
    pk_PTo1 (pressure tolerance): 0.01
    pk_lRatLimit (equilibrium-ratio limit): 0.008
    pk_stepLimit (step limit): 2000000
    pk_procCode (packing-procedure code): 0 (boundary contraction)
    pk_nc (grain-cloud porosity): 0.58
Boundary-contraction group:
    pk_fricCA (material friction coef. during confinement application): 0
    pk_vLimit (servo velocity limit): 1
    _pkORmaxLimit (overlap-ratio maximum limit): 0.25
    _pkORUpdateRate (overlap-ratio update rate, number of cycles): 100
```
Material-Genesis Procedure (packing phase)

```python
def mpSetPackingParams
    ; Set packing parameters.
    pk_Pm = 150.0e3
    pk_procCode = 0
    pk_nc = 0.58
    ; Boundary-contraction group:
    pk_fricCA = 0.0
    pk_vLimit = 1.0
end
@mpSetPackingParams
```

pfc3d>@mpListMicroProps
## Material Microproperties:  

**Packing group:**
- pk_seed (seed of random-number generator): 10000
- pk_Pm (material pressure): 150000
- pk_PCtol (pressure tolerance): 0.01
- pk_zerolim (equilibrium-ratio limit): 0.008
- pk_stepLimit (step limit): 2000000
- pk_procCode (packing-procedure code): 0 (boundary contraction)
- pk_nc (grain-cloud porosity): 0.58

**Boundary-contraction group:**
- pk_fricCA (material friction coef. during confinement application): 0
- pk_vLimit (servo velocity limit): 1
- pkORmaxLimit (overlap-ratio maximum limit): 0.25
- pkORupdateRate (overlap-ratio update rate, number of cycles): 100
Material-Genesis Procedure (packing phase)

Modify \texttt{pk\_fricCA} from 0.0 to 0.4 to increase final specimen porosity from 0.38 to 0.42.

```
def mpSetPackingParams
    ; Set packing parameters.
    pk_Pm = 150.0e3
    pk_procCode = 0
    pk_nc = 0.58
    ; Boundary-contraction group:
    pk_fricCA = 0.0
    pk_vLimit = 1.0
end
@mpSetPackingParams
```

```
pfc3d>@mpListMicroProps
## Material Microproperties:  

Packing group:
    pk_seed (seed of random-number generator): 10000
    pk_Pm (material pressure): 150000
    pk_PTol (pressure tolerance): 0.01
    pk_lRelLimit (equilibrium-ratio limit): 0.008
    pk_stepLimit (step limit): 2000000
    pk_procCode (packing-procedure code): 0 (boundary contraction)
    pk_nc (grain-cloud porosity): 0.58

Boundary-contraction group:
    pk_fricCA (material friction coef. during confinement application): 0
    pk_vLimit (servo velocity limit): 1
    _pkORmaxLimit (overlap-ratio maximum limit): 0.25
    _pkORupdateRate (overlap-ratio update rate, number of cycles): 100
```
Material-Genesis Procedure (finalization phase)

During the finalization phase:
  A. the final material properties are assigned to the grain-grain contacts, and
  B. additional material properties are specified that will be assigned to new contacts that may form during subsequent motion.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Common material parameters are listed in Table 1.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Packing parameters are listed in Table 7.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Parallel-bonded material group:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Linear group:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>[\ldots]</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parallel-bond group:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>[\ldots]</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Linear material group</strong> (for grain-grain contacts that may form subsequent to material finalization):</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Material-Genesis Procedure (finalization phase)

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

\[ g_i = 0 \]

\[ g_i = \delta \]
Material-Genesis Procedure (finalization phase)

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

Increasing the installation gap, increases the grain connectivity.
Material-Genesis Procedure (finalization phase)

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

Increasing the installation gap, increases the grain connectivity, which increases the material modulus and strength.
Material-Genesis Procedure (finalization phase)

For the bonded materials, the material properties are set to establish reference surfaces that do not overlap.

- There are no forces or moments in the material.
Material-Genesis Procedure (finalization phase)

reference surfaces

g_v > 0

g_v = 0

g_v < 0

bonded

unbonded

epoxy-cemented glass beads

The above-left case corresponds with the beads having been separated at the time of epoxy installation.
Material-Genesis Procedure (finalization phase)

For the bonded materials, the grain-vessel interface is smoothed.
- There are no forces at the grain-wall interface.

Before smoothing

After smoothing
Material-Genesis Procedure (completed)

The specimen remains within the material vessel, and the model state is saved.

For bonded materials, the specimen is removed from the material vessel, and the model state is saved.
Material-Genesis Procedure (completed)

The specimen remains within the material vessel, and the model state is saved.

For bonded materials, the specimen is removed from the material vessel, and the model state is saved.

Create contact-bonded material, demonstrate the two save states, and grain-scaling procedure.
Material-Genesis *(microstructural properties)*

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

- **Grain Size and Packing Information.** Number of grains in the model, grain-size distribution (discussed below), average and median grain diameters, vessel resolutions w.r.t. the average and median grain diameters,\(^{25}\) measurement-based porosity (defined in Section 5.1), and overlap ratios.\(^{26}\)

- **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 \((c_b)\).\(^{27}\) 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 2.7.2).
The microstructural properties of the material are computed and listed by `mpListMicroStrucProps` and include the following items.

- **Grain Size and Packing Information.** Number of grains in the model, grain-size distribution (discussed below), average and median grain diameters, vessel resolutions w.r.t. the average and median grain diameters, measurement-based porosity (defined in Section 5.1), and overlap ratios.

- **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 \( (c_b) \). 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 2.7.2).

Increasing the bond coordination number, increases the material modulus and strength.

Bond coordination number is increased by either: increasing the material pressure, or increasing the installation gap.
Material-Genesis (microstructural properties)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>mp_nGN</td>
<td>835</td>
</tr>
<tr>
<td>mp_Davg</td>
<td>0.0170003</td>
</tr>
<tr>
<td>mp_D50</td>
<td>0.0178</td>
</tr>
<tr>
<td>mp_PhiVavg</td>
<td>9.99983</td>
</tr>
<tr>
<td>mp_PhiV50</td>
<td>9.55059</td>
</tr>
<tr>
<td>mv_mn</td>
<td>0.382552</td>
</tr>
<tr>
<td>mp_ORS</td>
<td>{0.00211051, 5.38026e-07, 0.000554342}</td>
</tr>
<tr>
<td>mp_nLNC</td>
<td>360</td>
</tr>
<tr>
<td>mp_nLNgg</td>
<td>0</td>
</tr>
<tr>
<td>mp_nLNgw</td>
<td>360</td>
</tr>
</tbody>
</table>
Material-Genesis (microstructural properties)

bonded material

pfc3d> @mpListMicroStrucProps
## Material Microstructural Properties [# is "number of"]:
Grain Size and Packing Information:
   mp_nGN (# grains): 1276
   Grain-size distribution (GSD) via gsdMeasure(numBins) to create table GSD, which is displayed in view pl-GSD.
   mp_Davg (average grain diameter): 0.00488862
   mp_D50 (median grain diameter): 0.00518062
   mp_PhiVavg (vessel resolution w.r.t. mp_Davg): 10.2278
   mp_PhiV50 (vessel resolution w.r.t. mp_D50): 9.65135
   mv_mn (measurement-based porosity): 0.303652
   mp_ORs (overlap ratios {max, min, avg}): {0.0971667, 1.12196e-05, 0.019791}
Contact Information:
   mp_nLNC (# active linear-based contacts): 0
   mp_nLNgg (# active linear-based grain-grain contacts): 0
   mp_nLNgw (# active linear-based grain-wall contacts): 0
Bonded-Material Information:
   mp_CNb (bond coordination number via bcnMeasure): 6.60502
   mp_nCBb (# contact-bonded bonds): 0
   mp_nPBb (# parallel-bonded bonds): 0
   mp_nSBB (# soft-bonded bonds): 4214
   mp_nFJc (# flat-jointed contacts): 0
   mp_nFJe (# flat-jointed elements): 0
   mp_nFJb (# flat-jointed bonds): 0
# Materials (common material properties)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_{m}$, cm_matName</td>
<td>STR</td>
<td>NA</td>
<td>PFCmat</td>
<td>material name (for model title)</td>
</tr>
<tr>
<td>$N_{m5}$, cm_matNameSAV</td>
<td>STR</td>
<td>NA</td>
<td>PFCmat</td>
<td>material name (for SAV file names)</td>
</tr>
<tr>
<td>$T_{m}$, cm_matType</td>
<td>INT</td>
<td>[0,5]</td>
<td>0</td>
<td>material-type code</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0. linear</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1. contact-bonded</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2. parallel-bonded</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3. soft-bonded</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4. flat-jointed</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5. user-defined</td>
</tr>
<tr>
<td>$N_{cm}$, cm_modName</td>
<td>STR</td>
<td>NA</td>
<td>NA</td>
<td>contact-model name ($T_{m} = 5$, also redefine ft_setMatBehavior)</td>
</tr>
<tr>
<td>$\alpha$, cm_localDampFac</td>
<td>FLT</td>
<td>[0.0,0.7]</td>
<td>0.0</td>
<td>local-damping factor (for local damping)</td>
</tr>
</tbody>
</table>
# Materials (common material properties)

<table>
<thead>
<tr>
<th>Property</th>
<th>Type</th>
<th>Default Range</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_p$, cm_densityCode</td>
<td>INT</td>
<td>{0,1}</td>
<td>0</td>
</tr>
<tr>
<td>density code</td>
<td></td>
<td></td>
<td>0, grain 1, bulk</td>
</tr>
<tr>
<td>density value</td>
<td></td>
<td>$\rho$, $C_p = 0$</td>
<td></td>
</tr>
<tr>
<td>$\rho_v$, cm_densityVal</td>
<td>FLT</td>
<td>(0.0, $\infty$)</td>
<td>NA</td>
</tr>
<tr>
<td>$V_v$ is volume of vessel, and $V_g$ is total volume of grains</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Grain shape &amp; size distribution group:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$S_g$, cm_shape</td>
<td>INT</td>
<td>{0,1}</td>
<td>0</td>
</tr>
<tr>
<td>$n_{SD}$, cm_nSD</td>
<td>INT</td>
<td>$n_{SD} \geq 1$</td>
<td>NA</td>
</tr>
<tr>
<td>number of size distributions</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$T_{SD}$, cm_typeSD($n_{SD}$)</td>
<td>STR</td>
<td>{0,1}</td>
<td>0</td>
</tr>
<tr>
<td>size-distribution type</td>
<td></td>
<td>0, uniform, 1, gaussian</td>
<td></td>
</tr>
<tr>
<td>$N_s^{(j)}$, cm_ctName($n_{SD}$)</td>
<td>STR</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>$D_l^{(j)}$, cm_Dlo($n_{SD}$)</td>
<td>FLT</td>
<td>(0.0, $\infty$)</td>
<td>NA</td>
</tr>
<tr>
<td>diameter range (lower)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_u^{(j)}$, cm_Dup($n_{SD}$)</td>
<td>FLT</td>
<td>$D_u^{(j)} \geq D_l^{(j)}$</td>
<td>NA</td>
</tr>
<tr>
<td>diameter range (upper)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\phi^{(j)}$, cm_Vfrac($n_{SD}$)</td>
<td>FLT</td>
<td>(0.0,1.0]</td>
<td>NA</td>
</tr>
<tr>
<td>volume fraction ($\sum \phi^{(j)} = 1.0$)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{env}$, cm_Emult</td>
<td>FLT</td>
<td>(0.0, $\infty$)</td>
<td>1.0</td>
</tr>
<tr>
<td>diameter multiplier (shifts the size distribution)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Project**

- myMatGen.p3dvr
- myParams.p3dat
- mpParams.p3dat
- ft.p3fis

**ITASCA**
Materials (common material properties)

```python
def mpSetCommonParams
    ; Set common parameters.
    cm_matName = 'SS_ContactBonded'
    ; ** Typical sandstone (contact-bonded material).
    cm_matType = 1
    cm_localDampFac = 0.7
    cm_densityCode = 1
    cm_densityVal = 1960.0

    ; Grain shape & size distribution group:
    cm_nSD = 1
    cm_typeSD = array.create(cm_nSD)
    cm_cName = array.create(cm_nSD)
    cm_Dlo = array.create(cm_nSD)
    cm_Dup = array.create(cm_nSD)
    cm_Vfrac = array.create(cm_nSD)
    cm_Dlo(1) = 4.0e-3
    cm_Dup(1) = 6.0e-3
    cm_Vfrac(1) = 1.0
@end
```

pfc3d>mpListMicroProps
## Material Microproperties:
### Common group:
- **cm_matName**: SS_ContactBonded
- **cm_matType**: 1 (contact-bonded)
- **cm_localDampFac**: 0.7
- **cm_densityCode**: 1 (cm_densityVal is bulk density)
- **cm_densityVal**: 1960

### Grain shape & size distribution group:
- **cm_shape**: 0 (all balls)
- **cm_nSD**: 1
- **cm_typeSD**: 0 (uniform)
- **cm_Ilo**: 0.004
- **cm_Up**: 0.006
- **cm_Vfrac**: 1
- **cm_Dmult**: 1

Restore contact-bonded material, show the material name in view headers.
A given grain-size distribution (GSD) can be matched by specifying the volume fractions corresponding with the range of grain sizes — i.e., by breaking the given GSD into a finite number of uniform distributions (see Figure 14).

Restore cbonded material, change size dist. to half 1-2mm & half 4-6mm, show GSD plot.
Materials (grain-size distribution)

A given grain-size distribution (GSD) can be matched by specifying the volume fractions corresponding with the range of grain sizes — i.e., by breaking the given GSD into a finite number of uniform distributions (see Figure 14).

Restore cbonded material, shift size dist. by setting cm_Dmult = 2, show GSD plot.
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.

Figure image on next slide.

Figure 15  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).
**Material-Genesis** (microstructural plot sets)

Glass beads cemented with epoxy

Holt et al. (2005)
Material-Genesis (microstructural plot sets)

Flat-jointed material, “faced grain” plot set

Grains in the microstructural box
## Materials (linear material)

**Table 2  Linear Material Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E^*$, $\lnm_{\text{emod}}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>effective modulus</td>
</tr>
<tr>
<td>$\kappa^*$, $\lnm_{\text{krat}}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>stiffness ratio</td>
</tr>
<tr>
<td>$\mu$, $\lnm_{\text{fric}}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>friction coefficient</td>
</tr>
</tbody>
</table>

Material microproperties are listed via `@mpListMicroProps`.

Common material parameters are listed in Table 1.

Packing parameters are listed in Table 7.

**Linear material group:**

$$ (k_n, k_s) $$

---

**Edit mpParams.p3dat**

```plaintext
50 def mpSetLinParams
51 ; Set linear material parameters.
52 ; Common group (set in mpSetCommonParams)
53 ; Packing group (set in mpSetPackingParams)
54 ; Linear material group:
55  $\lnm_{\text{emod}} = 500\times10^6$
56  $\lnm_{\text{krat}} = 1.5$
57  $\lnm_{\text{fric}} = 0.5$
58 end
59 @mpSetLinParams
```

```
pfc3d>@mpListMicroProps
## Material Microproperties:

- $\lnm_{\text{emod}}$ (effective modulus): $5 \times 10^8$
- $\lnm_{\text{krat}}$ (stiffness ratio): 1.5
- $\lnm_{\text{fric}}$ (friction coefficient): 0.5
```

---

**Project**

**Data Files**

- `myMatGen.p3dvr`
- `mvParams.p3dat`
- `mpParams.p3dat`
Materials (contact-bonded material)

### Table 3  Contact-Bonded Material Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E^*$, cbm_emod</td>
<td>FLT</td>
<td>[0.0, $\infty$)</td>
<td>0.0</td>
<td>effective modulus</td>
</tr>
<tr>
<td>$\kappa^*$, cbm_krat</td>
<td>FLT</td>
<td>[0.0, $\infty$)</td>
<td>0.0</td>
<td>stiffness ratio</td>
</tr>
<tr>
<td>$\mu$, cbm_fric</td>
<td>FLT</td>
<td>[0.0, $\infty$)</td>
<td>0.0</td>
<td>friction coefficient</td>
</tr>
</tbody>
</table>

Material microproperties are listed via `@mpListMicroProps`. Common material parameters are listed in Table 1. Packing parameters are listed in Table 7.
### Materials (contact-bonded material)

#### Contact-bond group:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_i$, cbm_igap</td>
<td>FLT</td>
<td>$[0.0, \infty)$</td>
<td>0.0</td>
</tr>
<tr>
<td>$(I_\sigma)_{\text{m,sd}}$</td>
<td>FLT</td>
<td>$[0.0, \infty)$</td>
<td>0.0</td>
</tr>
<tr>
<td>cbm_tens_{m, sd}</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(S_\sigma)_{\text{m,sd}}$</td>
<td>FLT</td>
<td>$[0.0, \infty)$</td>
<td>0.0</td>
</tr>
<tr>
<td>cbm_shears_{m, sd}</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Linear material group (for grain-grain contacts that may form subsequent to material finalization):

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E^e$, lnm_emod</td>
<td>FLT</td>
<td>$[0.0, \infty)$</td>
<td>0.0</td>
</tr>
<tr>
<td>$\kappa^e$, lnm_krat</td>
<td>FLT</td>
<td>$[0.0, \infty)$</td>
<td>0.0</td>
</tr>
<tr>
<td>$\mu^e$, lnm_fric</td>
<td>FLT</td>
<td>$[0.0, \infty)$</td>
<td>0.0</td>
</tr>
</tbody>
</table>
**Materials** *(parallel-bonded material)*

### Table 4  Parallel-Bonded Material Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>E</em>, <em>pbm_emod</em></td>
<td>FLT</td>
<td>[0.0, ∞)</td>
<td>0.0</td>
<td>effective modulus</td>
</tr>
<tr>
<td><em>κ</em>, <em>pbm_krat</em></td>
<td>FLT</td>
<td>[0.0, ∞)</td>
<td>0.0</td>
<td>stiffness ratio</td>
</tr>
<tr>
<td><em>μ</em>, <em>pbm_fric</em></td>
<td>FLT</td>
<td>[0.0, ∞)</td>
<td>0.0</td>
<td>friction coefficient</td>
</tr>
</tbody>
</table>

Material microproperties are listed via `@mpListMicroProps`. Common material parameters are listed in Table 1. Packing parameters are listed in Table 7.

**Parallel-bonded material group:**

**Linear group:**

- *E*, *pbm_emod*  
- *κ*, *pbm_krat*  
- *μ*, *pbm_fric*
# Materials (parallel-bonded material)

## Parallel-bond group:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Variable</th>
<th>Type</th>
<th>Range</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g$, $p_{bm_igap}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>installation gap</td>
<td></td>
</tr>
<tr>
<td>$\lambda$, $p_{bm_rmul}$</td>
<td>FLT</td>
<td>$(0.0,\infty)$</td>
<td>1.0</td>
<td>radius multiplier</td>
<td></td>
</tr>
<tr>
<td>$E^*$, $p_{bm_bemod}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>bond effective modulus</td>
<td></td>
</tr>
<tr>
<td>$\kappa^*$, $p_{bm_bkrat}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>1.0</td>
<td>bond stiffness ratio</td>
<td></td>
</tr>
<tr>
<td>$\beta$, $p_{bm_mcf}$</td>
<td>FLT</td>
<td>$[0.0,1.0]$</td>
<td>0.0</td>
<td>moment-contribution factor</td>
<td></td>
</tr>
<tr>
<td>$(\sigma_c)<em>{\text{m,sd}}$, $p</em>{bm_ten_{m,sd}}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>${0.0,0.0}$</td>
<td>tensile-strength dist. [stress] (mean and std. deviation)</td>
<td></td>
</tr>
<tr>
<td>$(\bar{c})<em>{\text{m,sd}}$, $p</em>{bm_coh_{m,sd}}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>${0.0,0.0}$</td>
<td>cohesion dist. [stress] (mean and std. deviation)</td>
<td></td>
</tr>
<tr>
<td>$\phi$, $p_{bm_fa}$</td>
<td>FLT</td>
<td>$[0.0,90.0]$</td>
<td>0.0</td>
<td>friction angle [degrees]</td>
<td></td>
</tr>
</tbody>
</table>

## Linear material group (for grain-grain contacts that may form subsequent to material finalization):

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Variable</th>
<th>Type</th>
<th>Range</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_n^*$, $lnm_emod$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>effective modulus</td>
<td></td>
</tr>
<tr>
<td>$\kappa_n^*$, $lnm_krat$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>stiffness ratio</td>
<td></td>
</tr>
<tr>
<td>$\mu_n$, $lnm_fric$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>friction coefficient</td>
<td></td>
</tr>
</tbody>
</table>
# Materials (soft-bonded material)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g$, $\text{sbm_igap}$</td>
<td>FLT</td>
<td>$[0.0, \infty)$</td>
<td>0.0</td>
<td>installation gap</td>
</tr>
<tr>
<td>$\lambda$, $\text{sbm_rmul}$</td>
<td>FLT</td>
<td>$(0.0, \infty)$</td>
<td>1.0</td>
<td>radius multiplier</td>
</tr>
<tr>
<td>$E^*$, $\text{sbm_emod}$</td>
<td>FLT</td>
<td>$(0.0, \infty)$</td>
<td>0.0</td>
<td>effective modulus</td>
</tr>
<tr>
<td>$\kappa^*$, $\text{sbm_krat}$</td>
<td>FLT</td>
<td>$(0.0, \infty)$</td>
<td>0.0</td>
<td>stiffness ratio</td>
</tr>
<tr>
<td>$\beta$, $\text{sbm_mcf}$</td>
<td>FLT</td>
<td>$[0.0,1.0]$</td>
<td>0.0</td>
<td>moment-contribution factor</td>
</tr>
<tr>
<td>$(\sigma_{t})_{\text{ten_m,sd}}$</td>
<td>FLT</td>
<td>$(0.0, \infty)$</td>
<td>{0.0}</td>
<td>tensile-strength dist. [stress] (mean and std. deviation)</td>
</tr>
<tr>
<td>$(c)_{\text{coh_m,sd}}$</td>
<td>FLT</td>
<td>$(0.0, \infty)$</td>
<td>{0.0}</td>
<td>cohesion dist. [stress] (mean and std. deviation)</td>
</tr>
<tr>
<td>$\phi$, $\text{sbm_fa}$</td>
<td>FLT</td>
<td>$[0.0,90.0]$</td>
<td>0.0</td>
<td>friction angle [degrees]</td>
</tr>
<tr>
<td>$\zeta$, $\text{sbm_soft}$</td>
<td>FLT</td>
<td>$(0.0, \infty)$</td>
<td>0.0</td>
<td>softening factor ($\zeta = 0$ is no softening)</td>
</tr>
<tr>
<td>$\gamma$, $\text{sbm_cut}$</td>
<td>FLT</td>
<td>$[0.0,1.0]$</td>
<td>0.0</td>
<td>strength-reduction factor ($\gamma = 0/1$ is full/no softening)</td>
</tr>
</tbody>
</table>

Soft-bonded material group:

Table 5: Soft-Bonded Material Parameters

Common material parameters are listed in Table 1.

Packing parameters are listed in Table 8.

Material microproperties are listed via `@mpListMicroProps`.  

Data Files:
- myMatGen.p3dvr
- mvParams.p3dat
- mpParams.p3dat
- ft.p3fis
**Materials (soft-bonded material)**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$, $\text{sbm_fric}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>friction coefficient (when unbonded)</td>
</tr>
<tr>
<td>$\lambda_b$, $\text{sbm_bmul}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>bending-friction multiplier (when unbonded)</td>
</tr>
<tr>
<td>$\lambda_t$, $\text{sbm_tmul}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>twisting-friction multiplier (when unbonded)</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_n', \text{lnm_emod}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>effective modulus</td>
</tr>
<tr>
<td>$\kappa_n', \text{lnm_krat}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>stiffness ratio</td>
</tr>
<tr>
<td>$\mu_n$, $\text{lnm_fric}$</td>
<td>FLT</td>
<td>$[0.0,\infty)$</td>
<td>0.0</td>
<td>friction coefficient</td>
</tr>
</tbody>
</table>
## Materials (flat-jointed material)

Table 6: Flat-Jointed Material Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{jk}$, $fjm_trackMS$</td>
<td>BOOL</td>
<td>true, false</td>
<td>false</td>
<td>microstructure-tracking flag (draw microstructure with the faced grain plot set)</td>
</tr>
<tr>
<td>$g$, $fjm_igap$</td>
<td>FLT</td>
<td>[0.0, $\infty$)</td>
<td>0.0</td>
<td>installation gap</td>
</tr>
<tr>
<td>$\phi^*, fjm_B_frac$</td>
<td>FLT</td>
<td>[0.0,1.0]</td>
<td>NA</td>
<td>bonded fraction</td>
</tr>
<tr>
<td>$\phi^*, fjm_G_frac$</td>
<td>FLT</td>
<td>[0.0,1.0]</td>
<td>NA</td>
<td>gapped fraction</td>
</tr>
<tr>
<td>$(g_x)_{(u_sd)}$, $fjm_G_[m, sd]$</td>
<td>FLT</td>
<td>[0.0, $\infty$)</td>
<td>{0.0,0.0}</td>
<td>initial surface-gap distribution (mean and std. deviation)</td>
</tr>
<tr>
<td>$N$, $fjm_Nr$</td>
<td>INT</td>
<td>[1,$\infty$)</td>
<td>2</td>
<td>elements in radial direc. (2D model: total elements)</td>
</tr>
<tr>
<td>$N_s$, $fjm_Nal$</td>
<td>INT</td>
<td>[3,$\infty$)</td>
<td>4</td>
<td>elements in circumf. direc. (3D model only)</td>
</tr>
<tr>
<td>$C$, $fjm_rmulCode$</td>
<td>INT</td>
<td>{0,1,2}</td>
<td>0</td>
<td>radius-multiplier code</td>
</tr>
<tr>
<td>$\lambda$, $fjm_rmulVal$</td>
<td>FLT</td>
<td>(0.0, $\infty$)</td>
<td>1.0</td>
<td>radius-multiplier value</td>
</tr>
<tr>
<td>$\epsilon$, $fjm_emod$</td>
<td>FLT</td>
<td>[0.0, $\infty$)</td>
<td>0.0</td>
<td>effective modulus</td>
</tr>
<tr>
<td>$\kappa$, $fjm_krat$</td>
<td>FLT</td>
<td>[0.0, $\infty$)</td>
<td>0.0</td>
<td>stiffness ratio</td>
</tr>
</tbody>
</table>
# Materials (flat-jointed material)

<table>
<thead>
<tr>
<th>Name</th>
<th>Type</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$, fjm_frict</td>
<td>FLT</td>
<td>[0.0, $\infty$]</td>
<td>friction coefficient</td>
</tr>
<tr>
<td>$(\sigma_c)_{\text{mod}}$</td>
<td>FLT</td>
<td>{0.0,0.0}</td>
<td>tensile-strength dist. [stress] (mean and std. deviation)</td>
</tr>
<tr>
<td>fjm_ten_{m, sd}</td>
<td>FLT</td>
<td>{0.0,0.0}</td>
<td>cohesion dist. [stress] (mean and std. deviation)</td>
</tr>
<tr>
<td>$(c)_{\text{mod}}$</td>
<td>FLT</td>
<td>{0.0,0.0}</td>
<td>cohesion to tensile strength ratio</td>
</tr>
<tr>
<td>fjm_coh_{m, sd}</td>
<td>FLT</td>
<td>{0.0,0.0}</td>
<td>If $\gamma=0.0$, then $(c)_{\text{mod}}$ is used.</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>FLT</td>
<td>[0.0, $\infty$]</td>
<td>cohesion to tensile strength ratio</td>
</tr>
<tr>
<td>fjm_cohTenRatio</td>
<td>FLT</td>
<td>0.0</td>
<td>at each contact, set $c = \gamma \sigma_c$.</td>
</tr>
<tr>
<td>$c_r$</td>
<td>FLT</td>
<td>[0.0, $\infty$]</td>
<td>residual cohesion [stress]</td>
</tr>
<tr>
<td>fjm_cohres</td>
<td>FLT</td>
<td>0.0</td>
<td>shear-drop residual mode</td>
</tr>
<tr>
<td>$M$, fjm_resmode</td>
<td>INT</td>
<td>{0.1}</td>
<td>friction angle [degrees]</td>
</tr>
<tr>
<td>$\phi$, fjm_fa</td>
<td>FLT</td>
<td>[0.0,90.0]</td>
<td>friction angle [degrees]</td>
</tr>
</tbody>
</table>

**Linear material group** (for grain-grain contacts during packing, that are not flat-jointed, and that may form subsequent to material finalization):

<table>
<thead>
<tr>
<th>Name</th>
<th>Type</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E^*$, lnm_emod</td>
<td>FLT</td>
<td>[0.0, $\infty$]</td>
<td>effective modulus</td>
</tr>
<tr>
<td>$\kappa^*$, lnm_krat</td>
<td>FLT</td>
<td>[0.0, $\infty$]</td>
<td>stiffness ratio</td>
</tr>
<tr>
<td>$\mu^*$, lnm_fric</td>
<td>FLT</td>
<td>[0.0, $\infty$]</td>
<td>friction coefficient</td>
</tr>
</tbody>
</table>

+ Slit fraction: $\phi_s = 1 - \phi_x - \phi_o$ (0 ≤ $\phi_s$ ≤ 1).
Materials (flat-jointed material)

Microstructural Validity, valid if grain facets do not overlap

$C_{\lambda} = 0$  
$\lambda = 1$

$C_{\lambda} = 1$  
$\lambda$ varies

$C_{\lambda} = 2$  
$\lambda = 0.54$

Figure 12  The three types of flat-jointed microstructures produced by the material-modeling support package. The left-most images have invalid microstructures, while the middle and right images have valid microstructures. Only a single faced grain is shown for the 3D case (bottom).
Crack-Monitoring Package

Damage in the bonded materials consists of bond breakages, which we denote as cracks. Crack data is stored as a Discrete Fracture Network (DFN), and the DFN plot item supports visualization of the cracks. Each crack has a type (contact bonded, parallel bonded, flat jointed or smooth jointed) and failure mode (tensile or shear).

The type and failure mode of all cracks are stored in the group name of the CrackData-DFN, and the numbers of these items are stored in the crack count global variables.

\[
\text{ck}_n\text{All, } \text{ck}_n\{\text{CB, PB, SB, FJ, SJ}\}\{t, s\}
\]
Crack-Monitoring Package

A crack is a disk for the 3D model and a segment of unit-thickness depth for the 2D model.
Crack-Monitoring Package

A crack is a disk for the 3D model and a segment of unit-thickness depth for the 2D model.

<table>
<thead>
<tr>
<th>Ball group 1</th>
<th>Fracture group 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Balls (1276)</td>
<td>Fractures (88)</td>
</tr>
<tr>
<td>ttGripBottom</td>
<td>CB-tenFail</td>
</tr>
<tr>
<td>ttGripTop</td>
<td></td>
</tr>
</tbody>
</table>

**PFC3D 6.00**
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Mechanical step: 8267

SS ContactBonded material, Direct-tension test (eRate = 0.05 s⁻¹), end of load stage 1.
Tension Test Specimen
Crack-Monitoring Package

A crack is a disk for the 3D model and a segment of unit-thickness depth for the 2D model.
Crack-Monitoring Package

“crack” plot set, displays cracks with thickness proportional to gap.

Figure 17 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.
Crack-Monitoring Package

“crack” plot set, displays cracks with thickness proportional to gap.

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 18  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.
Lab-Testing Procedures (stress-strain-porosity)

### Table 8 Material-Vessel Stress, Strain and Porosity Quantities

<table>
<thead>
<tr>
<th>Quantity, FISH</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>${\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz}}$, mv_ms{xx,yy,zz,xy,xz,yz}</td>
<td>material stress&lt;br&gt;(2D model: $\sigma_{zz} \equiv \sigma_{xz} \equiv \sigma_{yz} \equiv 0$)</td>
</tr>
<tr>
<td>${\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{xy}, \varepsilon_{xz}, \varepsilon_{yz}}$, mv_me{xx,yy,zz,xy,xz,yz}</td>
<td>material strain&lt;br&gt;(2D model: $\varepsilon_{zz} \equiv \varepsilon_{xz} \equiv \varepsilon_{yz} \equiv 0$)</td>
</tr>
<tr>
<td>${\sigma_a, \sigma_r}$, mv_ms{a,r}</td>
<td>axial &amp; radial stress</td>
</tr>
<tr>
<td>${\varepsilon_a, \varepsilon_r}$, mv_me{a,r}</td>
<td>axial &amp; radial strain</td>
</tr>
<tr>
<td>$\sigma_d$, mv_msd</td>
<td>deviator stress</td>
</tr>
<tr>
<td>$\sigma_m$, mv_msm</td>
<td>mean stress</td>
</tr>
<tr>
<td>$\varepsilon_d$, mv_med</td>
<td>deviator strain</td>
</tr>
<tr>
<td>$\varepsilon_v$, mv_mev</td>
<td>volumetric strain</td>
</tr>
<tr>
<td>$n$, mv_mn</td>
<td>measurement-based porosity</td>
</tr>
<tr>
<td>$n_w$, mv_wn</td>
<td>wall-based porosity</td>
</tr>
</tbody>
</table>

3 measurement spheres
Lab-Testing Procedures (stress-strain-porosity)

We denote stress and strain by

\[
\text{stress: } \left\{ \sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz} \right\} \\
\text{strain: } \left\{ \varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{xy}, \varepsilon_{xz}, \varepsilon_{yz} \right\}
\]

(4)

where \( \sigma_{ii} > 0 \) is tension and \( \varepsilon_{ii} > 0 \) is extension. For the 2D model, the out-of-plane stress and strain components are equal to zero so that stress is \( \left\{ \sigma_{xx}, \sigma_{yy}, \sigma_{xy} \right\} \) and strain is \( \left\{ \varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{xy} \right\} \).

The three measurement techniques measure the following quantities:

\[
\sigma_{ij}^m \quad \varepsilon_{ij}^m \quad \text{measurement-based} \quad (6 \text{ terms each, symmetric}) \\
\sigma_k^w \quad \varepsilon_k^w \quad \text{wall-based} \quad (3 \text{ terms each}) \\
\varepsilon_{ik}^g \quad (i,j=\{x,y,z\}, k=\{x,y,z,r\}) \quad \text{guage-based} \quad (3 \text{ terms})
\]
Lab-Testing Procedures (summary)

\[ |v| = \frac{1}{2} \dot{\varepsilon}_a h_o \]

\( h_o \) (initial ht. in axial direc.)

**Figure 23** Loading conditions of laboratory-testing procedures.
Lab-Testing Procedures (compression test)

The axial walls act as loading platens, and the velocities of the radial walls are controlled by a servomechanism to maintain a constant confining stress.

polyaxial loading  triaxial loading

Specimen may have been created in physical vessel or carved out of a material block.
Lab-Testing Procedures (compression test)

There is a seating phase followed by a loading phase.
- **Seating phase:** strains reset to zero, confining pressure applied.
- **Loading phase:** strains reset to zero, axial strain applied.

The loading phase may consist either of a single stage that ends when the applied deviatoric stress falls below a specified fraction of its peak value or multiple stages during which the axial-strain increments are specified.

During the test, the crack-monitoring package is on (for bonded materials), and specimen behavior is monitored using the history mechanism to store relevant quantities.
Lab-Testing Procedures (compression test)

**Table 10 Compression-Test Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
</table>
| $I, \text{ ct_testType}$ | INT | $\{0, 1, 2\}$ | 0 | test-type code
| $P, \text{ ct_Pc}$ | FLT | $(0.0, \infty)$ | NA | confining pressure ($P_c > 0$ is compression)
| $\dot{\varepsilon}, \text{ ct_eRate}$ | FLT | $(0.0, \infty)$ | NA | axial strain rate ($|\dot{\varepsilon}| = \frac{1}{2} \dot{\varepsilon} h, \varepsilon > 0$, see Figure 23 and Section 5.4)
| $C, \text{ ct_loadCode}$ | INT | $\{0, 1\}$ | 0 | loading-phase code
| $\sigma, \text{ ct_loadFac}$ | FLT | $(0.0, 1.0)$ | 0.9 | load-termination factor ($C_l = 0$) for termination criterion: $\sigma^2 \leq \alpha \sigma^2_{\text{lim}}$

**Servo-control group:**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
</table>
| $\varepsilon_p, \text{ ct_PTo1}$ | FLT | $(0.0, \infty)$ | pk_PTo1 | pressure tolerance $\frac{|P-P_c|}{P_c} \leq \varepsilon_p$
| $\epsilon_{\text{eq}}, \text{ ct_ARatLimit}$ | FLT | $(0.0, \infty)$ | $1 \times 10^{-3}$ | equilibrium-ratio limit (parameter of ft_equ)
| $n_{\text{eq}}, \text{ ct_stepLimit}$ | INT | $[1, \infty]$ | pk_stepLimit | step limit (parameter of ft_equ)
| $v_{\text{eq}}, \text{ ct_vLimit}$ | FLT | $(0.0, \infty)$ | $10 H \dot{\varepsilon}_a$ | servo velocity limit (see Table 9)

Material-vessel parameters are listed in Table 6.

Perform compression test on contact-bonded material.

axial strain rate, must be slow enough to obtain quasi-static response
Lab-Testing Procs. *(diametral-compression test)*

The specimen is compressed between walls that act as loading platens while monitoring the wall-based axial force & displacement.

**Table 11 Diametral-Compression Test Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( { !w, !d } ), dc_{{ !w, !d }}</td>
<td>FLT</td>
<td>(0.0, ( \infty ))</td>
<td>NA</td>
<td>platen width and depth (2D model: ( d = 1 ))</td>
</tr>
<tr>
<td>( g_0 ), dc_{g0}</td>
<td>FLT</td>
<td>(0.0, ( \infty ))</td>
<td>NA</td>
<td>initial platen gap</td>
</tr>
<tr>
<td>( E_p ), dc_{emod}</td>
<td>FLT</td>
<td>(0.0, ( \infty ))</td>
<td>( m_v ) _emod or NA</td>
<td>platen effective modulus (used by linear contact model)</td>
</tr>
<tr>
<td>( \varepsilon_\alpha ), dc_{erRate}</td>
<td>FLT</td>
<td>(0.0, ( \infty ))</td>
<td>NA</td>
<td>axial strain rate ( (</td>
</tr>
<tr>
<td>( C_j ), dc_{loadCode}</td>
<td>INT</td>
<td>{0, 1}</td>
<td>0</td>
<td>loading-phase code { 0. single stage \ 1. multiple stages }</td>
</tr>
<tr>
<td>( \varepsilon_{\text{term}} ), dc_{ARatLimit}</td>
<td>FLT</td>
<td>(0, ( \infty ))</td>
<td>( 1 \times 10^{-5} )</td>
<td>equilibrium-ratio limit (parameter of ft_eq)</td>
</tr>
<tr>
<td>( \alpha ), dc_{stepLimit}</td>
<td>INT</td>
<td>[1.0, ( \infty ))</td>
<td>( \text{pk \ stepLimit} ) or ( 2 \times 10^6 )</td>
<td>step limit (parameter of ft_eq)</td>
</tr>
</tbody>
</table>

**Static-equilibrium group:**

- \( \varepsilon_{\text{term}} \), dc_{ARatLimit}  
- \( \alpha \), dc_{stepLimit}  

**Figure 18 Loading configuration of diametral-compression test.**

Perform diametral-compression test on contact-bonded material.
Lab-Testing Procedures (direct-tension test)

The specimen is gripped at its end (via grip grains) and pulled apart slowly while monitoring the axial stress and strain using the measurement-based quantities.

**Table 12 Direct-Tension Test Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Range</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_g$, tt_tg</td>
<td>FLT</td>
<td>$(0.0, \infty)$</td>
<td>0.1H</td>
<td>grip thickness</td>
</tr>
<tr>
<td>$\dot{\varepsilon}_a$, tt_eRate</td>
<td>FLT</td>
<td>$(0.0, \infty)$</td>
<td>NA</td>
<td>axial strain rate</td>
</tr>
<tr>
<td>$C_l$, tt_loadCode</td>
<td>INT</td>
<td>{0,1}</td>
<td>0</td>
<td>loading-phase code</td>
</tr>
<tr>
<td>$\alpha$, tt_loadFac</td>
<td>FLT</td>
<td>$(0.0,1.0)$</td>
<td>0.9</td>
<td>load-termination factor $(C_l = 0)$</td>
</tr>
</tbody>
</table>

Material-vessel parameters are listed in Table 6.

Specimen may have been created in physical vessel or carved out of a material block.
Example Materials

Each example serves as a base case, and provides a material at the lowest resolution sufficient to demonstrate system behavior. There is a material-generation project for each material, and these projects are in the `fistPkgN/ExampleProjects/MatGen-M` directory. There are separate 2D and 3D projects for each material, and both projects are contained within the same example-project directory.
Example Materials

Each example serves as a base case, and provides a material at the lowest resolution sufficient to demonstrate system behavior. There is a material-genesis project for each material, and these projects are in the fistPkgN/ExampleProjects/MatGen-M directory. There are separate 2D and 3D projects for each material, and both projects are contained within the same example-project directory.

When constructing a PFC material, start with the corresponding example project and modify it as necessary.
Example Materials

Each example serves as a base case, and provides a material at the lowest resolution sufficient to demonstrate system behavior. There is a material-genesis project for each material, and these projects are in the fistPkgN/ExampleProjects/MatGen-M directory. There are separate 2D and 3D projects for each material, and both projects are contained within the same example-project directory.

When constructing a PFC material, start with the corresponding example project and modify it as necessary.

Clumped materials are created by calling mpParams-Clumped.p{2,3}dat.
Example Materials (linear material)

1.1 Linear Material Example

The linear material example is in the MatGen-Linear example-project directory. A linear material is created to represent a typical aggregate base layer of an asphalt-surface roadway (Potyondy et al., 2016). We denote our aggregate material as the AG_Linear material with microproperties listed in Table 1. The material is created in a cylindrical material vessel (of initial 240-mm height and 170-mm diameter, with a 500 MPa effective modulus) and packed at a 150 kPa material pressure via the boundary-contraction packing procedure as shown in Figure 1. The material is then subjected to triaxial testing. During the triaxial test, the confinement is 150 kPa, and a load-unload cycle is performed at an axial strain of 0.05% to measure the resilient modulus (see Figure 2). The hysteretic response is the expected behavior, and the resilient modulus is similar to the effective modulus of the linear material.
### Example Materials (linear material)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Common group:</strong></td>
<td></td>
</tr>
<tr>
<td>$N_m$</td>
<td>AG_Linear</td>
</tr>
<tr>
<td>$T_m$, $\alpha$, $C_p$, $\rho_v ,[\text{kg/m}^3]$</td>
<td>0, 0.7, 0, 2650</td>
</tr>
<tr>
<td>$S_g$, $T_{SD}$, ${D_{{i,u}} ,[\text{mm}], \phi}$, $D_{mult}$</td>
<td>0, 0, ${14,20,1}$, 1.0</td>
</tr>
<tr>
<td><strong>Packing group:</strong></td>
<td></td>
</tr>
<tr>
<td>$S_{RN}$, $P_m ,[\text{kPa}]$, $\varepsilon_p$, $\varepsilon_{lim}$, $n_{lim}$</td>
<td>100000, 150, $1 \times 10^{-2}$, $8 \times 10^{-3}$, $2 \times 10^6$</td>
</tr>
<tr>
<td>$C_p$, $n_c$, $\mu_{Ca}$, $v_{lim} ,[\text{m/s}]$</td>
<td>0, 0.58, 0, 1.0</td>
</tr>
<tr>
<td><strong>Linear material group:</strong></td>
<td></td>
</tr>
<tr>
<td>$E^* ,[\text{MPa}]$, $\kappa^*$, $\mu$</td>
<td>500, 1.5, 0.4</td>
</tr>
</tbody>
</table>

* Linear material parameters are defined in Table 2 of the base memo.
Example Materials (linear material)

Figure 1  AG_Linear material packed at 150 kPa material pressure at the end of material genesis.
Example Materials (linear material)

Figure 2  Deviator stress versus axial strain for AG_Linear material tested at 150 kPa confinement, and measurement of resilient modulus.

\[ P_c = 150 \text{ kPa}, \quad \dot{e}_a = 0.01 \text{ s}^{-1} \]

\[ M_R \approx \frac{7.7 \times 10^4 \text{ Pa}}{(5.0 - 0.75) \times 10^{-4}} \approx 181 \text{ MPa} \]
Example Materials (contact-bonded material)

1.3 Contact-Bonded Material Example

The contact-bonded material example is in the MatGen-ContactBonded example-project directory. A contact-bonded material is created to represent a typical sandstone, which we take to be Castlegate sandstone.\(^4\) We denote our sandstone material as the SS_ContactBonded material with microproperties listed in Table 5. The material is created in a cubic material vessel (of 50 mm side length, with a 3 GPa effective modulus). The grain-scaling packing procedure is used to pack the grains to a 30 MPa material pressure, and then contact bonds are added between all grains that are in contact with one another (see Figure 11). The material is then subjected to compression, diametral-compression and direct-tension tests. The test results are shown in Figures 12–18.

\(^4\) The following properties are typical of Castlegate sandstone: density of 1960 kg/m\(^3\); median grain size of 0.19 mm; direct-tension strength of 1.0 MPa; unconfined-compressive strength of 20.0 MPa; and Young’s modulus and Poisson’s ratio measured during unconfined-compression test of 2.9 GPa and 0.33, respectively.
Table 5  Microproperties of SS_ContactBonded Material*

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Common group:</td>
<td></td>
</tr>
<tr>
<td>$N_m$</td>
<td>SS_ContactBonded</td>
</tr>
<tr>
<td>$T_m$, $\alpha$, $C_p$, $\rho_v$ [$\text{kg/m}^3$]</td>
<td>1, 0.7, 1, 1960</td>
</tr>
<tr>
<td>$S_g$, $T_{sd}$, ${D_{l,w}}$ [mm], $\phi$, $D_{nlt}$</td>
<td>0, 0, ${4.0,6.0,1.0}$, 1.0</td>
</tr>
<tr>
<td>Packing group:</td>
<td></td>
</tr>
<tr>
<td>$S_{RN}$, $P_m$ [MPa], $\varepsilon_p$, $\varepsilon_{lim}$, $n_{lim}$</td>
<td>10000, 30, $1 \times 10^{-2}$, $8 \times 10^{-3}$, $2 \times 10^6$</td>
</tr>
<tr>
<td>$C_p$, $n_c$</td>
<td>1, 0.30</td>
</tr>
<tr>
<td>Contact-bonded material group:</td>
<td></td>
</tr>
<tr>
<td>Linear group:</td>
<td></td>
</tr>
<tr>
<td>$E^<em>$ [GPa], $\kappa^</em>$, $\mu$</td>
<td>3.0, 1.5, 0.4</td>
</tr>
<tr>
<td>Contact-bond group:</td>
<td></td>
</tr>
<tr>
<td>$g$, [mm]</td>
<td>0</td>
</tr>
<tr>
<td>$(T_\circ)<em>{(m,w)}$ [MPa], $(S</em>\circ)_{(m,w)}$ [MPa]</td>
<td>${10,0}$, ${20,0}$</td>
</tr>
<tr>
<td>Linear material group:</td>
<td></td>
</tr>
<tr>
<td>$E_n^<em>$ [GPa], $\kappa_n^</em>$, $\mu_n$</td>
<td>3.0, 1.5, 0.4</td>
</tr>
</tbody>
</table>

* Contact-bonded material parameters are defined in Table 3 of the base memo.
Example Materials (contact-bonded material)

$E_v^* = 3.0 \text{ GPa}$

cube, $s = 50 \text{ mm}$

$P_m = 30 \text{ MPa}$
$g_i = 0$

**SS** ContactBonded
1276 grains, $c_b = 6.1$
$\tilde{D} = 4.8 \text{ mm}$, $D_{50} = 5.1 \text{ mm}$

cube, $s = 20 \text{ mm}$

contact bonds as lines

*Figure 11*  SS ContactBonded material at the end of material genesis with grains and contact bonds in the microstructural box.
**Example Materials** *(contact-bonded material)*

**Increasing the bond coordination number, increases the material modulus and strength.**

\[
E_v^* = 3.0 \text{ GPa}
\]

\[
P_m = 30 \text{ MPa}
\]

\[
g_i = 0
\]

Bond coordination number is increased by either: increasing the material pressure, or increasing the installation gap.
Example Materials (contact-bonded material)

\[ P_c = 0, \ \dot{\varepsilon}_a = 0.05 \text{ s}^{-1} \]

Figure 12  SS_ContactBonded material at the end of the fully unconfined test with grains and cracks.
Example Materials (contact-bonded material)

Figure 13  Deviator stress versus axial strain for SS_ContactBonded material tested fully unconfined, and measurement of peak strength and Young’s modulus.
Example Materials (contact-bonded material)

Figure 14  Radial strain versus axial strain for SS_ConactBonded material tested fully unconfined, and measurement of Poisson’s ratio.
Example Materials (contact-bonded material)

Figure 15  SS_ContactBonded material at the end of diametral-compression test with grains and cracks.
Example Materials (contact-bonded material)

**Figure 16** Axial force versus axial displacement for SS_ContactBonded material during the diametral-compression test, and measurement of Brazilian tensile strength.
Example Materials (contact-bonded material)

*Figure 17*  *SS_CondtBonded material at the end of the direct-tension test with grains and cracks.*
Example Materials (contact-bonded material)

Figure 18  Axial stress versus axial strain for SS_ConactBonded material during the direct-tension test, and measurement of tensile strength.
Conclusion

The PFC model provides a synthetic material consisting of an assembly of rigid grains that interact at contacts. This synthetic material encompasses a vast microstructural space, and only a small portion of this space has been explored.

The PFC FISHTank provides a state of the art embodiment of four well-defined materials and a user-defined material to support:

- **practical applications** (via boundary-value models made from these materials), and
- **scientific inquiry** (via further exploration of this microstructural space).
Future Webinars

- **Future webinars** will introduce the BPM methodology, and discuss how to calibrate a BPM to match behavior of a particular rock.
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*Stay tuned for more...*

For now, calibration notes and material behavior: