Material-Modeling Support for PFC

David Potyondy

Originally: Itasca Webinar (December 14, 2017)
Updated for fistPkg26 & fistPkg6.N
April 5, 2019

Preamble

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

Potyondy, D.O. (2015) "The Bonded-Particle Model as a Tool for Rock Mechanics Research and Application: Current Trends and Future Directions," *Geosystem Engineering*, ***18****(1)*, 1–28.

Preamble

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

Potyondy, D. (2017) "Material-Modeling Support in PFC [fistPkg25]," Itasca Consulting Group, Inc., Technical Memorandum ICG7766-L (March 16, 2017), Minneapolis, Minnesota.

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

fistPkg for PFC version 6 is fistPkg6.N, where N is package version number

Potyondy, D. (2019) "Material-Modeling Support in PFC [fistPkg6.5]," Itasca Consulting Group, Inc., Technical Memorandum ICG7766-L (April 5, 2019), Minneapolis, Minnesota.

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:

Potyondy, D. (2018) "Calibration of the Flat-Jointed Material," PowerPoint Slide Set (April, 13, 2018).

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.

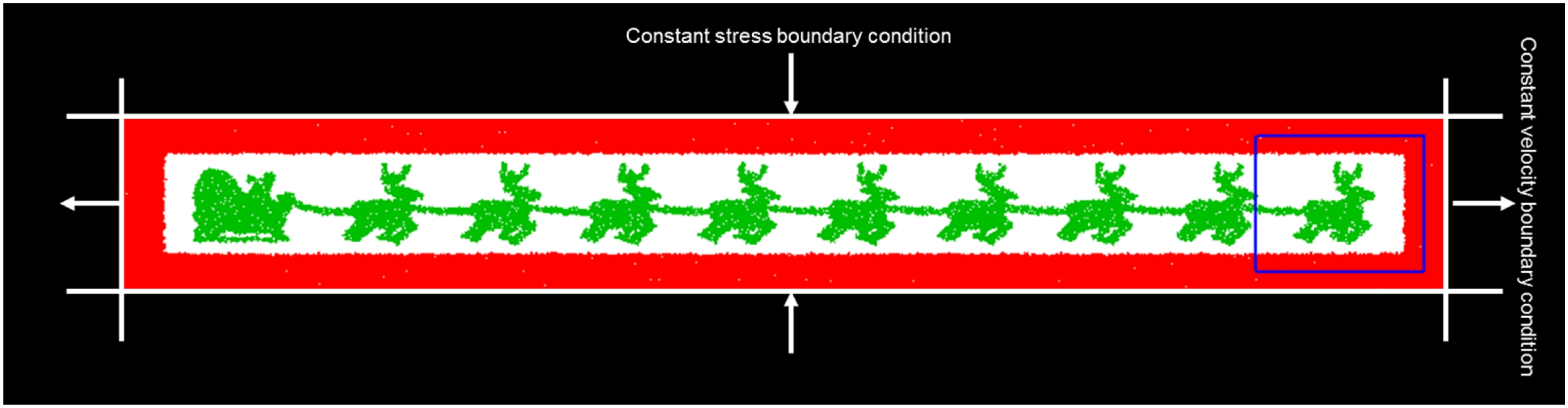
Overview

Bonded-Particle Modeling (Essential Features)

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

Material-Modeling Support Package (Hands-On, usage)

Bonded-Particle Modeling (Essential Features)



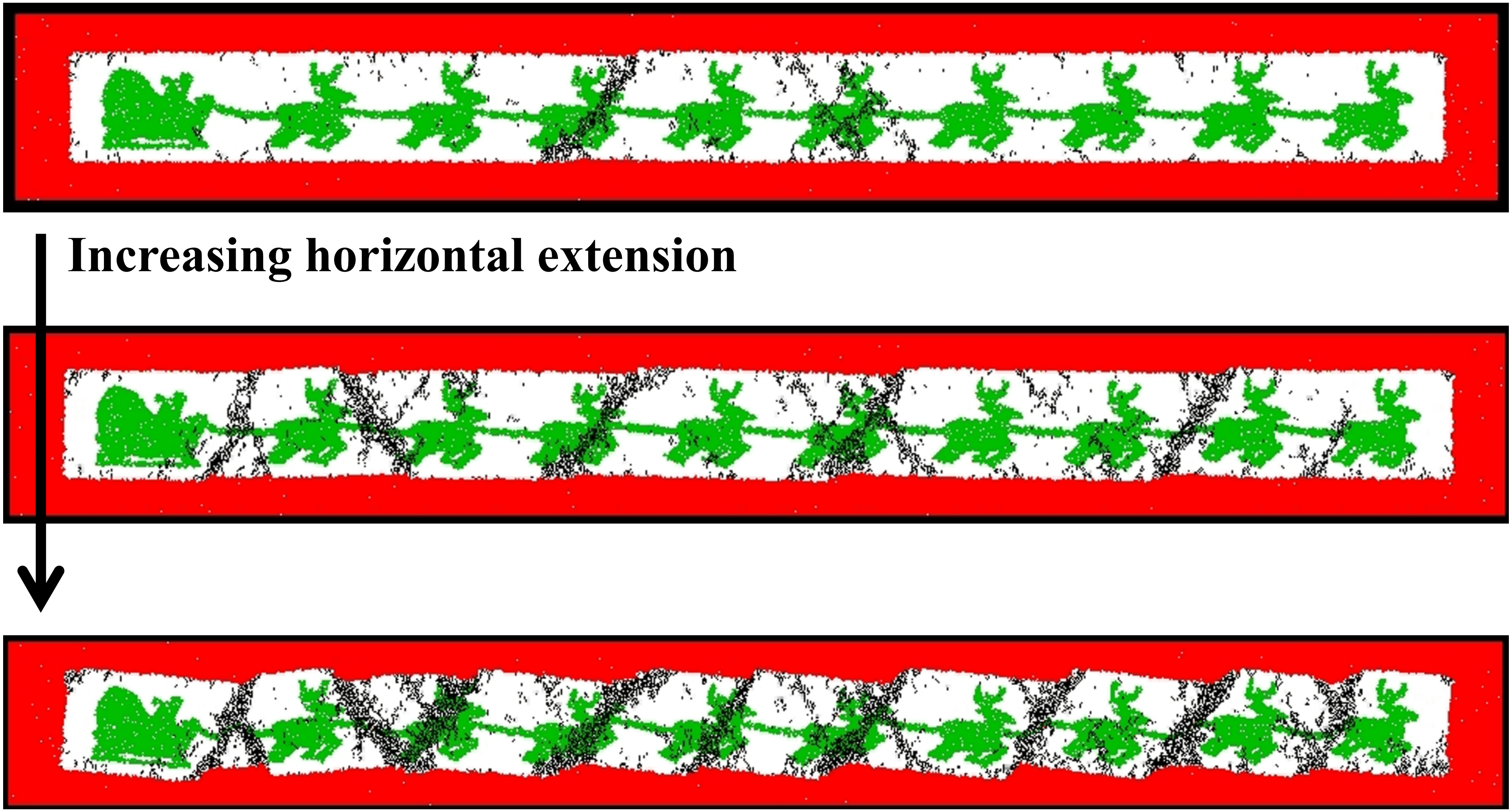
From Martin Schöpfer

■ ■

Structural-geology application

Schöpfer, M.P.J. et al. (2017) “The Emergence of Asymmetric Normal Fault Systems under Symmetric Boundary Conditions,” *Journal of Structural Geology*, ***104***, 159–171.

Bonded-Particle Modeling (Essential Features)



Bonded-Particle Modeling (Essential Features)

6

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.

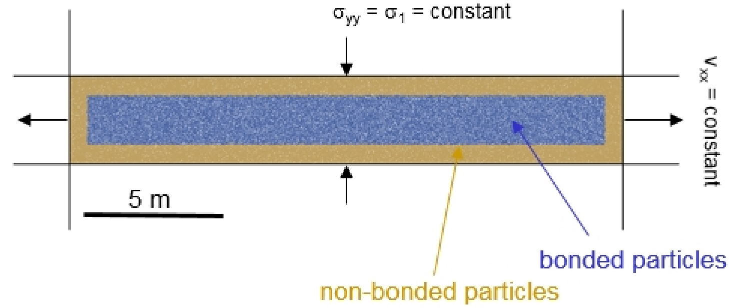
Symmetric fault system

Photo: B. Grasemann Quartzitic Marble, Serifos, Greece

Asymmetric fault system

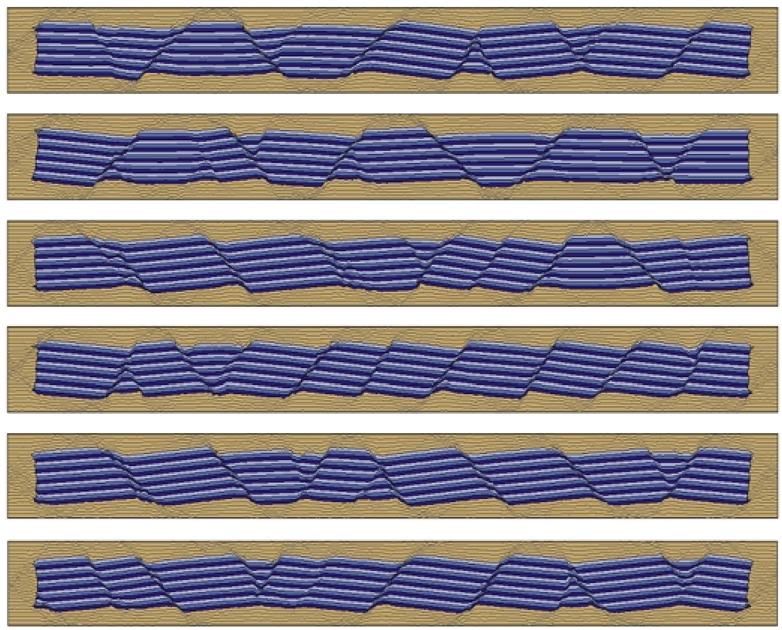
Photo: B. Grasemann Pegmatitic dyke in marble, Naxos, Greece

2D DEM model boundary conditions



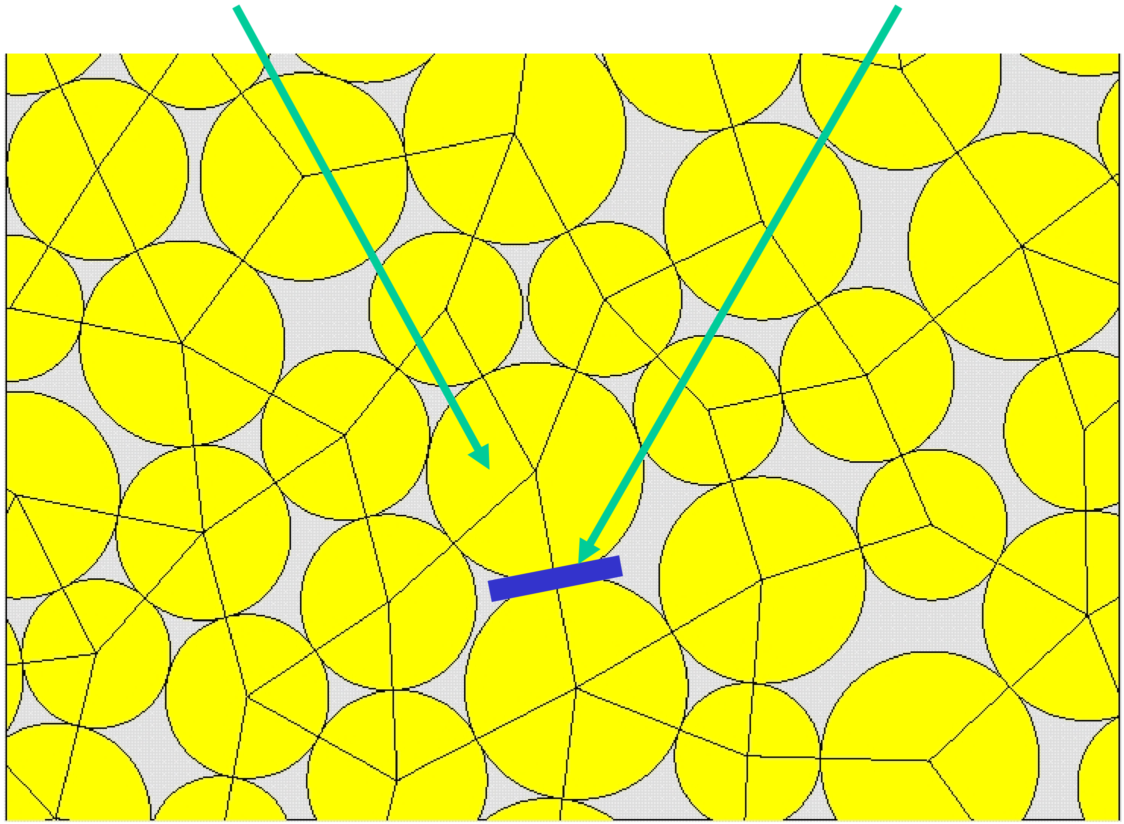
Six realisations at 10% extension

Passive markers obtained by intersecting triangulation of particle centres with initially horizontal lines



From Martin Schöpfer: science

Essential Features of a BPM

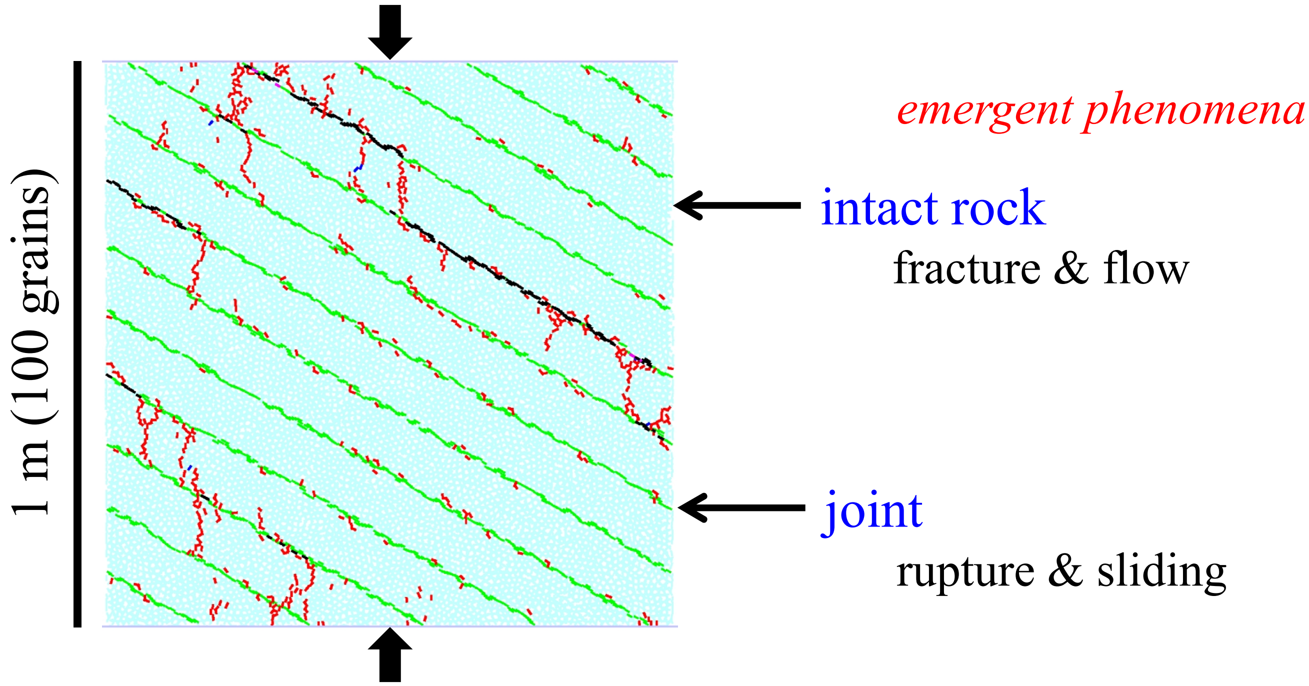


Damage consists of bond breakages.

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

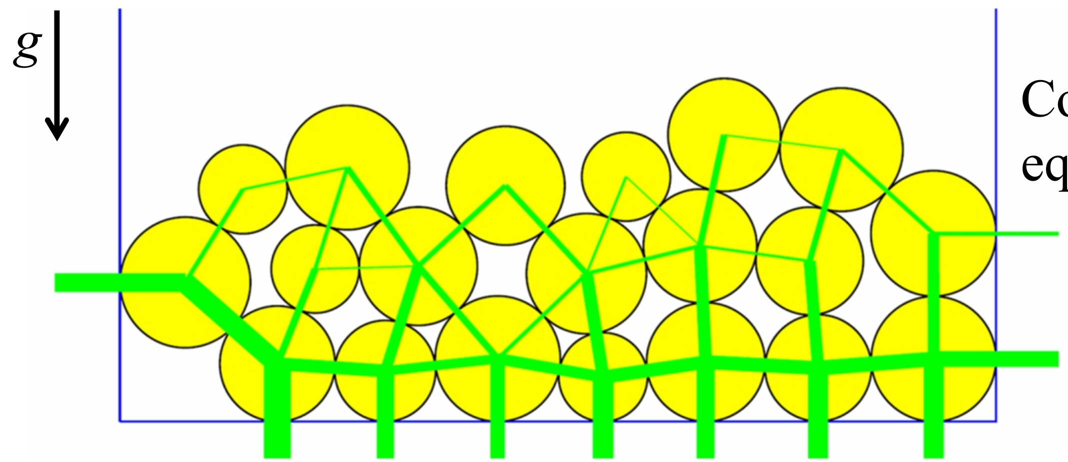


Damage consists of bond breakages.

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.

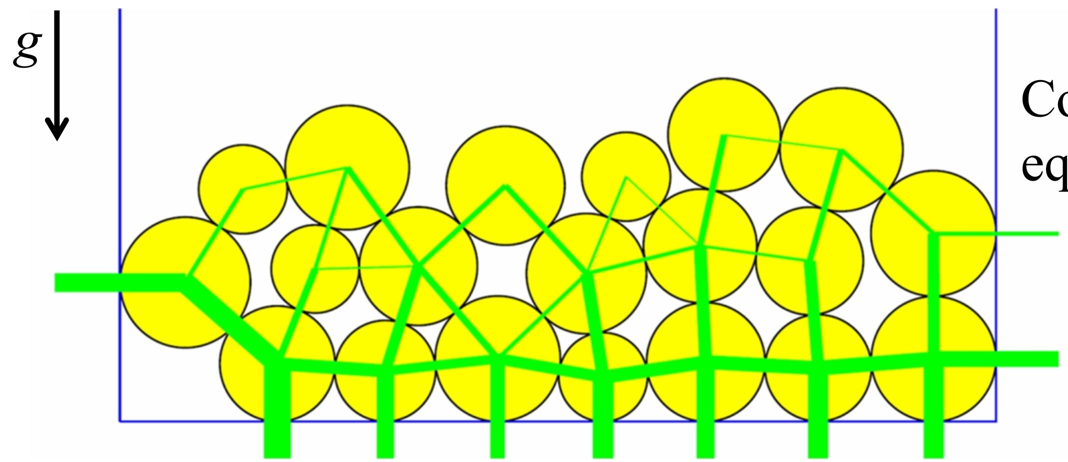


Contact forces are equal & opposite

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.

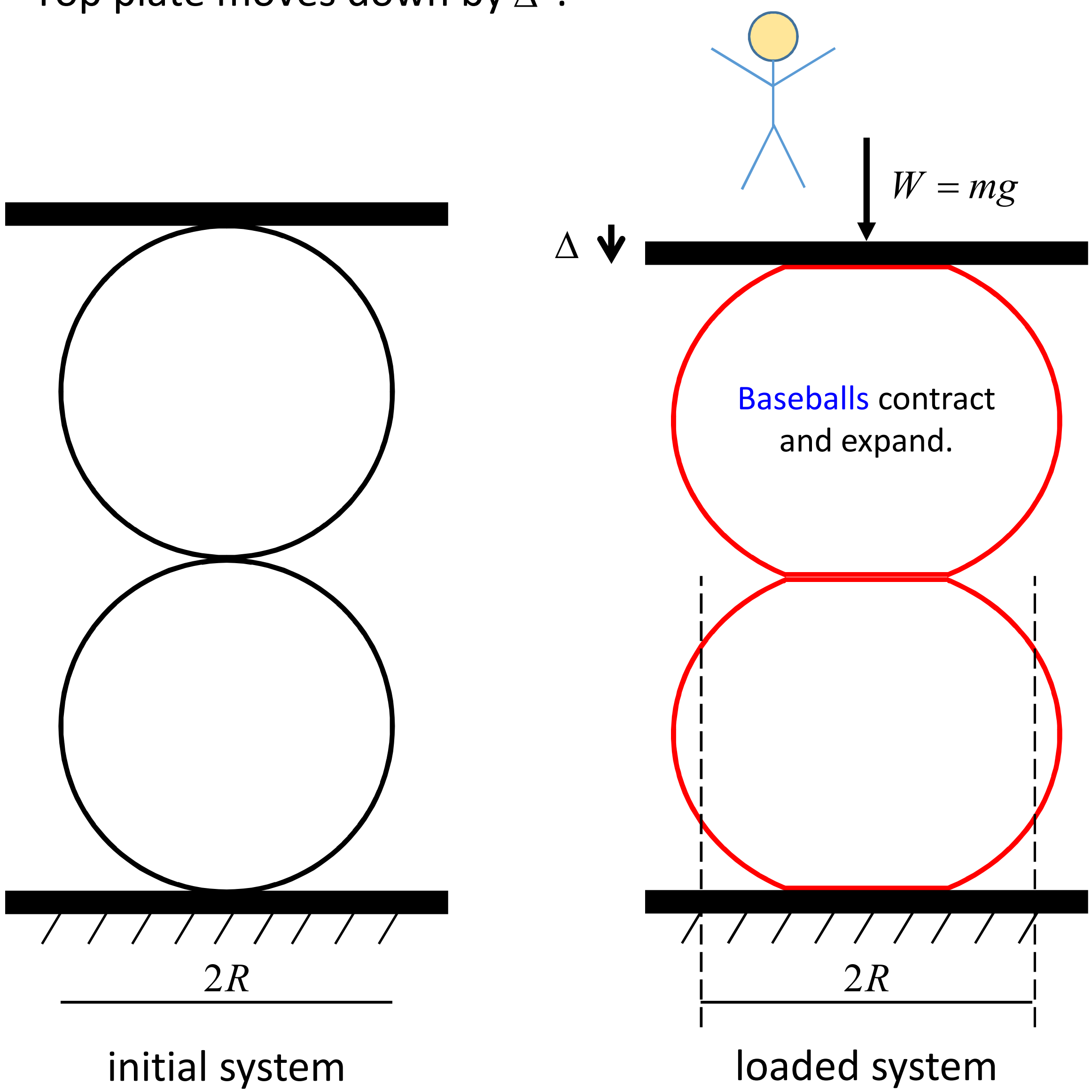
Contact mechanics is embodied in particle-interaction laws that employ a soft-contact approach for which all deformation occurs at the contacts between the rigid bodies. The particle-interaction law (contact model) updates the internal force and moment.



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 Δ .



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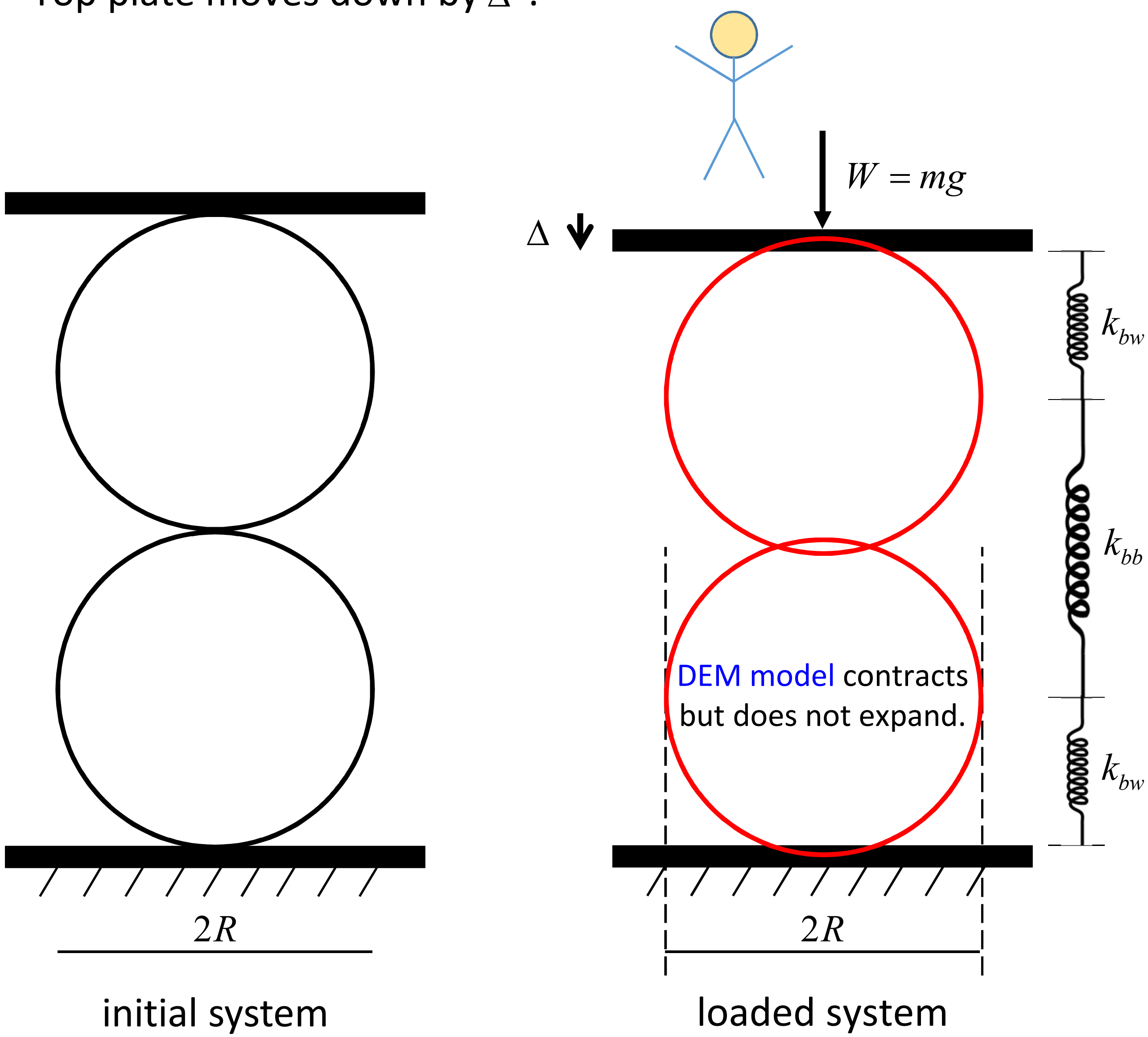


DEM model employs a "soft contact" approach:

all deformation occurs at the contacts between the rigid bodies.

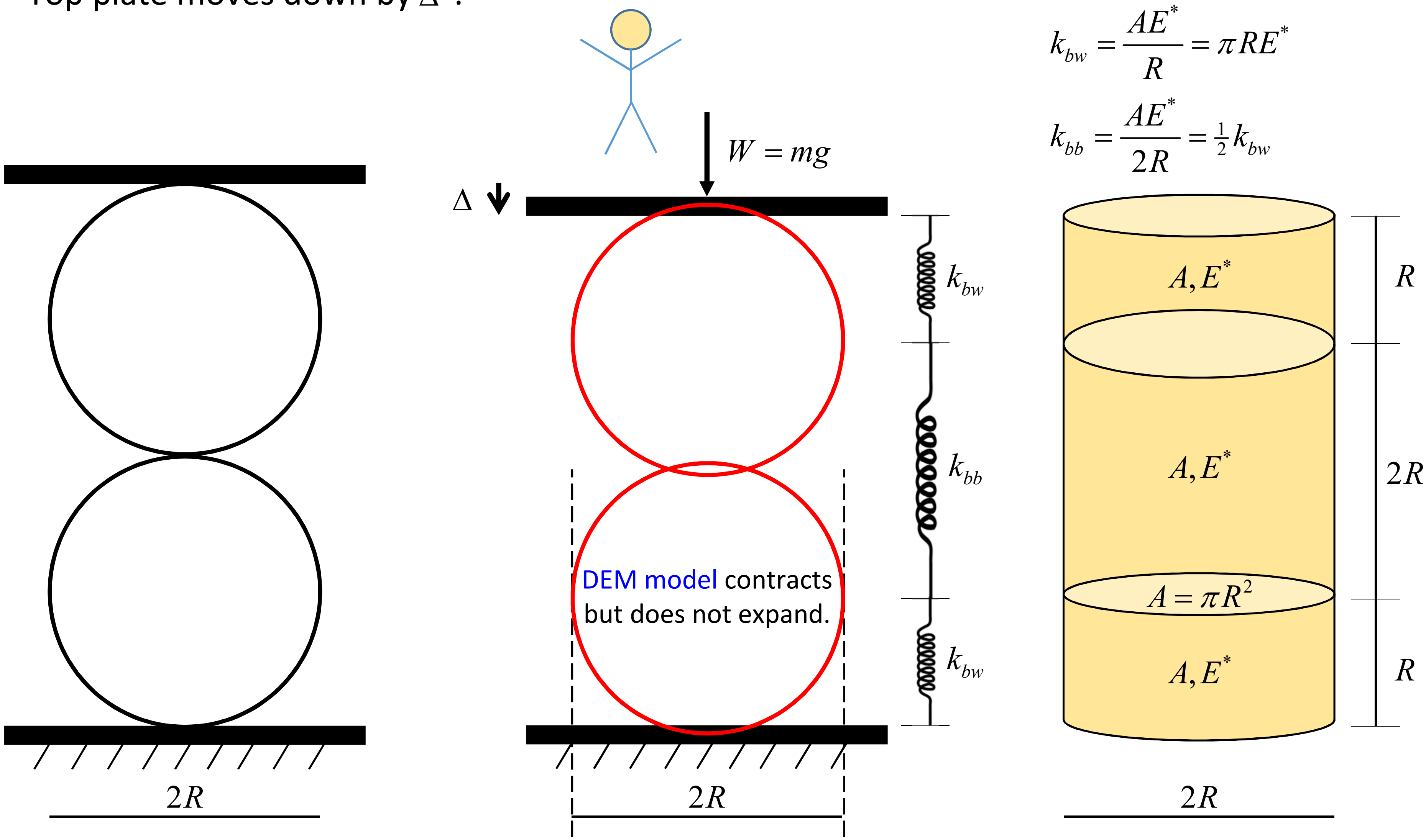
The stiffnesses can be related to the effective modulus of an equivalent continuum. . .

soft-contact approach

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

$$k_{bw} = \frac{AE^*}{R} = \pi R E^*$$

$$k_{bb} = \frac{AE^*}{2R} = \tfrac{1}{2} k_{bw}$$



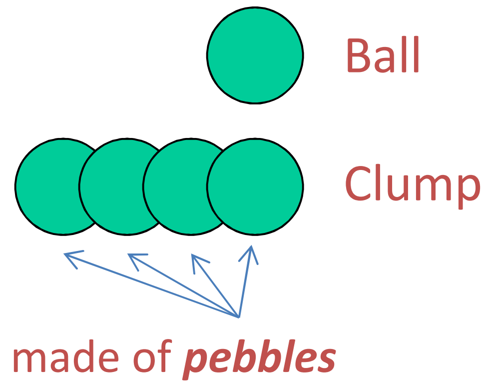
initial system loaded system equivalent continuum

Bonded-Particle Modeling Methodology (PFC model)

PFC model provides three basic entities:

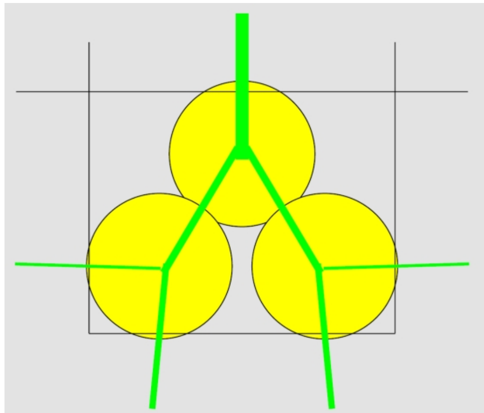
balls and clumps

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



walls

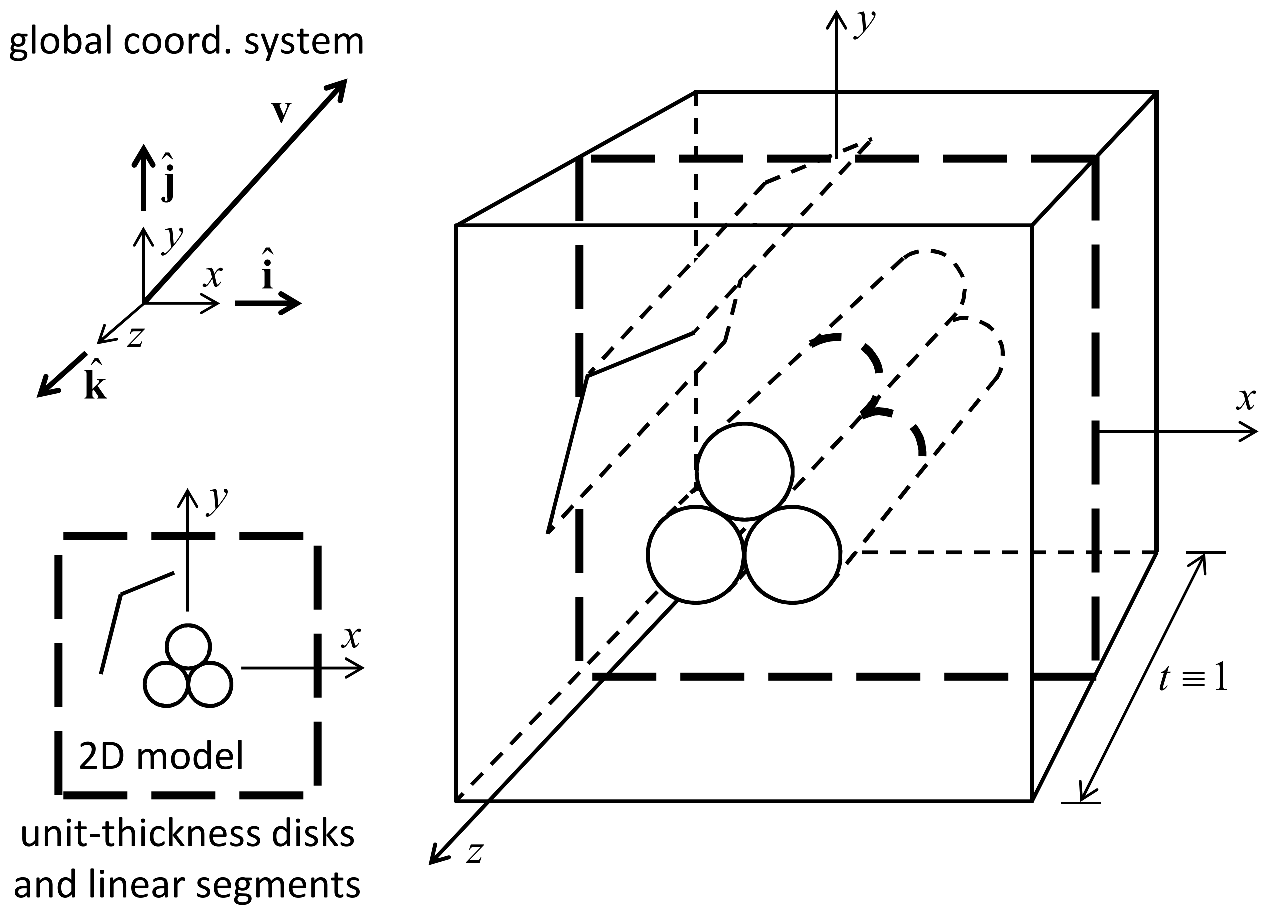
- do not obey laws of motion
- used to apply velocity boundary conditions
- interact *only* with balls and clumps
- made of facets



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

Bonded-Particle Modeling Methodology (PFC model)

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.

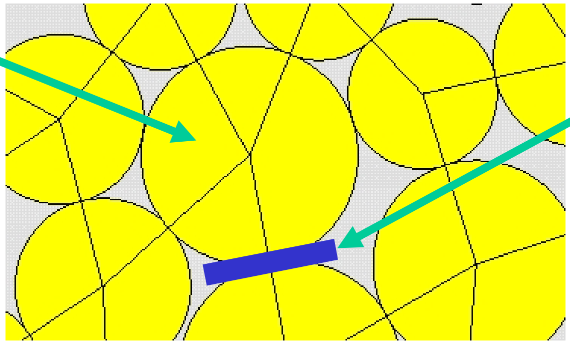
The most up-to-date incarnation of the PFC model is provided in the form of the linear, contact-bonded, parallel-bonded, and flat-jointed materials to support:

- 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-bonded contact
- parallel-bonded contact
- flat-jointed contact

When bond breaks, behaves as linear contact.

cement can be

- contact-bonded contact
- parallel-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!

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

Material-Modeling Support Package (Hands-on, usage)

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 6 is fistPkg6.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).

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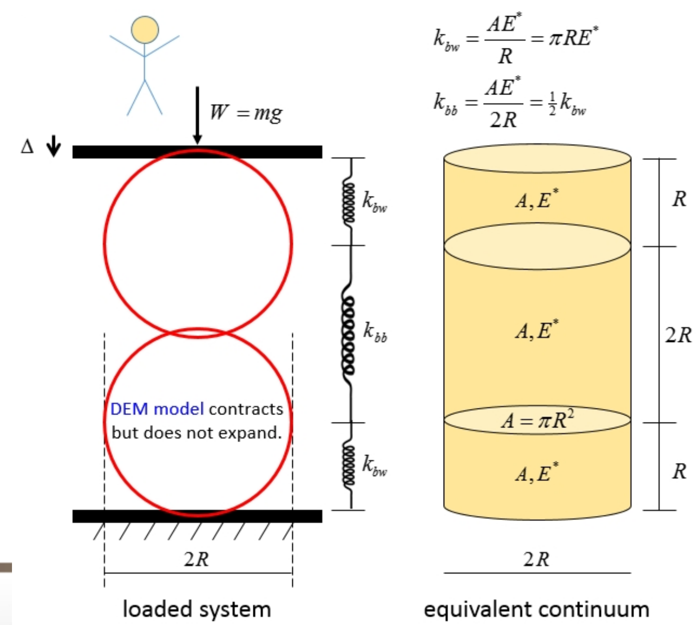
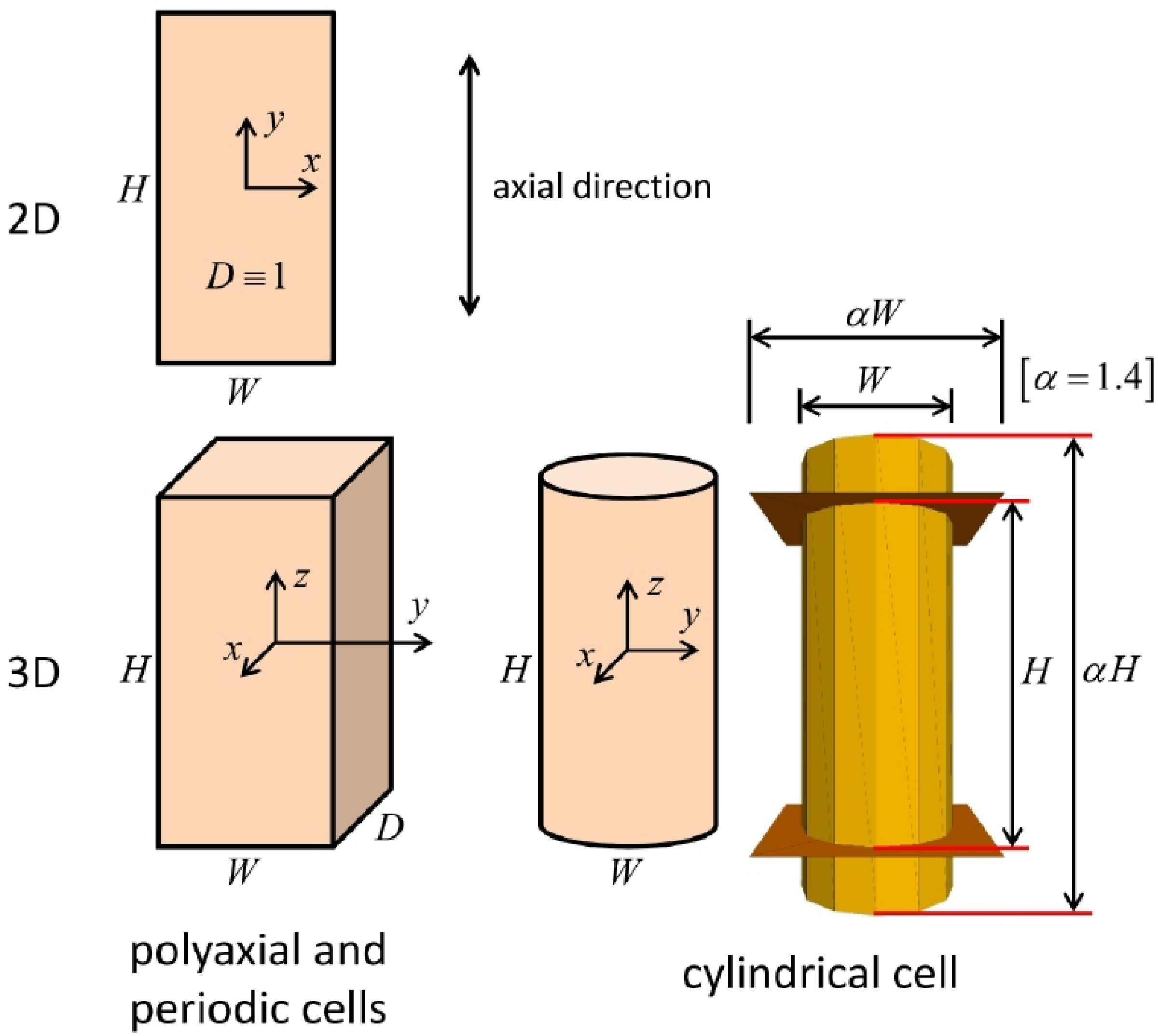
Should be greater than or equal to modulus of the material.



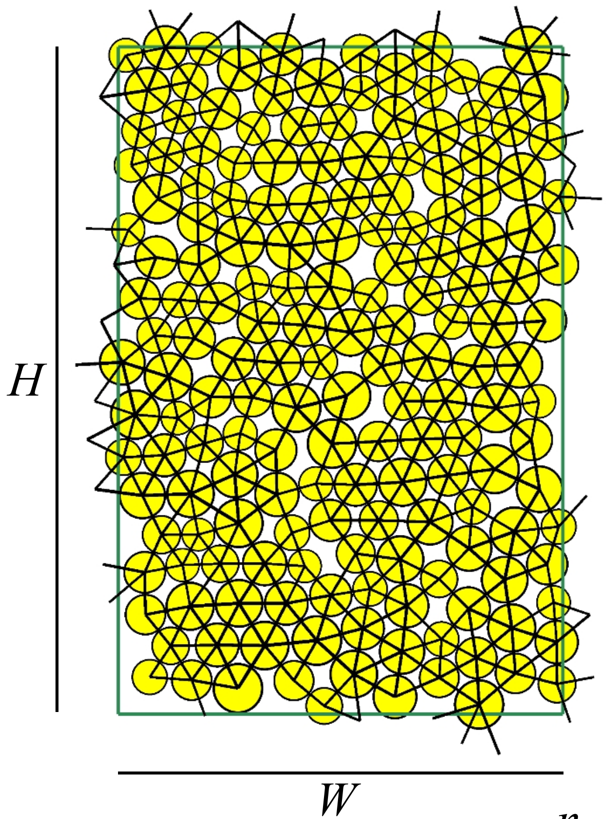
Material Vessels



Material Vessels (periodic vessel)

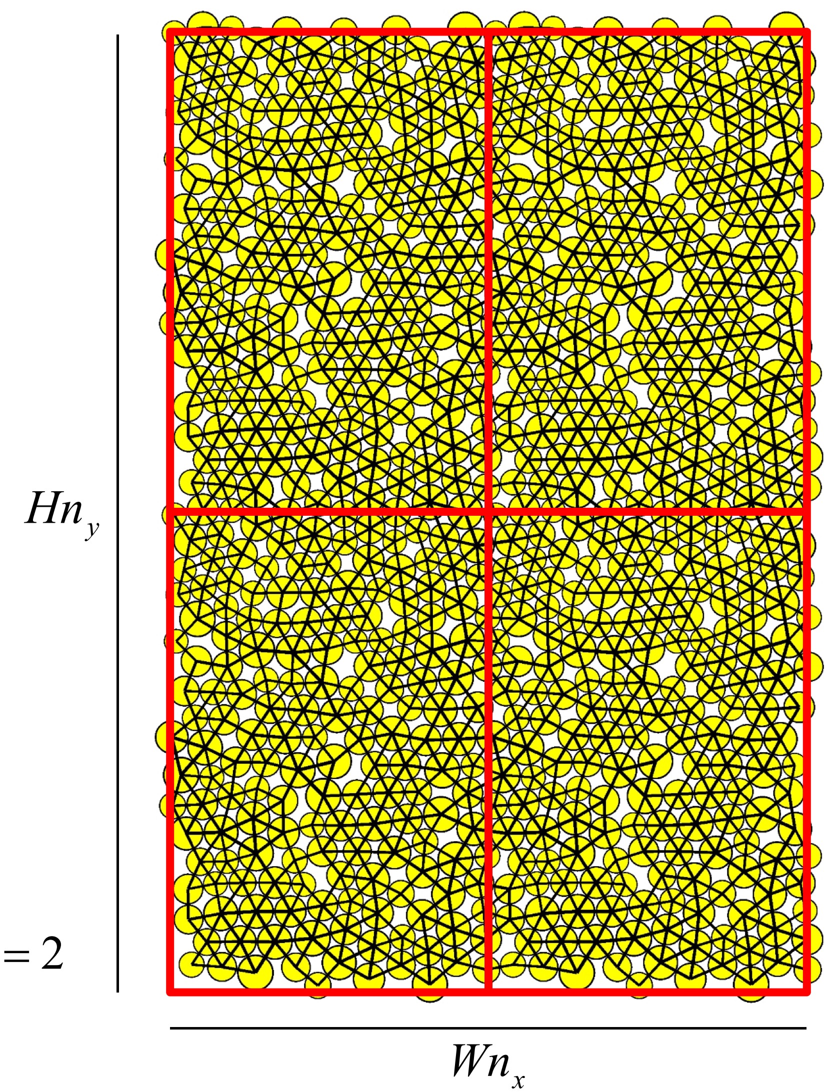
Bricks are assembled into a perfectly packed ensemble, may have installed stress.

periodic brick



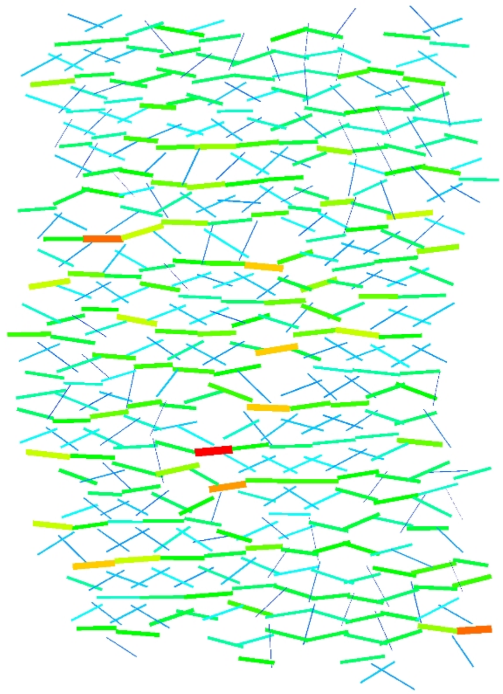
$n_x = n_y = 2$

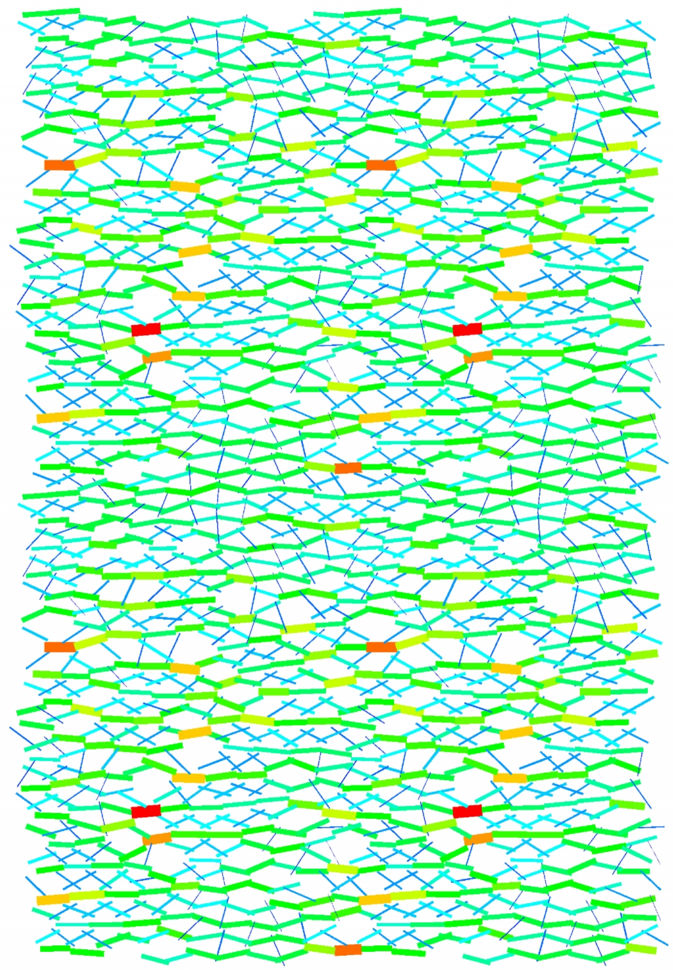
assembled specimen

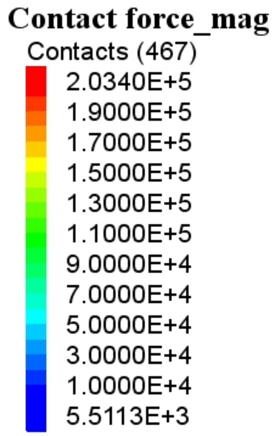


Material Vessels (periodic vessel)

Installed stress: Sxx = -78 MPa, Syy = -19.5 MPa





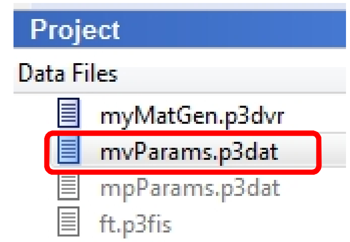


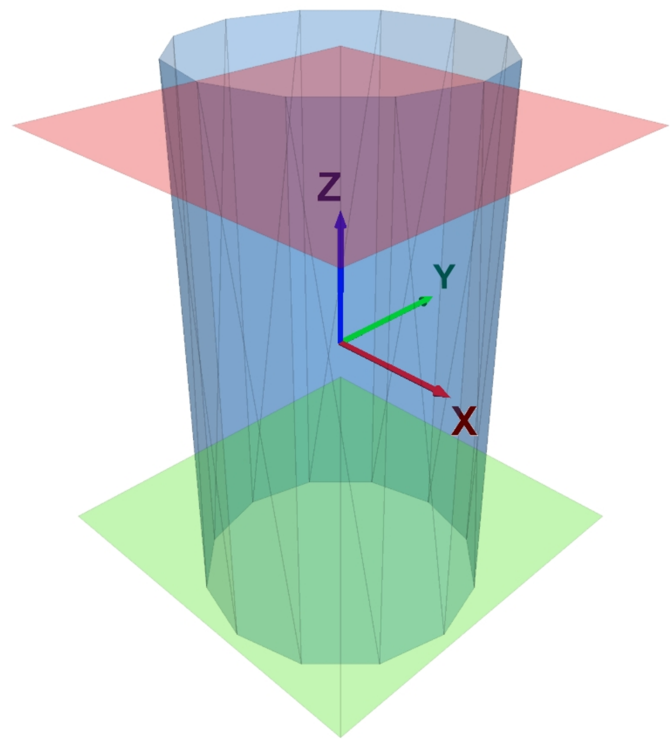
Force chains in bonded ensemble

Material Vessels

Table 6 Material-Vessel Parameters

Parameter, FISH	Type	Range	Default	Description
Material-vessel properties (including current vessel dimensions) are listed via `@mvListProps`.				
T_v, `mv_type`	INT	$\{0,1\}$	0	vessel-type code $\begin{cases} 0, & \text{physical} \\ 1, & \text{periodic} \end{cases}$
S_v, `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: $S_v \equiv 0$)
$\{H,W,D\}$, `mv_{H,W,D}`	FLT	$(0.0,\infty)$	NA	height, width and depth (sphere diameter is H ; 2D model: $D \equiv 1$, see Figure 2)
α, `mv_expandFac`	FLT	$[1.0,\infty)$	1.2	expansion factor of physical vessel
$\{\alpha_l,\alpha_d\}$, `mv_inset{L,D}Fac`	FLT	$(0.0,1.0]$	$\{0.8, 0.8\}$	inset factors of measurement regions
E_v^*, `mv_emod`	FLT	$(0.0,\infty)$	NA	effective modulus of physical vessel





Material Vessels

Edit mvParams.p3dat*

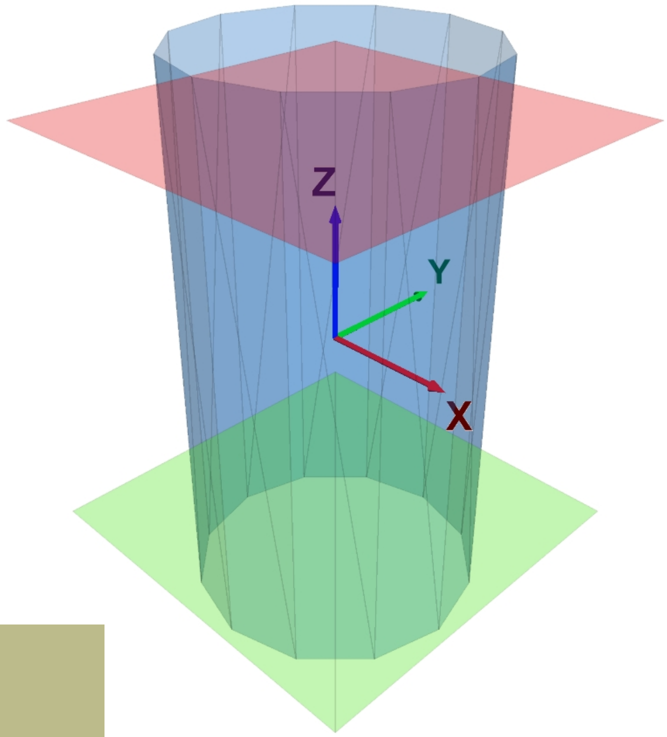
```
;fname: mvParams.p3dat

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, _wdz} (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): 5e+08
     mv_insetLFac (measurement region spanning-length factor): 0.8
     mv_insetDFac (measurement region diameter factor): 0.8
```



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SI units, for legends of plots

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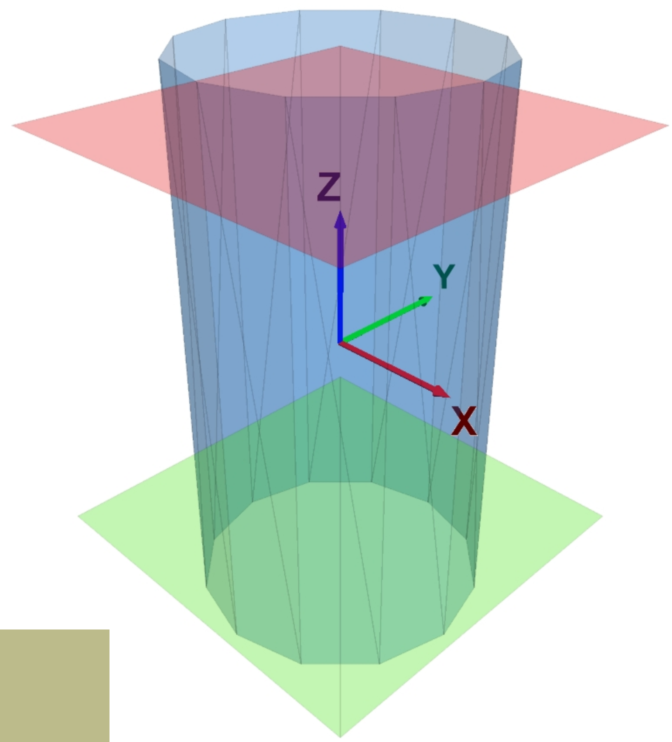

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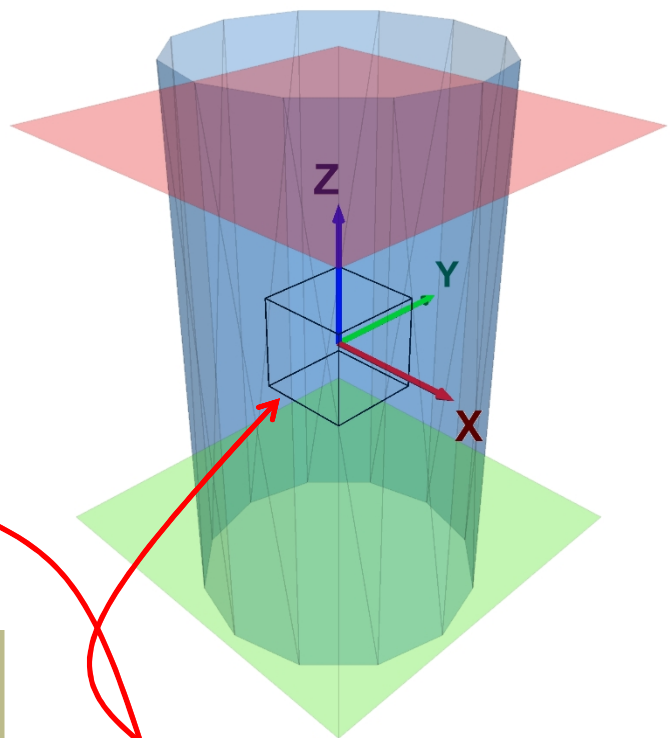

microstructural box

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 μ_{CA} to obtain dense or loose packing]

grain scaling:

grain sizes are scaled iteratively

[$\mu \equiv 0$ to obtain dense packing]

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[$\mu \equiv 0$ to obtain dense packing]

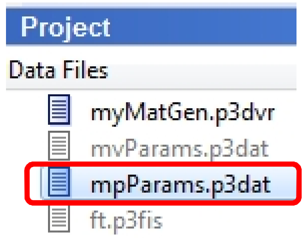
$$\mu_{CA} = 0 \ \left(\text{dense}\right)$$

$$\mu_{CA} = \mu_m \ \left(\text{loose}\right)$$

Material-Genesis Procedure (packing phase)

Table 7 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_PTol**	FLT	$(0.0, \infty)$	1×10^{-2}	pressure tolerance $\left(\frac{\lvert P - P_m \rvert}{P_m} \leq \varepsilon_P \right)$ where P is current pressure
$\varepsilon_{\lim}$, **pk_ARatLimit**	FLT	$(0.0, \infty)$	8×10^{-3}	equilibrium-ratio limit (parameter of `ft_eq`)
$n_{\lim}$, **pk_stepLimit**	INT	$[1, \infty)$	25000	step limit (parameter of `ft_eq`)
C_p, **pk_procCode**	INT	$\{0, 1\}$	0	packing-procedure code $\begin{cases} 0, & \text{boundary contraction} \\ 1, & \text{grain scaling} \end{cases}$
n_c, **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 9)



Material-Genesis Procedure (packing phase)

Project

Data Files

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

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$\varepsilon_{\lim}$, **pk_ARatLimit**	FLT	$(0.0, \infty)$	8×10^{-3}	equilibrium-ratio limit (parameter of **ft_eq**)
$n_{\lim}$, **pk_stepLimit**	INT	$[1, \infty)$	25000	step limit (parameter of **ft_eq**)
C_p, **pk_procCode**	INT	$\{0,1\}$	0	packing-procedure code $\begin{cases} 0, & \text{boundary contraction} \\ 1, & \text{grain scaling} \end{cases}$
n_c, **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 9)

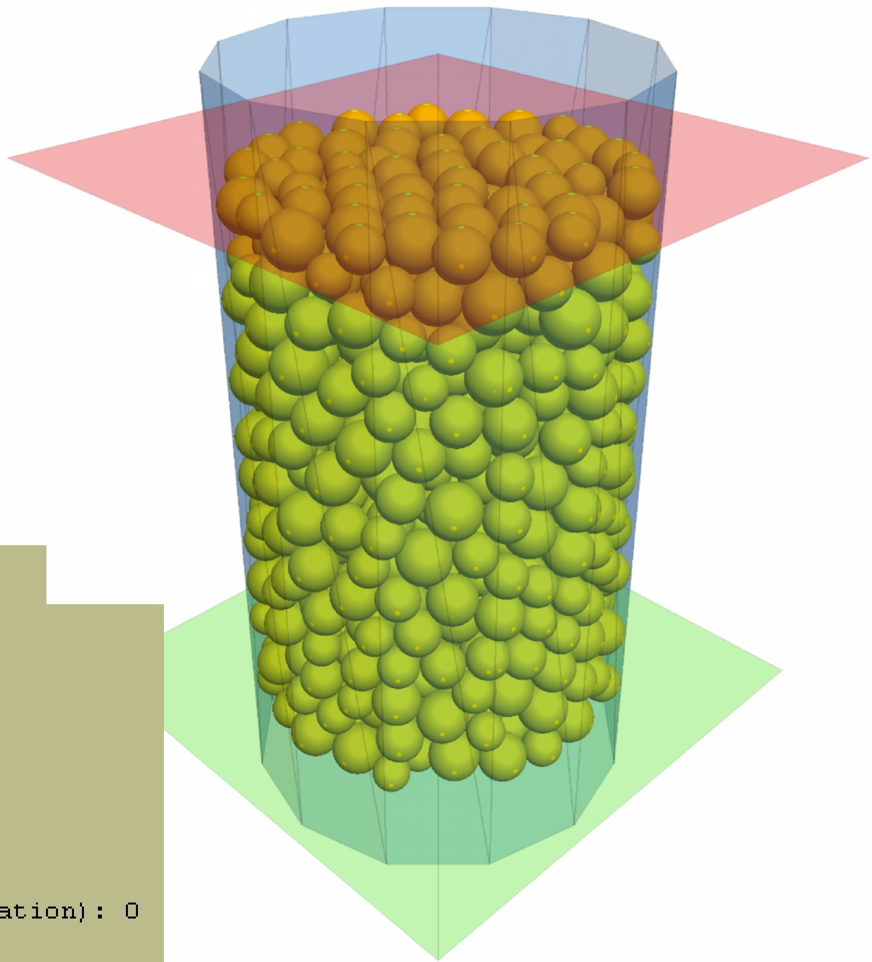
pk_seed: affects particle arrangement

Material-Genesis Procedure (packing phase)

Edit mpParams.p3dat

```
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_ARatLimit (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
```

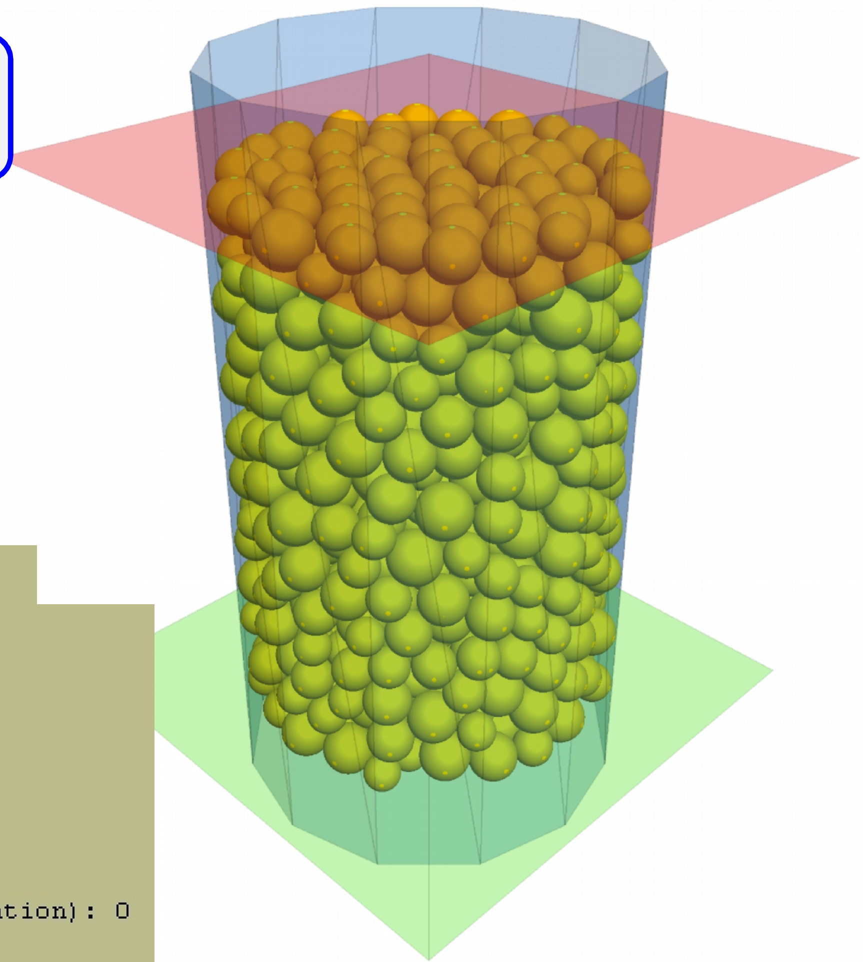


Material-Genesis Procedure (packing phase)

```
Edit mpParams.p3dat
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
```

Other parameters have default values.

```
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_ARatLimit (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
```



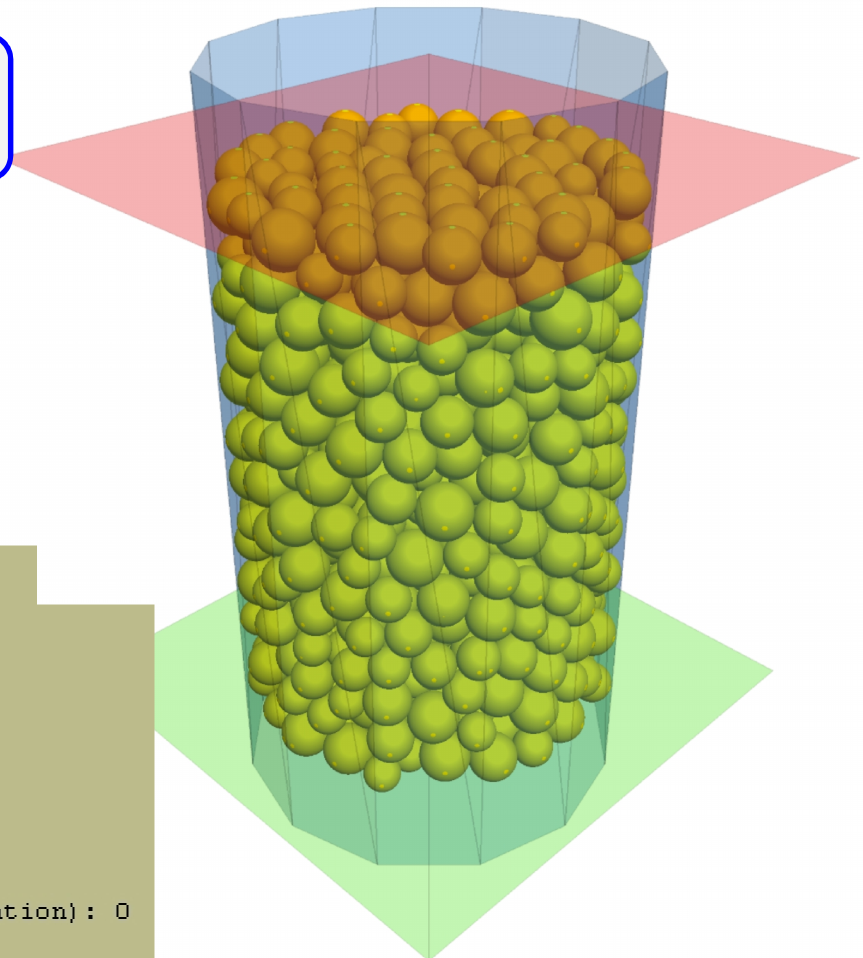
Material-Genesis Procedure (packing phase)

Edit mpParams.p3dat

```
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
```

Other parameters have default values.

```
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_ARatLimit (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
```



Modify **pk_fricCA** from 0.0 to 0.4 to increase final specimen porosity from 0.38 to 0.42.

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 3 Parallel-Bonded Material Parameters

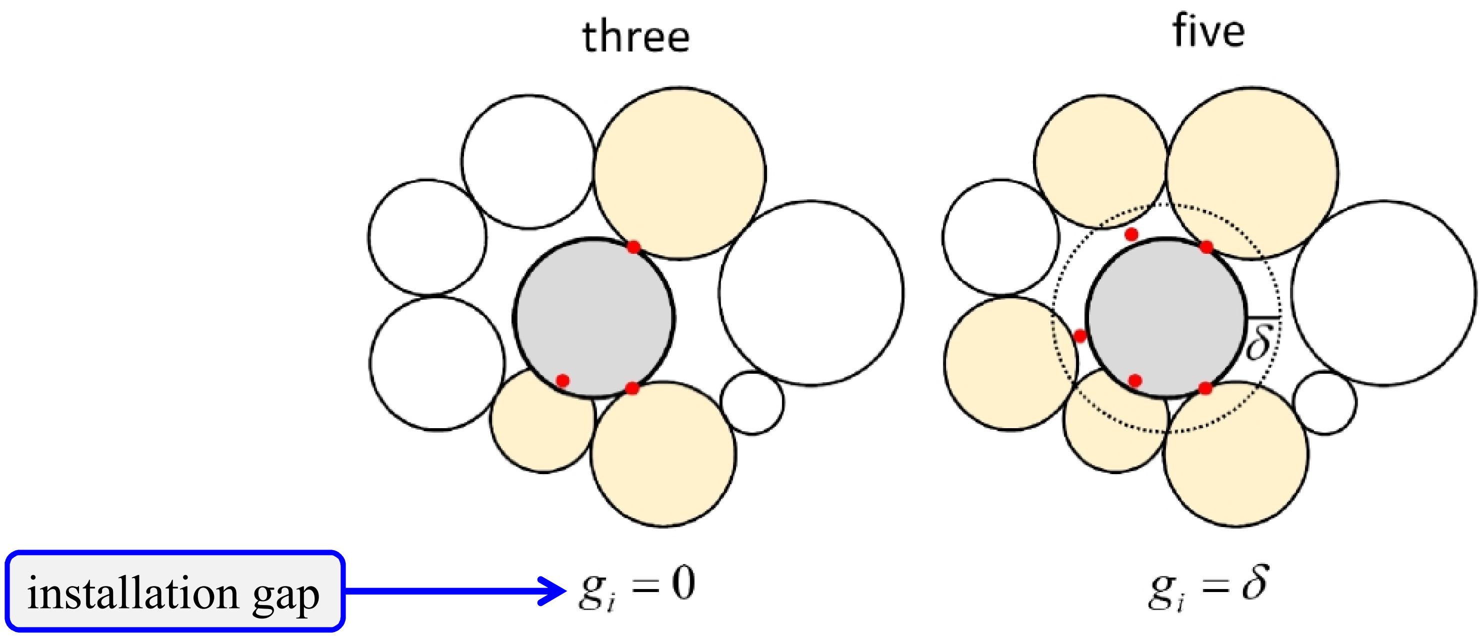
Parameter	Type	Range	Default	Description
Common material parameters are listed in Table 1.				
Packing parameters are listed in Table 7.				
Parallel-bonded material group:				
Linear group:				
• • •				
Parallel-bond group:				
• • •				
Linear material group (for grain-grain contacts that may form subsequent to material finalization):				

A

B

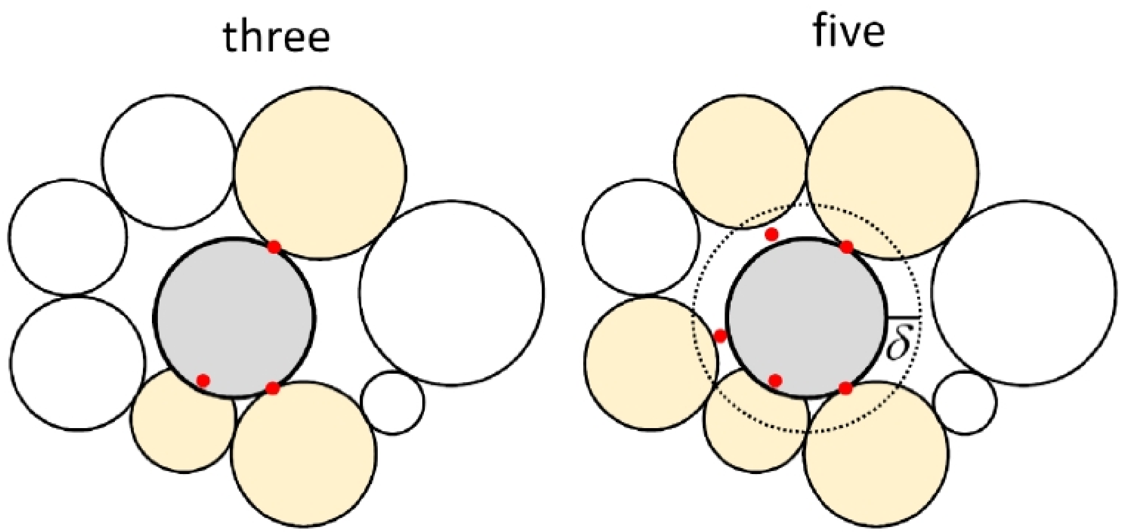
Material-Genesis Procedure (finalization phase)

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



Material-Genesis Procedure (finalization phase)

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

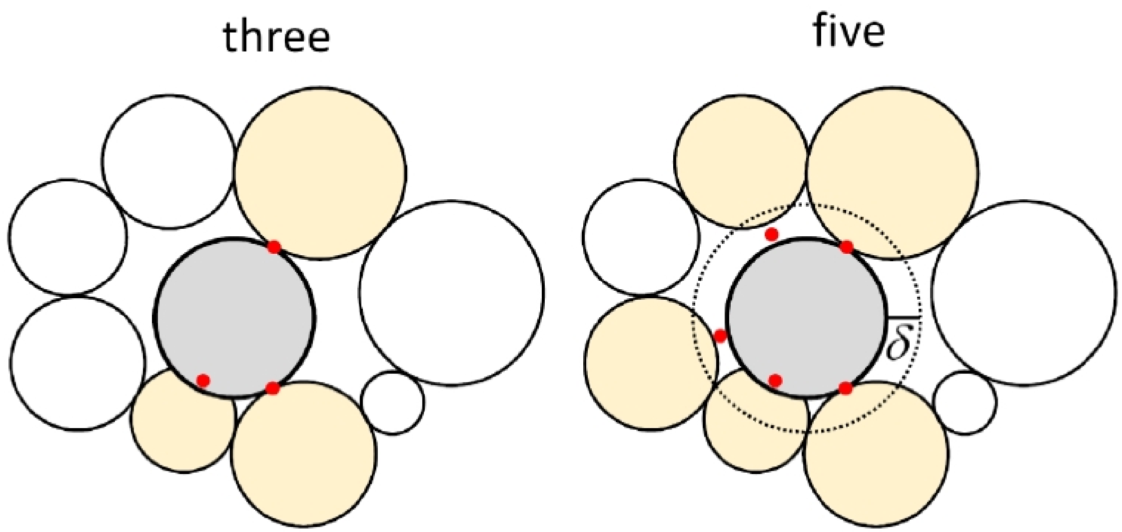


installation gap → $g_i = 0$ $g_i = \delta$

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!



installation gap → $g_i = 0$ $g_i = \delta$

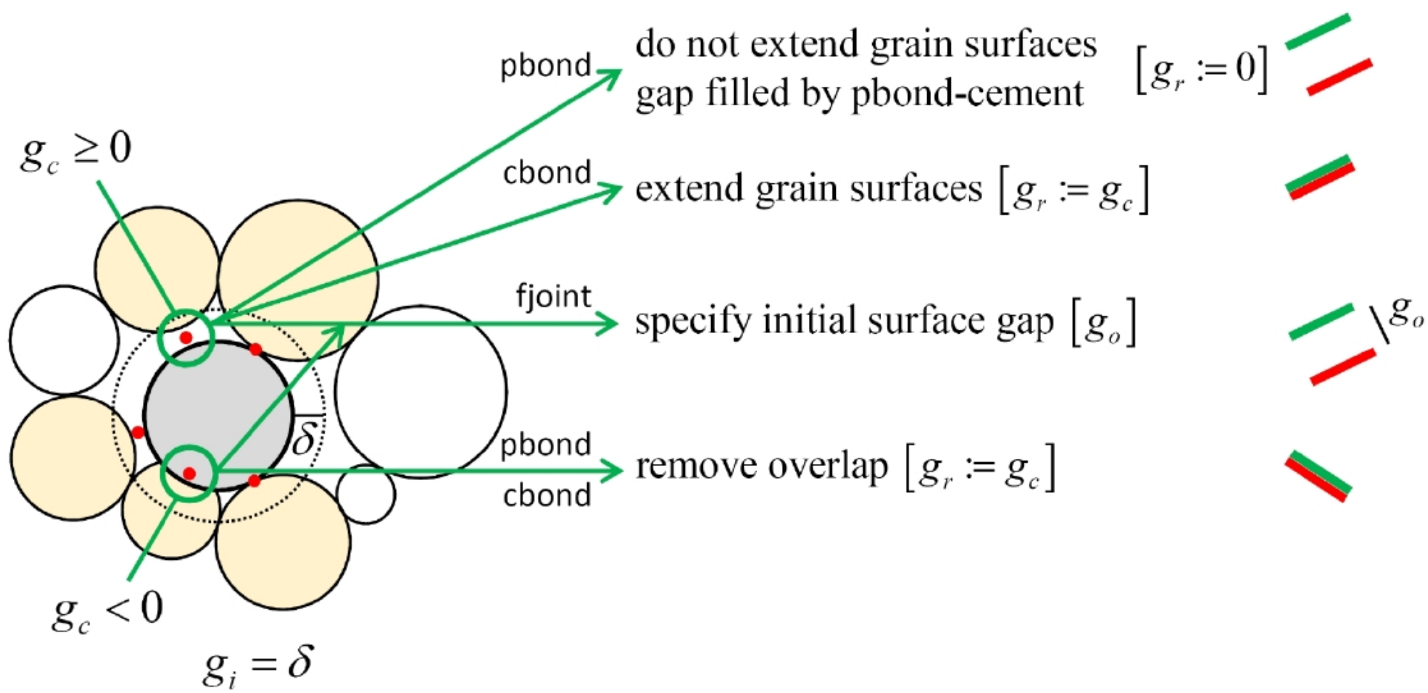
Increasing the installation gap, increases the grain connectivity,

which increases the material modulus and strength.

Material-Genesis Procedure (finalization phase)

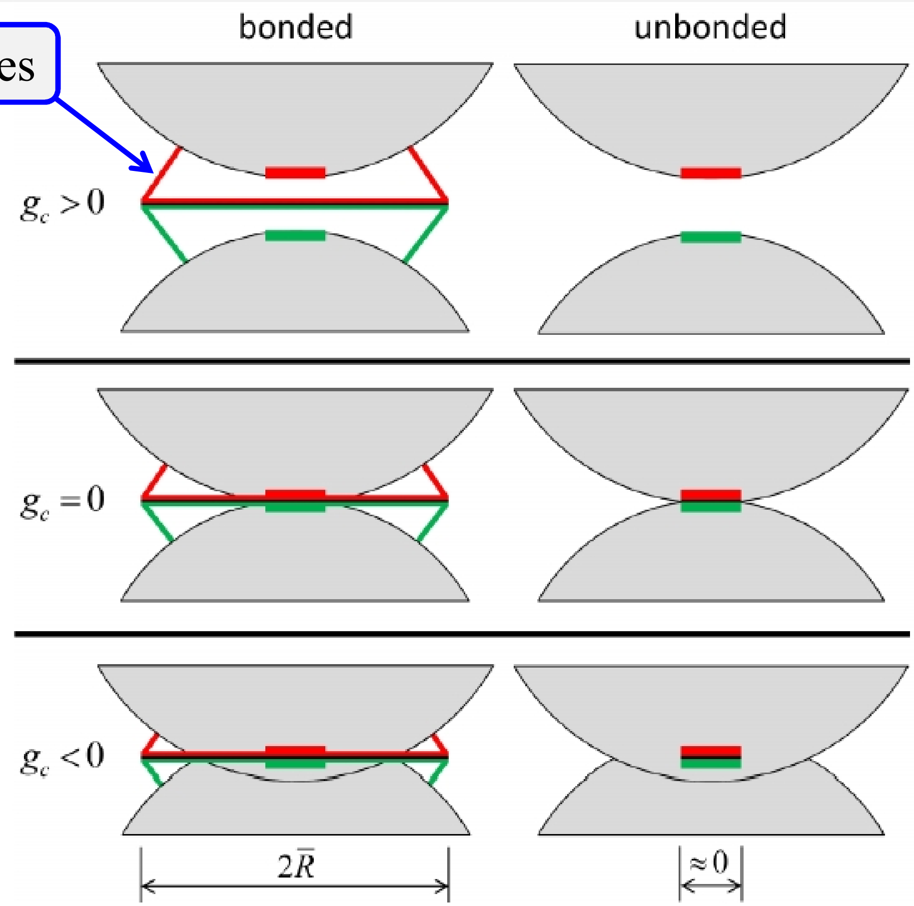
For the bonded materials, the material properties are set to establish reference surfaces that do not overlap.

- There are no forces or moments in the material.

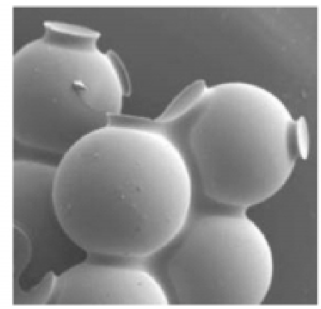


Material-Genesis Procedure (finalization phase)

reference surfaces



epoxy-cemented glass beads

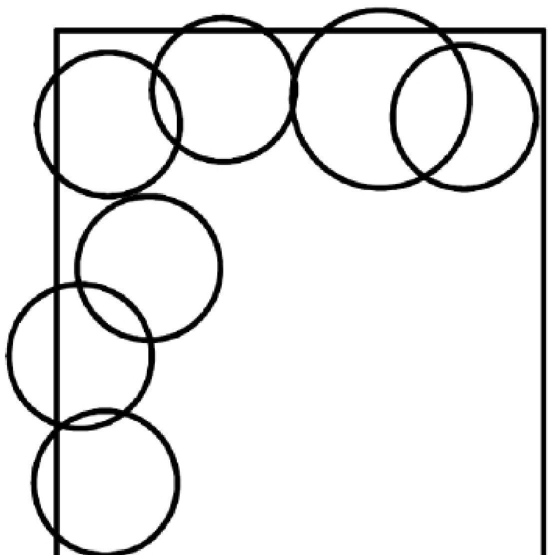


The above-left case corresponds with the beads having been separated at the time of epoxy installation.

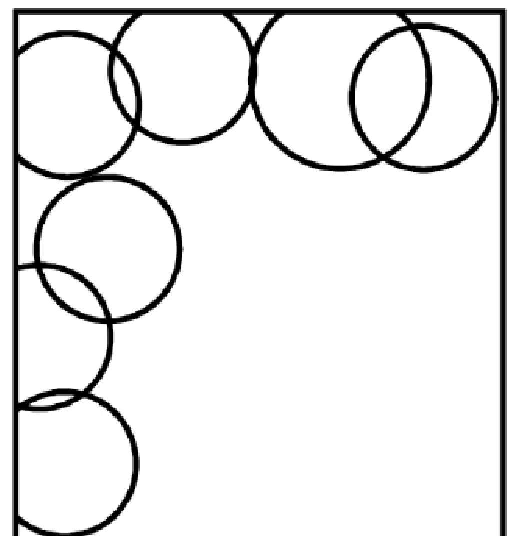
Material-Genesis Procedure (finalization phase)

For the bonded materials, the grain-vessel interface is smoothed.

- There are no forces at the grain-wall interface.



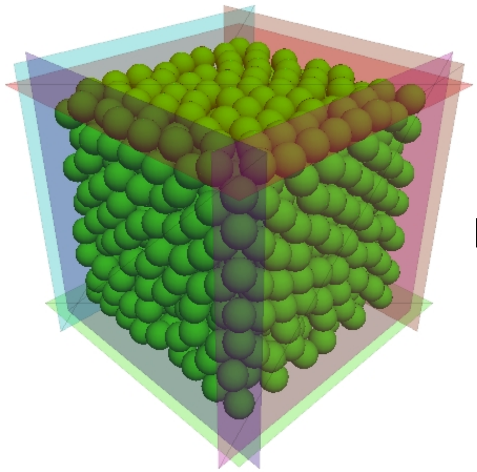
Before smoothing



After smoothing

Material-Genesis Procedure (completed)

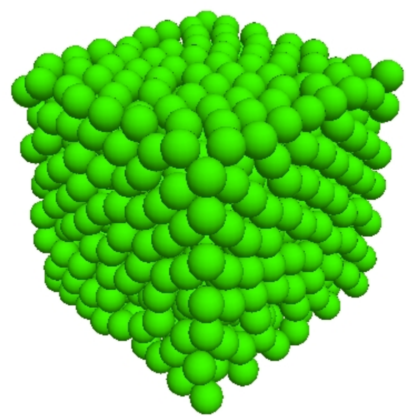
The specimen remains within the material vessel, and the model state is saved.



materials testing

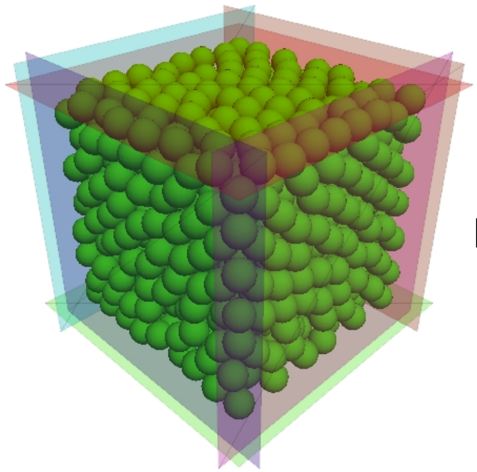
For bonded materials, the specimen is removed from the material vessel, and the model state is saved.

boundary-value simulation



Material-Genesis Procedure (completed)

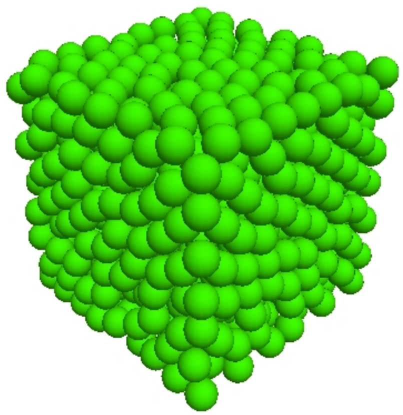
The specimen remains within the material vessel, and the model state is saved.



materials testing

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

boundary-value simulation



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,[24] measurement-based porosity (defined in Section 5.1), and overlap ratios.[25]
- **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).[26] Number of contact-bonded bonds, parallel-bonded bonds, flat-jointed contacts, flat-jointed elements, and flat-jointed bonds. The initial microstructural types of the flat-jointed material (defined in Section 2.6.2).

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,[24] measurement-based porosity (defined in Section 5.1), and overlap ratios.[25]
- **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).[26] Number of contact-bonded bonds, parallel-bonded bonds, flat-jointed contacts, flat-jointed elements, and flat-jointed bonds. The initial microstructural types of the flat-jointed material (defined in Section 2.6.2).

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)

granular material

```
pfc3d>@mpListMicroStrucProps
## Material Microstructural Properties [# is "number of"]:
   Grain Size and Packing Information:
     mp_nGN (# grains): 835
     Grain-size distribution (GSD) via gsdMeasure(numBins) to create table GSD,
       which is displayed in view pl-GSD.
     mp_Davg               (average grain diameter): 0.0170003
     mp_D50                ( median grain diameter): 0.0178
     mp_PhiVavg (vessel resolution w.r.t. mp_Davg ): 9.99983
     mp_PhiV50  (vessel resolution w.r.t. mp_D50  ): 9.55059
     mv_mn (measurement-based porosity): 0.382552
     mp_ORs (overlap ratios {max, min, avg}): {0.00211051,5.38026e-07,0.000554342}
   Contact Information:
     mp_nLNc  (# active linear-based             contacts): 360
     mp_nLNgg (# active linear-based grain-grain contacts): 0
     mp_nLNgw (# active linear-based grain-wall  contacts): 360
```

Material-Genesis (microstructural properties)

bonded material

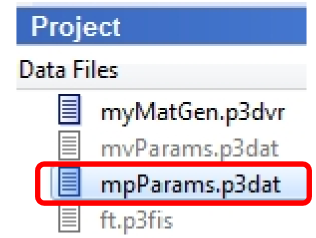
```
pfc3d>@mpListMicroStrucProps

## Material Microstructural Properties [# is "number of"]:
   Grain Size and Packing Information:
     mp_nGN (# grains): 1183
     Grain-size distribution (GSD) via gsdMeasure(numBins) to create table GSD,
       which is displayed in view pl-GSD.
     mp_Davg               (average grain diameter): 0.00486063
     mp_D50                ( median grain diameter): 0.00514904
     mp_PhiVavg (vessel resolution w.r.t. mp_Davg ): 10.2867
     mp_PhiV50  (vessel resolution w.r.t. mp_D50  ): 9.71054
     mv_mn (measurement-based porosity): 0.365802
     mp_ORs (overlap ratios (max, min, avg)): (0.000663431,-0.126217,-0.0136422)
   Contact Information:
     mp_nLNc  (# active linear-based             contacts): 4446
     mp_nLNgg (# active linear-based grain-grain contacts): 4446
     mp_nLNgw (# active linear-based grain-wall  contacts): 0
   Bonded-Material Information:
     mp_CNb (bond coordination number via bcnMeasure): 7.51648
     mp_nCBb  (# contact-bonded  bonds): 4446
     mp_nPBb  (# parallel-bonded bonds): 0
     mp_nFJc  (# flat-jointed contacts): 0
     mp_nFJe  (# flat-jointed elements): 0
     mp_nFJb  (# flat-jointed    bonds): 0
```

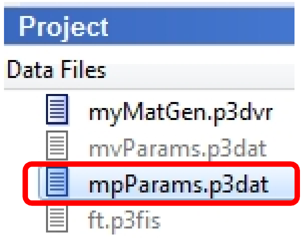
Materials (common material properties)

Table 1 Common Parameters

Parameter	Type	Range	Default	Description
N_m , **cm_matName**	STR	NA	**PFCmat**	material name
T_m , **cm_matType**	INT	$[0,4]$	0	material-type code $\begin{cases} 0, & \text{linear} \\ 1, & \text{contact-bonded} \\ 2, & \text{parallel-bonded} \\ 3, & \text{flat-jointed} \\ 4, & \text{user-defined} \end{cases}$
N_{cm} , **cm_modName**	STR	NA	NA	contact-model name ($T_m = 4$, also provide **udm_setMatBehavior**)
α , **cm_localDampFac**	FLT	$[0.0, 0.7]$	0.0	local-damping factor (for local damping)
C_ρ , **cm_densityCode**	INT	$\{0,1\}$	0	density code $\begin{cases} 0, & \text{grain} \\ 1, & \text{bulk} \end{cases}$
ρ_v , **cm_densityVal**	FLT	$(0.0, \infty)$	NA	density value (set grain density: $\rho_g = \begin{cases} \rho_v, & C_\rho = 0 \\ \rho_v V_v / V_g, & C_\rho = 1 \end{cases}$ V_v is volume of vessel, and V_g is total volume of grains)



Materials (common material properties)



Grain shape & size distribution group:

S_g, `cm_shape`	INT	$\{0,1\}$	0	grain-shape code $\begin{cases} 0, & \text{all balls} \\ 1, & \text{all clumps} \end{cases}$
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	$(0.0, \infty)$	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	$(0.0, 1.0]$	NA	volume fraction $\left(\sum \phi^{(j)} = 1.0\right)$
D_{mult}, `cm_Dmult`	FLT	$(0.0, \infty)$	1.0	diameter multiplier (shifts the size distribution)

Materials (common material properties)

Edit mpParams.p3dat

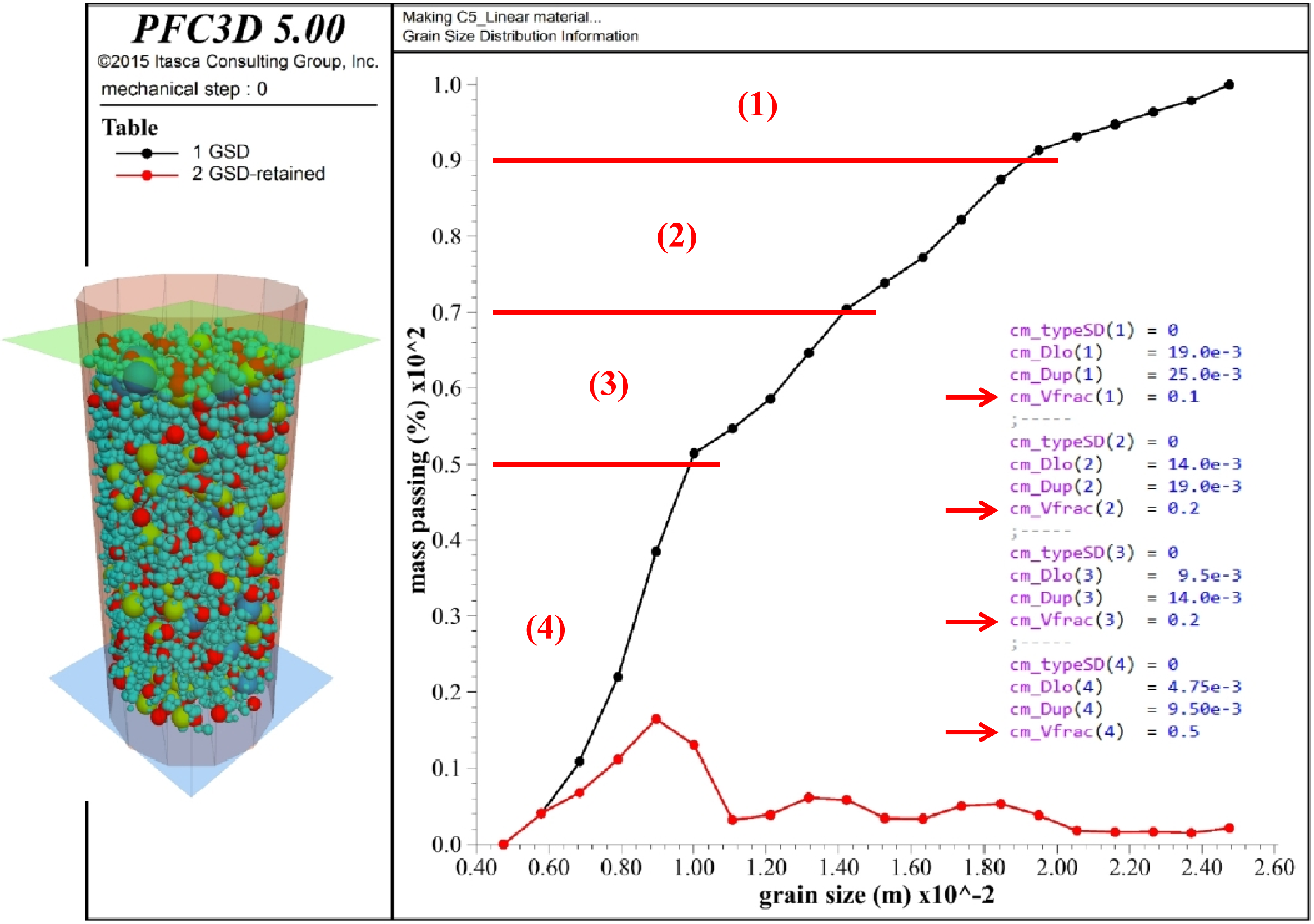
```
def mpSetCommonParams
; Set common parameters.
  cm_matName = 'SS_ContactBonded'
  ; ** Typical sandstone (contact-bonded material).
  cm_matType = 1
  cm_localDampFac = 0.7
  cm_densityCode = 1
  cm_densityVal = 1960.0

  ; Grain shape & size distribution group:
    cm_nSD = 1
    cm_typeSD = array.create(cm_nSD)
    cm_ctName = 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
@mpSetCommonParams
```

```
pfc3d>@mpListMicroProps
## Material Microproperties:
   Common group:
     cm_matName (material name): SS_ContactBonded
     cm_matType (material-type code): 1 (contact-bonded)
     cm_localDampFac (local-damping factor): 0.7
     cm_densityCode: 1 (cm_densityVal is bulk density)
     cm_densityVal: 1960
     Grain shape & size distribution group:
       cm_shape (grain-shape code): 0 (all balls)
       cm_nSD (number of size distributions): 1
         cm_typeSD(1): 0 (uniform)
         cm_Dlo(1): 0.004
         cm_Dup(1): 0.006
         cm_Vfrac(1): 1
       cm_Dmult (diameter multiplier): 1
```


Restore contact-bonded material, show the material name in view headers.

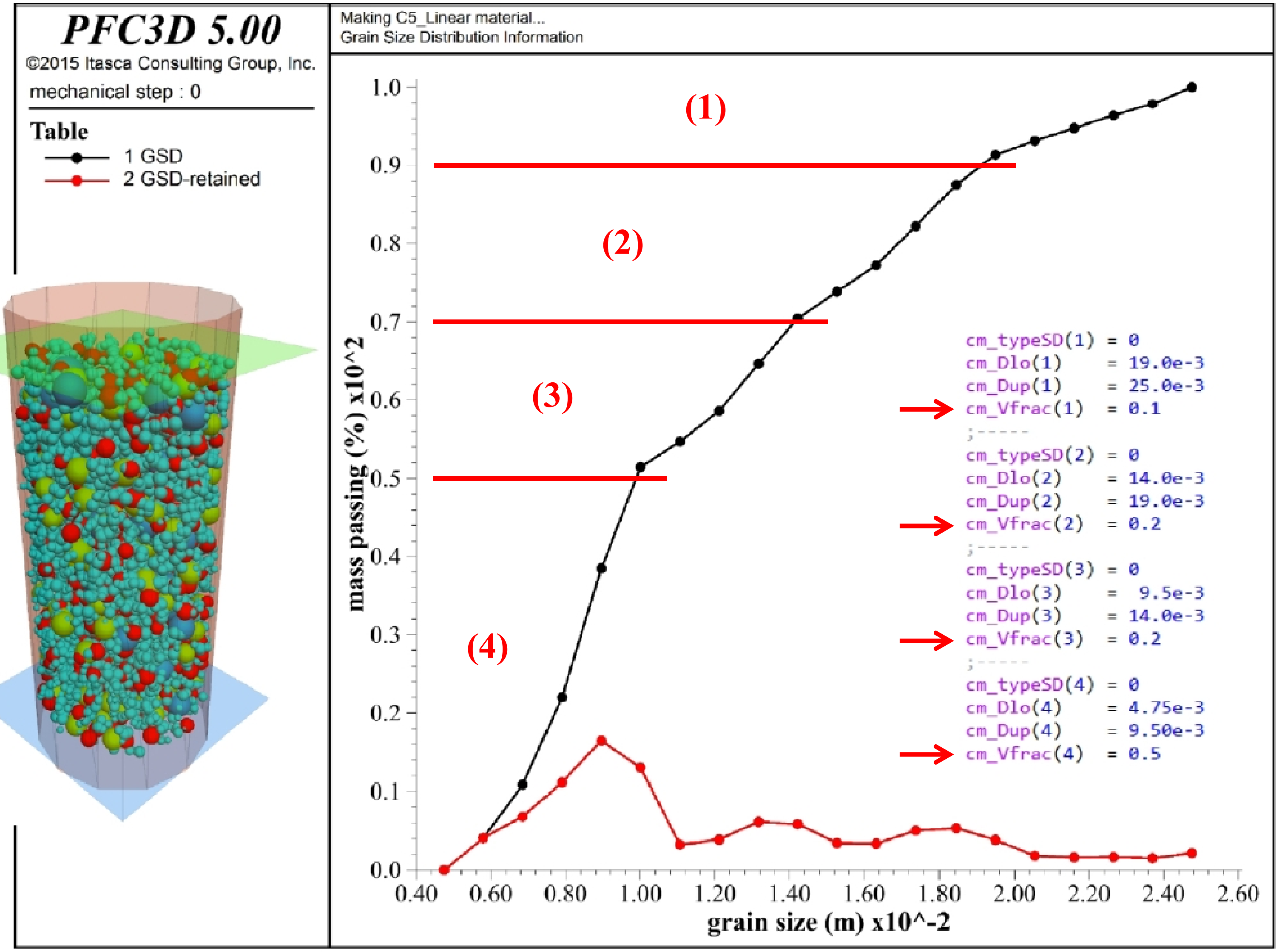
Materials (grain-size distribution)



[10] 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)



[10] 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).

ITASCA

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

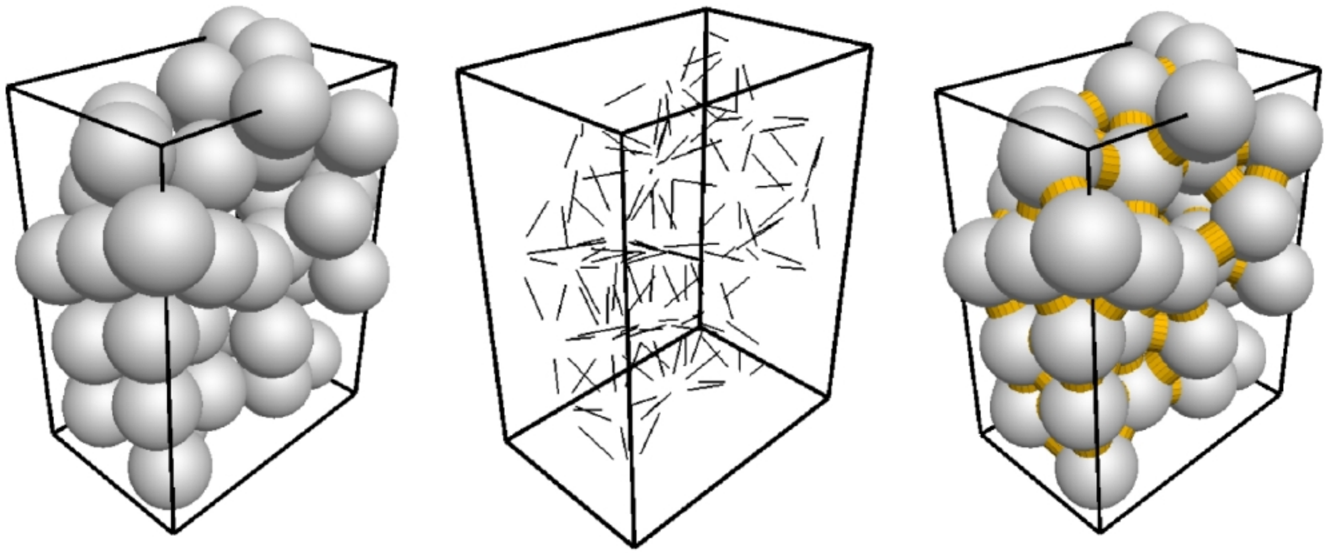
Microstructural Plot Sets

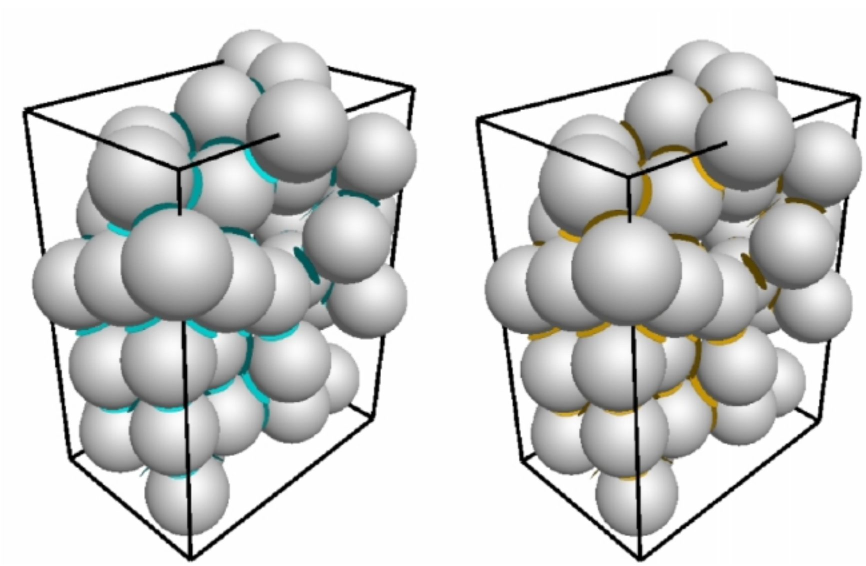
Microstructural plot sets are provided for the bonded materials to display the material microstructure and thereby reveal how the evolution of the microstructure influences the macroscopic behavior. The microstructural plot sets include depictions of the grains and the grain-grain interfaces, and when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

Figure image on next slide.

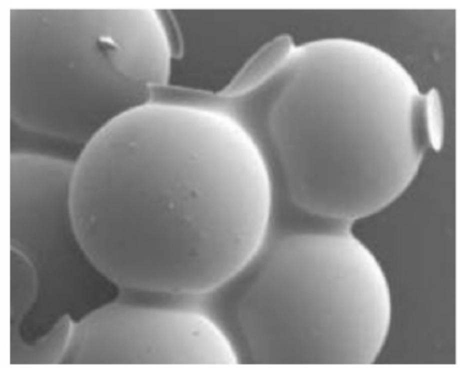
Figure 15 Microstructural plot sets for bonded materials with the same initial packing showing (clockwise from upper left): microstructural box and grains in the box (grey); contact-bonded material with contact bonds in the box; parallel-bonded material with parallel-bond cement (gold, 50% size) and parallel-bond interfaces (gold, 50% size); and flat-jointed material with flat-jointed interfaces (blue, 50% size).

Material-Genesis (microstructural plot sets)

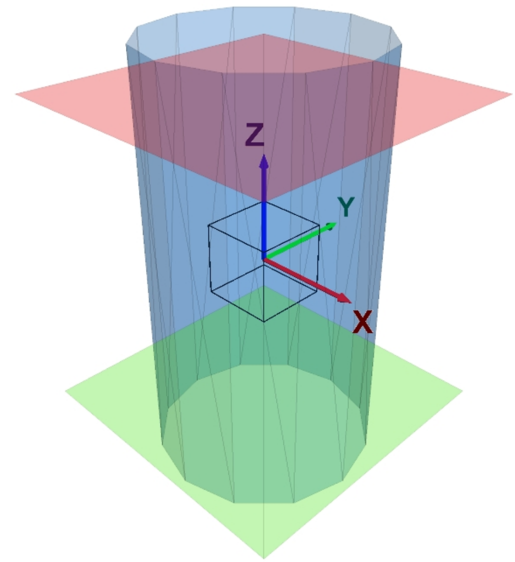




Glass beads cemented with epoxy



Holt et al. (2005)



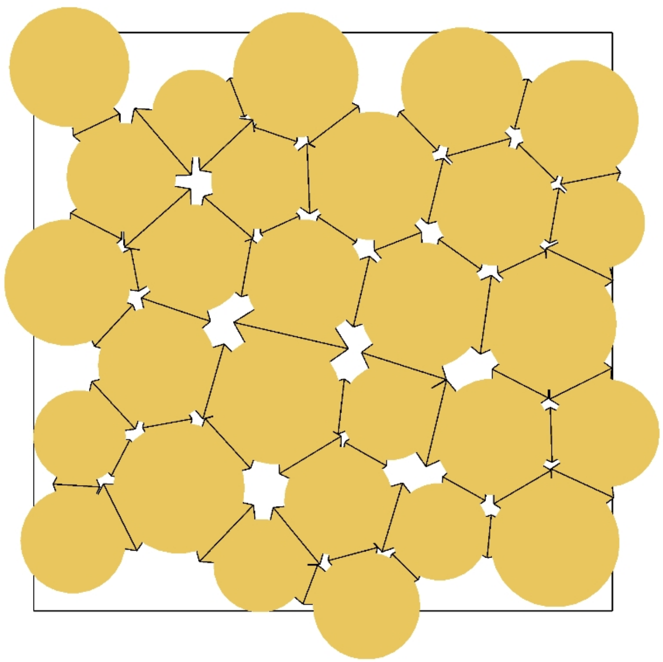
microstructural box

Restore cbonded material, {@msOn}, show box, ballsIn & cbonds.

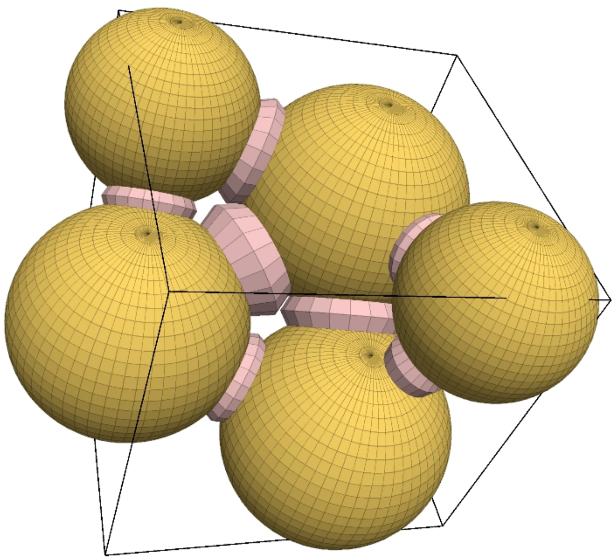
Material-Genesis (microstructural plot sets)

Flat-jointed material, "faced grain" plot set

PFC2D



PFC3D



Grains in the microstructural box

Materials (linear material)

Table 2 Linear 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 7.				
Linear material group:				
E^*, **lnm_emod**	FLT	$[0.0,\infty)$	0.0	effective modulus
κ^*, **lnm_krat**	FLT	$[0.0,\infty)$	0.0	stiffness ratio
μ, **lnm_fric**	FLT	$[0.0,\infty)$	0.0	friction coefficient

$$\mapsto (k_n, k_s)$$

Project

Data Files

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

Edit mpParams.p3dat*

```
def mpSetLinParams
; Set linear material parameters.
  ; Common group (set in mpSetCommonParams)
  ; Packing group (set in mpSetPackingParams)
  ; Linear material group:
    lnm_emod = 500e6
    lnm_krat = 1.5
    lnm_fric = 0.5
end
@mpSetLinParams
```

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

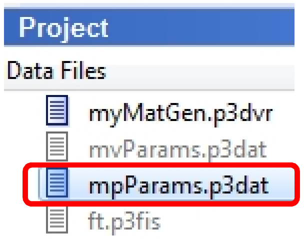
• • •

```
  Linear material group:
    lnm_emod (effective modulus): 5e+08
    lnm_krat (stiffness ratio): 1.5
    lnm_fric (friction coefficient): 0.5
```

Materials (contact-bonded material)

Table 3 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 7.				
Contact-bonded material group:				
Linear group:				
E^*, **cbm_emod**	FLT	$[0.0, \infty)$	0.0	effective modulus
κ^*, **cbm_krat**	FLT	$[0.0, \infty)$	0.0	stiffness ratio
μ, **cbm_fric**	FLT	$[0.0, \infty)$	0.0	friction coefficient



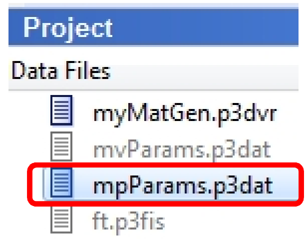
Materials (contact-bonded material)

Contact-bond group:				
g_i, `cbm_igap`	FLT	$[0.0,\infty)$	0.0	installation gap
$(T_\sigma)_{\{msd\}}$ `cbm_tens_{m,sd}`	FLT	$[0.0,\infty)$	$\{0.0,0.0\}$	tensile-strength dist. [stress] (mean and std. deviation)
$(S_\sigma)_{\{msd\}}$ `cbm_shears_{m,sd}`	FLT	$[0.0,\infty)$	$\{0.0,0.0\}$	shear-strength dist. [stress] (mean and std. deviation)
Linear material group (for grain-grain contacts that may form subsequent to 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

Materials (parallel-bonded material)

Table 4 Parallel-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 7.				
Parallel-bonded material group:				
Linear group:				
E^*, **pbm_emod**	FLT	$[0.0, \infty)$	0.0	effective modulus
κ^*, **pbm_krat**	FLT	$[0.0, \infty)$	0.0	stiffness ratio
μ, **pbm_fric**	FLT	$[0.0, \infty)$	0.0	friction coefficient



Materials (parallel-bonded material)

Parallel-bond group:

g_i, **pbm_igap**	FLT	$[0.0, \infty)$	0.0	installation gap
$\bar{\lambda}$, **pbm_rmul**	FLT	$(0.0, \infty)$	1.0	radius multiplier
$\bar{E}^*$, **pbm_bemod**	FLT	$[0.0, \infty)$	0.0	bond effective modulus
$\bar{\kappa}^*$, **pbm_bkrat**	FLT	$[0.0, \infty)$	1.0	bond stiffness ratio
$\bar{\beta}$, **pbm_mcf**	FLT	$[0.0, 1.0]$	0.0	moment-contribution factor
$(\bar{\sigma}_c)_{\{\mathrm{m,sd}\}}$ **pbm_ten_{m,sd}**	FLT	$[0.0, \infty)$	$\{0.0, 0.0\}$	tensile-strength dist. [stress] (mean and std. deviation)
$(\bar{c})_{\{\mathrm{m,sd}\}}$ **pbm_coh_{m,sd}**	FLT	$[0.0, \infty)$	$\{0.0, 0.0\}$	cohesion dist. [stress] (mean and std. deviation)
$\bar{\phi}$, **pbm_fa**	FLT	$[0.0, 90.0)$	0.0	friction angle [degrees]

Linear material group (for grain-grain contacts that may form subsequent to 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

Materials (flat-jointed material)

Table 5 Flat-Jointed 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 7.				
Flat-jointed material group:				
g_i, `fjm_igap`	FLT	$[0.0, \infty)$	0.0	installation gap
$\phi_B{}^+$, `fjm_B_frac`	FLT	$[0.0, 1.0]$	NA	bonded fraction
$\phi_G{}^+$, `fjm_G_frac`	FLT	$[0.0, 1.0]$	NA	gapped fraction
$(g_o)_{\{m,sd\}}$, `fjm_G_{m,sd}`	FLT	$[0.0, \infty)$	$\{0.0, 0.0\}$	initial surface-gap distribution (mean and std. deviation)
N_r, `fjm_Nr`	INT	$[1, \infty)$	2	elements in radial direc. (2D model: total elements)
N_α, `fjm_Nal`	INT	$[3, \infty)$	4	elements in circumf. direc. (3D model only)
C_λ, `fjm_rmulCode`	INT	$\{0, 1\}$	0	radius-multiplier code $\begin{cases} 0, & \text{fixed} \\ 1, & \text{varying} \end{cases}$

Project

Data Files

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

Materials (flat-jointed material)

λ_{ν}, `fjm_rmulVal`	FLT	$(0.0, \infty)$	1.0	radius-multiplier value $\begin{cases} \lambda_f, & C_\lambda = 0 \\ \lambda_o, & C_\lambda = 1 \end{cases}$ λ_f is fixed value, and λ_o is starting value
E^*, `fjm_emod`	FLT	$[0.0, \infty)$	0.0	effective modulus
κ^*, `fjm_krat`	FLT	$[0.0, \infty)$	0.0	stiffness ratio
μ, `fjm_fric`	FLT	$[0.0, \infty)$	0.0	friction coefficient
$(\sigma_c)_{\{m,sd\}}$ `fjm_ten_{m,sd}`	FLT	$[0.0, \infty)$	$\{0.0, 0.0\}$	tensile-strength dist. [stress] (mean and std. deviation)
$(c)_{\{m,sd\}}$ `fjm_coh_{m,sd}`	FLT	$[0.0, \infty)$	$\{0.0, 0.0\}$	cohesion dist. [stress] (mean and std. deviation)
ϕ, `fjm_fa`	FLT	$[0.0, 90.0)$	0.0	friction angle [degrees]
Linear material group (for grain-grain contacts that are not flat-jointed and that may form subsequent to 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: $\phi_S = 1 - \phi_B - \phi_G \ (0 \le \phi_S \le 1)$.

Materials (flat-jointed material)

Microstructural Validity, valid if grain facets do not overlap

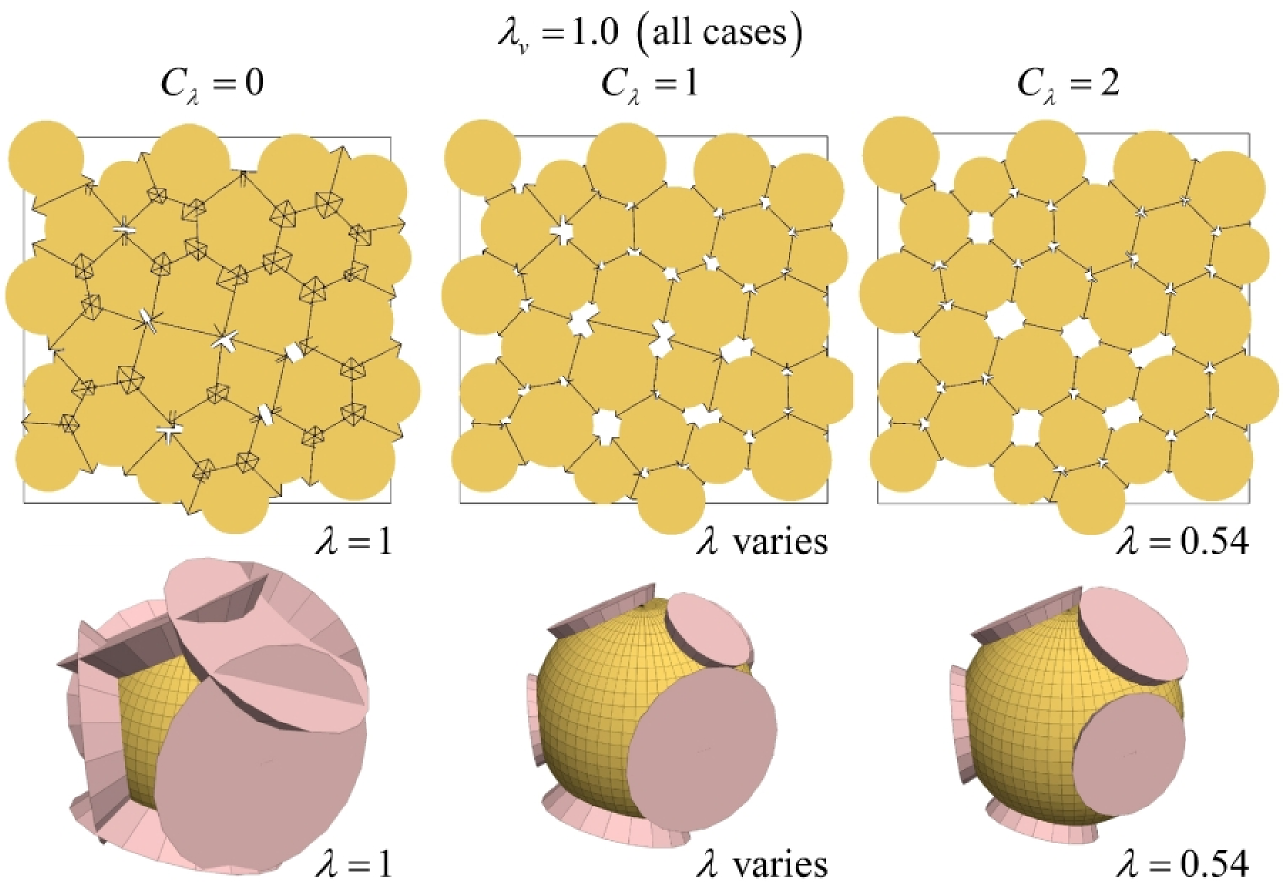


Figure 12 The three types of flat-jointed microstructures produced by the material-modeling support package. The left-most images have invalid microstructures, while the middle and right images have valid microstructures. Only a single faced grain is shown for the 3D case (bottom).

Crack-Monitoring Package

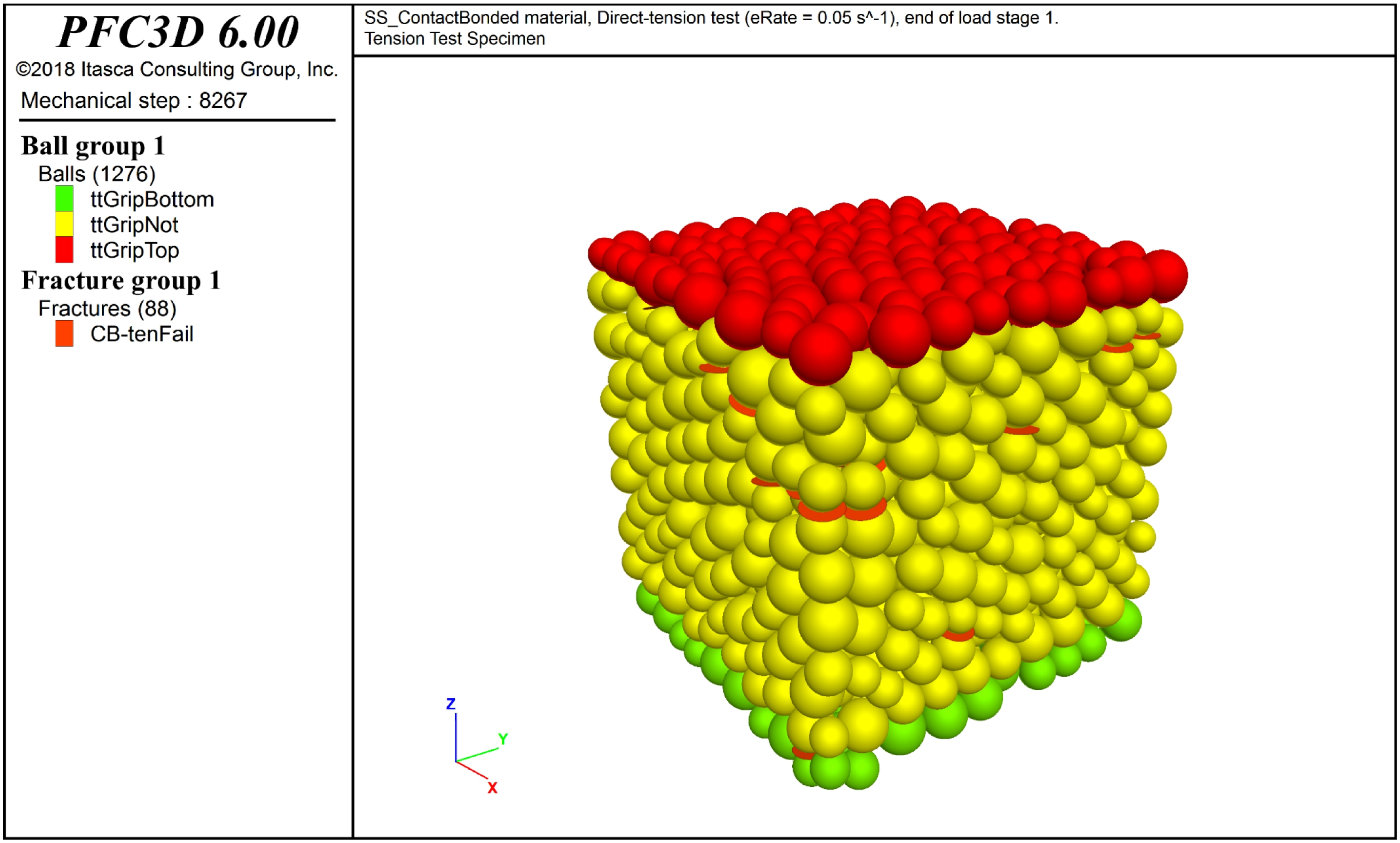
Damage in the bonded materials consists of bond breakages, which we denote as cracks. Crack data is stored as a Discrete Fracture Network (DFN), and the DFN plot item supports visualization of the cracks. Each crack has a type (contact bonded, parallel bonded, flat jointed or smooth jointed) and failure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

`ck_nAll`, `ck_n{CB,PB,FJ,SJ}{t,s}`

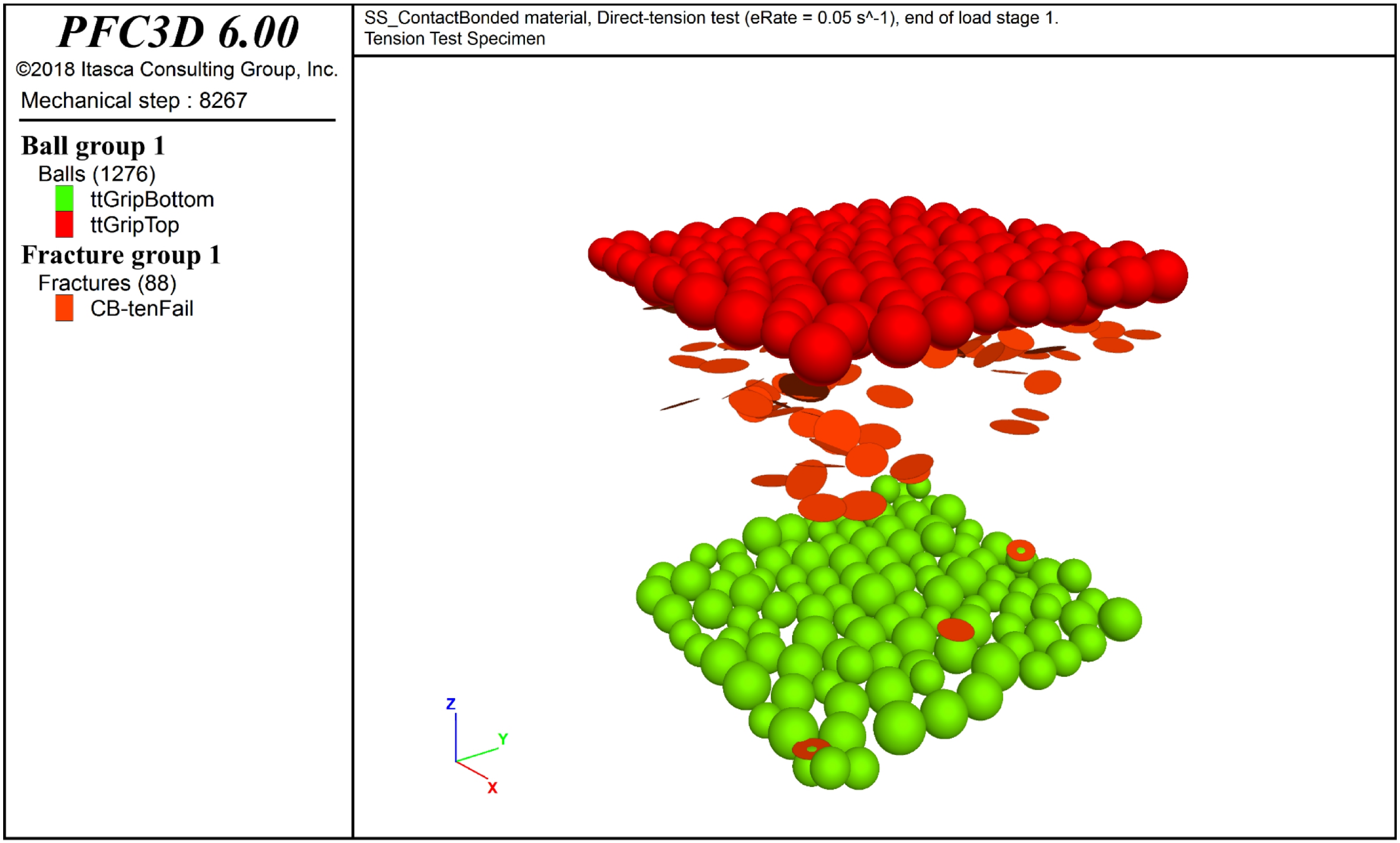
Crack-Monitoring Package

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



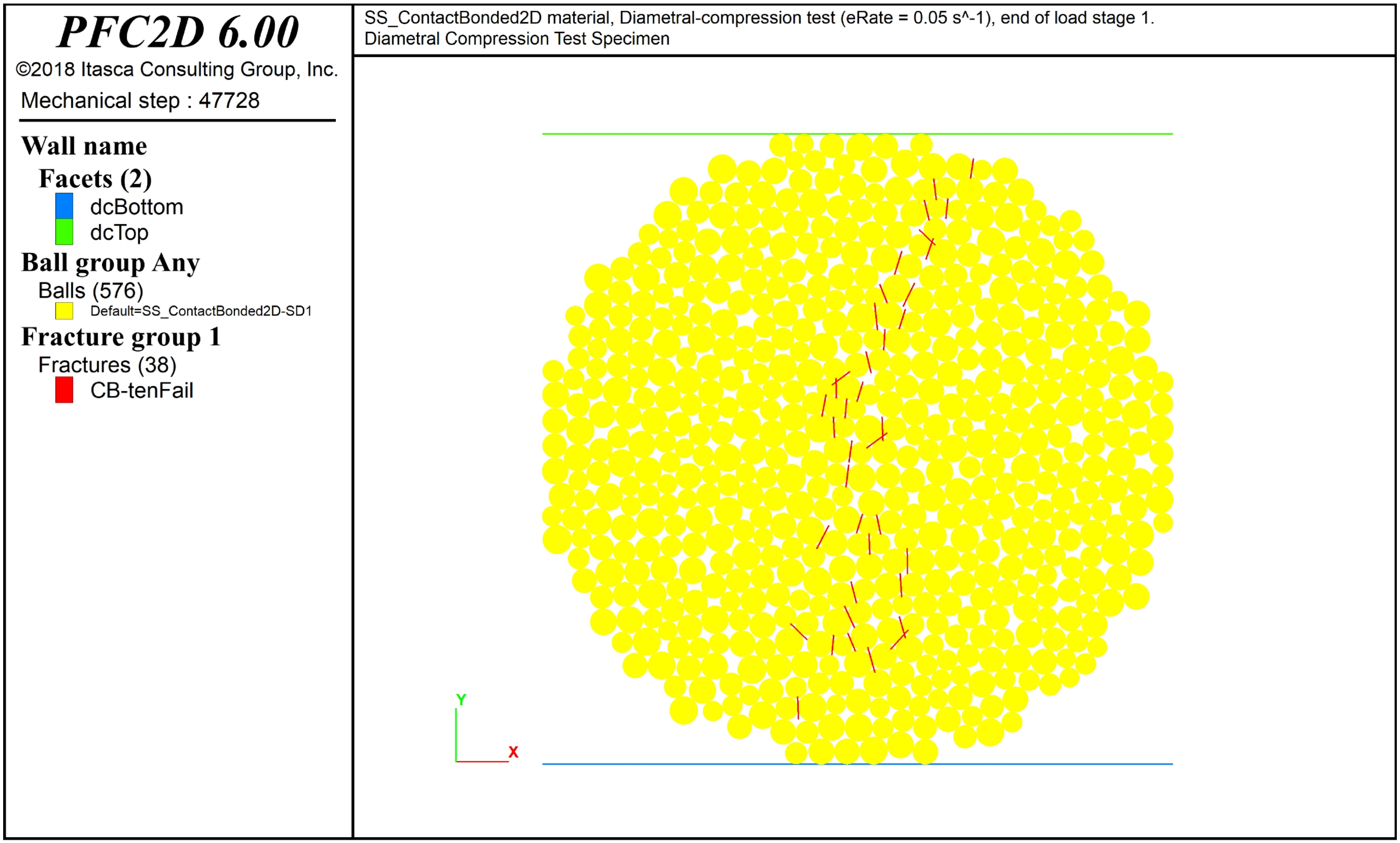
Crack-Monitoring Package

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



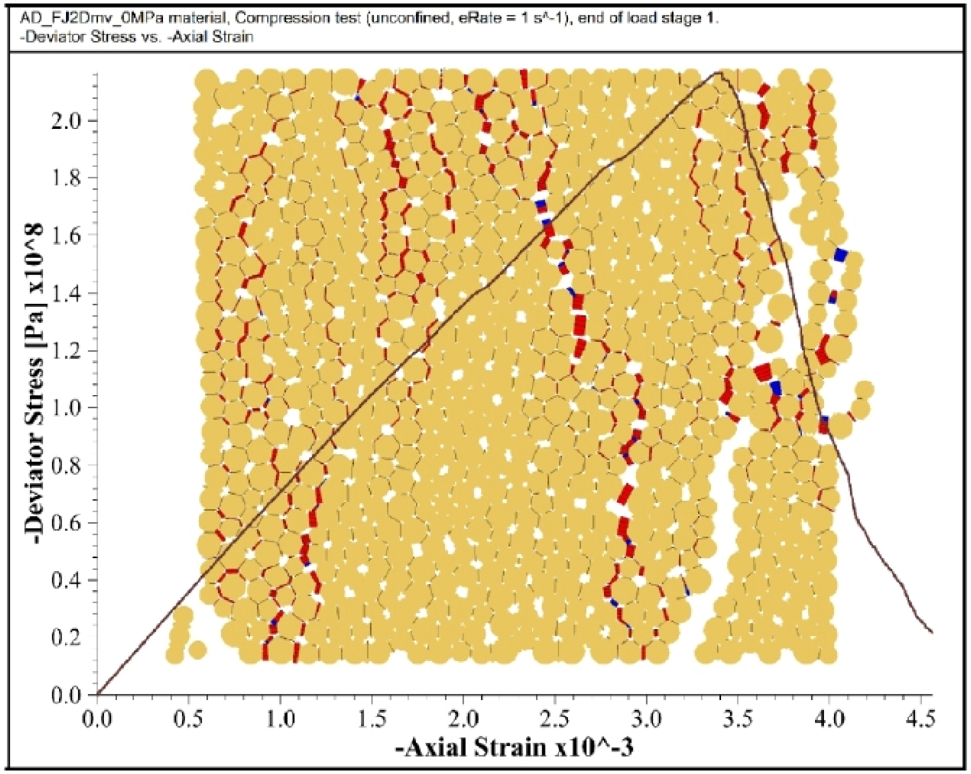
Crack-Monitoring Package

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.



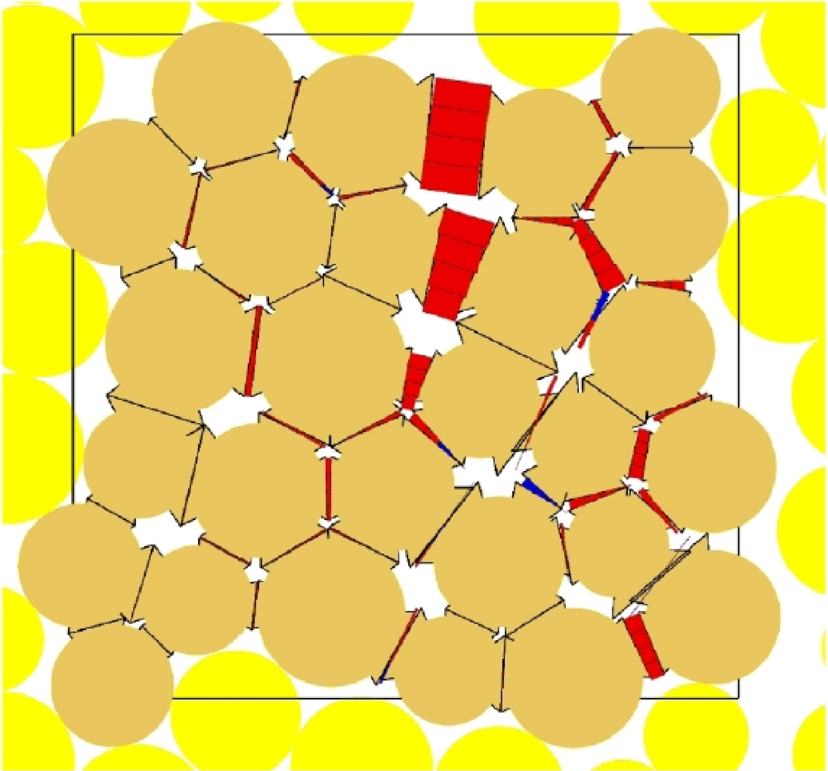


Figure 17 Crack and faced grain plot sets in 2D showing cracks, with crack thickness equal to gap, and cracks colored red/blue for tensile/shear failure. 2D flat-jointed material at end of UCS test as the specimen exhibits axial splitting.

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.

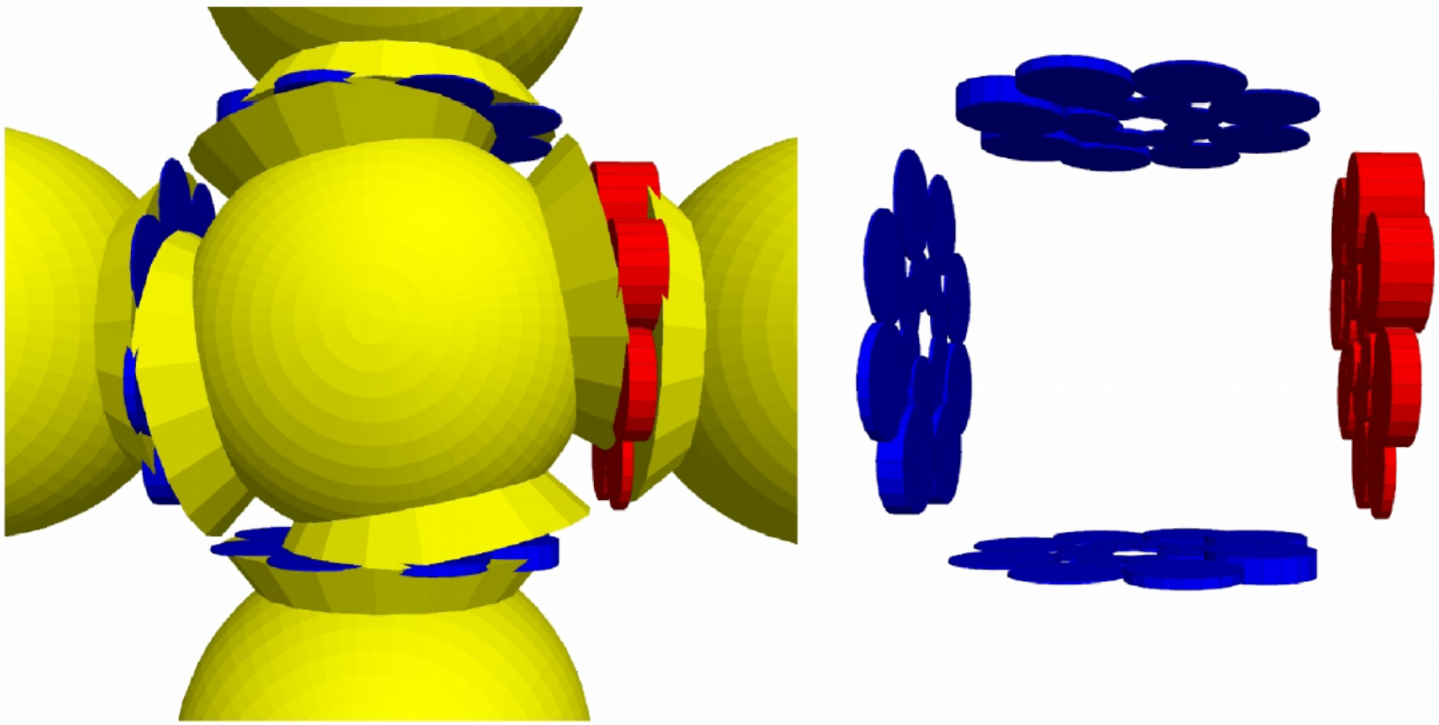
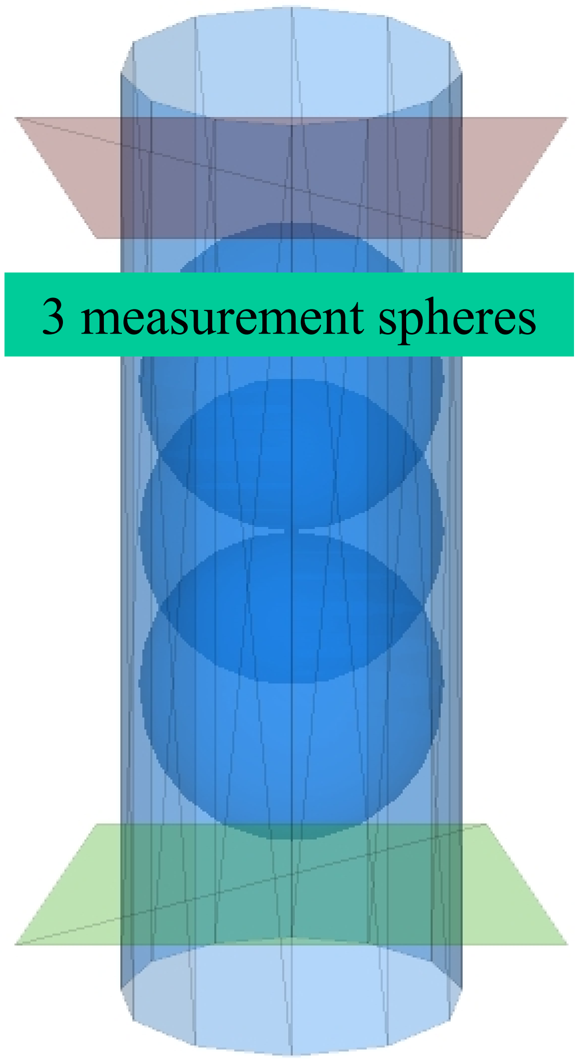


Figure 18 Crack and faced grain plot sets in 3D showing cracks, with crack thickness equal to gap, and cracks colored red/blue for tensile/shear failure.

Lab-Testing Procedures (stress-strain-porosity)

Table 8 Material-Vessel Stress, Strain and Porosity Quantities

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
σ_d , **mv_msd**	deviator stress
σ_m , **mv_msm**	mean stress
ε_d, **mv_med**	deviator strain
ε_v, **mv_mev**	volumetric strain
n, **mv_mn**	measurement-based porosity
n_w, **mv_wn**	wall-based porosity



Lab-Testing Procedures (stress-strain-porosity)

We denote stress and strain by

$$\begin{aligned} &\text{stress:} \quad \{\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz}\} \\ &\text{strain:} \quad \{\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{xy}, \varepsilon_{xz}, \varepsilon_{yz}\} \end{aligned} \tag{4}$$

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 $\{\sigma_{xx}, \sigma_{yy}, \sigma_{xy}\}$ and strain is $\{\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{xy}\}$.

The three measurement techniques measure the following quantities:

$$\begin{array}{ll} \sigma_{ij}^{m} \quad \varepsilon_{ij}^{m} & \boxed{\text{measurement-based}}\text{(6 terms each, symmetric)} \\ \sigma_{k}^{w} \quad \varepsilon_{k}^{w} & \boxed{\text{wall-based}}\text{(3 terms each)} \\ \underbrace{\qquad\quad \varepsilon_{k}^{g}}_{\substack{i,j=\{x,y,z\} \\ k=\{x,y,z,r\}}} & \text{guage-based (3 terms)} \end{array}$$

Lab-Testing Procedures (summary)

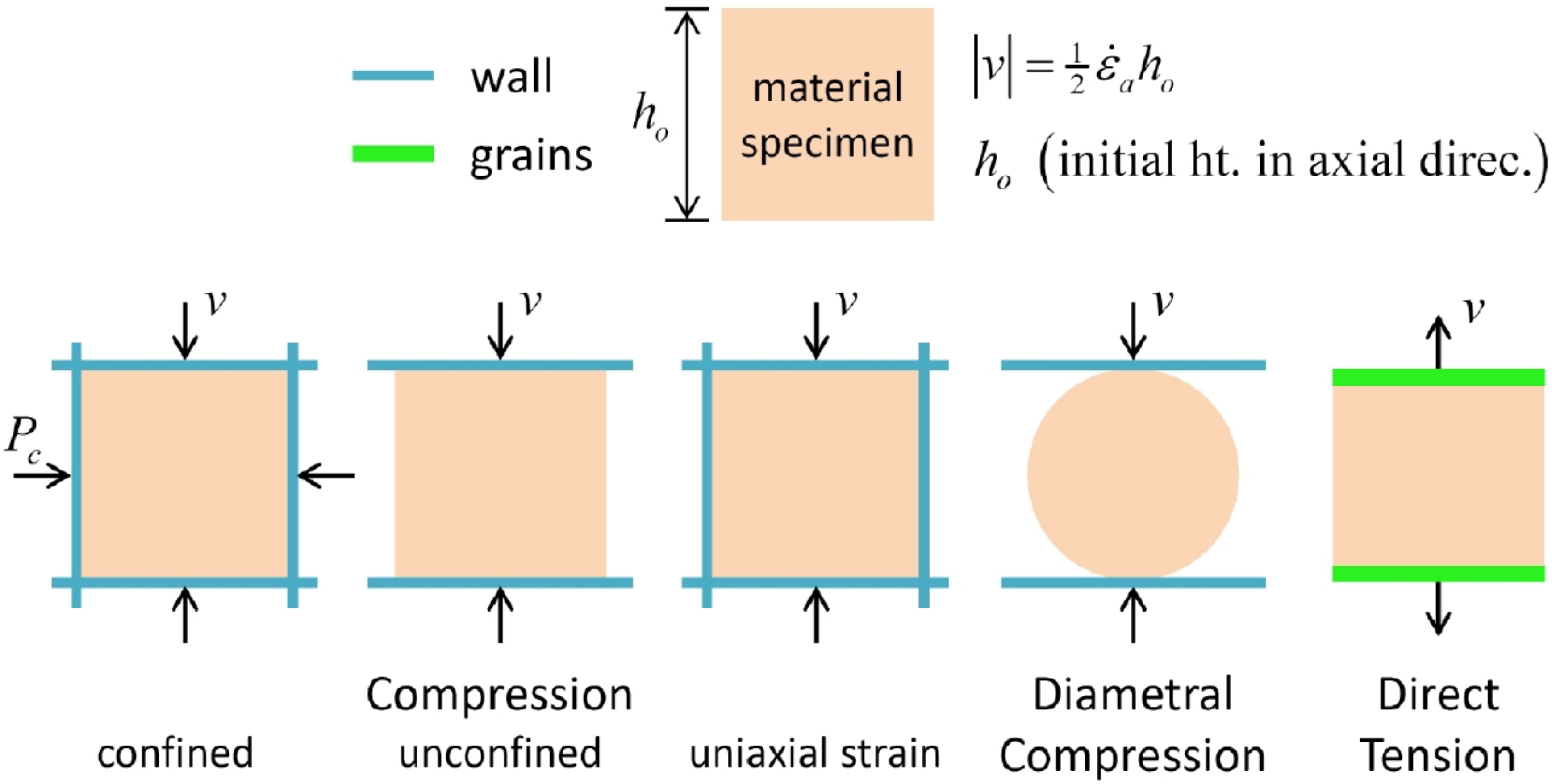
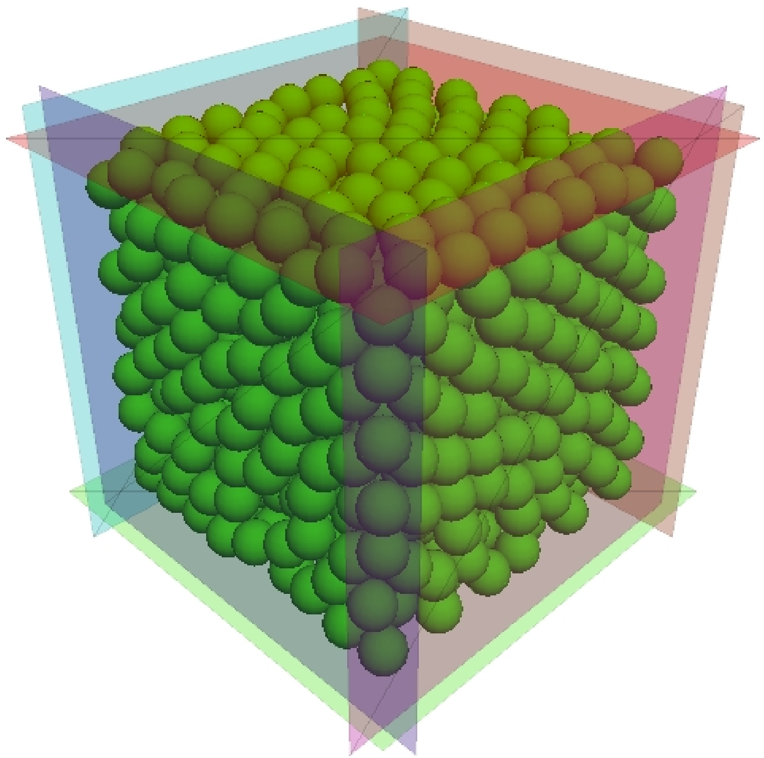


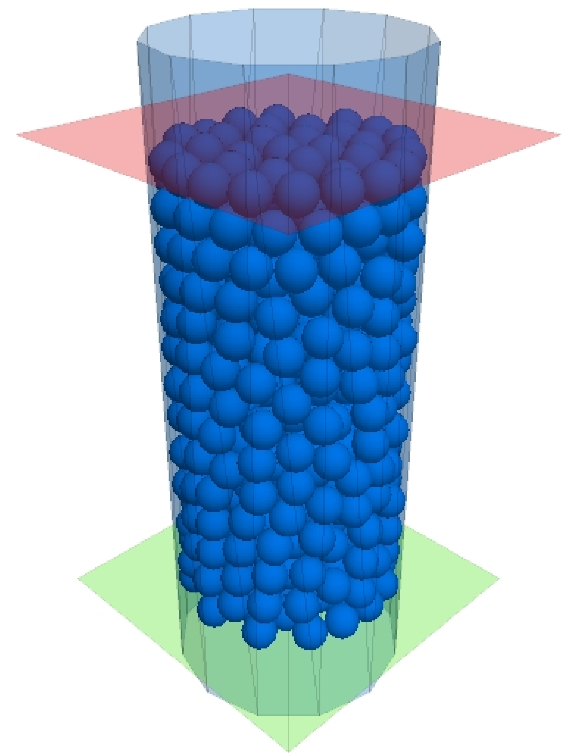
Figure 23 Loading conditions of laboratory-testing procedures.

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.

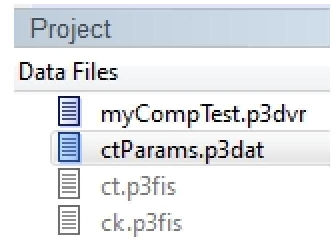
The loading phase may consist either of a single stage that ends when the applied deviatoric stress falls below a specified fraction of its peak value or multiple stages during which the axial-strain increments are specified.

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

Parameter	Type	Range	Default	Description
Material-vessel parameters are listed in Table 6.				
T_t, `ct_testType`	INT	$\{0,1,2\}$	0	test-type code 0, confined 1, unconfined 2, uniaxial strain
P_c, `ct_Pc`	FLT	$(0.0,\infty)$	NA	confining pressure ($P_c > 0$ is compression)
$\dot{\varepsilon}_a$, `ct_eRate`	FLT	$(0.0,\infty)$	NA	axial strain rate ($\lvert v\rvert = \frac{1}{2}\dot{\varepsilon}_a h_o$, $\dot{\varepsilon}_a > 0$, see Figure 23 and Section 5.4)
C_l, `ct_loadCode`	INT	$\{0,1\}$	0	loading-phase code 0, single stage 1, multiple stages
α, `ct_loadFac`	FLT	$(0.0,1.0)$	0.9	load-termination factor ($C_l = 0$) for termination criterion: $\lvert\sigma_d^w\rvert \le \alpha \lvert\sigma_d^w\rvert_{max}$
Servo-control group:				
ε_P, `ct_PTol`	FLT	$(0.0,\infty)$	`pk_PTol`	pressure tolerance $\left(\frac{\lvert P-P_c\rvert}{P_c} \le \varepsilon_P\right)$ where P is current pressure
$\varepsilon_{\lim}$, `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 9)



axial strain rate,
must be slow enough to obtain
quasi-static response

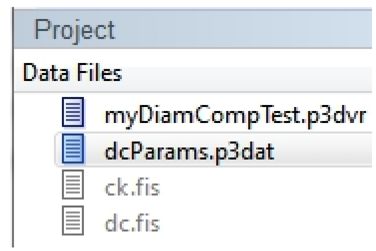
Perform compression test on contact-bonded material.

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

Parameter	Type	Range	Default	Description
$\{w,d\}$, `dc_{w,d}`	FLT	$(0.0,\infty)$	NA	platen width and depth (2D model: $d \equiv 1$)
g_o, `dc_g0`	FLT	$(0.0,\infty)$	NA	initial platen gap
E_p^*, `dc_emod`	FLT	$(0.0,\infty)$	`mv_emod` or NA	platen effective modulus (used by linear contact model)
$\dot{\varepsilon}_a$, `dc_eRate`	FLT	$(0.0,\infty)$	NA	axial strain rate ($\lvert v \rvert = \frac{1}{2}\dot{\varepsilon}_a g_o$, $\dot{\varepsilon}_a > 0$, see Figure 25 and Section 5.4)
C_l, `dc_loadCode`	INT	$\{0,1\}$	0	loading-phase code $\begin{cases} 0, & \text{single stage} \\ 1, & \text{multiple stages} \end{cases}$
α, `dc_loadFac`	FLT	$(0.0,1.0)$	0.9	load-termination factor ($C_l = 0$) for termination criterion: $\lvert F_a \rvert \le \alpha \lvert F_a \rvert_{\max}$
Static-equilibrium group:				
$\varepsilon_{\lim}$, `dc_ARatLimit`	FLT	$(0.0,\infty)$	1×10^{-5}	equilibrium-ratio limit (parameter of `ft_eq`)
α, `dc_stepLimit`	INT	$[1.0,\infty)$	`pk_stepLimit` or 2×10^{6}	step limit (parameter of `ft_eq`)



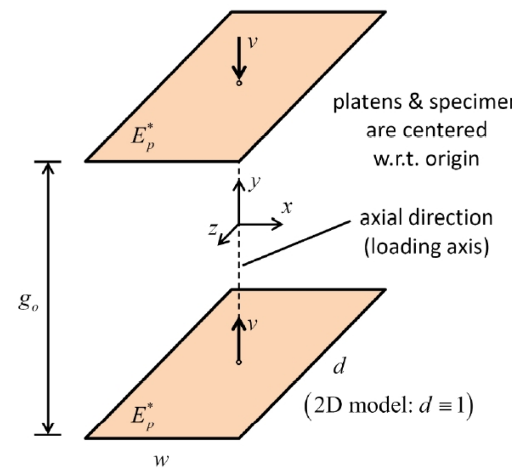


Figure 18 Loading configuration of diametral-compression test.

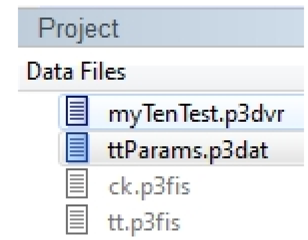
Perform diametral-compression test on contact-bonded material.

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

Parameter	Type	Range	Default	Description
Material-vessel parameters are listed in Table 6.				
t_g , `tt_tg`	FLT	$(0.0, \infty)$	$0.1H$	grip thickness
$\dot{\varepsilon}_a$, `tt_eRate`	FLT	$(0.0, \infty)$	NA	axial strain rate ($\lvert v \rvert = \frac{1}{2}\dot{\varepsilon}_a h_o$, $\dot{\varepsilon}_a > 0$, see Figure 17 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	$(0.0,1.0)$	0.9	load-termination factor ($C_l = 0$) for termination criterion: $\lvert \sigma_a^m \rvert \le \alpha \lvert \sigma_a^m \rvert_{\max}$



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

Perform direct-tension test on contact-bonded material.

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.

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).[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 1 Microproperties of AG_Linear Material

Property	Value
Common group:	
N_m	AG_Linear
$T_m,\ \alpha,\ C_\rho,\ \rho_v\ \left[\mathrm{kg/m^3}\right]$	$0,\ 0.7,\ 0,\ 2650$
$S_g,\ T_{SD},\ \left\{D_{\{l,u\}}\ [\mathrm{mm}],\ \phi\right\},\ D_{mult}$	$0,\ 0,\ \{14, 20, 1.0\},\ 1.0$
Packing group:	
$S_{RN},\ P_m\ [\mathrm{kPa}],\ \varepsilon_P,\ \varepsilon_{\lim},\ n_{\lim}$	$10000,\ 150,\ 1\times10^{-2},\ 8\times10^{-3},\ 2\times10^{6}$
$C_p,\ n_c,\ \mu_{CA},\ v_{\lim}\ [\mathrm{m/s}]$	$0,\ 0.58,\ 0,\ 1.0$
Linear material group:	
$E^*\ [\mathrm{MPa}],\ \kappa^*,\ \mu$	$500,\ 1.5,\ 0.4$

* Linear material parameters are defined in Table 2 of the base memo.

Example Materials (linear material)

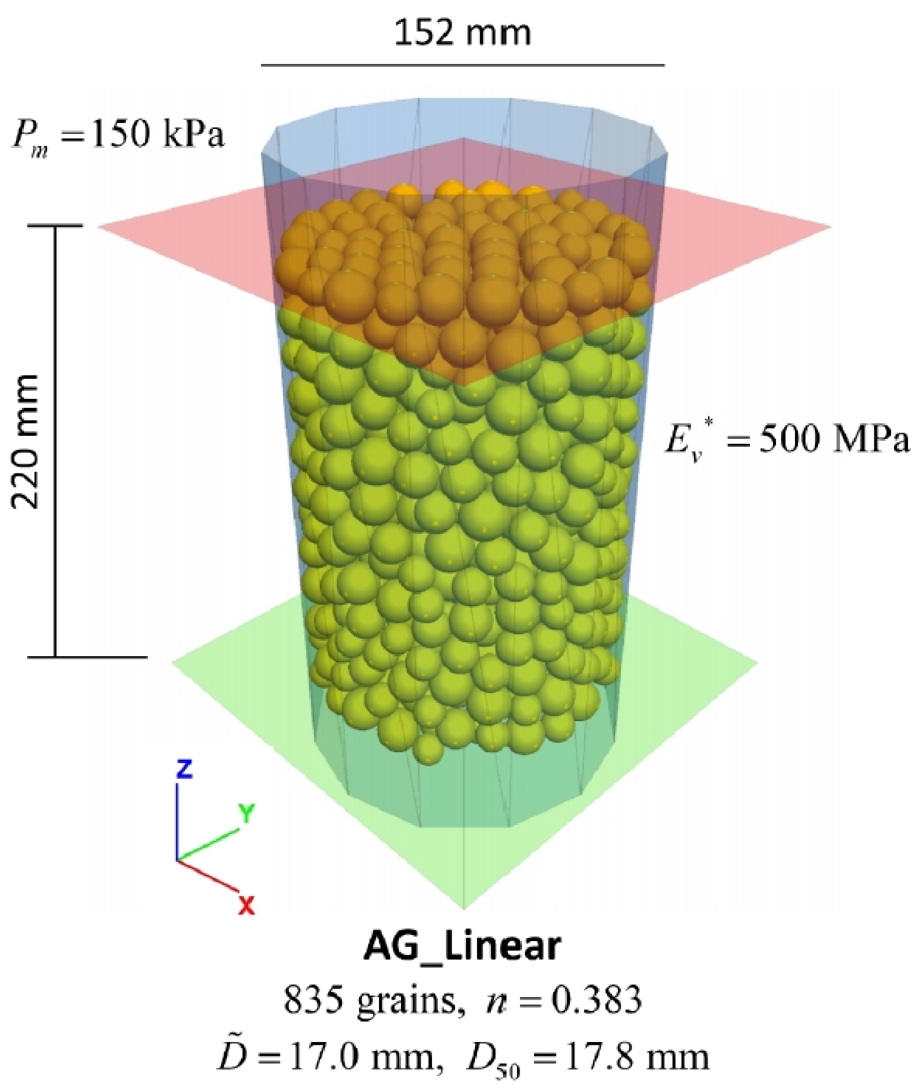


Figure 1 AG_Linear material packed at 150 kPa material pressure at the end of material genesis.

Example Materials (linear material)

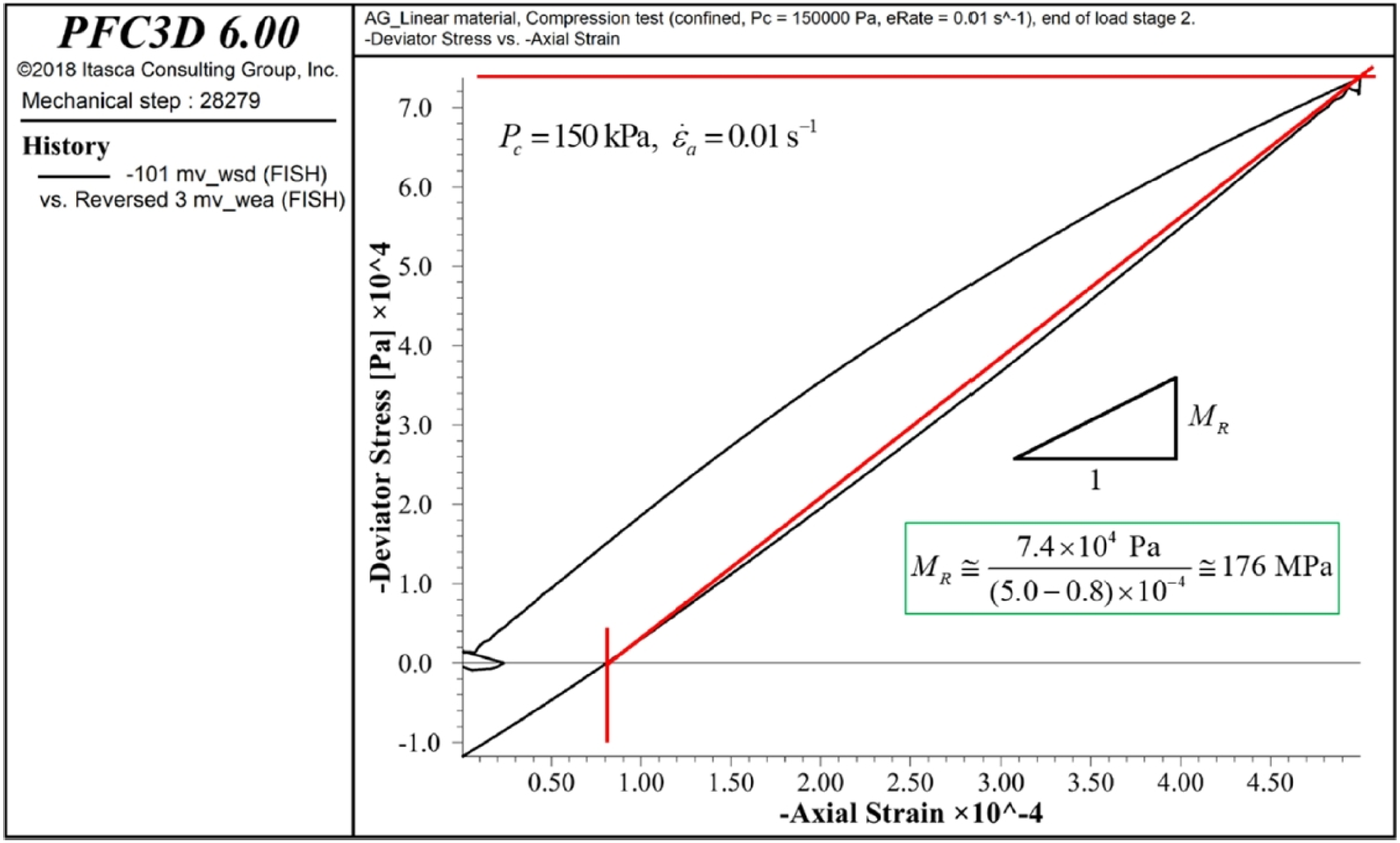


Figure 2 Deviator stress versus axial strain for AG_Linear material tested at 150 kPa confinement, and measurement of resilient modulus.

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 $\mathrm{kg/m^3}$; 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.

Example Materials (contact-bonded material)

*Table 5 Microproperties of SS_ContactBonded Material**

Property	Value
Common group:	
N_m	SS_ContactBonded
$T_m,\ \alpha,\ C_\rho,\ \rho_v\left[\mathrm{kg/m^3}\right]$	1, 0.7, 1, 1960
$S_g,\ T_{SD},\ \left\{D_{\{l,u\}}\,[\mathrm{mm}],\ \phi\right\},\ D_{mult}$	0, 0, $\{4.0, 6.0, 1.0\}$, 1.0
Packing group:	
$S_{RN},\ P_m\,[\mathrm{MPa}],\ \varepsilon_P,\ \varepsilon_{\lim},\ n_{\lim}$	10000, 30, 1×10^{-2}, 8×10^{-3}, 2×10^{6}
$C_p,\ n_c$	1, 0.30
Contact-bonded material group:	
Linear group:	
$E^*\,[\mathrm{GPa}],\ \kappa^*,\ \mu$	3.0, 1.5, 0.4
Contact-bond group:	
$g_i\,[\mathrm{mm}]$	0
$(T_\sigma)_{\{\mathrm{m,sd}\}}\,[\mathrm{MPa}],\ (S_\sigma)_{\{\mathrm{m,sd}\}}\,[\mathrm{MPa}]$	$\{1.0, 0\}$, $\{20.0, 0\}$
Linear material group:	
$E_n^*\,[\mathrm{GPa}],\ \kappa_n^*,\ \mu_n$	3.0, 1.5, 0.4

* Contact-bonded material parameters are defined in Table 3 of the base memo.

Example Materials (contact-bonded material)

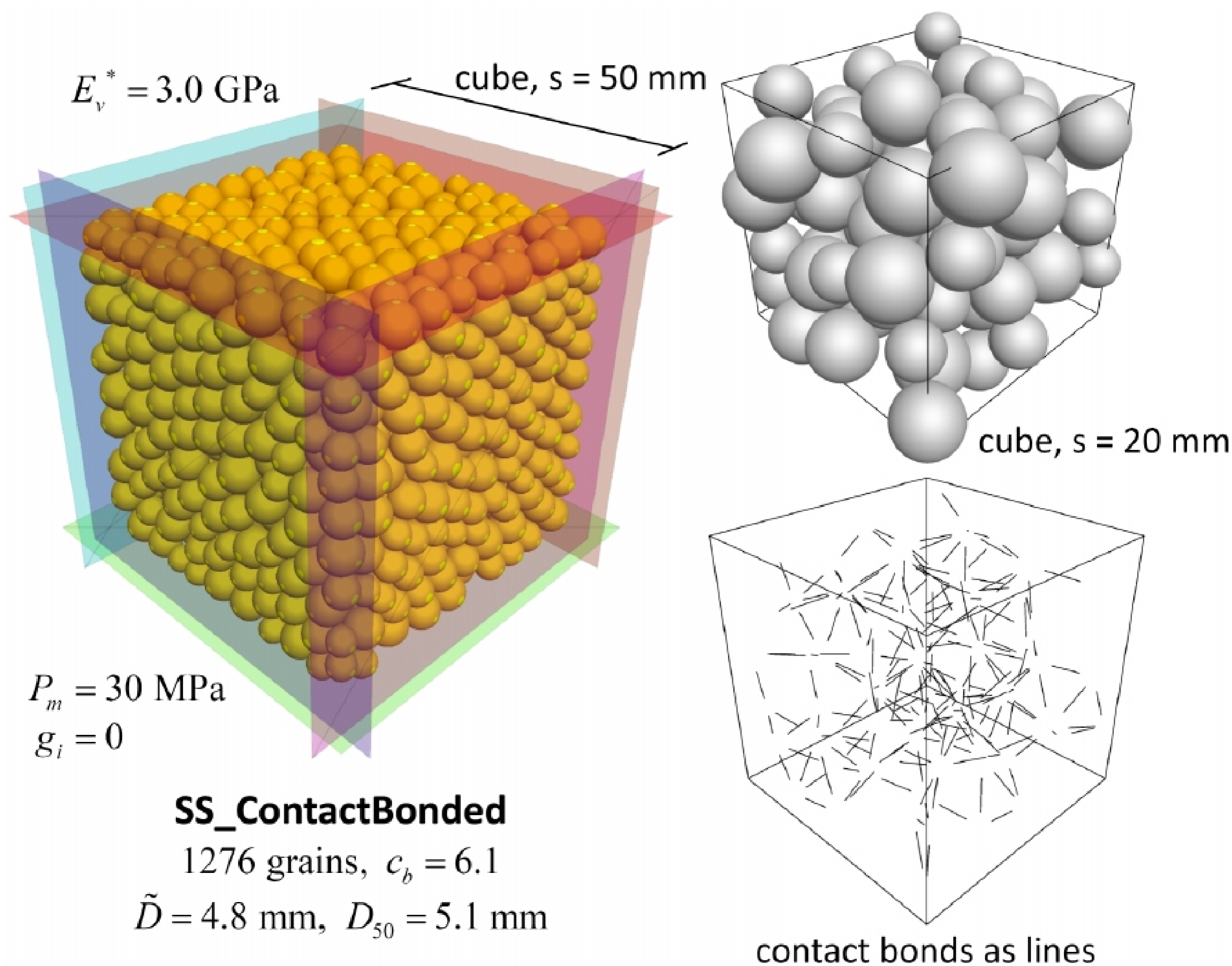
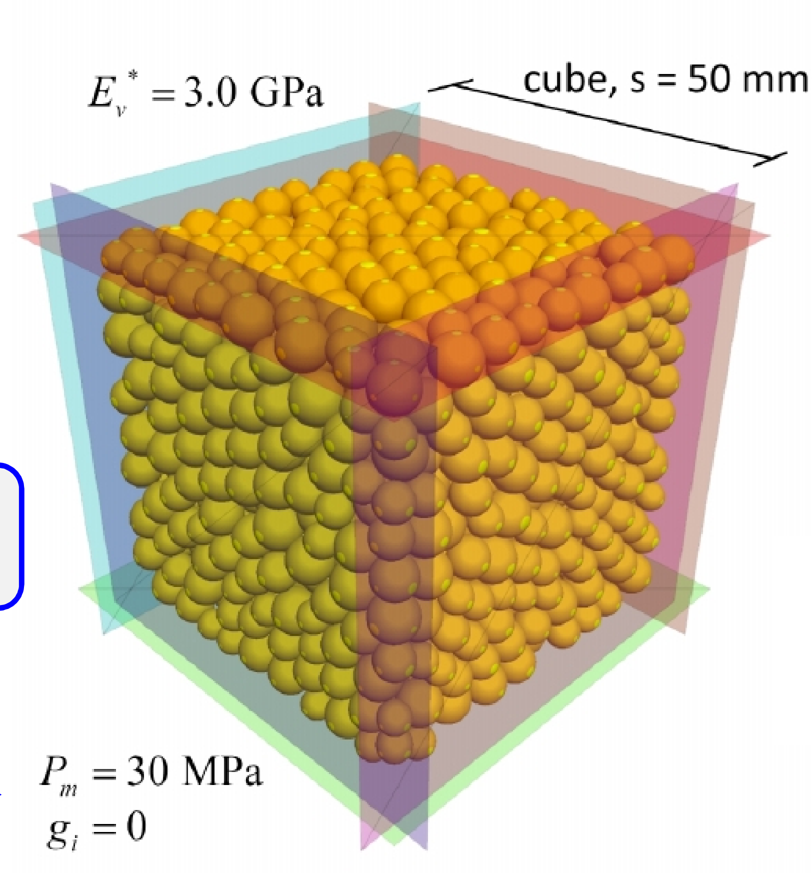


Figure 11 SS_ContactBonded material at the end of material genesis with grains and contact bonds in the microstructural box.

Example Materials (contact-bonded material)



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

Bond coordination number is increased by either: increasing the material pressure, or increasing the installation gap.

Example Materials (contact-bonded material)

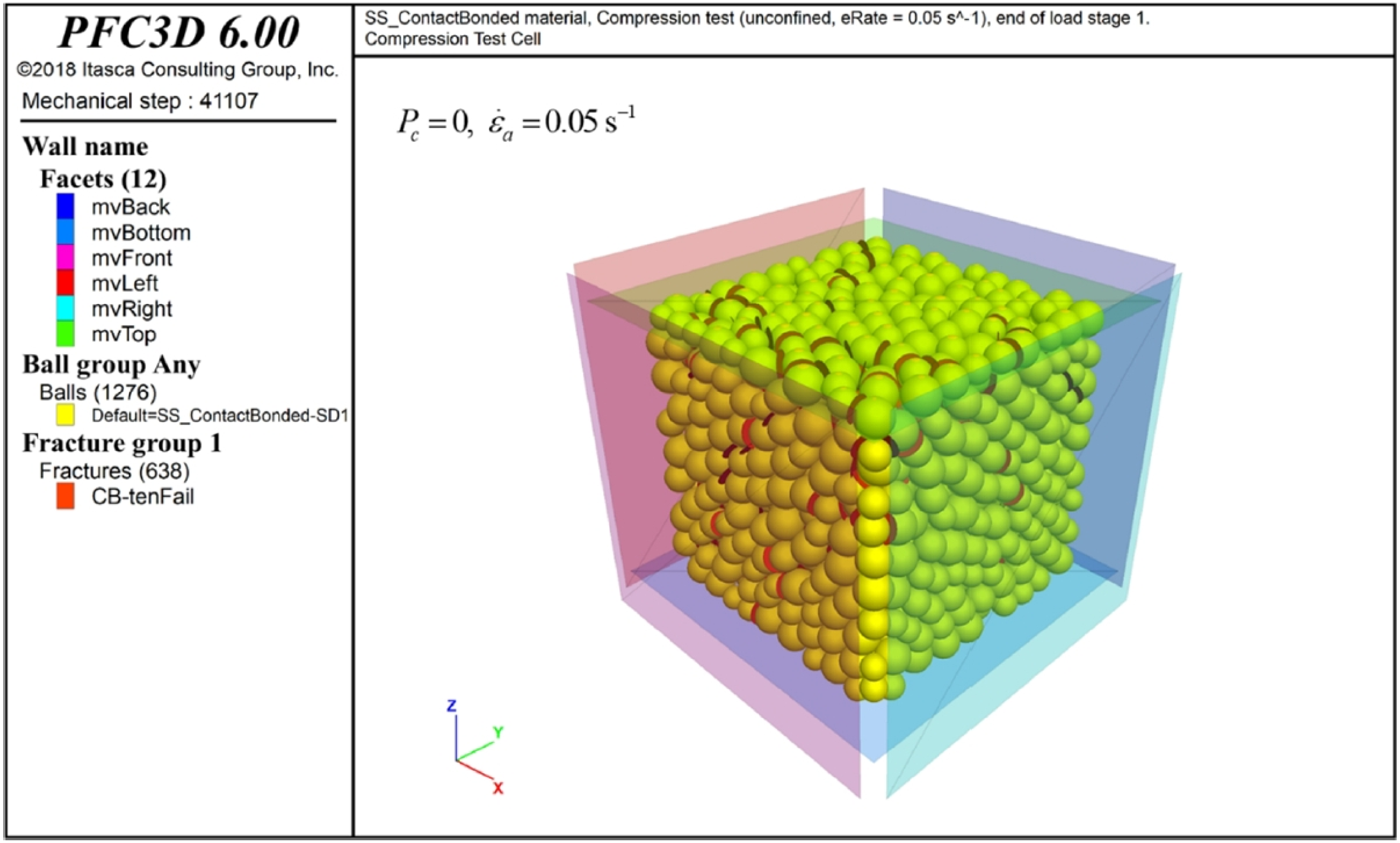


Figure 12 SS_ContactBonded material at the end of the fully unconfined test with grains and cracks.

Example Materials (contact-bonded material)

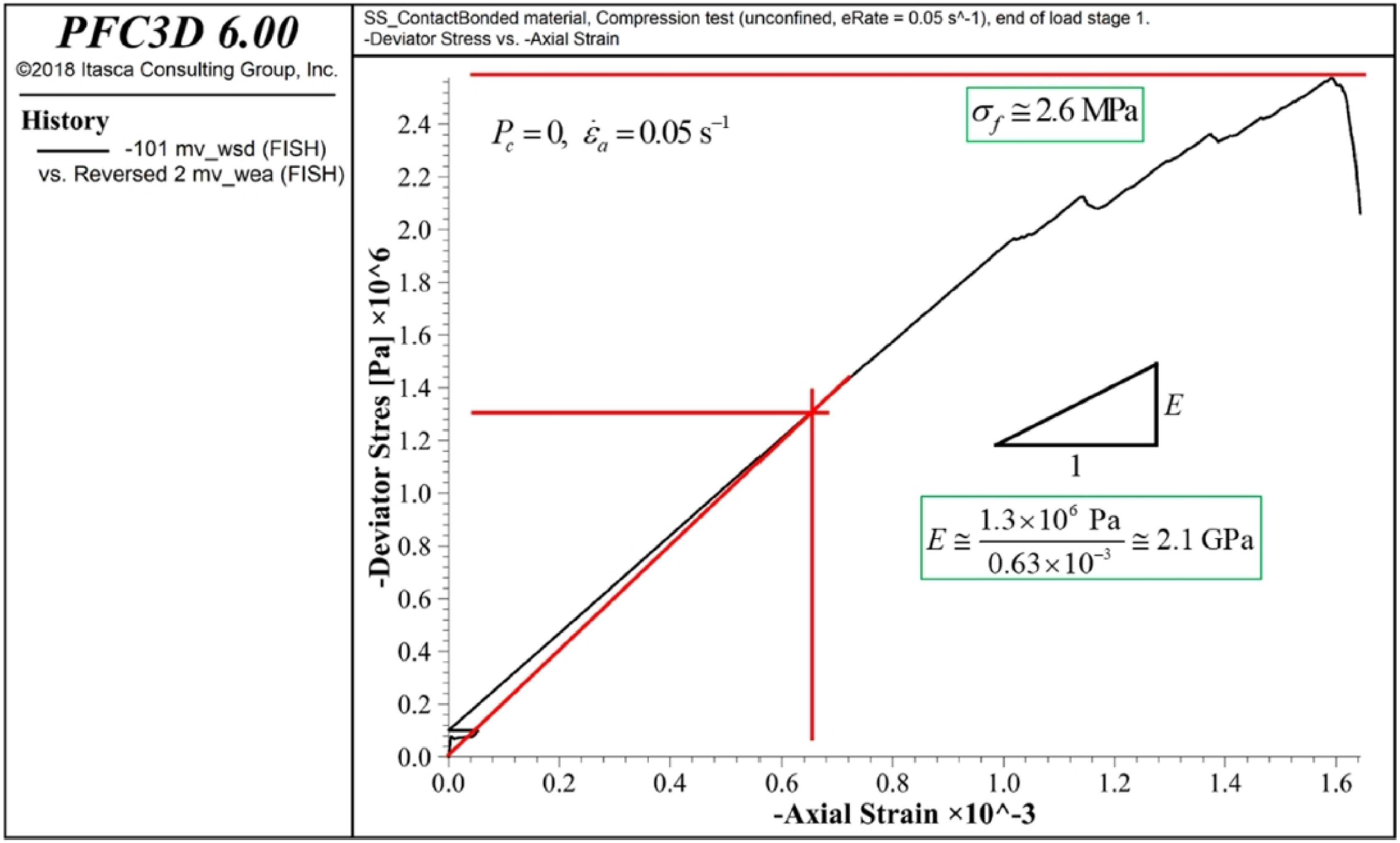


Figure 13 ***Deviator stress versus axial strain for SS_ContactBonded material tested fully unconfined, and measurement of peak strength and Young's modulus.***

Example Materials (contact-bonded material)

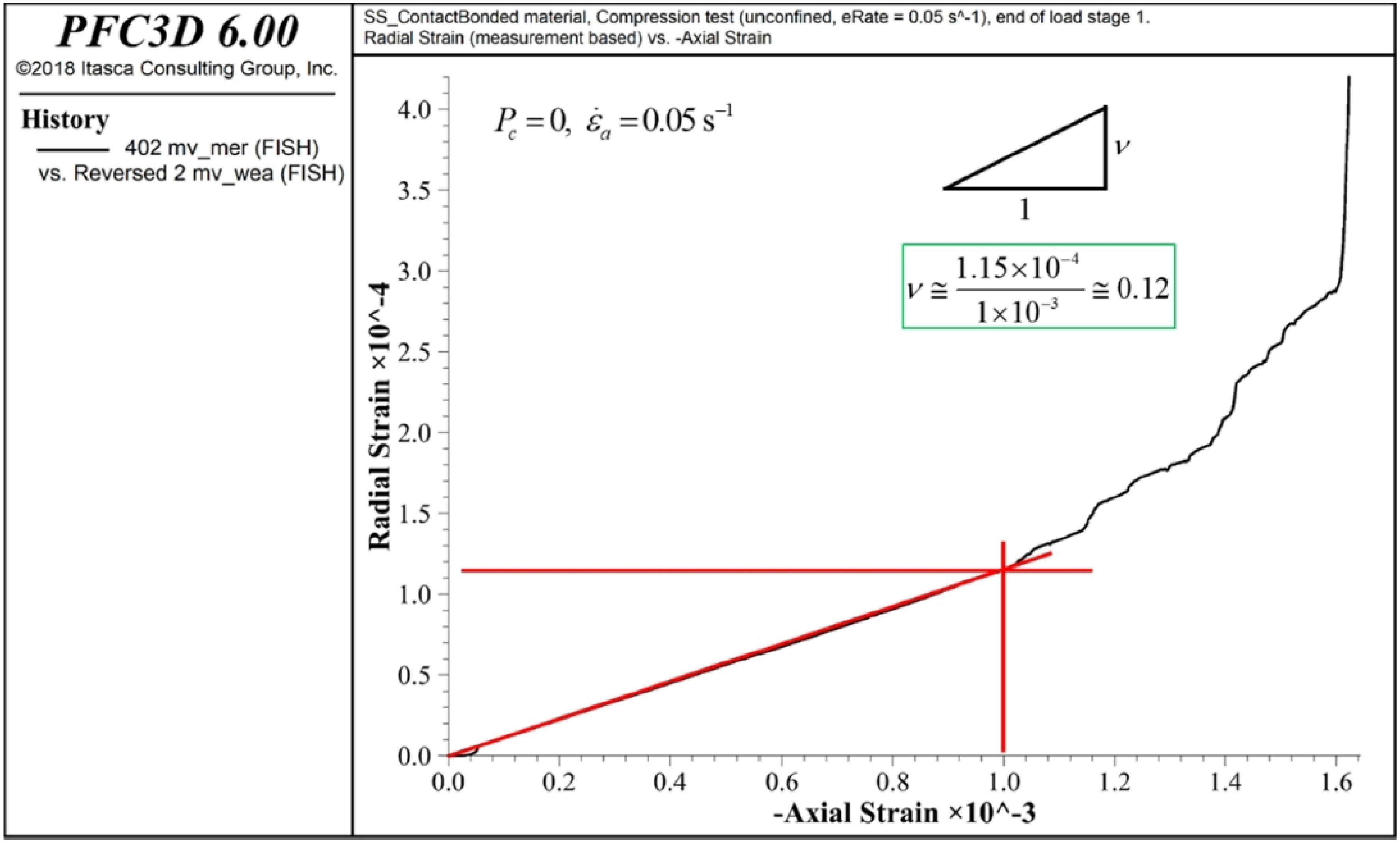


Figure 14 Radial strain versus axial strain for SS_ContactBonded material tested fully unconfined, and measurement of Poisson's ratio.

Example Materials (contact-bonded material)

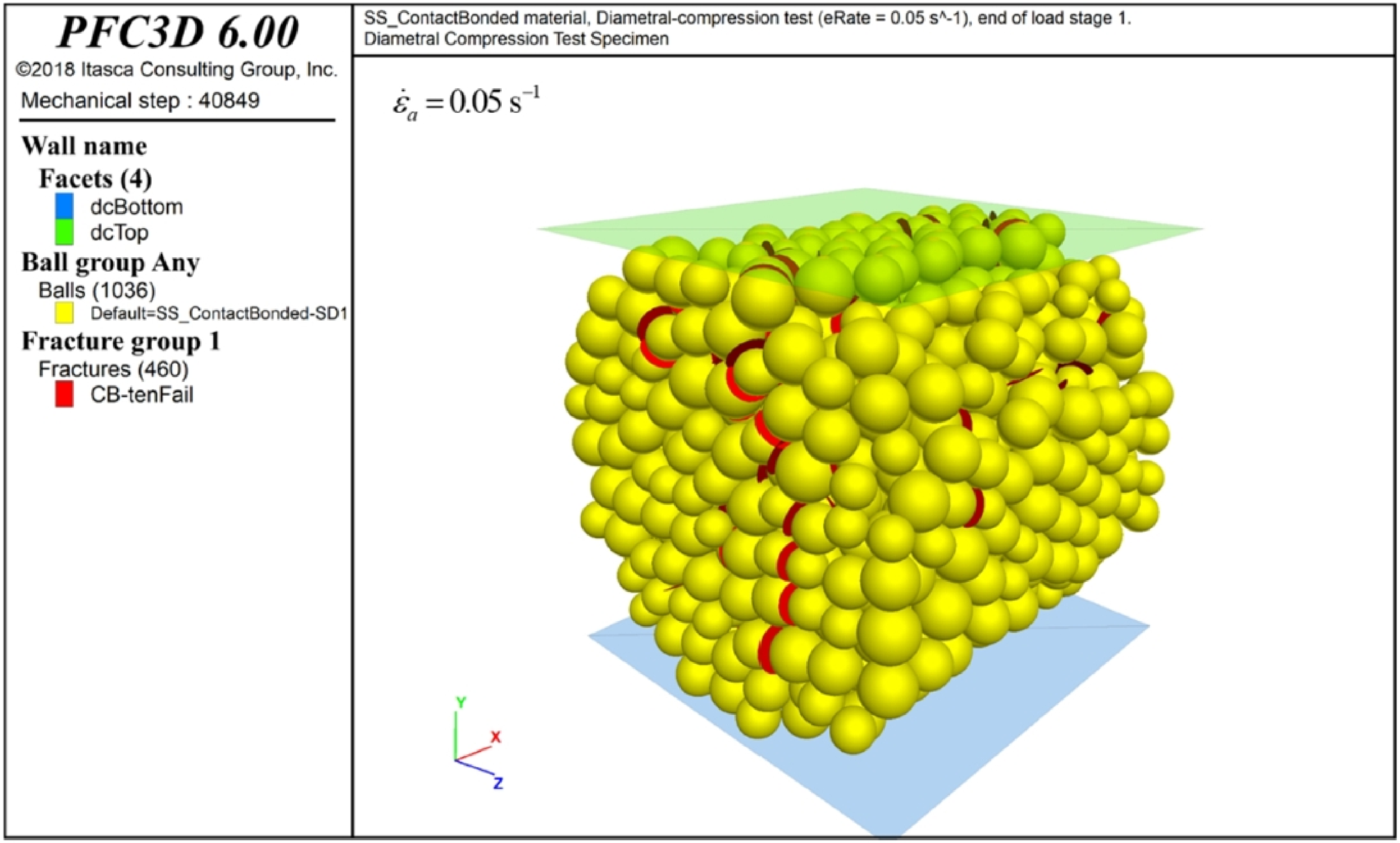


Figure 15 SS_ContactBonded material at the end of diametral-compression test with grains and cracks.

Example Materials (contact-bonded material)

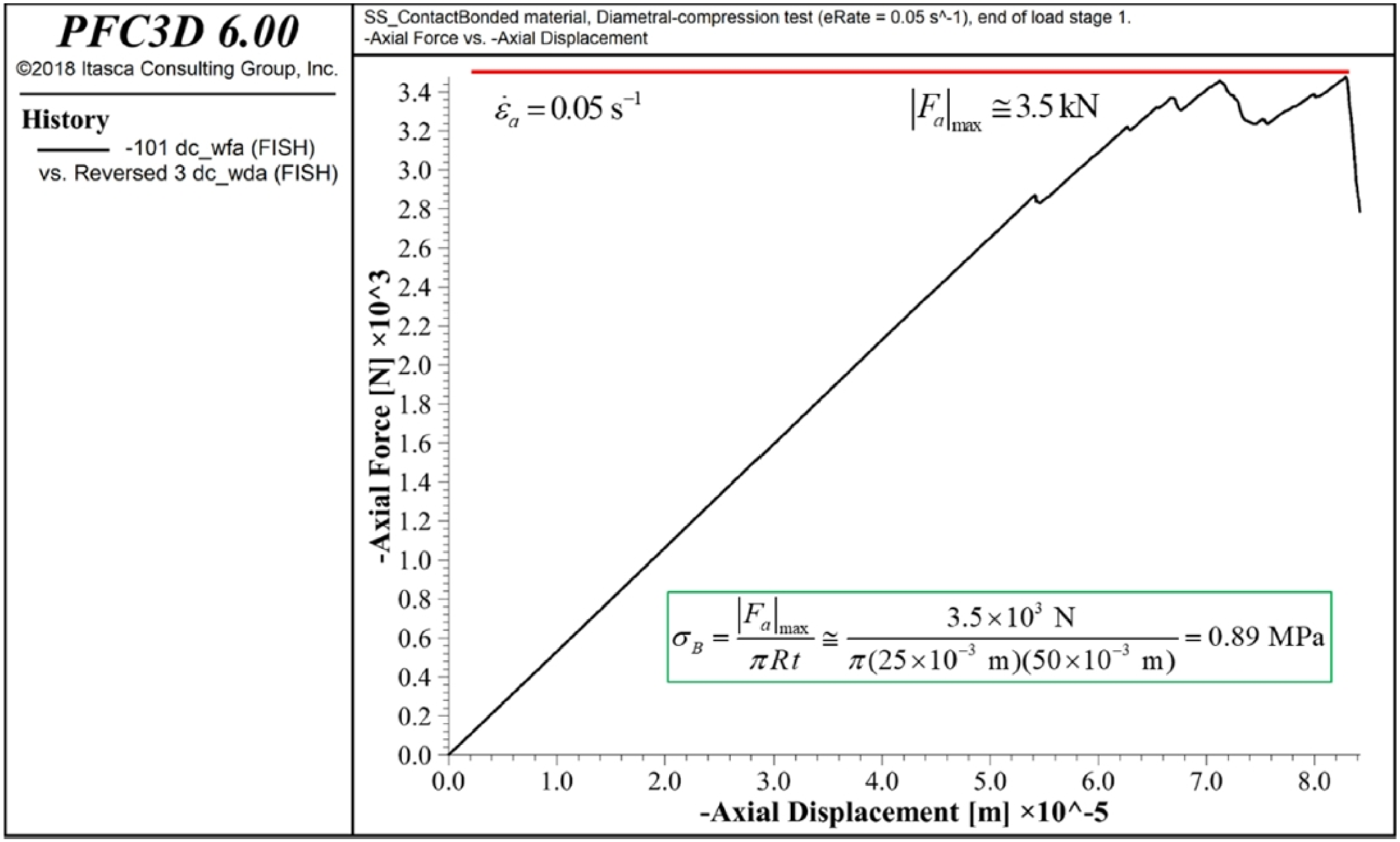


Figure 16 Axial force versus axial displacement for SS_ContactBonded material during the diametral-compression test, and measurement of Brazilian tensile strength.

Example Materials (contact-bonded material)

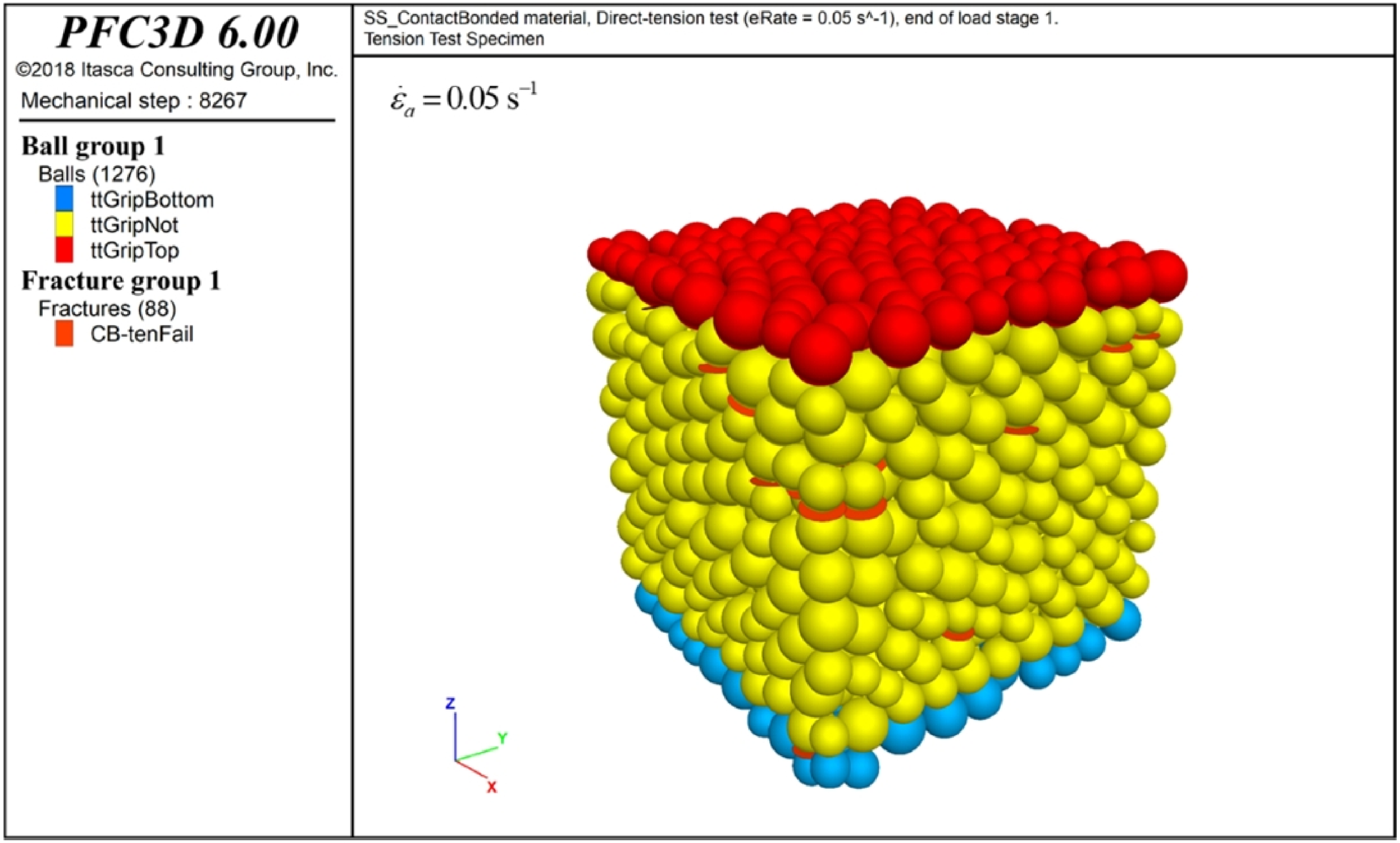


Figure 17 SS_ContactBonded material at the end of the direct-tension test with grains and cracks.

Example Materials (contact-bonded material)

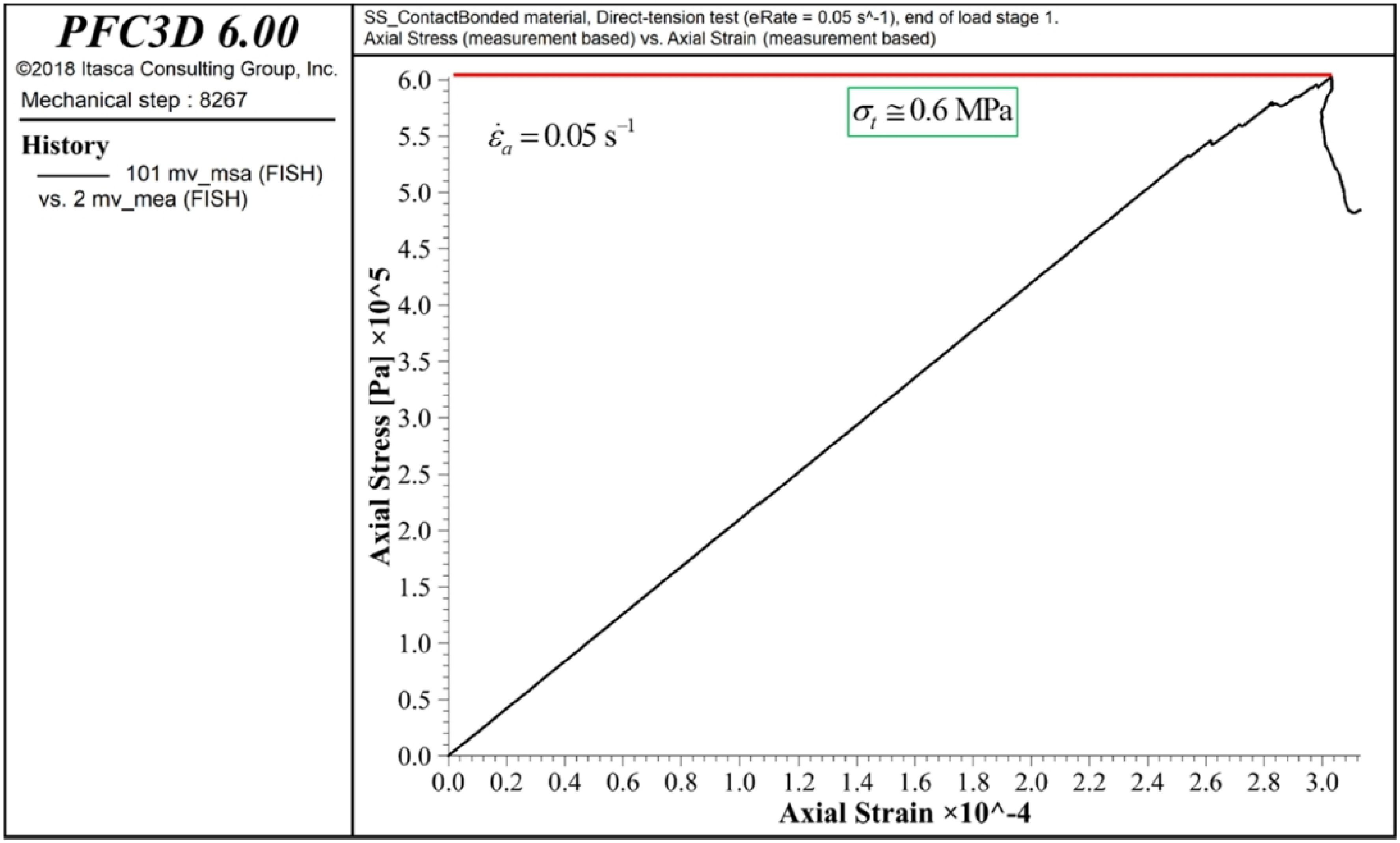


Figure 18 Axial stress versus axial strain for SS_ContactBonded material during the direct-tension test, and measurement of tensile strength.

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:

Potyondy, D. (2018) “Calibration of the Flat-Jointed Material,” PowerPoint Slide Set (April, 13, 2018).