Material-Modeling Support for PFC

David Potyondy

Originally: Itasca Webinar (December 14, 2017)
Updated for fistPkg26, fistPkg6.6, fistPkg{7.1, 7.2, 7.3}
June 29, 2023

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 7 is fistPkg7.N, where N is package version number

Potyondy, D. (2023) "Material-Modeling Support in PFC [fistPkg7.3]," Itasca Consulting Group, Inc., Technical Memorandum ICG7766-L (June 29, 2023), Minneapolis, Minnesota.

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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.
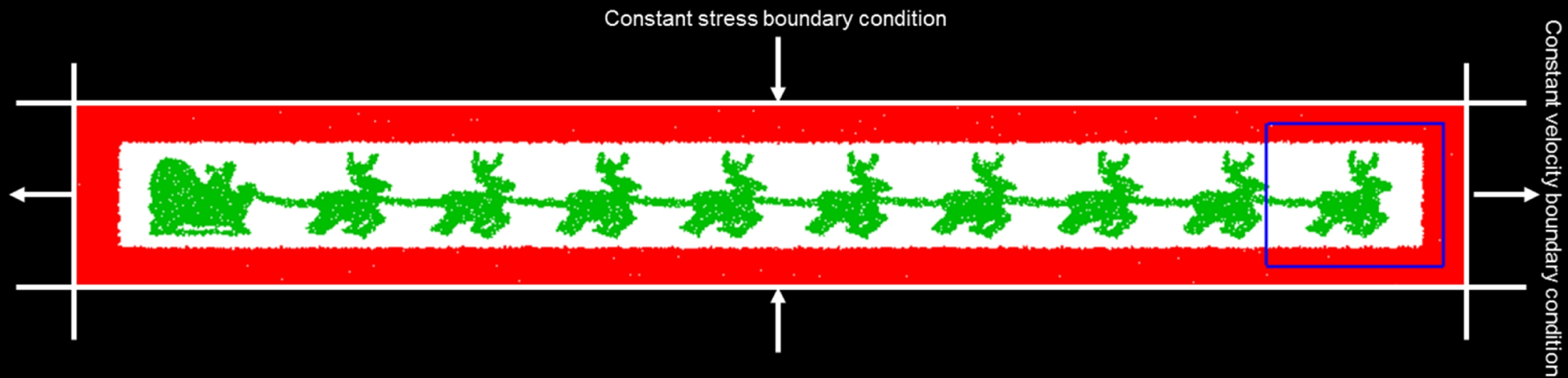
Overview

Bonded-Particle Modeling (Essential Features)

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

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

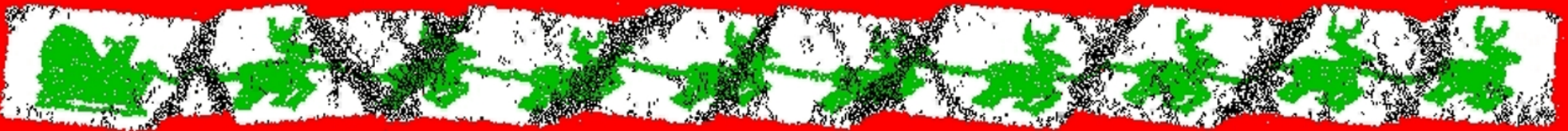# Bonded-Particle Modeling (Essential Features)

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.

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Bonded-Particle Modeling (Essential Features)

Increasing horizontal extension

From Martin Schöpfer: animation

Bonded-Particle Modeling (Essential Features)

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

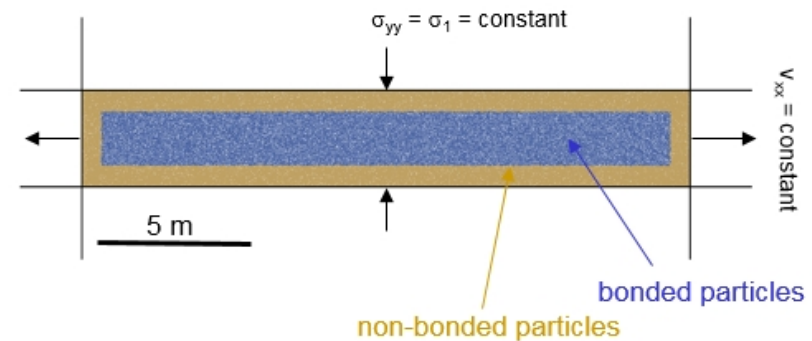Photo: B. Grasemann   Quartzitic Marble, Serifos, Greece

Asymmetric fault system

Shear?
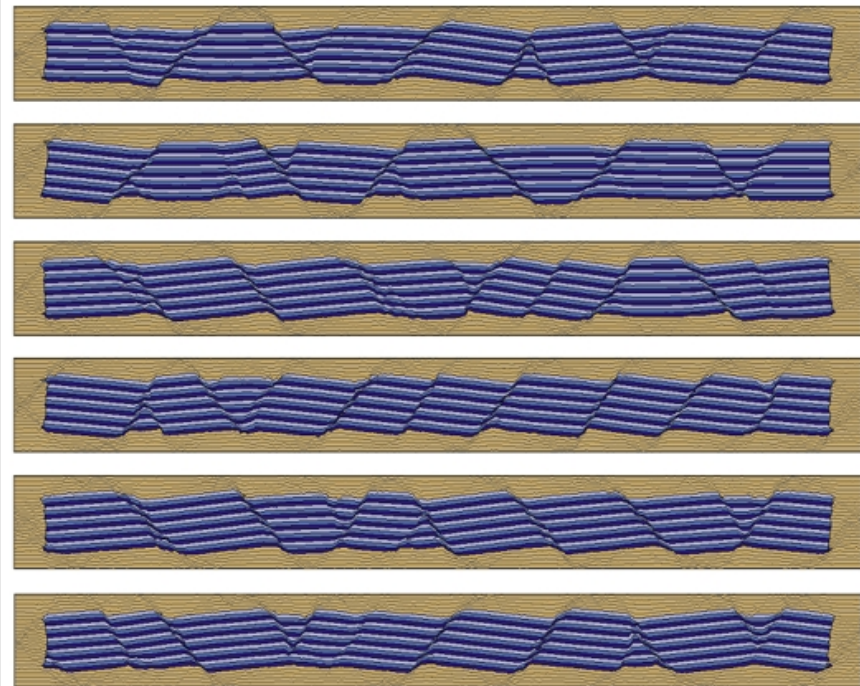
fig. 11

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

2D DEM model boundary conditions

$\sigma_{yy} = \sigma_1 = $ constant

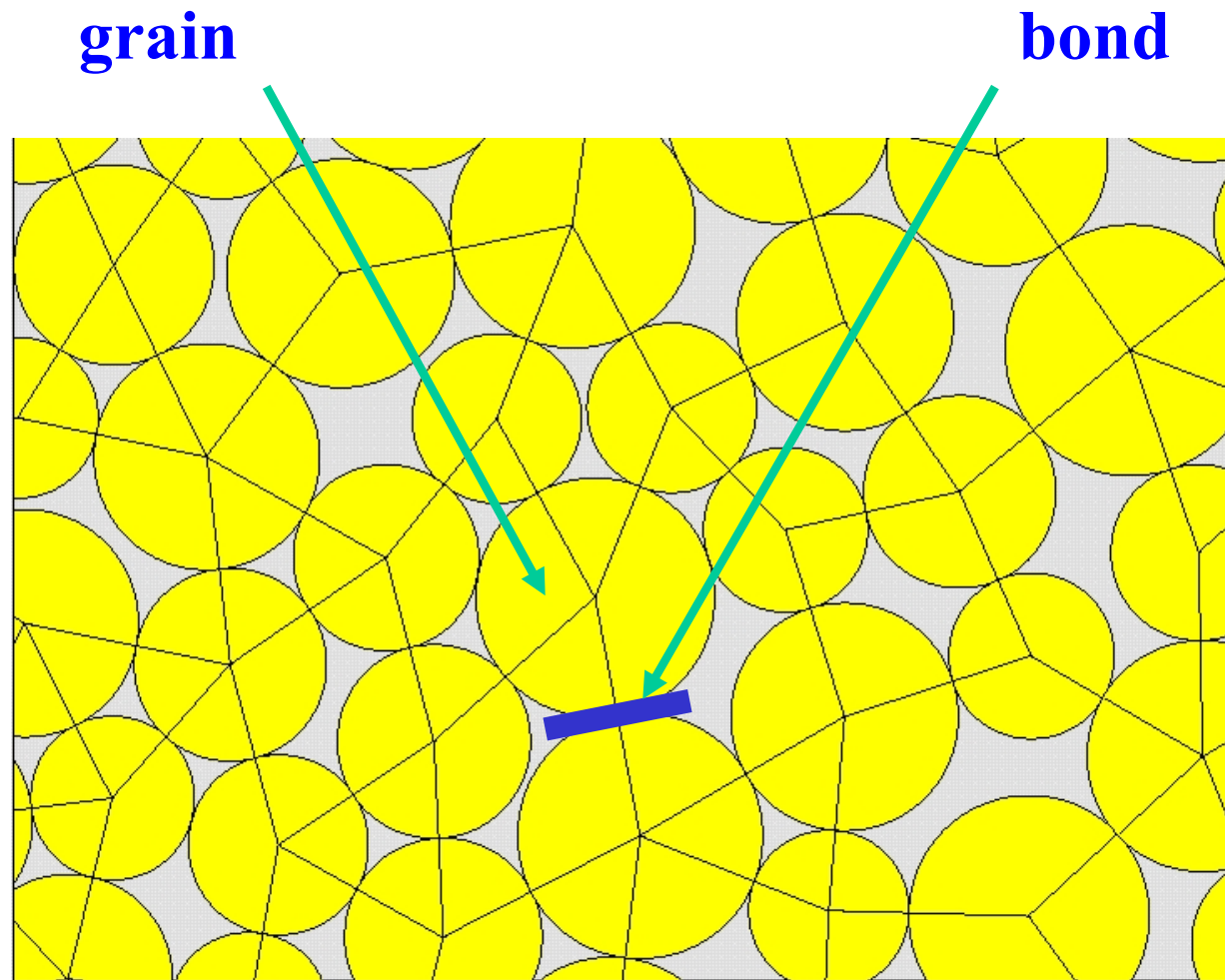$V_{xx} = $ constant

5 m

bonded particles

non-bonded particles

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

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From Martin Schöpfer: science
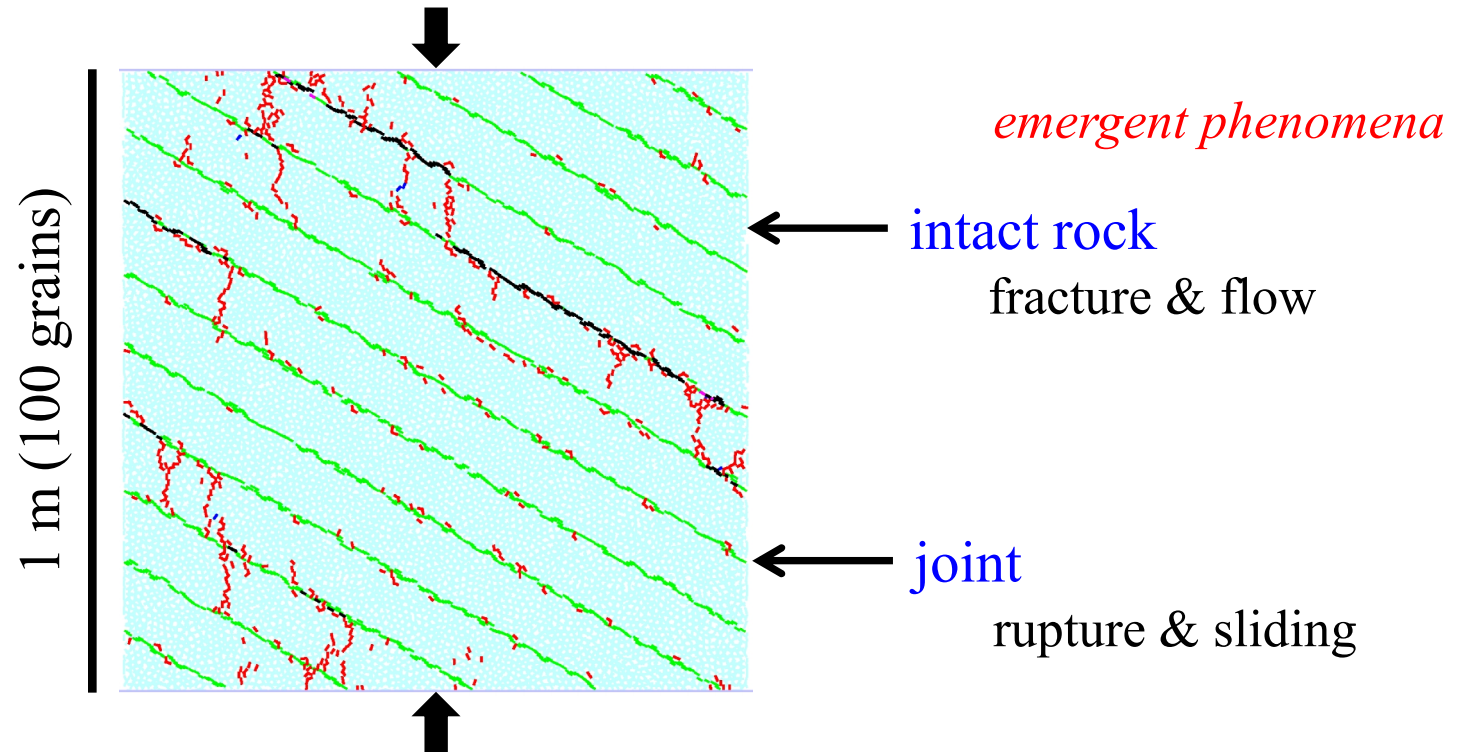
Essential Features of a BPM

grain   bond

Damage consists of bond breakages.

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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

1 m (100 grains)

emergent phenomena

intact rock
fracture & flow

joint
rupture & sliding

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
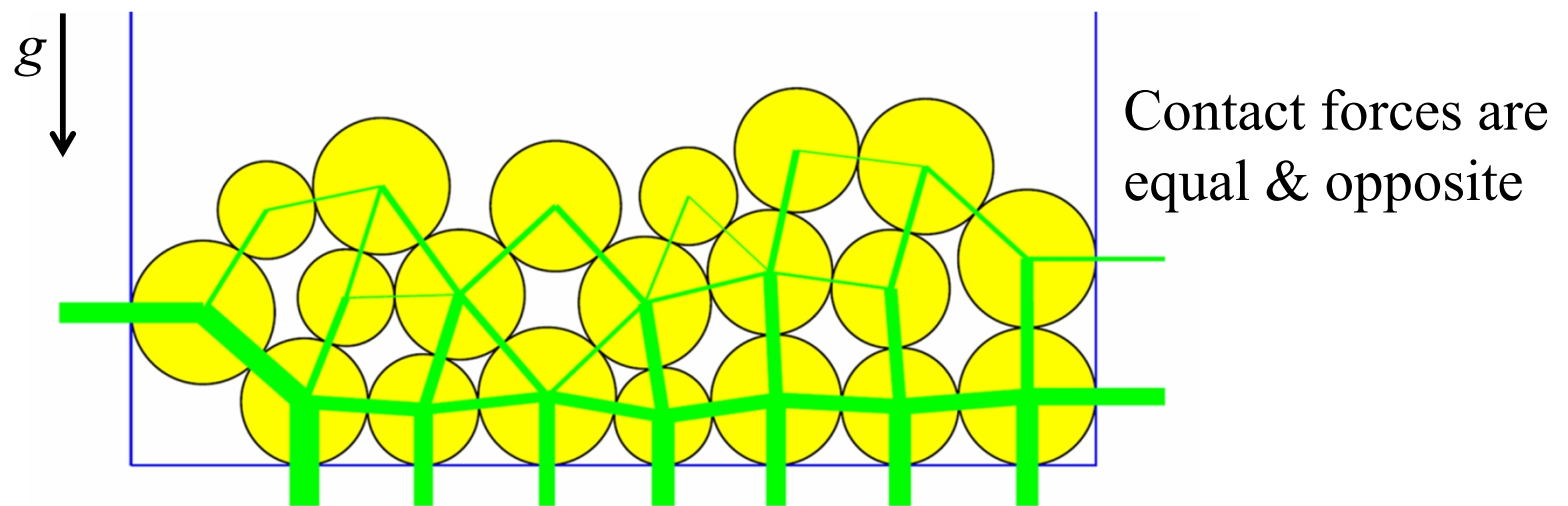
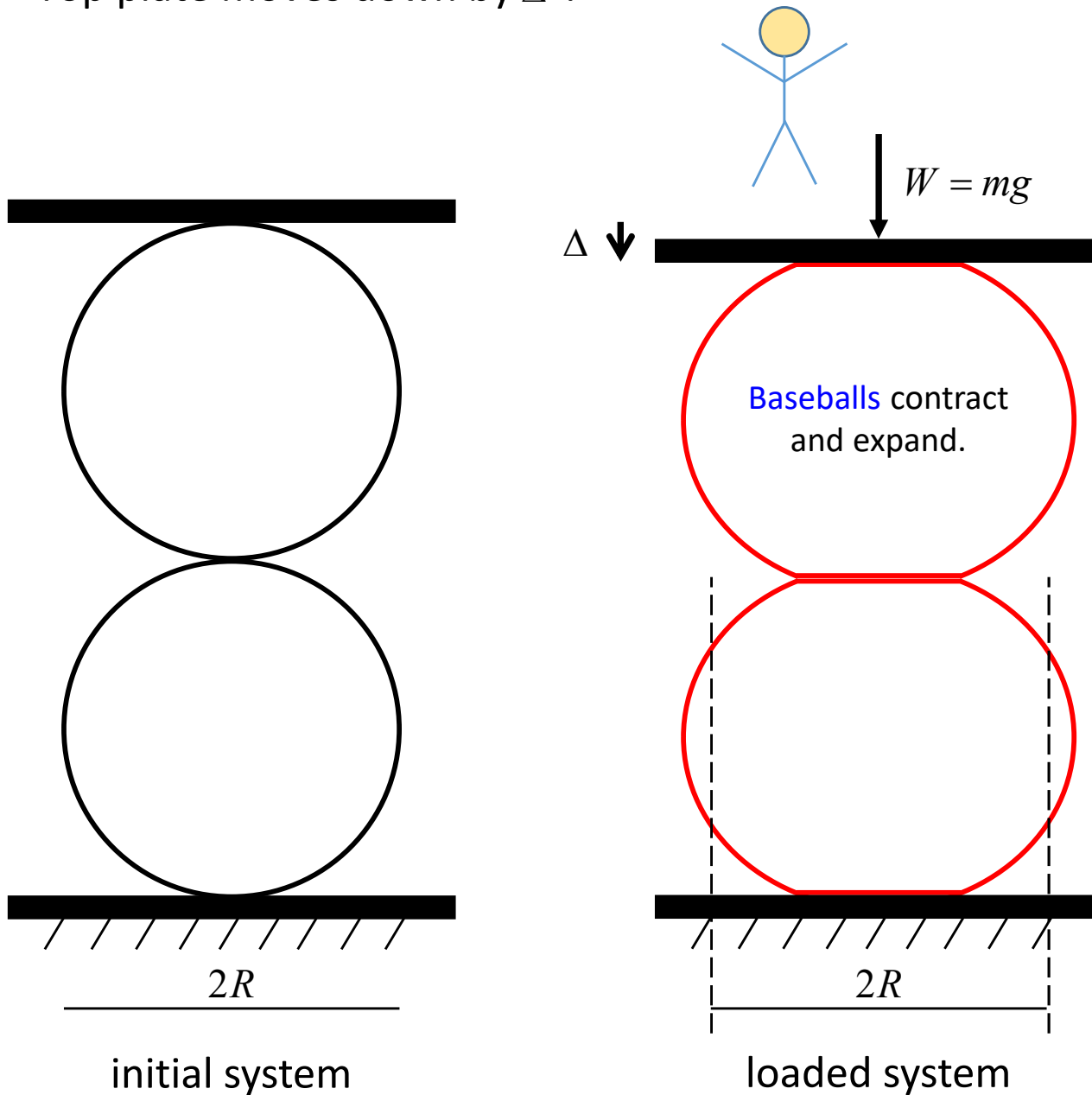# Bonded-Particle Modeling Methodology (PFC model)

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.
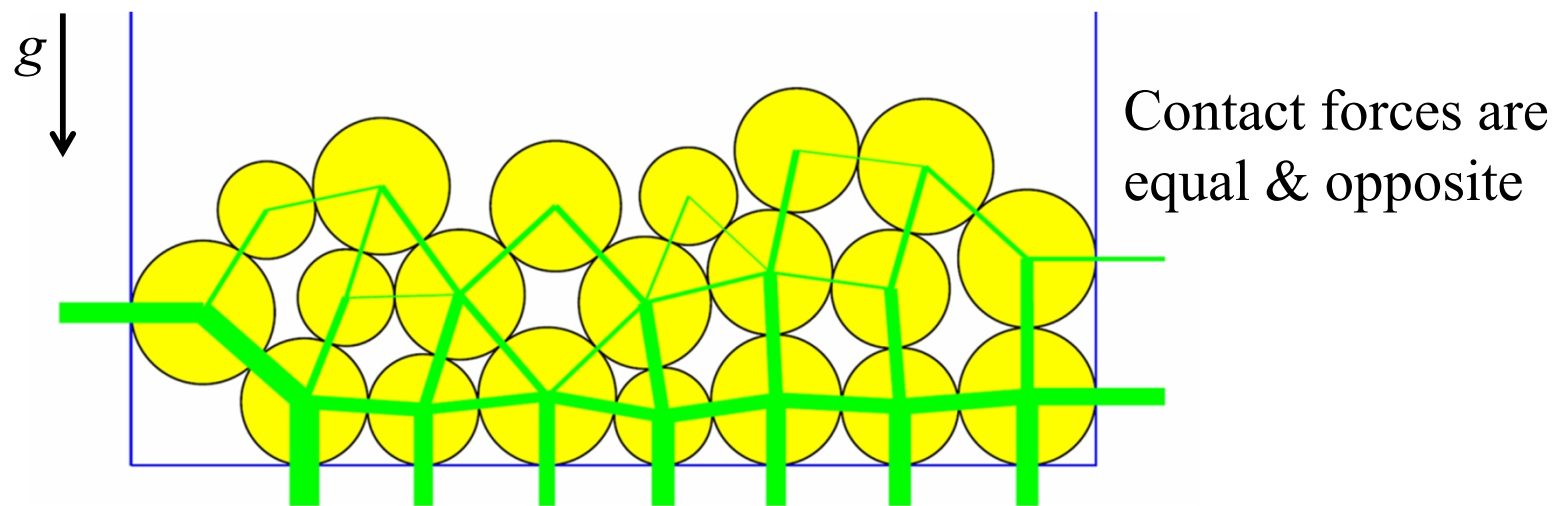
g

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 .

$W = mg$

Δ

Baseballs contract
and expand.

$2R$

$2R$

initial system

loaded system

soft-contact approach

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

$W = mg$

Δ

k_{bw}

k_{bb}

DEM model contracts but does not expand.

k_{bw}

$2R$

$2R$

initial system

loaded system

DEM model employs a
"soft contact" approach:

all deformation
occurs at the contacts
between the rigid
bodies.

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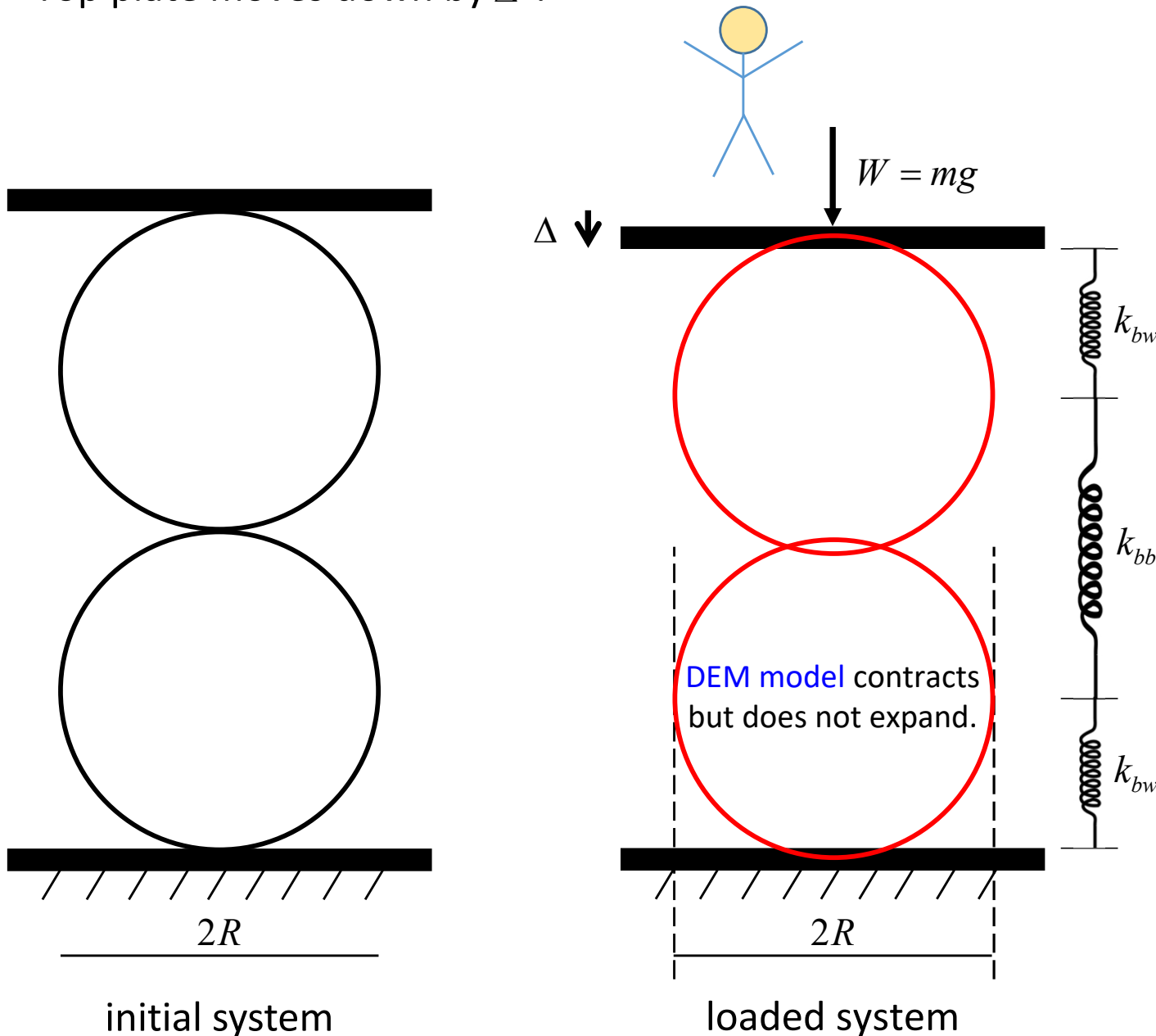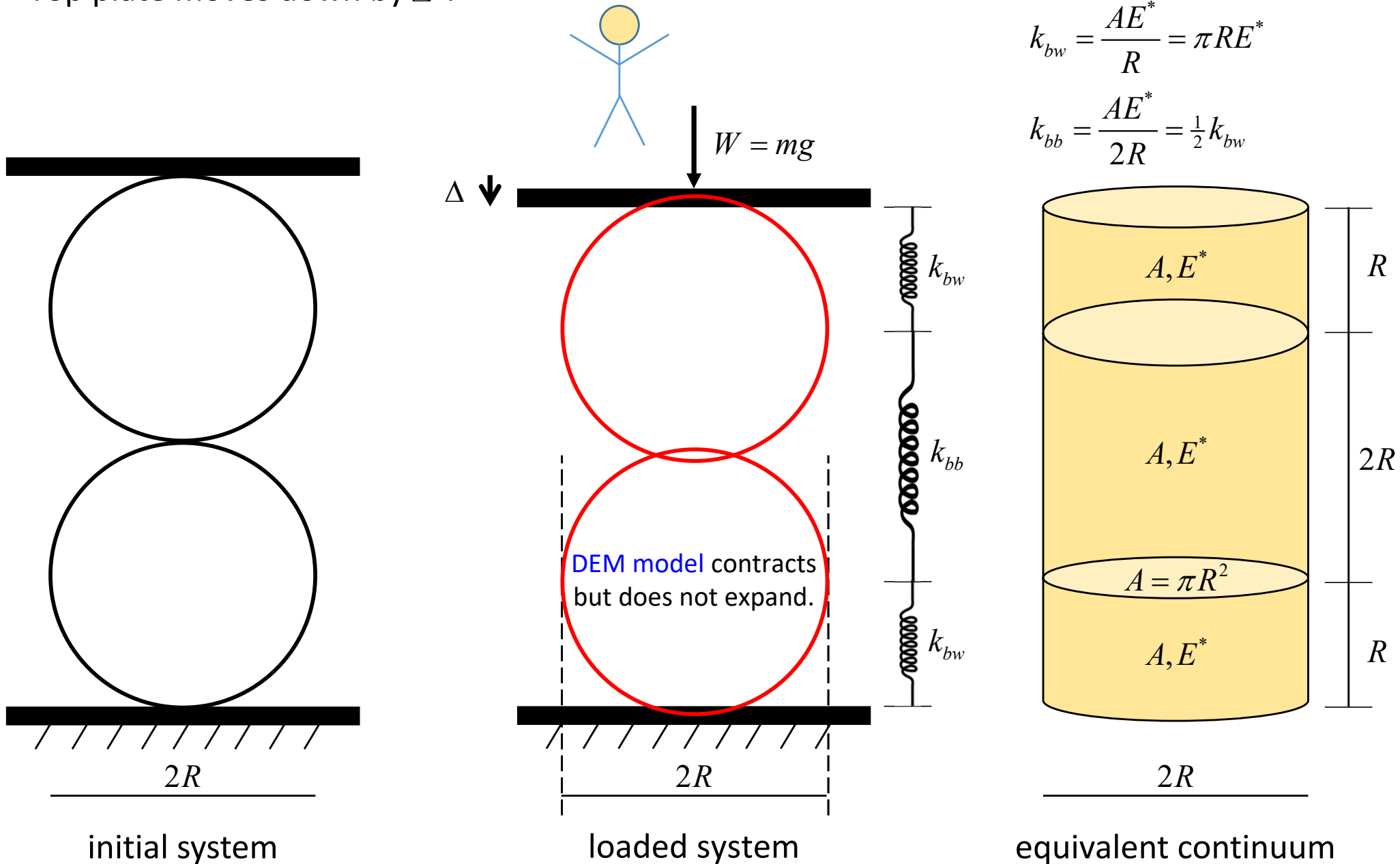related to the effective
modulus of an equivalent
continuum. . .

soft-contact approach

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

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

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

$W = mg$

Δ

k_{bw}

k_{bb}

DEM model contracts but does not expand.

k_{bw}

A, E^*

A, E^*

$A = \pi R^2$

A, E^*

R

$2R$

R

$2R$

$2R$

$2R$

initial system
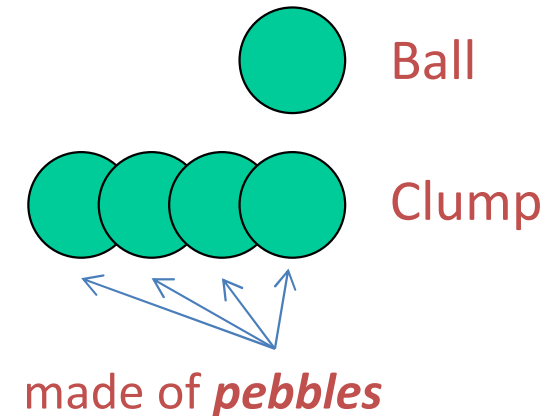
loaded system

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
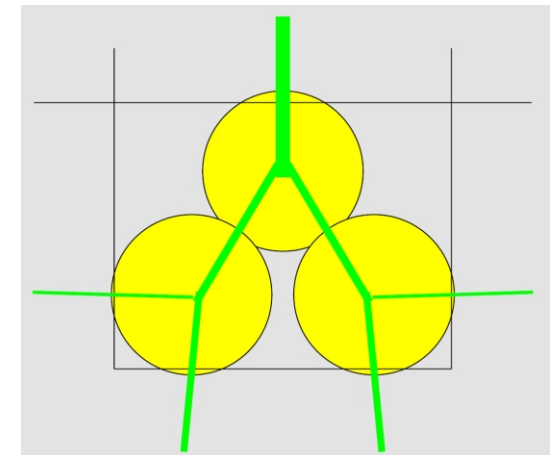
Ball

Clump

made of *pebbles*

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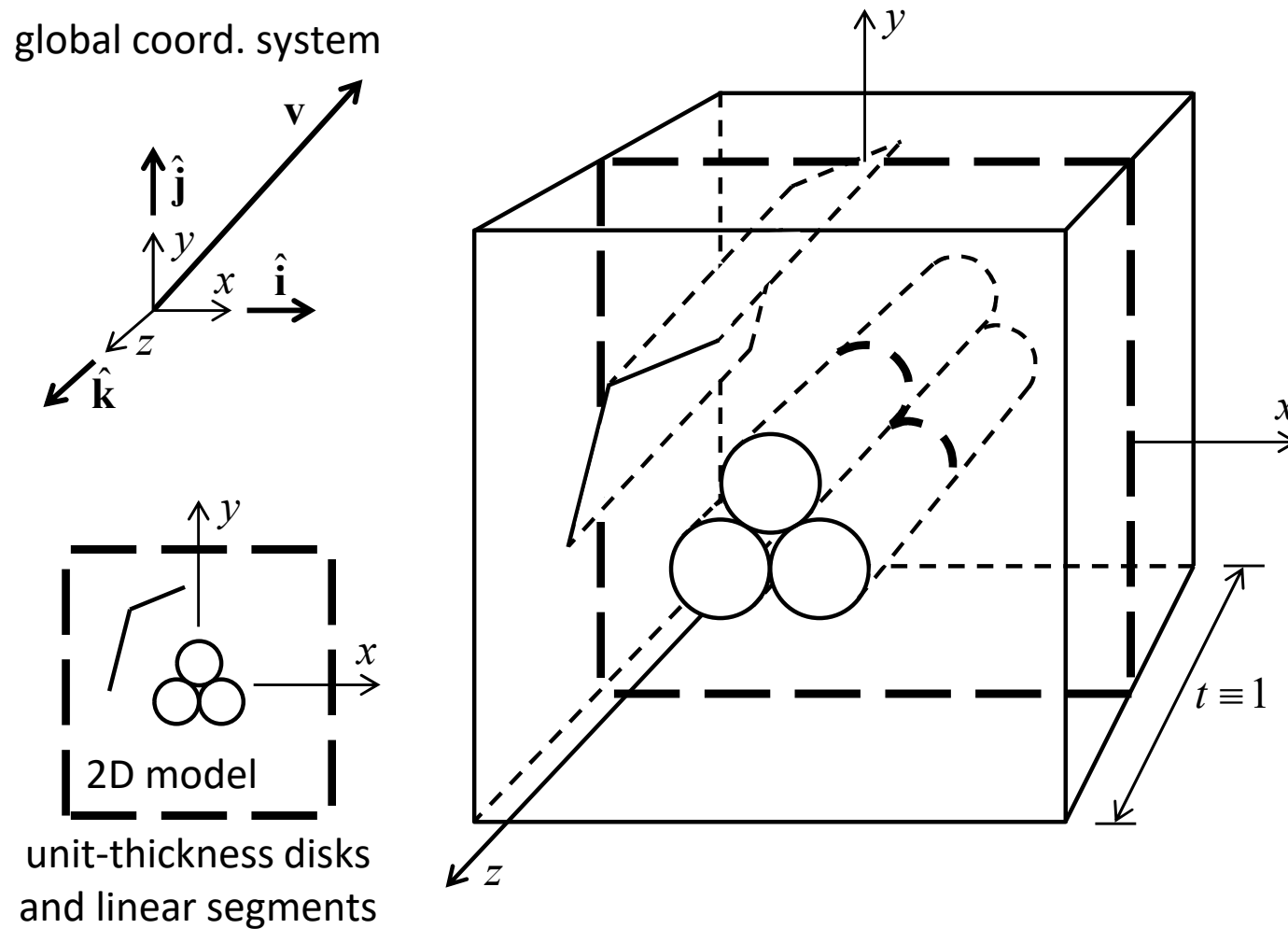- used to apply velocity boundary conditions
- interact *only* with balls and clumps
- made of facets

These entities interact at contacts.
Each contact stores force & moment that act on the two contacting entities.

Bonded-Particle Modeling Methodology (PFC model, 2D)

global coord. system

2D model

unit-thickness disks and linear segments

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**
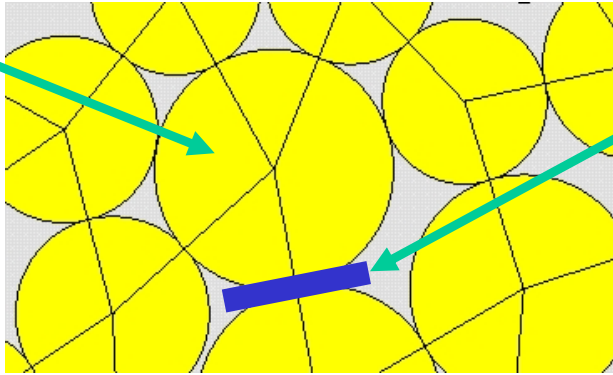
grains can be balls, clumps or rigid blocks

cement can be

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

Also soft-bonded & subspring network contacts

When bond breaks, behaves as linear contact.

cement can be

- **contact-bonded** contact
- **parallel-bonded** contact
- **flat-joint** contact

Also soft-bonded & subspring network contacts

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, soft-bonded, flat-jointed or SNed.

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 ⟶ No time, future webinar!
Linear Parallel Bond Model & Soft Bond Model
Flat-Joint Model & Subspring Network Model

Potyondy, D. (2021) "Material-Modeling Support for PFC [fistPkg7.2]," Itasca Consulting Group, Inc., Technical Memorandum ICG7766-L (June 24, 2021), Minneapolis, Minnesota.

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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 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.
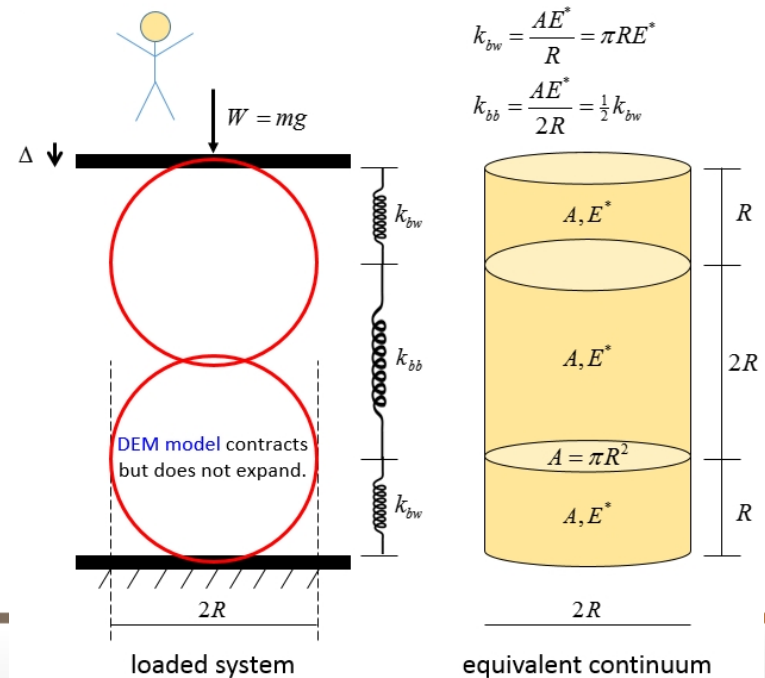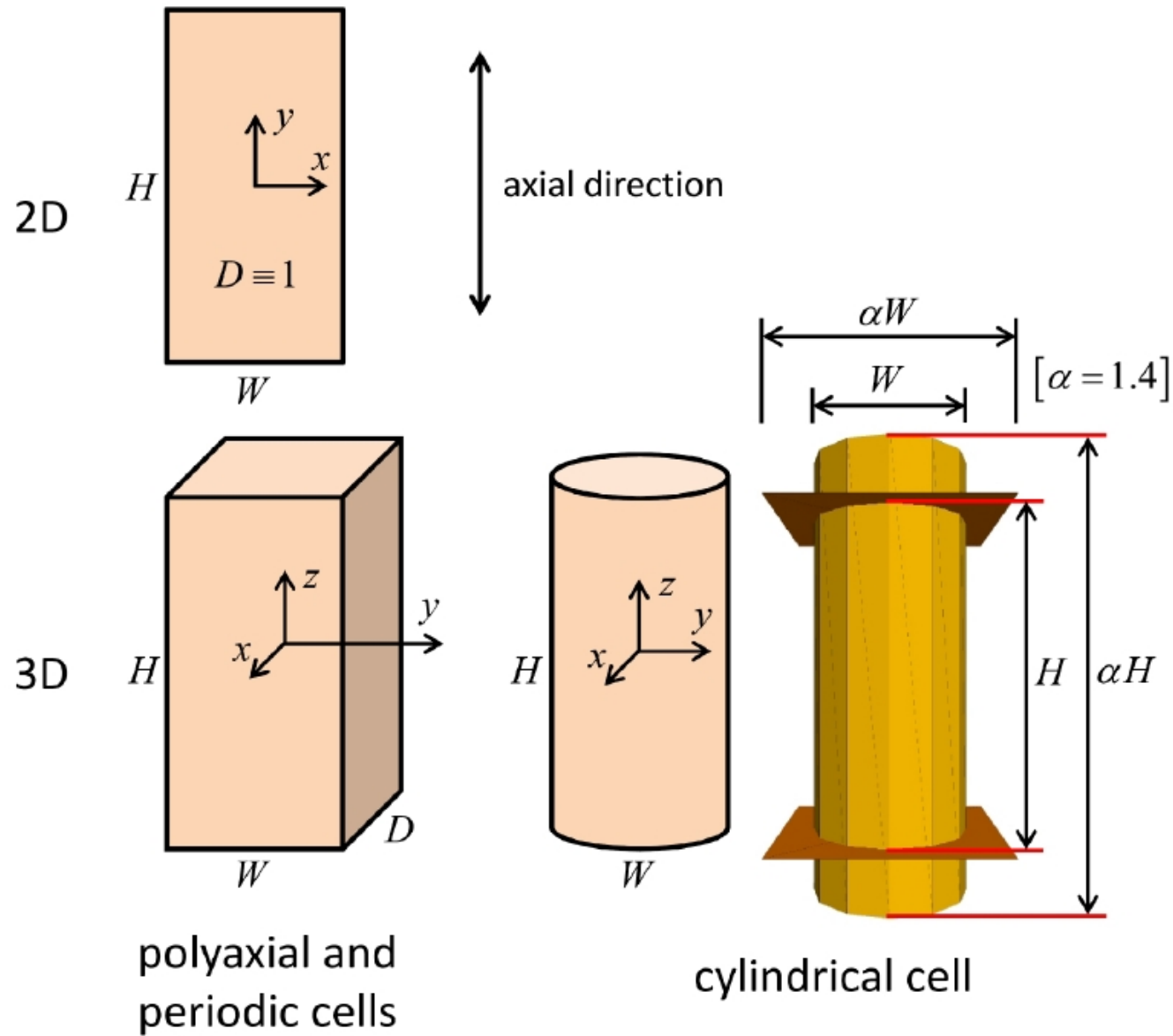
The linear contact model is installed at the grain-wall contacts. The walls are frictionless, and grain-wall contact stiffness is set based on a specified contact deformability (effective modulus).

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

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

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

$W = mg$

k_{bw}

k_{bb}

DEM model contracts but does not expand.

k_{bw}

A, E^* R

A, E^* $2R$

$A = \pi R^2$

A, E^* R

2R

2R

loaded system

equivalent continuum

Material Vessels

2D — H, $D \equiv 1$, W, axial direction

3D — H, W, D — polyaxial and periodic cells

H, W — cylindrical cell

αW, W, $[\alpha = 1.4]$, H, αH
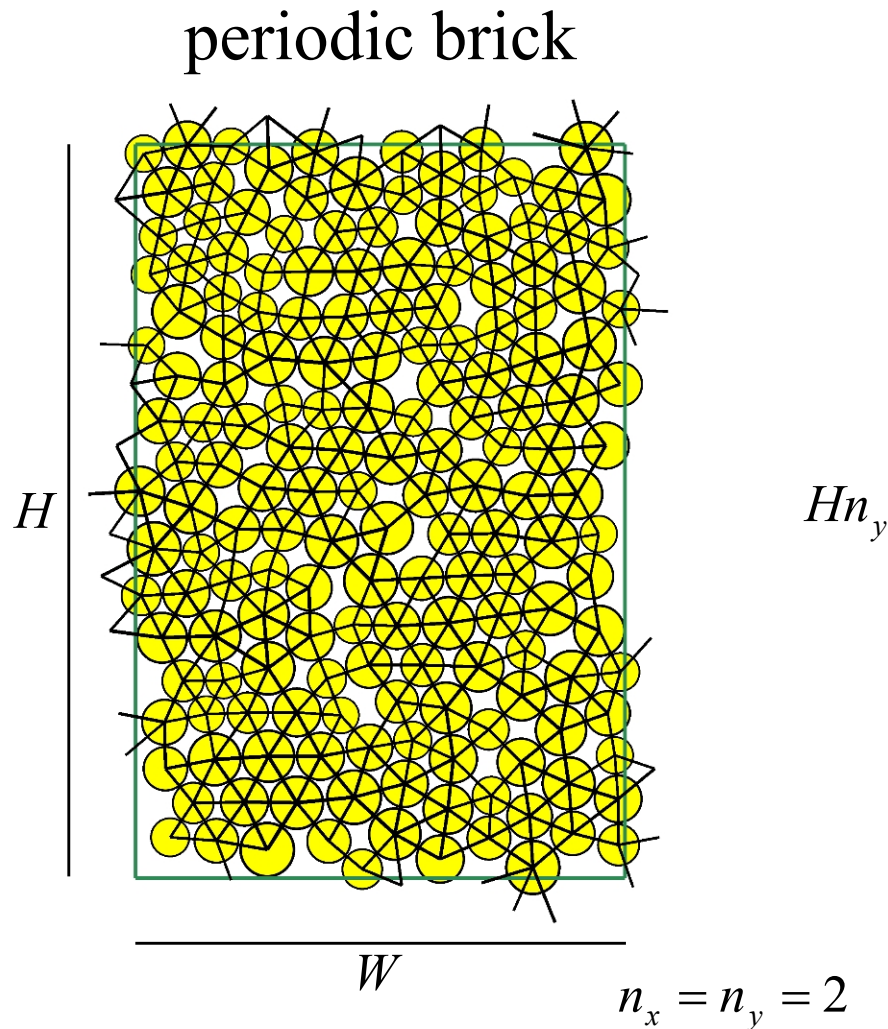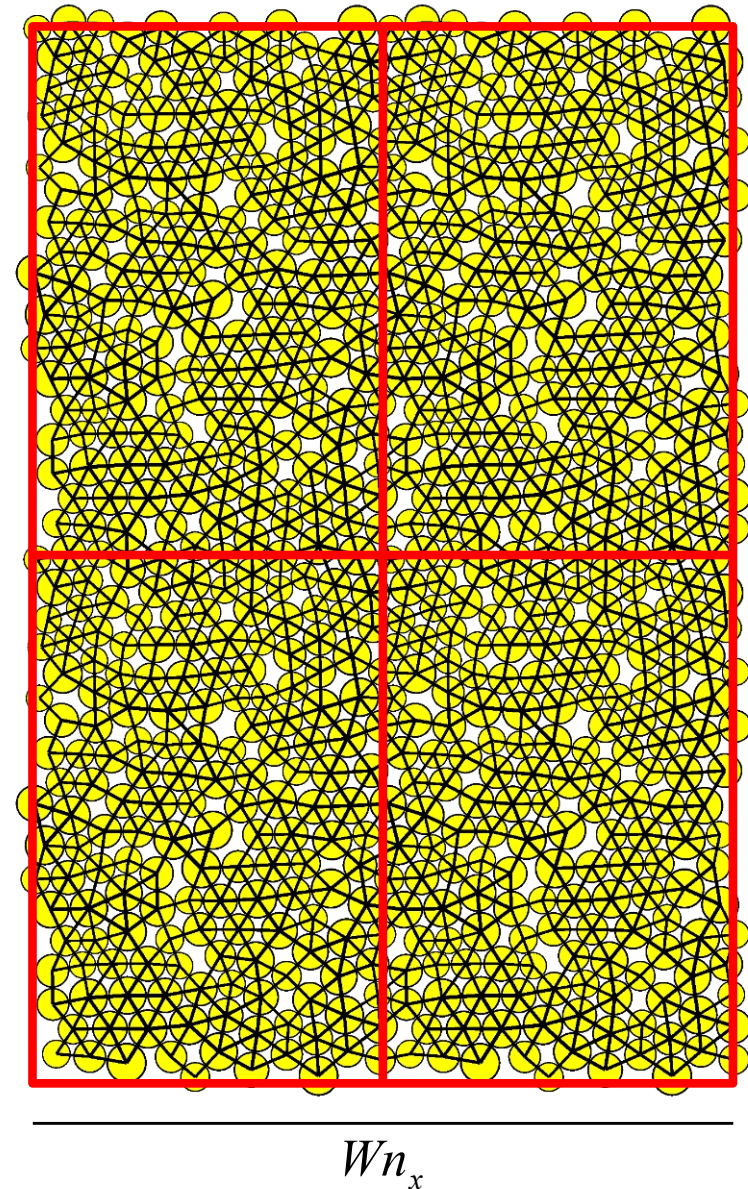
Material Vessels (periodic vessel)

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

periodic brick

assembled specimen

H

W

$n_x = n_y = 2$

Hn_y

Wn_x

Material Vessels (periodic vessel)

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

Contact force_mag

Contacts (467)

2.0340E+5
1.9000E+5
1.7000E+5
1.5000E+5
1.3000E+5
1.1000E+5
9.0000E+4
7.0000E+4
5.0000E+4
3.0000E+4
1.0000E+4
5.5113E+3
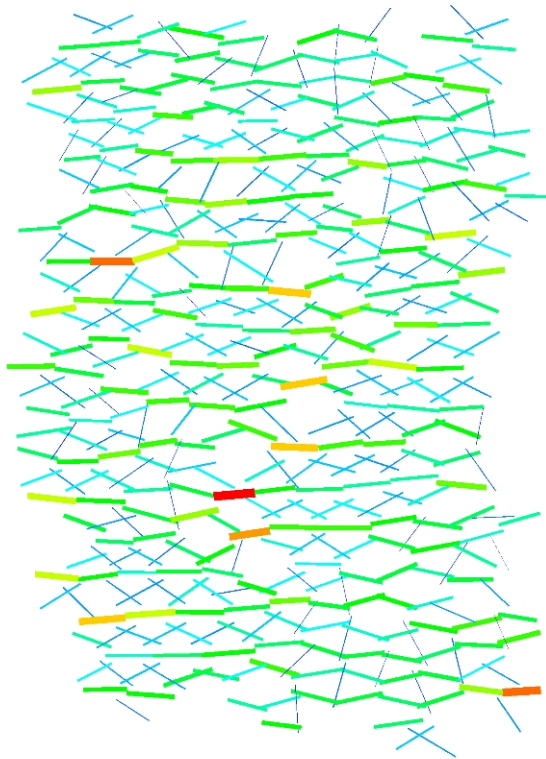
Force chains in bonded ensemble

Material Vessels
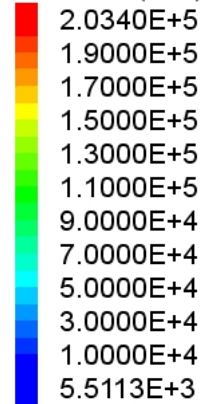
Project
Data Files
  myMatGen.p3dvr
  mvParams.p3dat
  mpParams.p3dat
  ft.p3fis

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
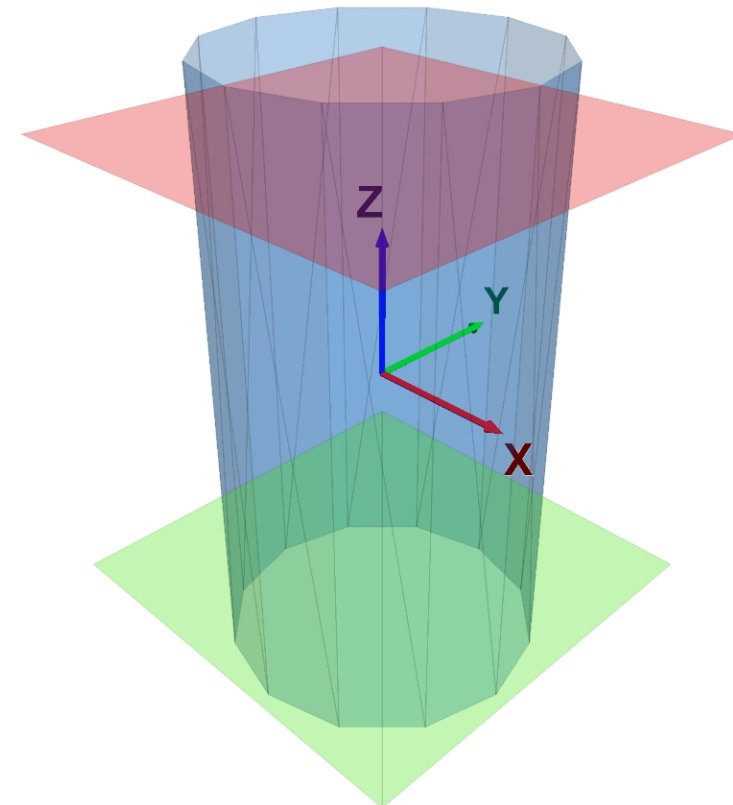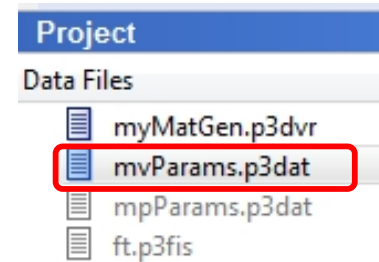
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Material Vessels


```
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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Material Vessels


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```

SI units, for legends of plots

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```
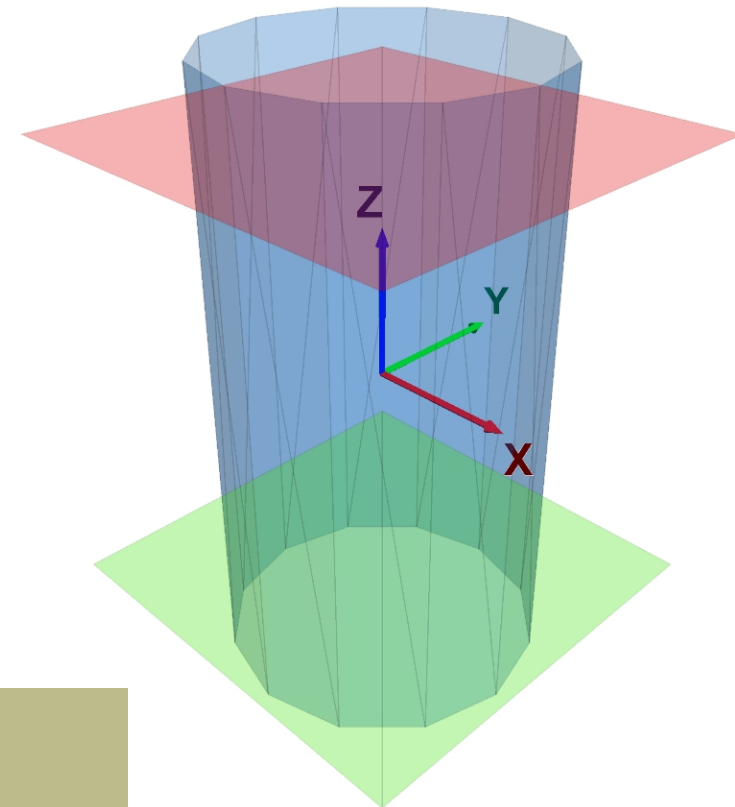
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Material Vessels

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    {mv_W, _wdr} (diameter {initial, current},  lies in xy-plane): {0.17,0.152297}
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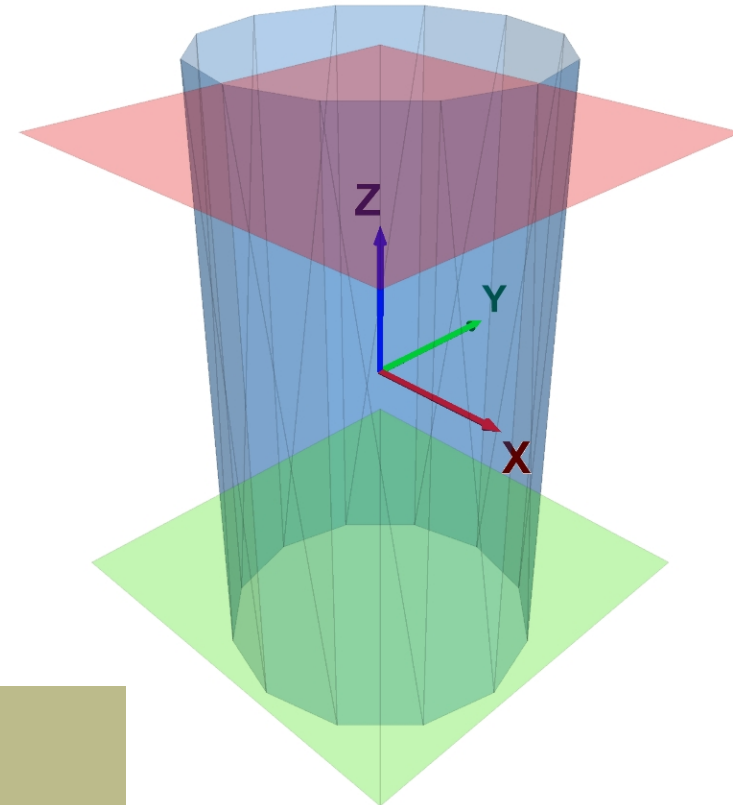
microstructural box

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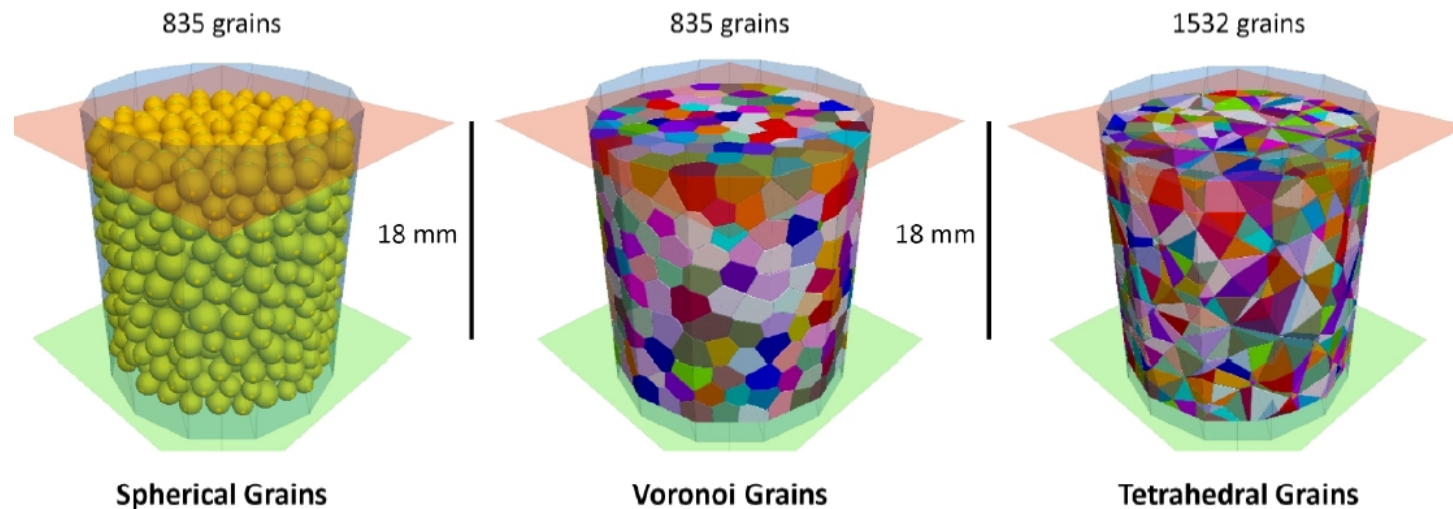
Figure 7 *The three flat-jointed materials with spherical, Voronoi and tetrahedral grains at specimen resolutions of 10.* (From Fig. 9 of Potyondy et al. [2020])

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 μ_{CA} to obtain dense or loose packing$]$

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

Material-Genesis Procedure (packing phase)

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grain sizes are scaled iteratively

$\left[\mu \equiv 0 \text{ to obtain dense packing}\right]$

$$\mu_{CA} = 0 \; (\text{dense})$$
$$\mu_{CA} = \mu_m \; (\text{loose})$$

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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 $\left(\dfrac{|P - P_m|}{P_m} \leq \varepsilon_P \right)$ where P is current pressure
ε_{lim}, pk_ARatLimit	FLT	$(0.0, \infty)$	8×10^{-3}	equilibrium-ratio limit (parameter of ft_eq)
n_{lim}, pk_stepLimit	INT	$[1, \infty)$	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	$(0.0, 1.0)$	$\begin{cases} \begin{cases} 0.58, & \text{3D} \\ 0.25, & \text{2D} \end{cases}, & C_p = 0 \\ \begin{cases} 0.35, & \text{3D} \\ 0.08, & \text{2D} \end{cases}, & C_p = 1 \end{cases}$	grain-cloud porosity

Boundary-contraction group ($C_p = 0$):

Parameter	Type	Range	Default	Description
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)

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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 $\left(\dfrac{|P - P_m|}{P_m} \leq \varepsilon_P \right)$ 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	$(0.0, 1.0)$	$\begin{cases} \begin{cases} 0.58, \text{3D} \\ 0.25, \text{2D} \end{cases}, C_p = 0 \\ \begin{cases} 0.35, \text{3D} \\ 0.08, \text{2D} \end{cases}, C_p = 1 \end{cases}$	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)

Project
Data Files
- myMatGen.p3dvr
- mvParams.p3dat
- mpParams.p3dat
- ft.p3fis

pk_seed: affects particle arrangement

ITASCA

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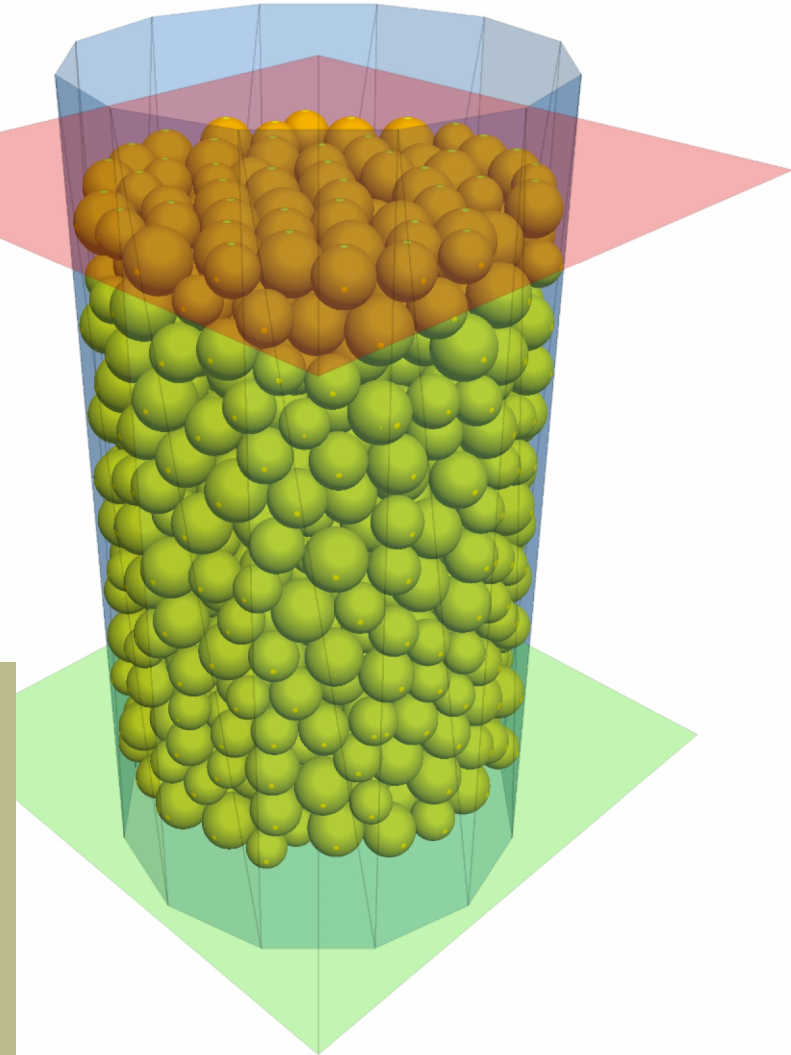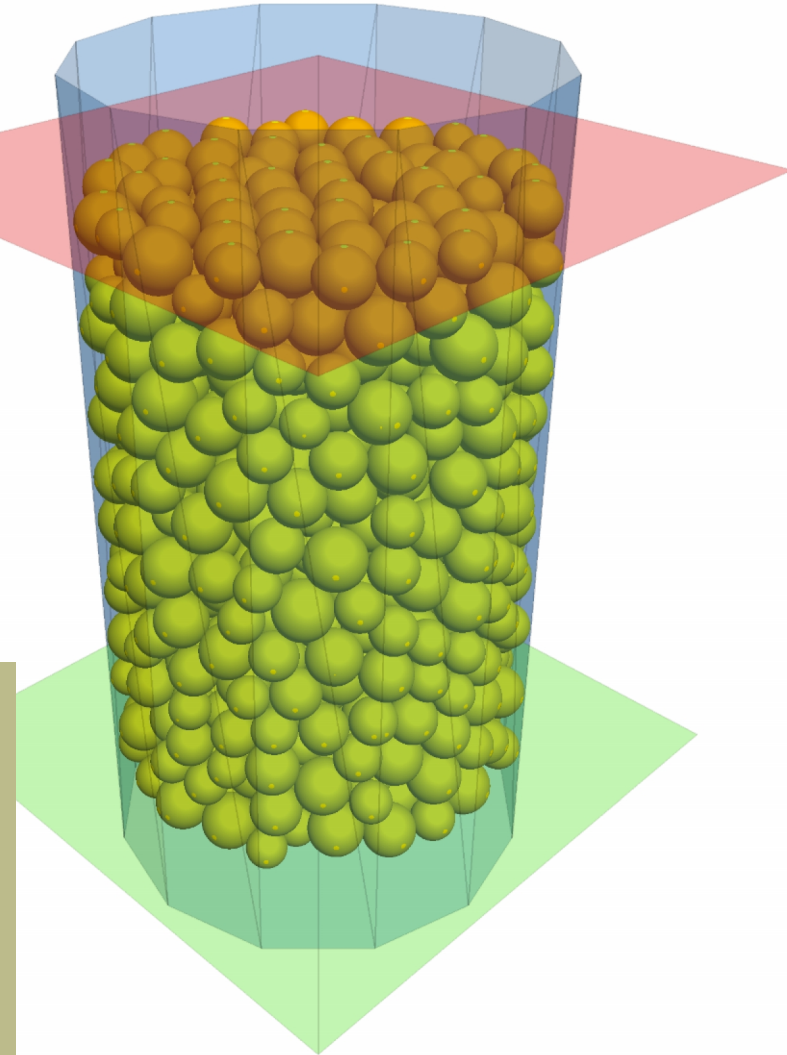
Modify **pk_fricCA** from 0.0 to 0.4 to increase final specimen porosity from 0.38 to 0.42.

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 — Parallel-bonded material group through Parallel-bond group

B — Linear material group (for grain-grain contacts that may form subsequent to material finalization)

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Material-Genesis Procedure (finalization phase)

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

three

five

installation gap $\longrightarrow$ $g_i = 0$ $\qquad$ $g_i = \delta$

Material-Genesis Procedure (finalization phase)

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

three

five

installation gap $\longrightarrow$ $g_i = 0$

$g_i = \delta$
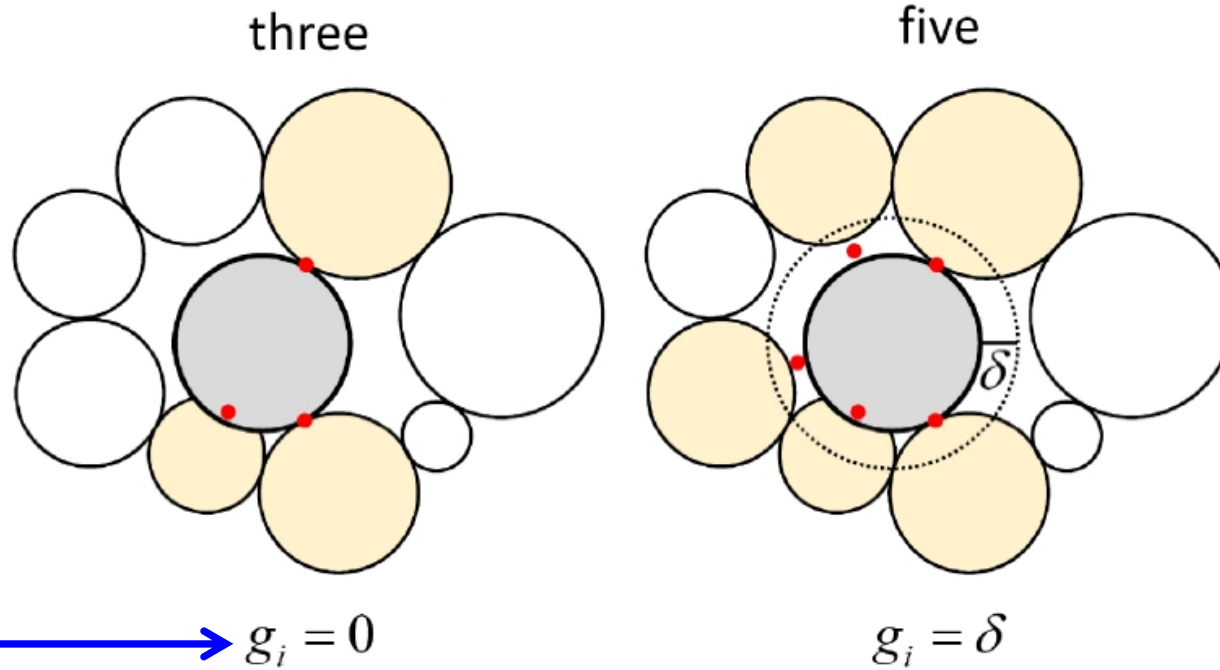
Increasing the installation gap, increases the grain connectivity.

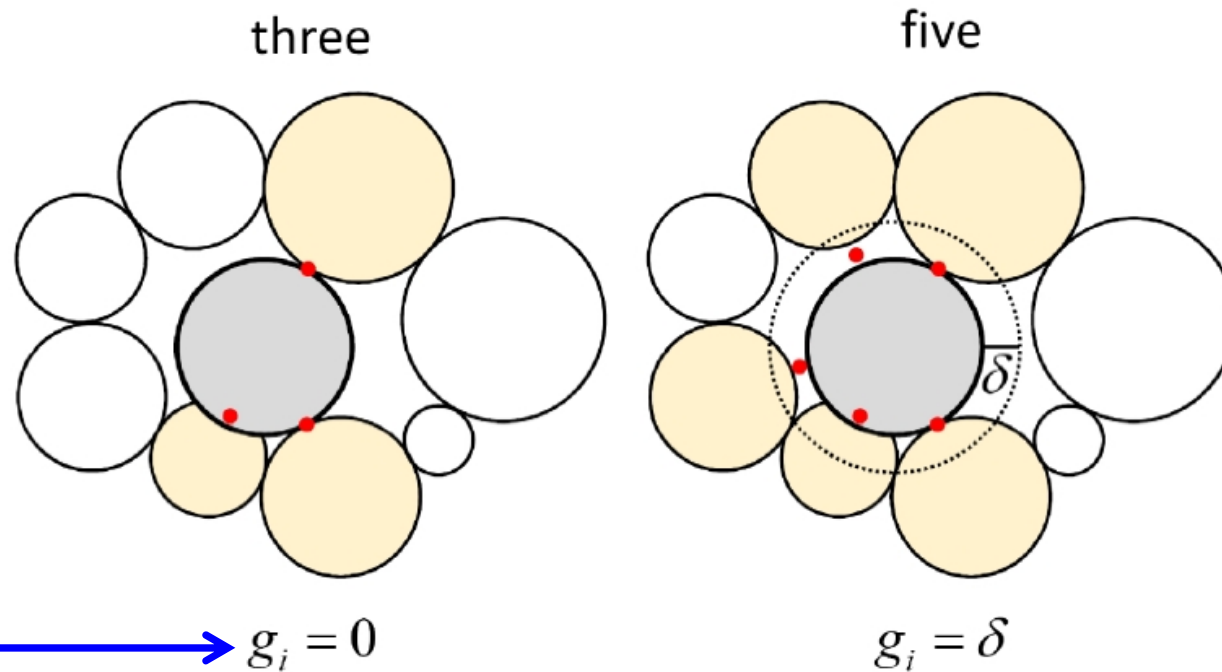# Material-Genesis Procedure (finalization phase)

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

three   five

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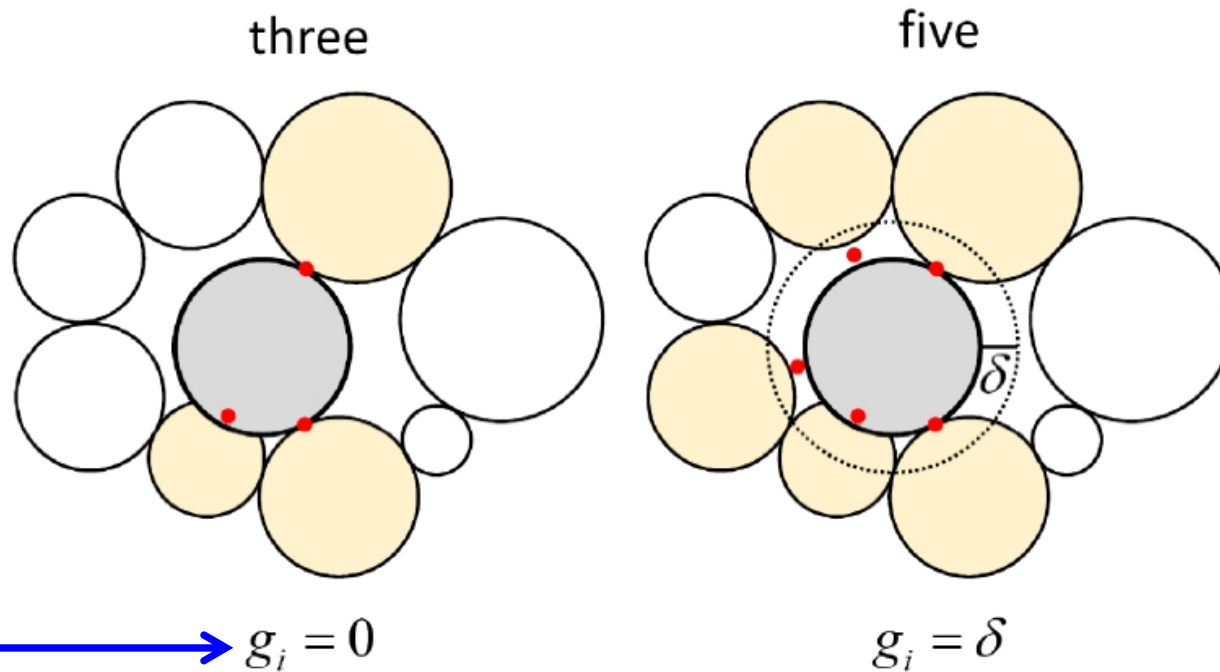
installation gap

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.
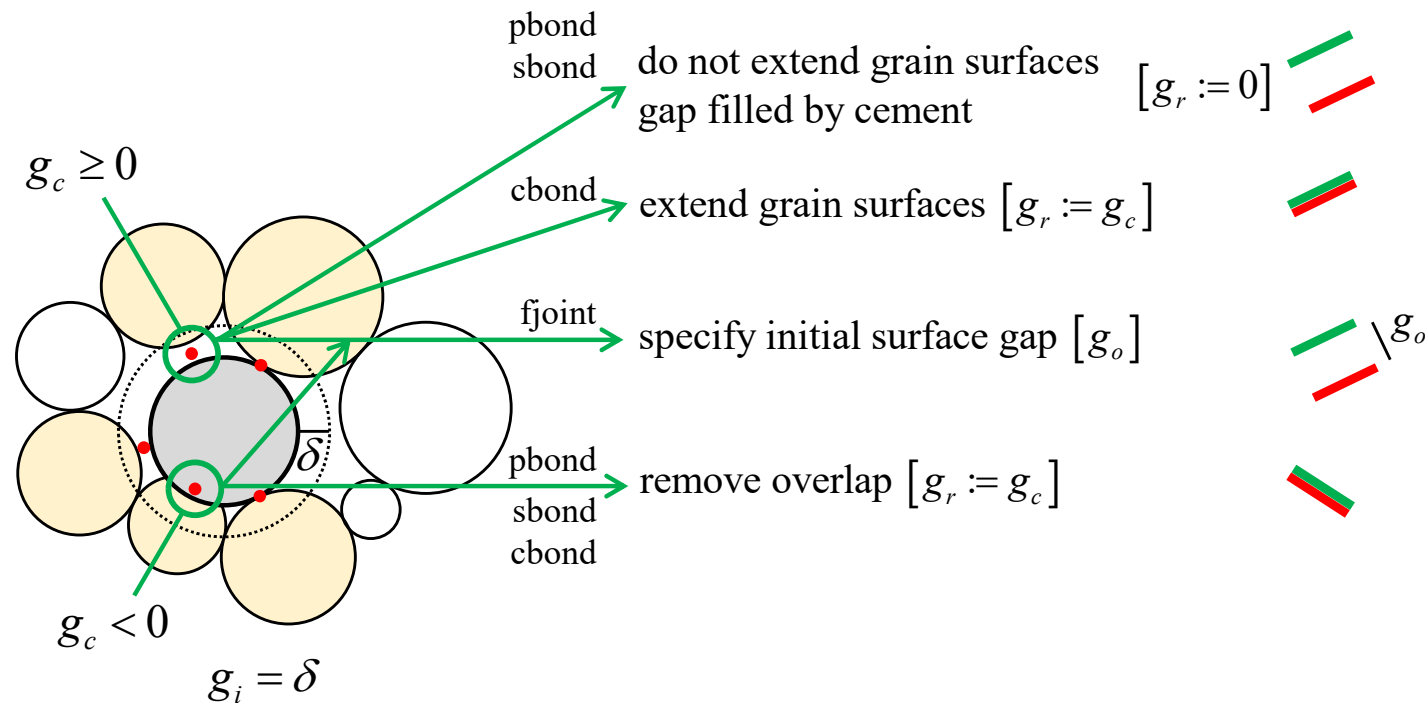
pbond
sbond — do not extend grain surfaces gap filled by cement $\left[g_r := 0\right]$

cbond — extend grain surfaces $\left[g_r := g_c\right]$

fjoint — specify initial surface gap $\left[g_o\right]$

pbond
sbond
cbond — remove overlap $\left[g_r := g_c\right]$

$g_c \geq 0$

$g_c < 0$

$g_i = \delta$

δ

g_o

Material-Genesis Procedure (finalization phase)

reference surfaces

bonded   unbonded

$g_c > 0$

$g_c = 0$

$g_c < 0$

$2\bar{R}$

$|\approx 0|$

epoxy-cemented glass beads

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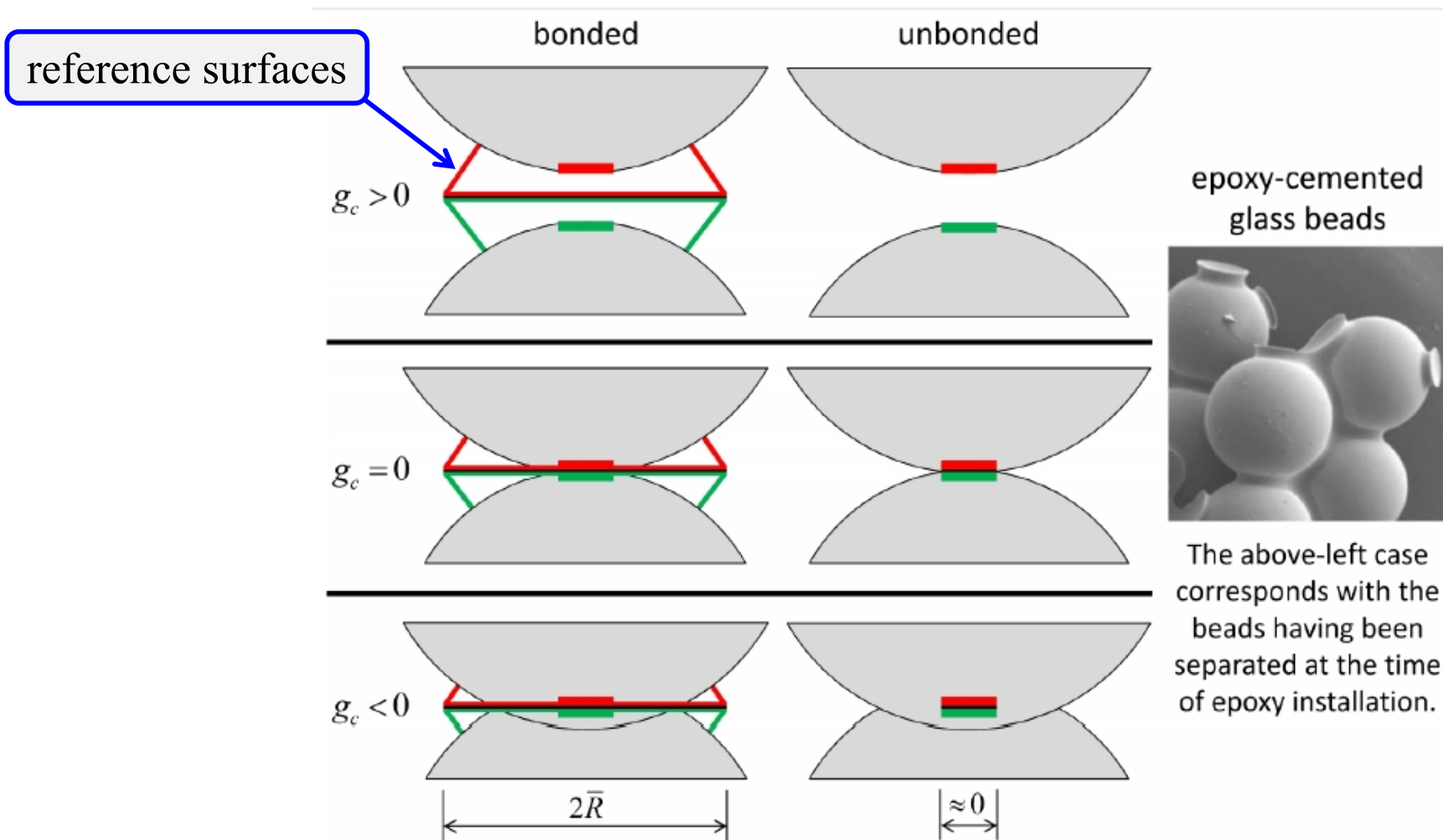
Material-Genesis Procedure (finalization phase)

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

- There are no forces at the grain-wall interface.
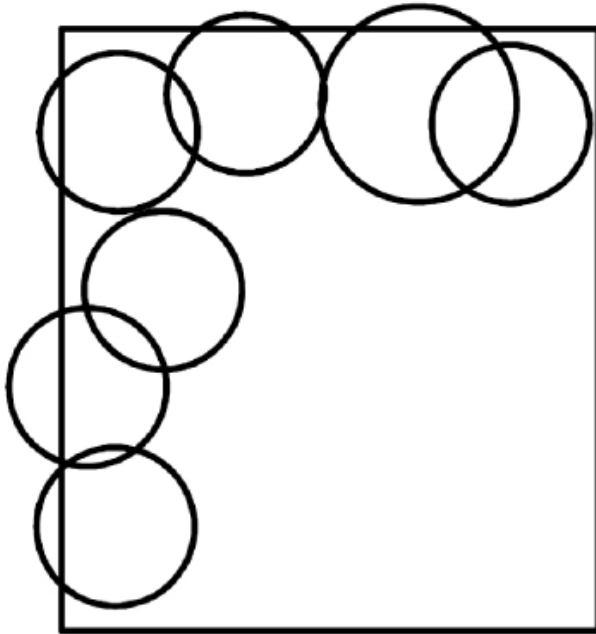
Before smoothing   After smoothing

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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 ←

Material-Genesis (microstructural properties)

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

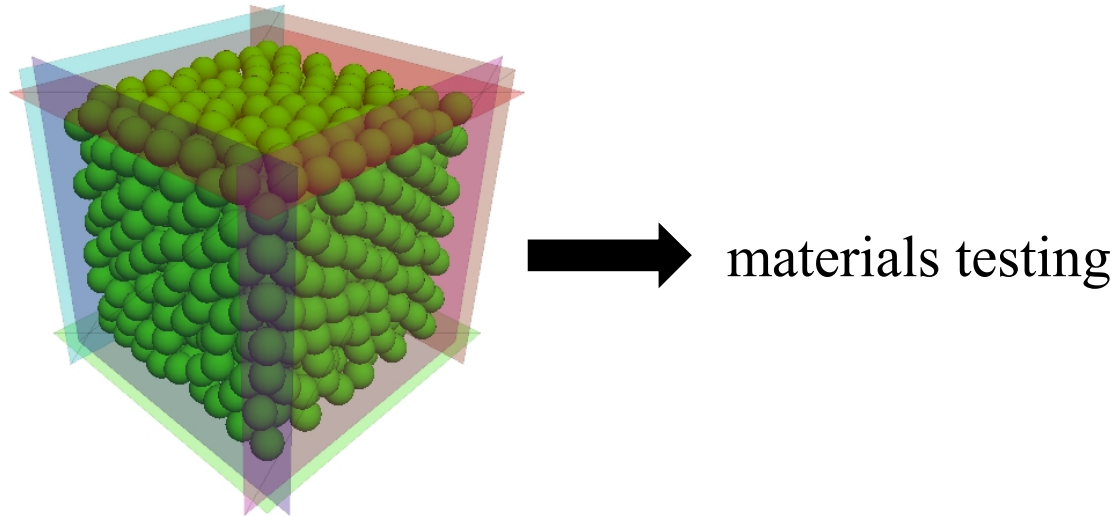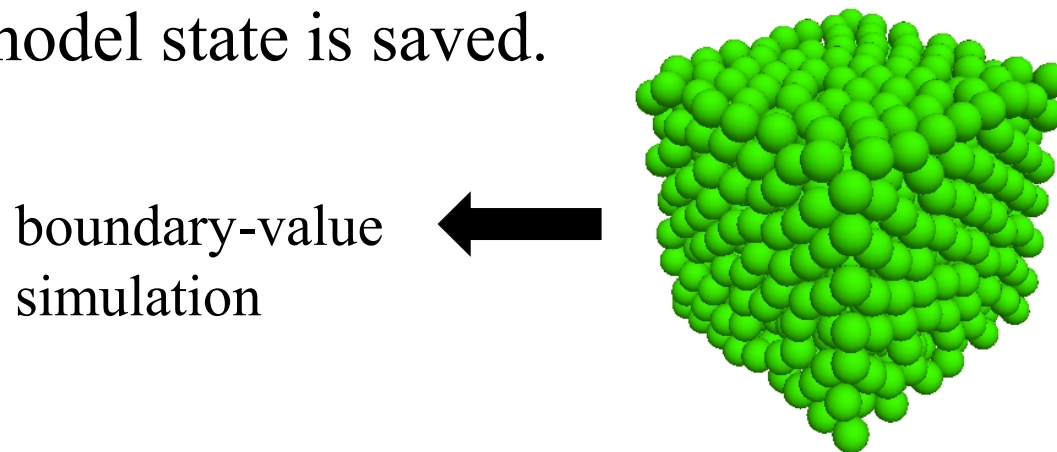- **Grain Size and Packing Information.** Number of grains in the model, grain-size distribution (discussed below), average and median grain diameters, vessel resolutions w.r.t. the average and median grain diameters,[25] measurement-based porosity (defined in Section 5.1), and overlap ratios.[26]

- **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).

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).

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): 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
```

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Materials (common material properties)

Project

Data Files
- myMatGen.p3dvr
- mvParams.p3dat
- **mpParams.p3dat**
- ft.p3fis

Table 1   Common Parameters

Parameter	Type	Range	Default	Description
N_{mt} , cm_matName	STR	NA	PFCmat	material name (for model title)
N_{ms} , cm_matNameSAV	STR	NA	PFCmat	material name (for SAV file names)
T_m , cm_matType	INT	$[0,5]$	0	material-type code 0, linear 1, contact-bonded 2, parallel-bonded 3, soft-bonded 4, flat-jointed 5, user-defined
N_{cm} , cm_modName	STR	NA	NA	contact-model name ($T_m = 5$, also redefine ft_setMatBehavior)
α , cm_localDampFac	FLT	$[0.0,0.7]$	0.0	local-damping factor (for local damping)

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Materials (common material properties)

C_p, `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)	

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)

Project

Data Files

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

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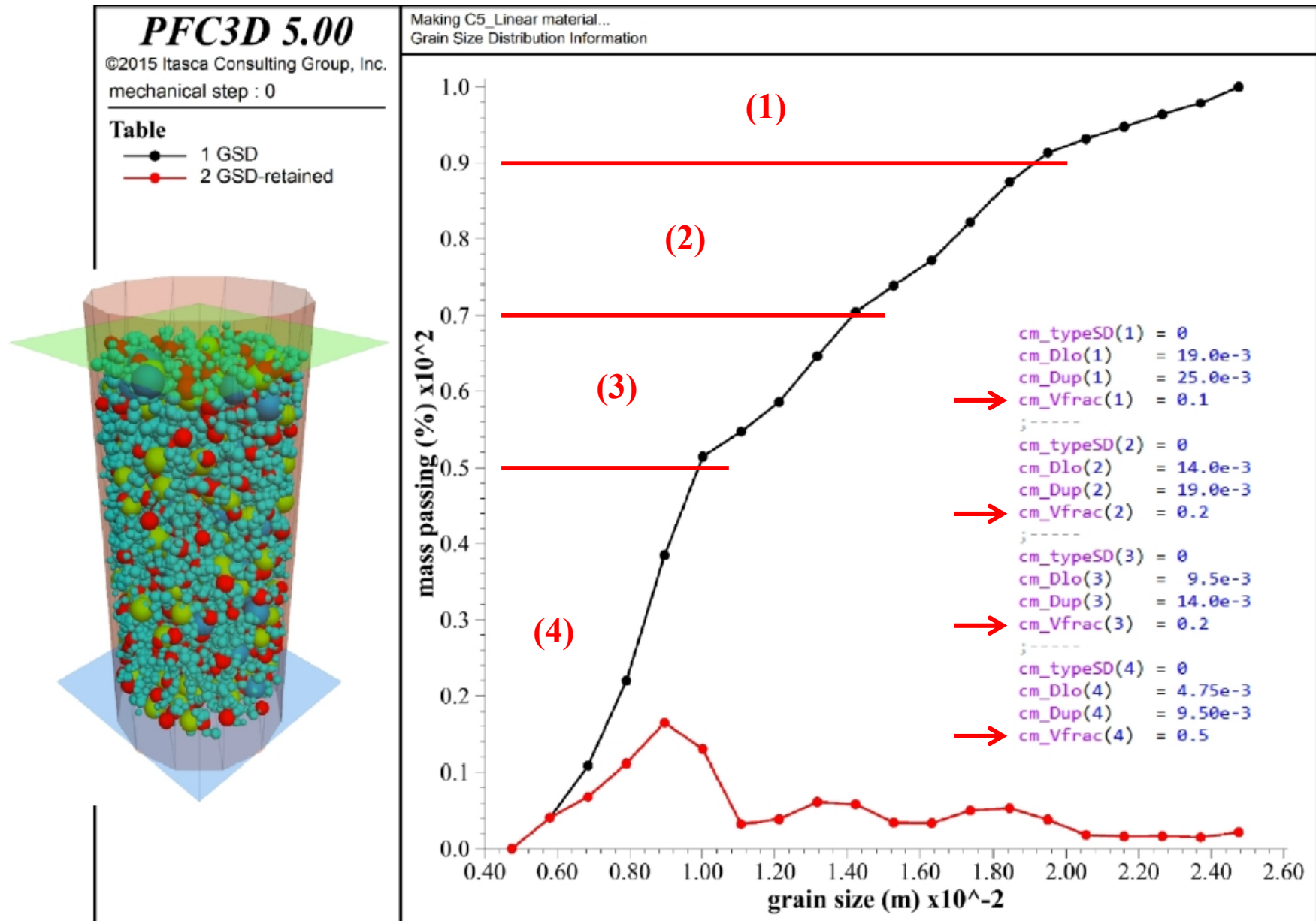
Restore contact-bonded material, show the material name in view headers.

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).

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

Materials (grain-size distribution)

PFC3D 5.00

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mechanical step : 0

Table
- 1 GSD
- 2 GSD-retained

Making C5_Linear material...
Grain Size Distribution Information

```
cm_typeSD(1) = 0
cm_Dlo(1)    = 19.0e-3
cm_Dup(1)    = 25.0e-3
cm_Vfrac(1)  = 0.1
;-----
cm_typeSD(2) = 0
cm_Dlo(2)    = 14.0e-3
cm_Dup(2)    = 19.0e-3
cm_Vfrac(2)  = 0.2
;-----
cm_typeSD(3) = 0
cm_Dlo(3)    =  9.5e-3
cm_Dup(3)    = 14.0e-3
cm_Vfrac(3)  = 0.2
;-----
cm_typeSD(4) = 0
cm_Dlo(4)    = 4.75e-3
cm_Dup(4)    = 9.50e-3
cm_Vfrac(4)  = 0.5
```

[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).

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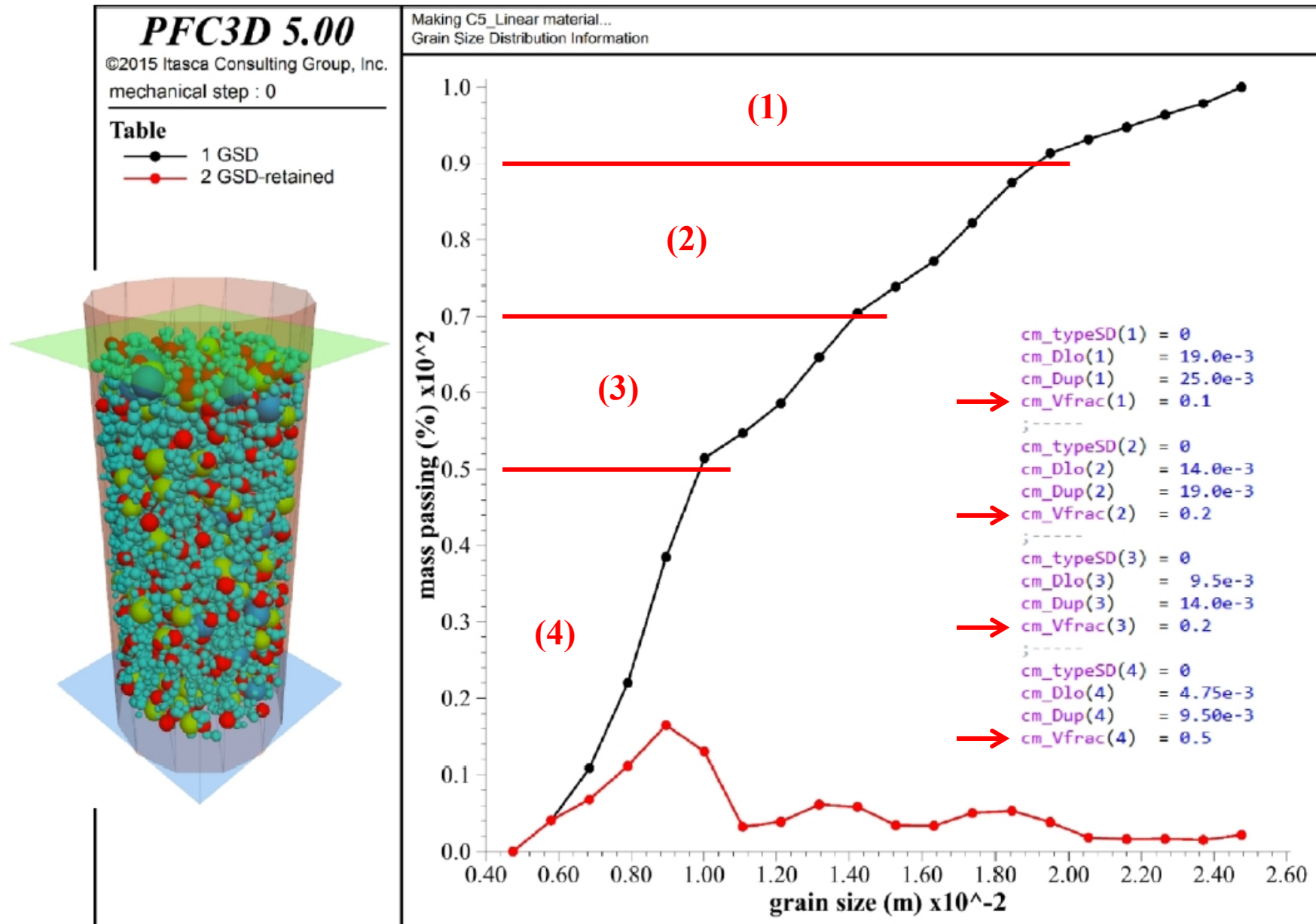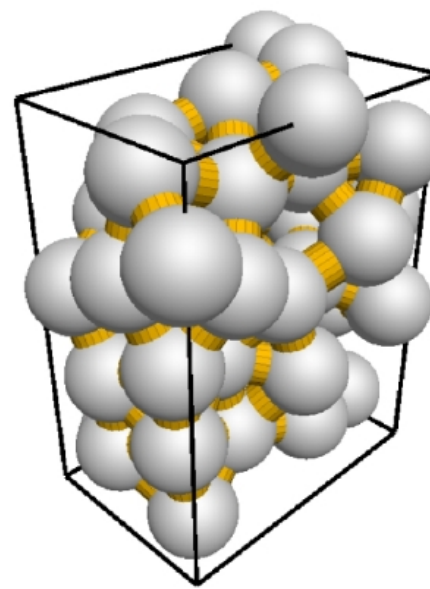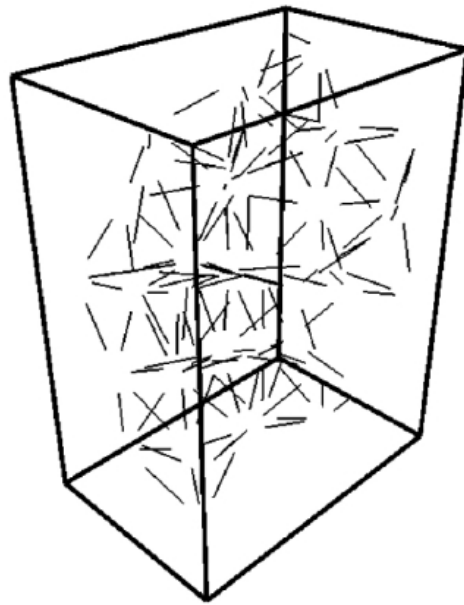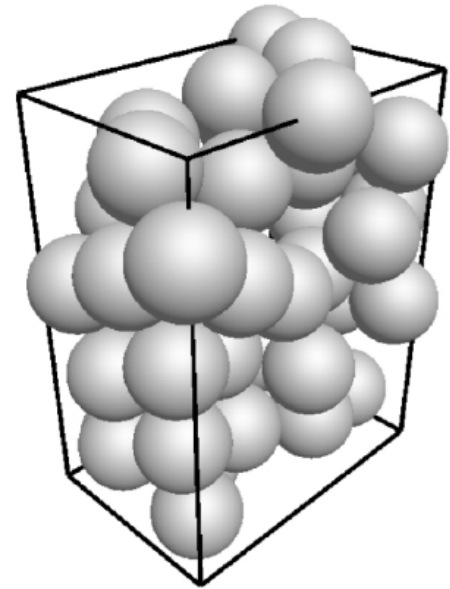
Microstructural Plot Sets

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
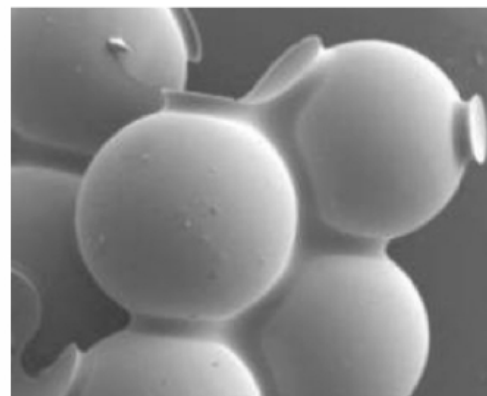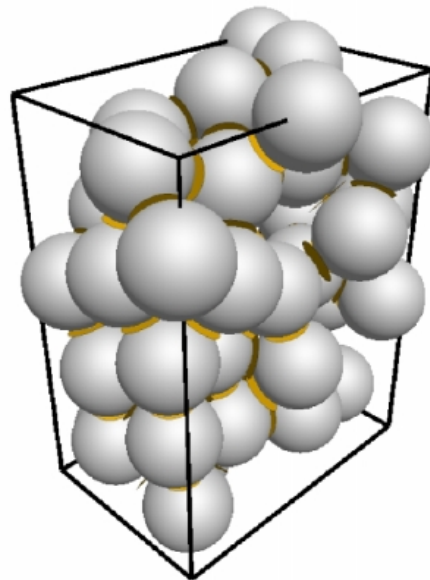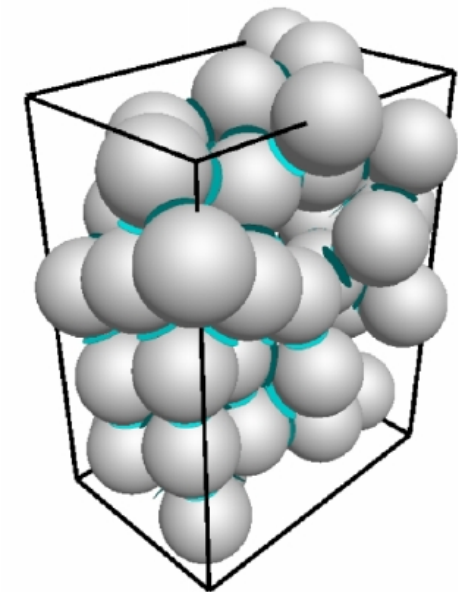
Holt et al. (2005)

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)
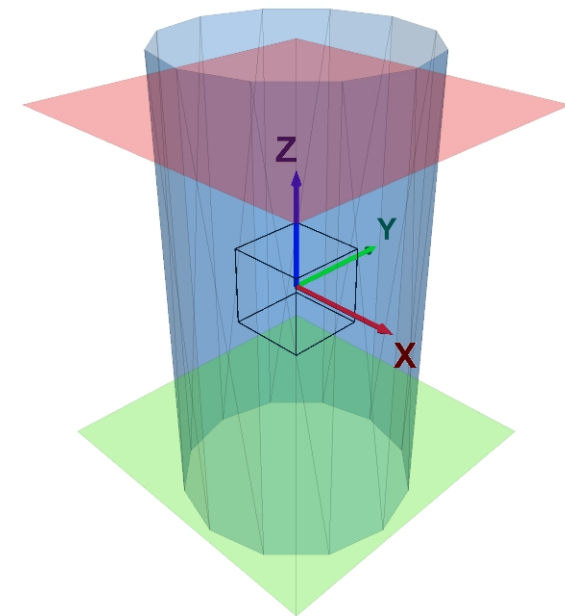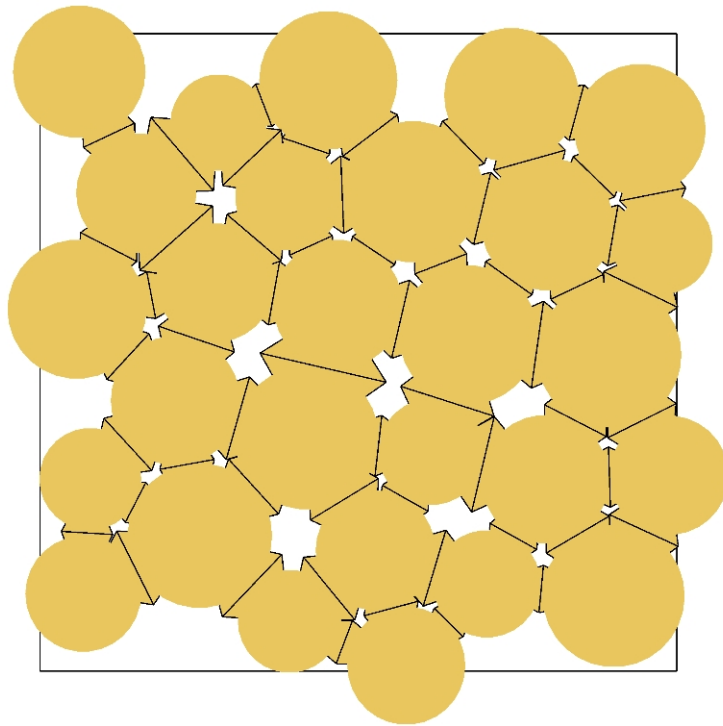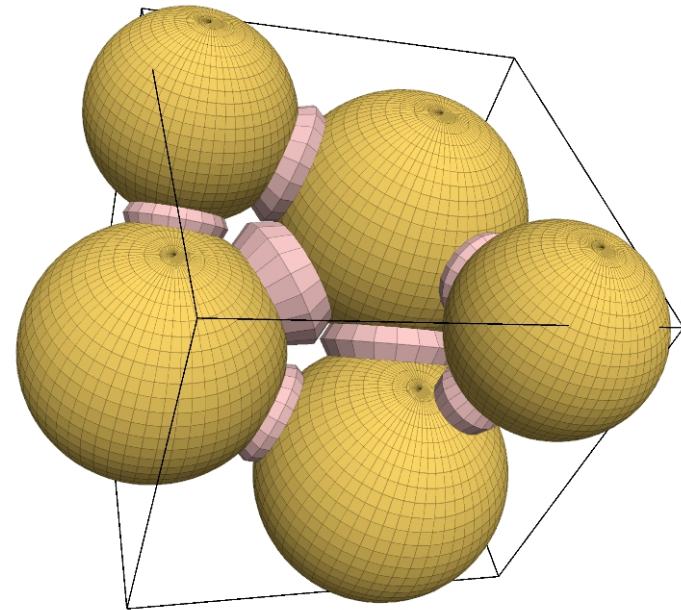
Table 2 Linear Material Parameters

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

$$\longmapsto (k_n, k_s)$$

```
Edit mpParams.p3dat*
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_emod = 500e6
56       lnm_krat = 1.5
57       lnm_fric = 0.5
58 end
59 @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
```

ITASCA

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

Project

Data Files

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

ITASCA
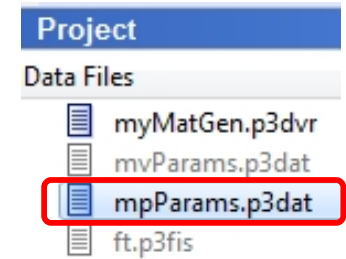
Materials (contact-bonded material)

Contact-bond group:

g, 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)
γ cbm_shearsTensRatio	FLT	$[0.0, \infty)$	0.0	(At each contact, set $S_\sigma = \gamma T_\sigma$. If $\gamma = 0.0$, then $(S_\sigma)_{\{msd\}}$ is used.)

Linear material group (for grain-grain contacts during packing 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

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

Project

Data Files

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

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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
$(\bar{\sigma}_c)_{\{msd\}}$ pbm_ten_{m,sd}	FLT	$[0.0, \infty)$	$\{0.0, 0.0\}$		tensile-strength dist. [stress] (mean and std. deviation)
$(\bar{c})_{\{m,sd\}}$ pbm_coh_{m,sd}	FLT	$[0.0, \infty)$	$\{0.0, 0.0\}$		cohesion dist. [stress] (mean and std. deviation)
$\bar{\gamma}$ pbm_cohTenRatio	FLT	$[0.0, \infty)$	0.0		cohesion to tensile strength ratio (At each contact, set $\bar{c} = \bar{\gamma}\,\bar{\sigma}_c$. If $\bar{\gamma} = 0.0$, then $(\bar{c})_{\{m,sd\}}$ is used.)
$\bar{\phi}$, pbm_fa	FLT	$[0.0, 90.0)$	0.0		friction angle [degrees]

Linear material group (for grain-grain contacts during packing 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

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Materials (soft-bonded material)

Table 5 Soft-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 8.				
Soft-bonded material group:				
g_i, sbm_igap	FLT	$[0.0,\infty)$	0.0	installation gap
λ, sbm_rmul	FLT	$(0.0,\infty)$	1.0	radius multiplier
E^*, sbm_emod	FLT	$[0.0,\infty)$	0.0	effective modulus
κ^*, sbm_krat	FLT	$[0.0,\infty)$	0.0	stiffness ratio
β, sbm_mcf	FLT	$[0.0,1.0]$	0.0	moment-contribution factor
$(\sigma_c)_{\{m,sd\}}$ sbm_ten_{m,sd}	FLT	$[0.0,\infty)$	$\{0,0\}$	tensile-strength dist. [stress] (mean and std. deviation)
$(c)_{\{m,sd\}}$ sbm_coh_{m,sd}	FLT	$[0.0,\infty)$	$\{0,0\}$	cohesion dist. [stress] (mean and std. deviation)
γ sbm_cohTenRatio	FLT	$[0.0,\infty)$	0.0	(At each contact, set $c=\gamma\sigma_c$. If $\gamma=0.0$, then $(c)_{\{m,sd\}}$ is used.)
ϕ, sbm_fa	FLT	$[0.0,90.0)$	0.0	friction angle [degrees]
ζ, sbm_soft	FLT	$[0.0,\infty)$	0.0	softening factor ($\zeta=0$ is no softening)
γ, sbm_cut	FLT	$[0.0,1.0]$	0.0	strength-reduction factor ($\gamma=0/1$ is full/no softening)

Project

Data Files

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

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Materials (soft-bonded material)

μ, **sbm_fric**	FLT	$[0.0, \infty)$	0.0	friction coefficient (when unbonded)
λ_b, **sbm_bmul**	FLT	$[0.0, \infty)$	0.0	bending-friction multiplier (when unbonded)
λ_t, **sbm_tmul**	FLT	$[0.0, \infty)$	0.0	twisting-friction multiplier (when unbonded)

Linear material group (for grain-grain contacts during packing 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

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Materials (flat-jointed material)

Table 6 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 8.				
Flat-jointed material group:				
C_{MS}, **fjm_trackMS**	BOOL	$\{\text{true, false}\}$	false	microstructure-tracking flag (draw microstructure with the faced grain plot set)
g_i, **fjm_igap**	FLT	$[0.0, \infty)$	0.0	installation gap
ϕ_B^+, **fjm_B_frac**	FLT	$[0.0, 1.0]$	NA	bonded fraction
ϕ_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	$\{0, 1, 2\}$	0	radius-multiplier code $\begin{cases} 0, & \lambda \text{ constant (no valid check)} \\ 1, & \text{valid } (\lambda \text{ non-uniform reduce)} \\ 2, & \text{valid } (\lambda \text{ uniform reduce}) \end{cases}$
λ_v, **fjm_rmulVal**	FLT	$(0.0, \infty)$	1.0	radius-multiplier value $\lambda = \lambda_v = \begin{cases} \lambda_f, & C_\lambda = 0 \\ \lambda_b, & C_\lambda = \{1, 2\} \end{cases}$ 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

Project

Data Files
- myMatGen.p3dvr
- mvParams.p3dat
- **mpParams.p3dat**
- ft.p3fis

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Materials (flat-jointed material)

μ, **fjm_fric**	FLT	$[0.0, \infty)$	0.0	friction coefficient
$(\sigma_c)_{\{msd\}}$ **fjm_ten_{m,sd}**	FLT	$[0.0, \infty)$	$\{0.0, 0.0\}$	tensile-strength dist. [stress] (mean and std. deviation)
$(c)_{\{msd\}}$ **fjm_coh_{m,sd}**	FLT	$[0.0, \infty)$	$\{0.0, 0.0\}$	cohesion dist. [stress] (mean and std. deviation)
γ **fjm_cohTenRatio**	FLT	$[0.0, \infty)$	0.0	cohesion to tensile strength ratio (At each contact, set $c = \gamma \sigma_c$. If $\gamma = 0.0$, then $(c)_{\{msd\}}$ is used.)
c_r **fjm_cohres**	FLT	$[0.0, \infty)$	0.0	residual cohesion [stress]
M_r, **fjm_resmode**	INT	$\{0,1\}$	0	shear-drop residual mode
ϕ, **fjm_fa**	FLT	$[0.0, 90.0)$	0.0	friction angle [degrees]

Linear material group (for grain-grain contacts during packing, 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: $\phi_S = 1 - \phi_B - \phi_G \quad (0 \le \phi_S \le 1)$.

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Materials (flat-jointed material)

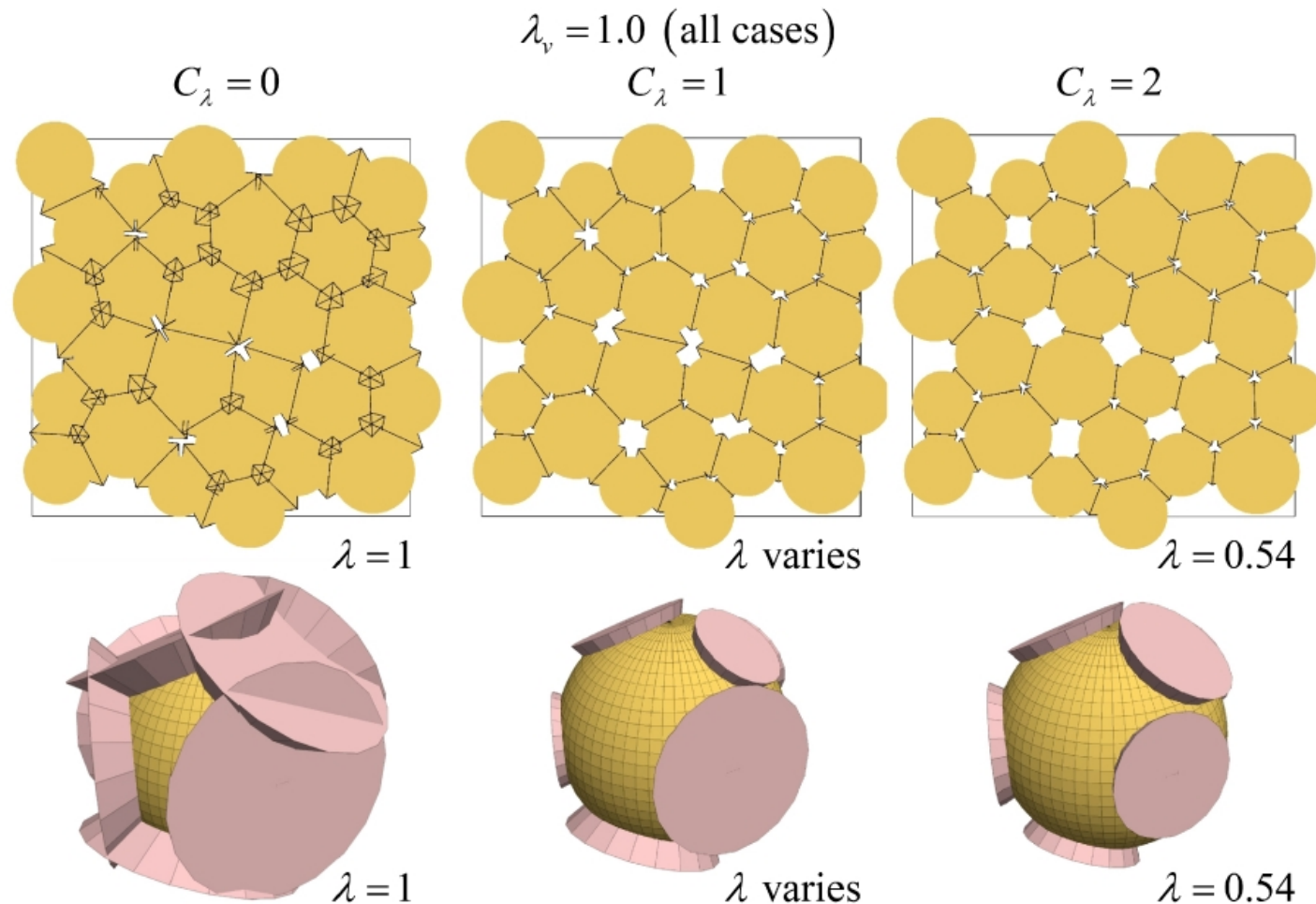Microstructural Validity, valid if grain facets do not overlap

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).
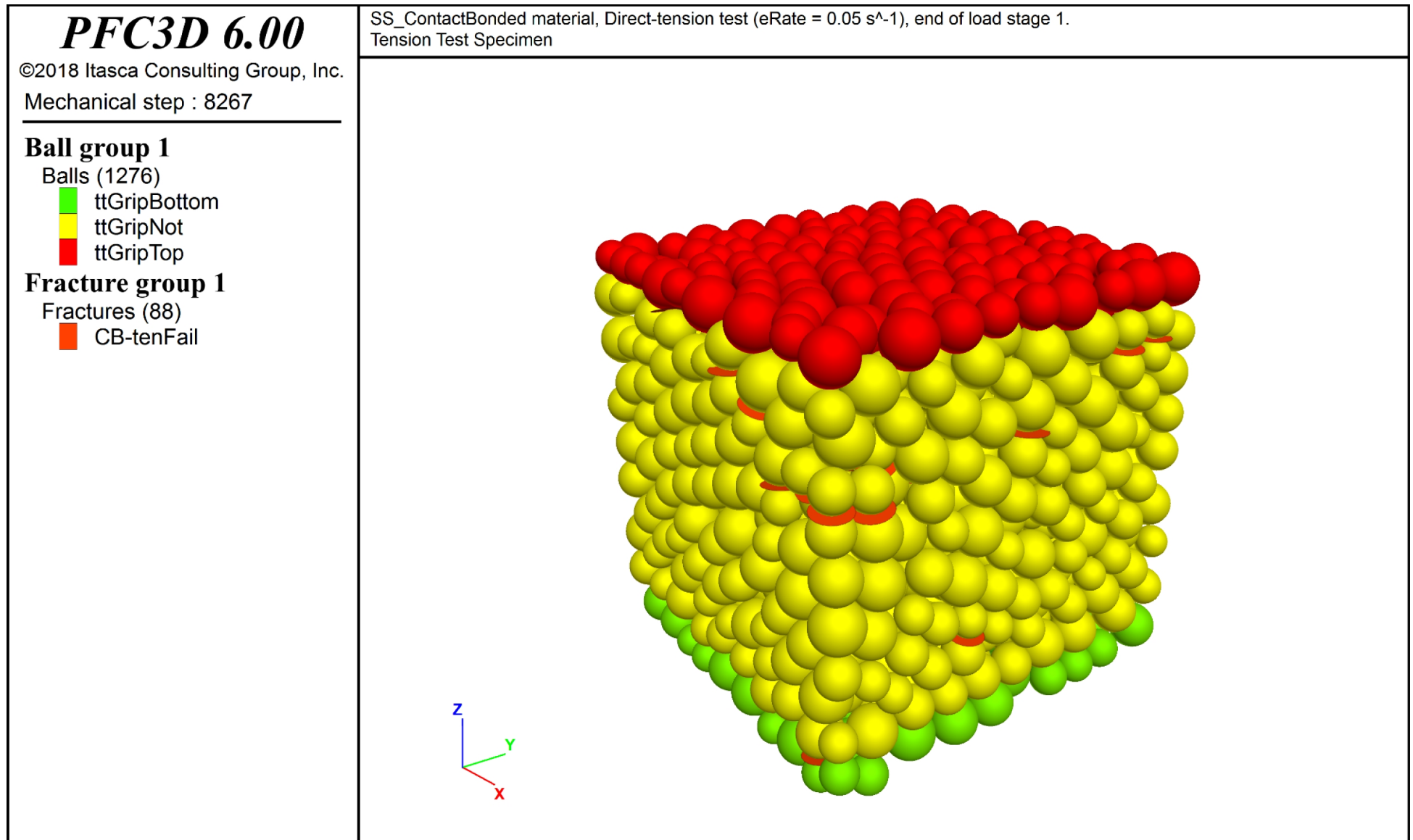
Crack-Monitoring Package

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.

$$\texttt{ck\_nAll}, \texttt{ck\_n\{CB,PB,SB,FJ,SJ\}\{t,s\}}$$

Crack-Monitoring Package

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

PFC3D 6.00

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Mechanical step : 8267

Ball group 1
Balls (1276)
- ttGripBottom
- ttGripNot
- ttGripTop

Fracture group 1
Fractures (88)
- CB-tenFail

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.
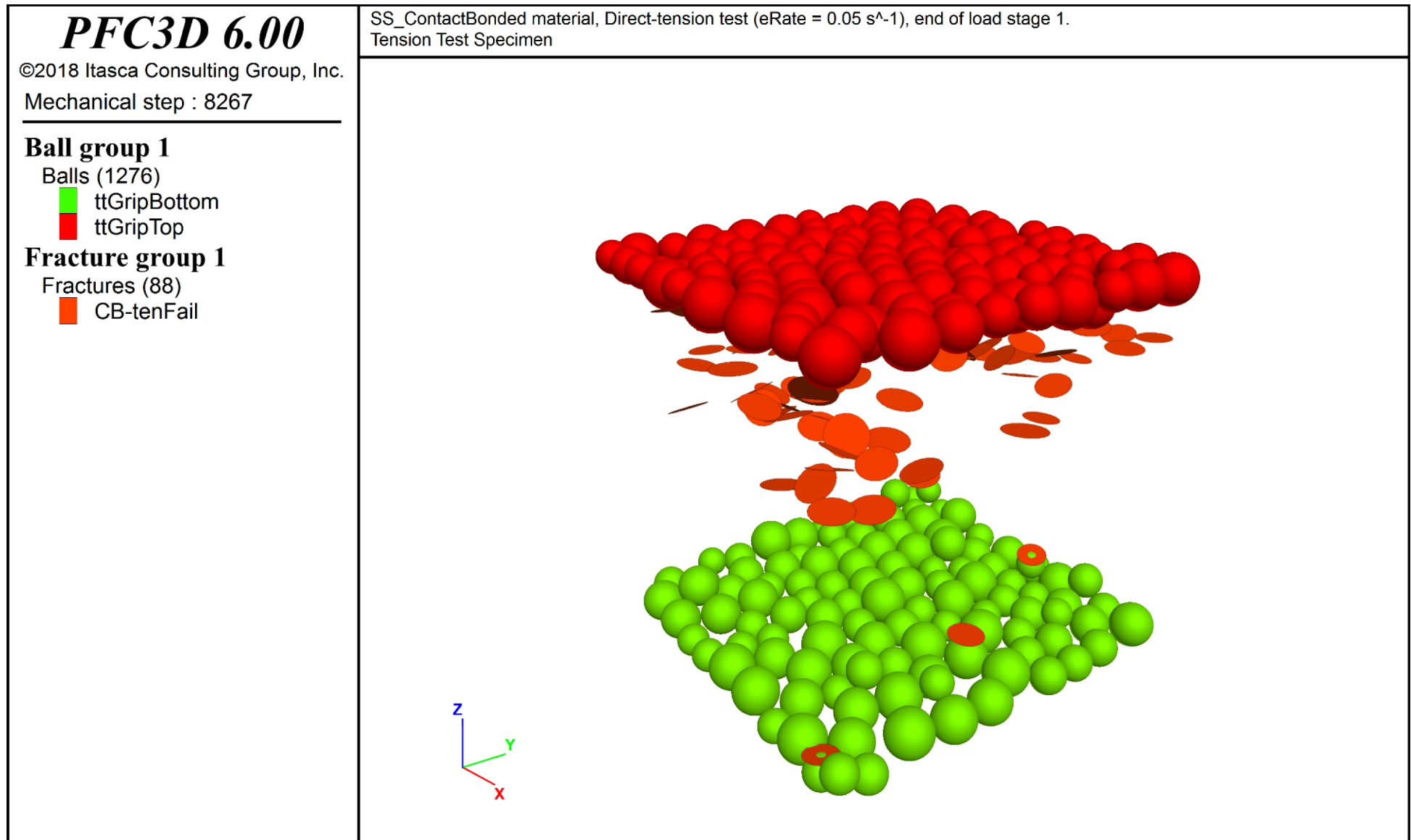
Crack-Monitoring Package

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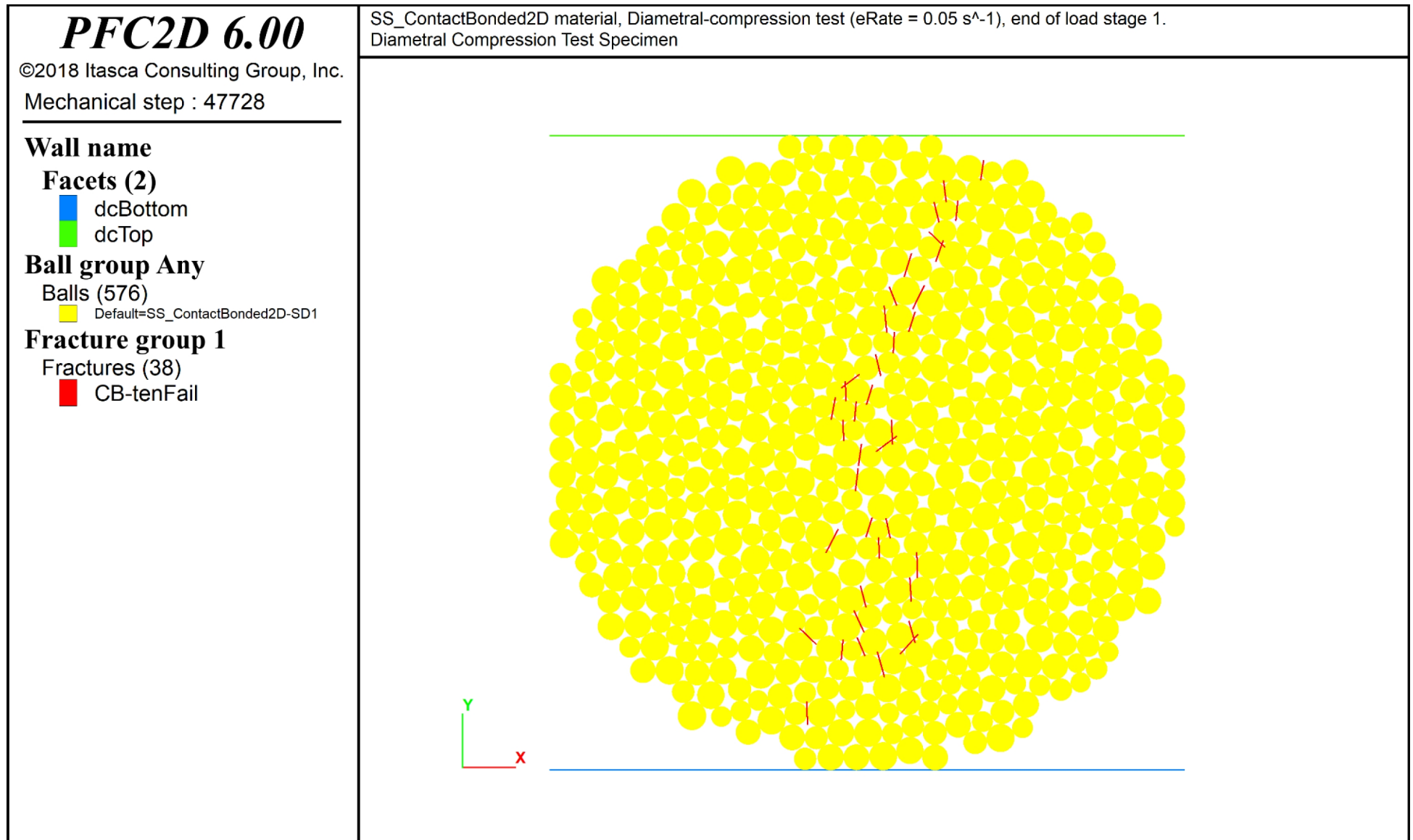
Crack-Monitoring Package

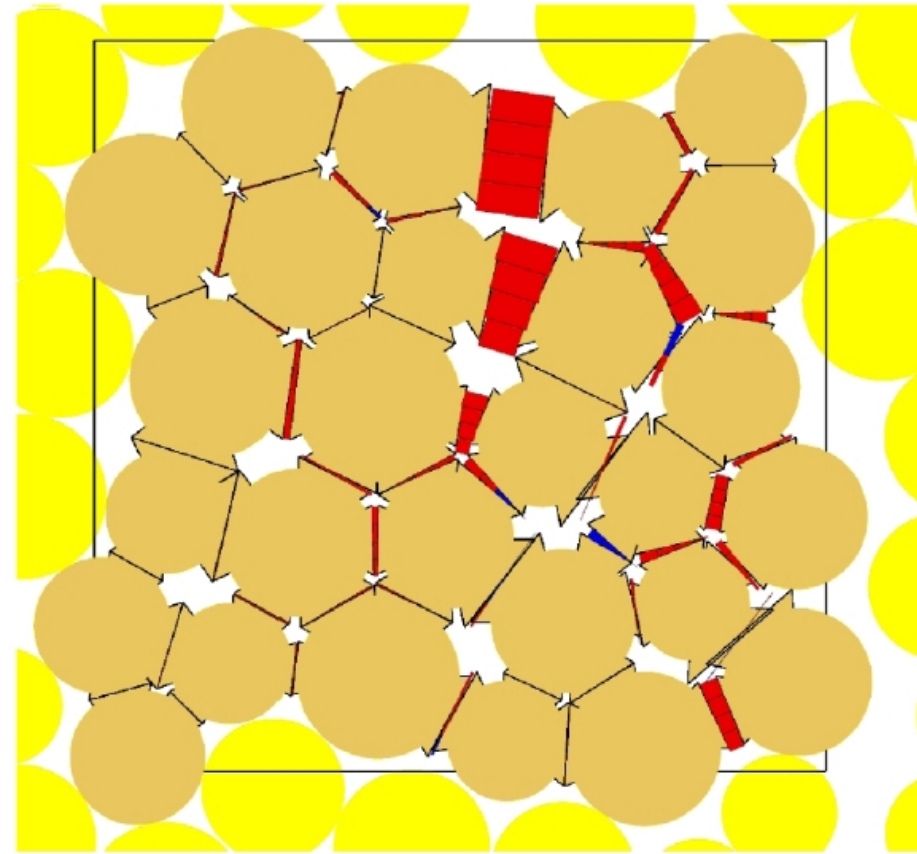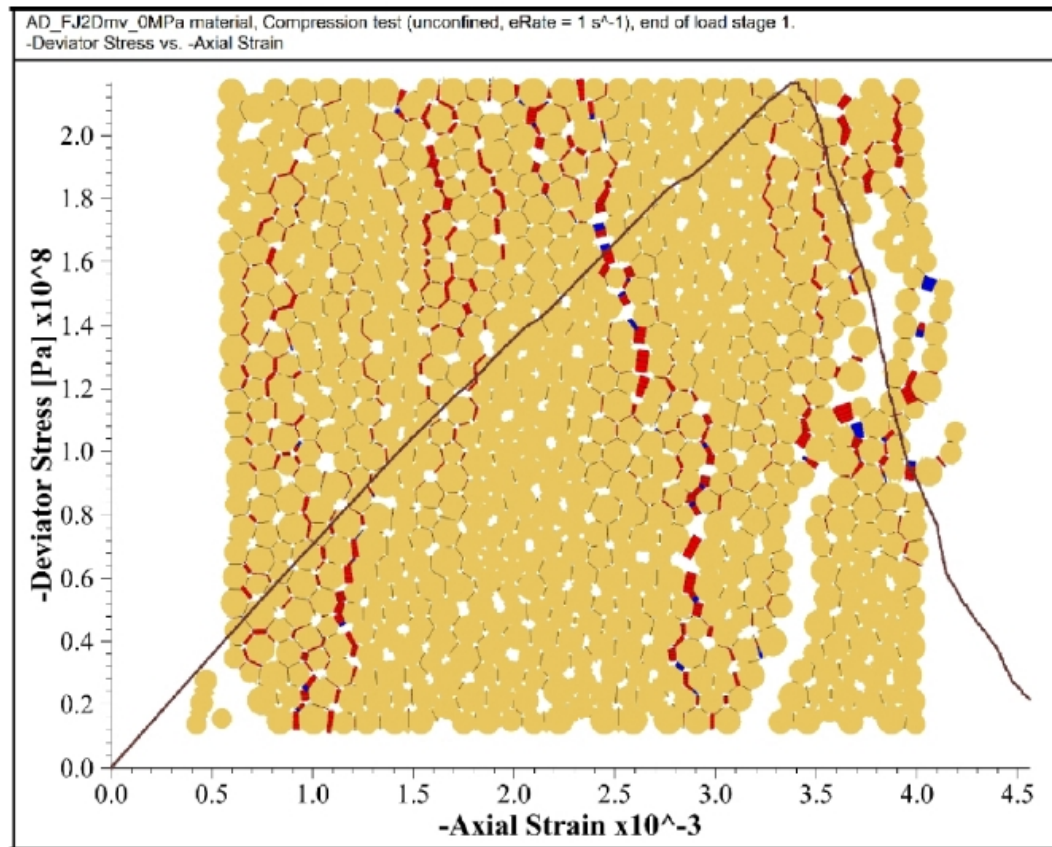"crack" plot set, displays cracks with thickness proportional to gap.

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.
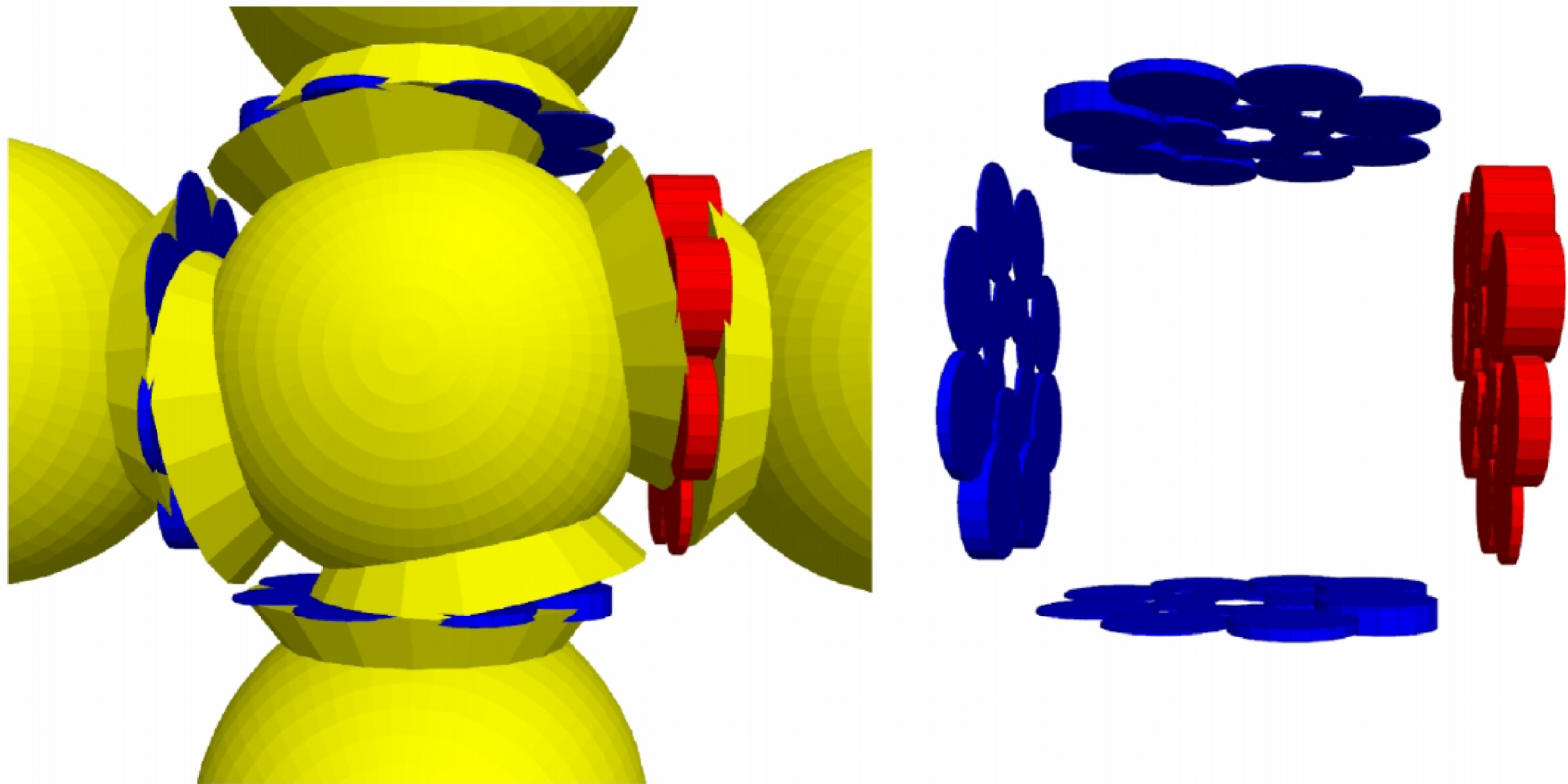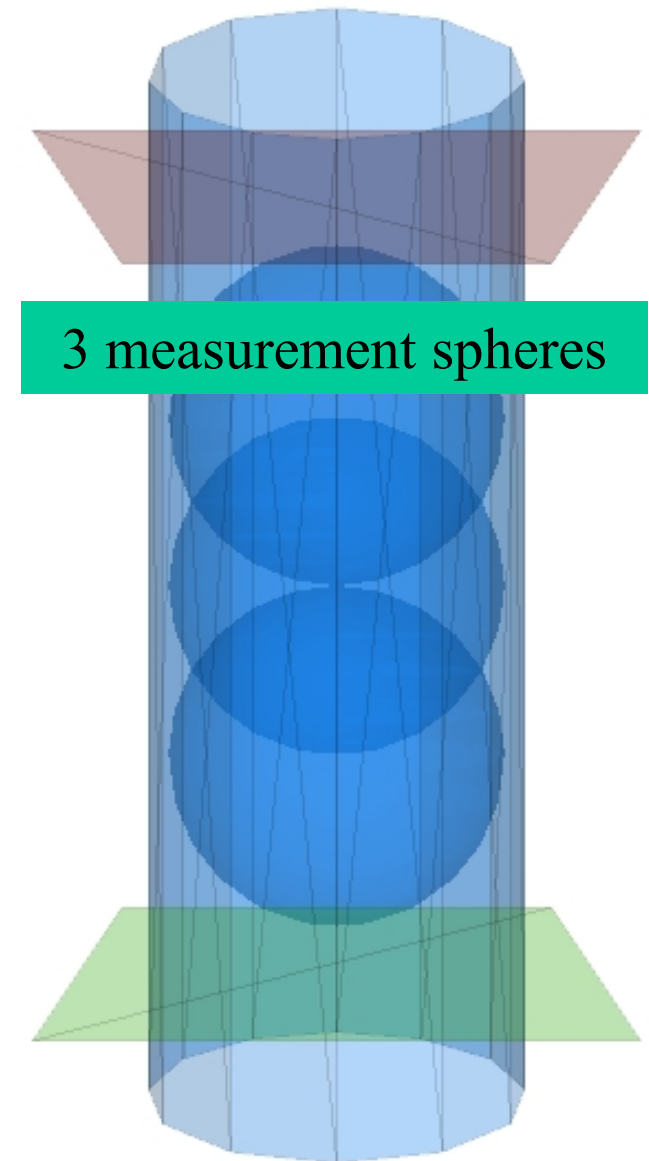

Figure 18   Crack and faced grain plot sets in 3D showing cracks, with crack thickness equal to gap, and cracks colored red/blue for tensile/shear failure.

Lab-Testing Procedures (stress-strain-porosity)

Table 8 Material-Vessel Stress, Strain and Porosity Quantities

Quantity, FISH	Description
$\left\{\sigma_{xx},\sigma_{yy},\sigma_{zz},\sigma_{xy},\sigma_{xz},\sigma_{yz}\right\}$, `mv_ms{xx,yy,zz,xy,xz,yz}`	material stress (2D model: $\sigma_{zz} \equiv \sigma_{xz} \equiv \sigma_{yz} \equiv 0$)
$\left\{\varepsilon_{xx},\varepsilon_{yy},\varepsilon_{zz},\varepsilon_{xy},\varepsilon_{xz},\varepsilon_{yz}\right\}$, `mv_me{xx,yy,zz,xy,xz,yz}`	material strain (2D model: $\varepsilon_{zz} \equiv \varepsilon_{xz} \equiv \varepsilon_{yz} \equiv 0$)
$\left\{\sigma_a,\sigma_r\right\}$, `mv_ms{a,r}`	axial & radial stress
$\left\{\varepsilon_a,\varepsilon_r\right\}$, `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

3 measurement spheres

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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:

$$\sigma_{ij}^{m} \quad \varepsilon_{ij}^{m} \quad \boxed{\text{measurement-based}} \text{ (6 terms each, symmetric)}$$

$$\sigma_{k}^{w} \quad \varepsilon_{k}^{w} \quad \boxed{\text{wall-based}} \text{ (3 terms each)}$$

$$\underbrace{\varepsilon_{k}^{g} \quad \text{guage-based (3 terms)}}_{\substack{i,j=\{x,y,z\} \\ k=\{x,y,z,r\}}}$$

Lab-Testing Procedures (summary)

wall

grains

material specimen

h_o

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

h_o (initial ht. in axial direc.)

P_c

confined

Compression unconfined

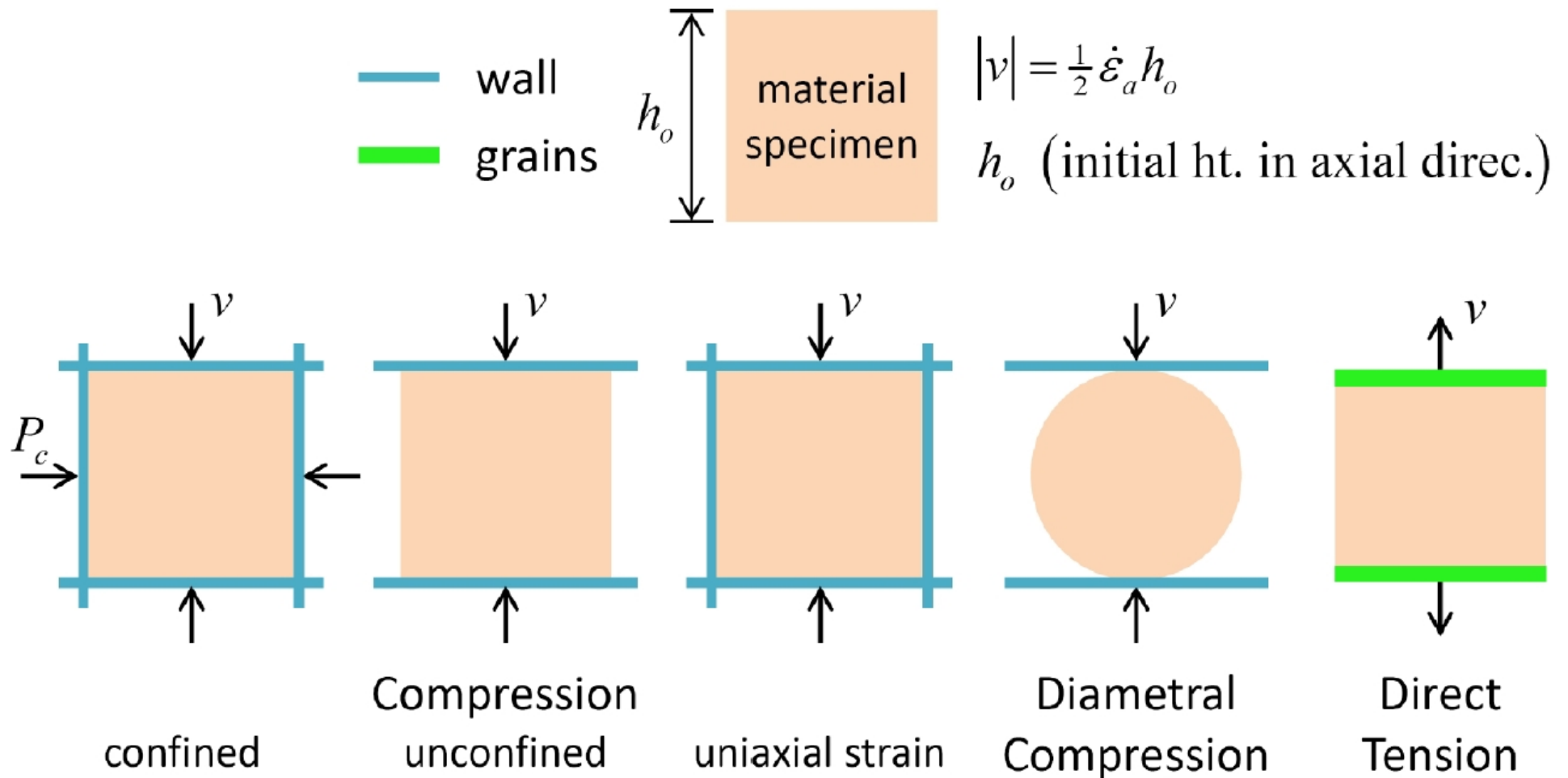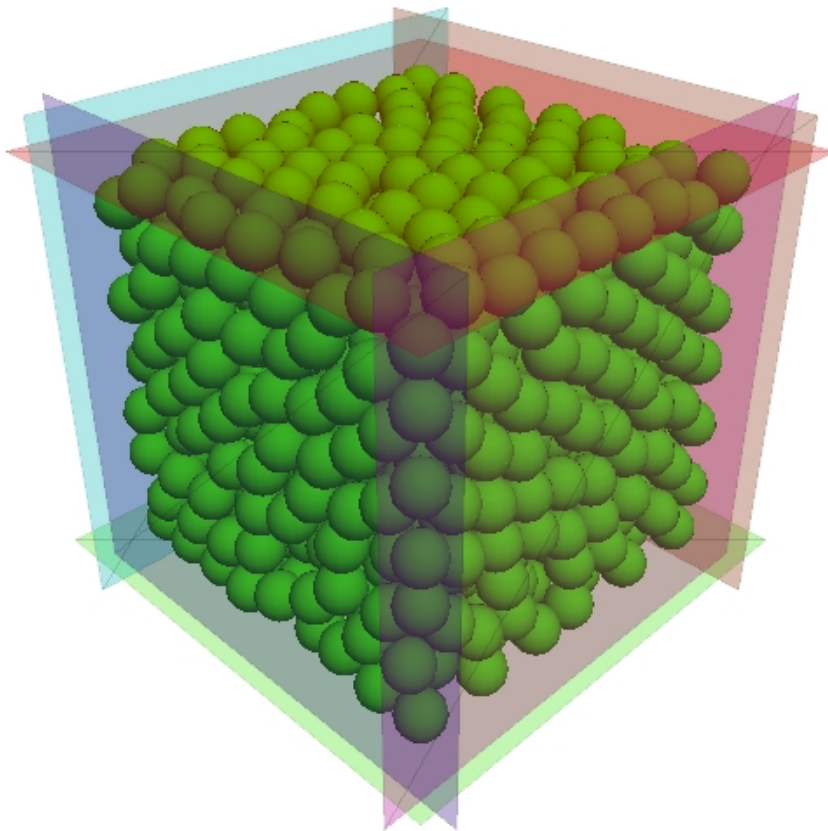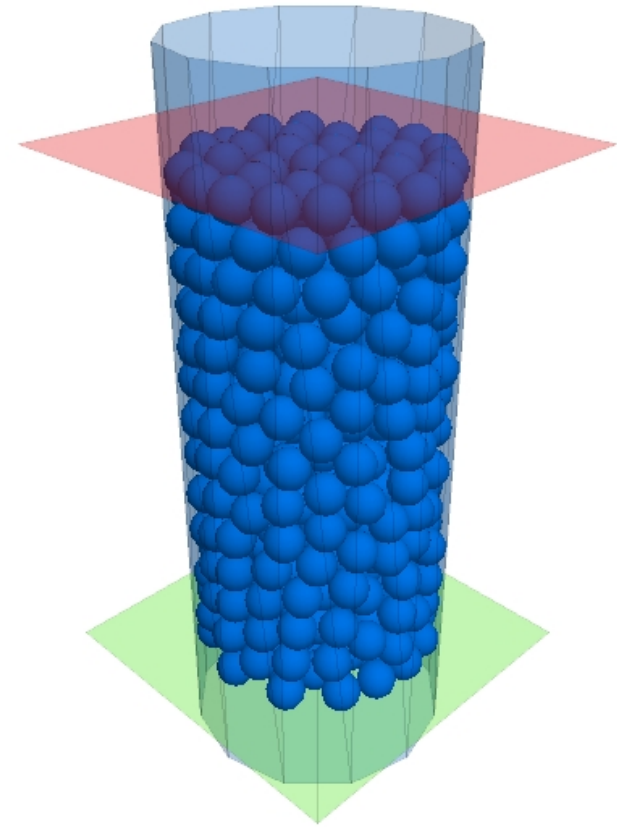uniaxial strain

Diametral Compression

Direct Tension

Figure 23   Loading conditions of laboratory-testing procedures.

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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 $\begin{cases} 0, & \text{confined} \\ 1, & \text{unconfined} \\ 2, & \text{uniaxial strain} \end{cases}$
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 ($|v| = \frac{1}{2}\dot{\varepsilon}_a h_o$, $\dot{\varepsilon}_a > 0$, see Figure 23 and Section 5.4)
C_l, **ct_loadCode**	INT	$\{0,1\}$	0	loading-phase code $\begin{cases} 0, & \text{single stage} \\ 1, & \text{multiple stages} \end{cases}$
α, **ct_loadFac**	FLT	$(0.0,1.0)$	0.9	load-termination factor ($C_l = 0$) for termination criterion: $\left|\sigma_d^w\right| \le \alpha \left|\sigma_d^w\right|_{max}$
Servo-control group:				
ε_p, **ct_PTol**	FLT	$(0.0,\infty)$	**pk_PTol**	pressure tolerance $\left(\dfrac{|P - P_c|}{P_c} \le \varepsilon_P\right)$ where P is current pressure
ε_{lim}, **ct_ARatLimit**	FLT	$(0.0,\infty)$	1×10^{-5}	equilibrium-ratio limit (parameter of **ft_eq**)
n_{lim}, **ct_stepLimit**	INT	$[1,\infty)$	**pk_stepLimit**	step limit (parameter of **ft_eq**)
v_{lim}, **ct_vLimit**	FLT	$(0.0,\infty)$	$10H\dot{\varepsilon}_a$	servo velocity limit (see Table 9)

Project
Data Files
- myCompTest.p3dvr
- ctParams.p3dat
- ct.p3fis
- ck.p3fis

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

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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 ($\|v\| = \frac{1}{2}\dot{\varepsilon}_a g_o$, $\dot{\varepsilon}_a > 0$, 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: $\|F_a\| \le \alpha \|F_a\|_{\max}$
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)

Project

Data Files

- myDiamCompTest.p3dvr
- dcParams.p3dat
- ck.fis
- dc.fis

platens & specimen are centered w.r.t. origin

axial direction (loading axis)

(2D model: $d \equiv 1$)
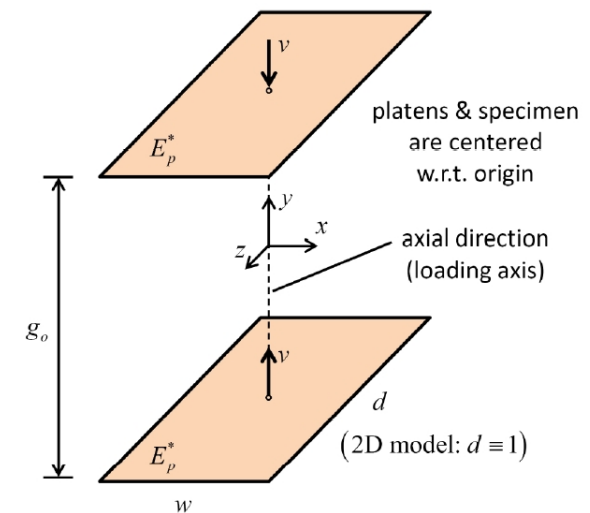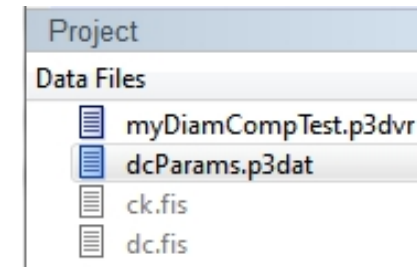
Figure 18   Loading configuration of diametral-compression test.

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 ($|v| = \frac{1}{2}\dot{\varepsilon}_a h_o$, $\dot{\varepsilon}_a > 0$, 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: $\left|\sigma_a^m\right| \leq \alpha \left|\sigma_a^m\right|_{\max}$

Project

Data Files

- myTenTest.p3dvr
- ttParams.p3dat
- ck.p3fis
- tt.p3fis

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

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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).[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, α, C_ρ, $\rho_v \left[\text{kg/m}^3 \right]$	0, 0.7, 0, 2650
S_g, T_{SD}, $\left\{ D_{\{l,u\}} \text{ [mm]}, \phi \right\}$, D_{mult}	0, 0, $\{14, 20, 1.0\}$, 1.0
Packing group:	
S_{RN}, $P_m \text{ [kPa]}$, ε_P, $\varepsilon_{\lim}$, $n_{\lim}$	10000, 150, 1×10^{-2}, 8×10^{-3}, 2×10^6
C_p, n_c, μ_{CA}, $v_{\lim} \text{ [m/s]}$	0, 0.58, 0, 1.0
Linear material group:	
$E^* \text{ [MPa]}$, κ^*, μ	500, 1.5, 0.4

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

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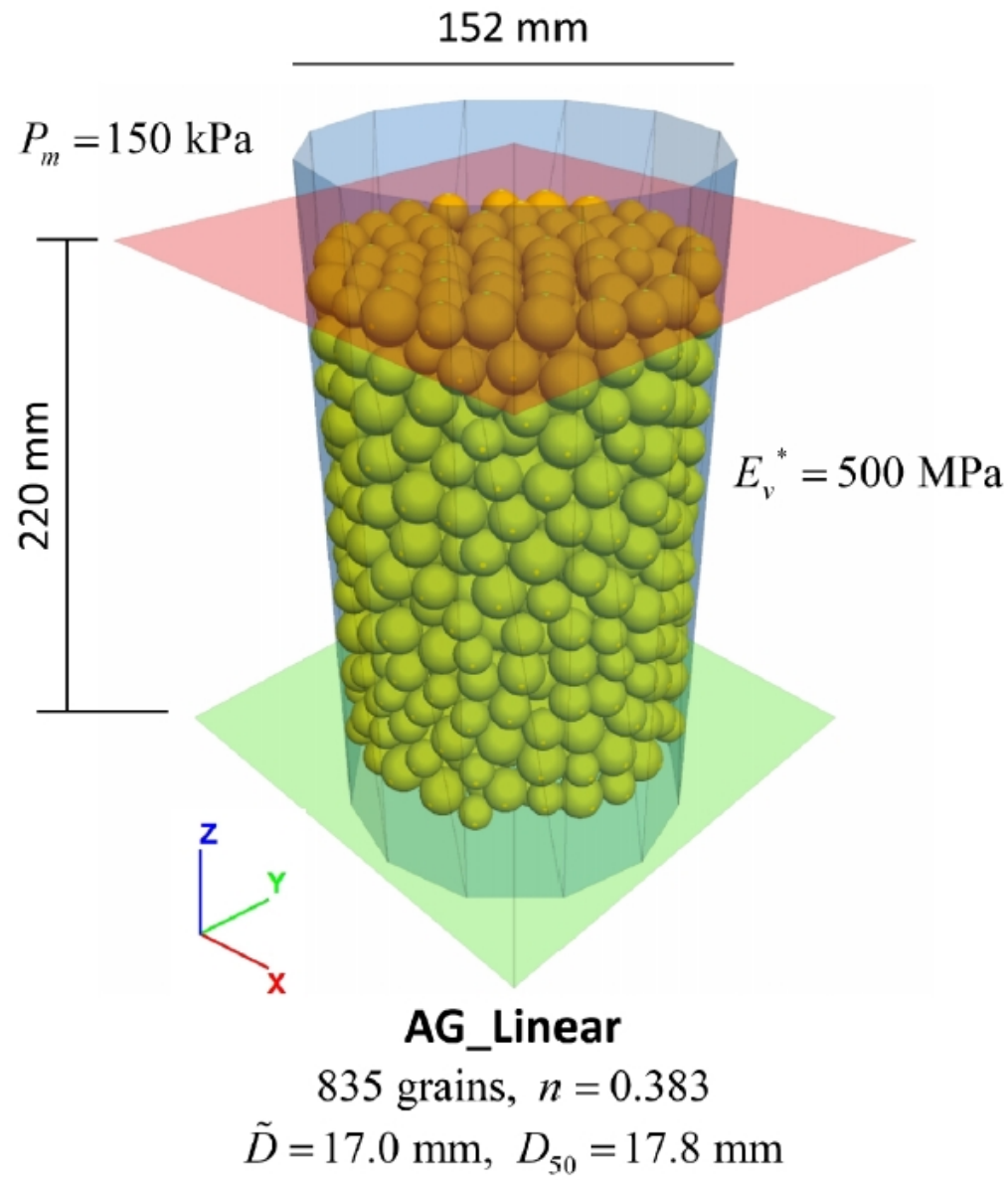
Figure 1   AG_Linear material packed at 150 kPa material pressure at the end of material genesis.

Example Materials (linear material)
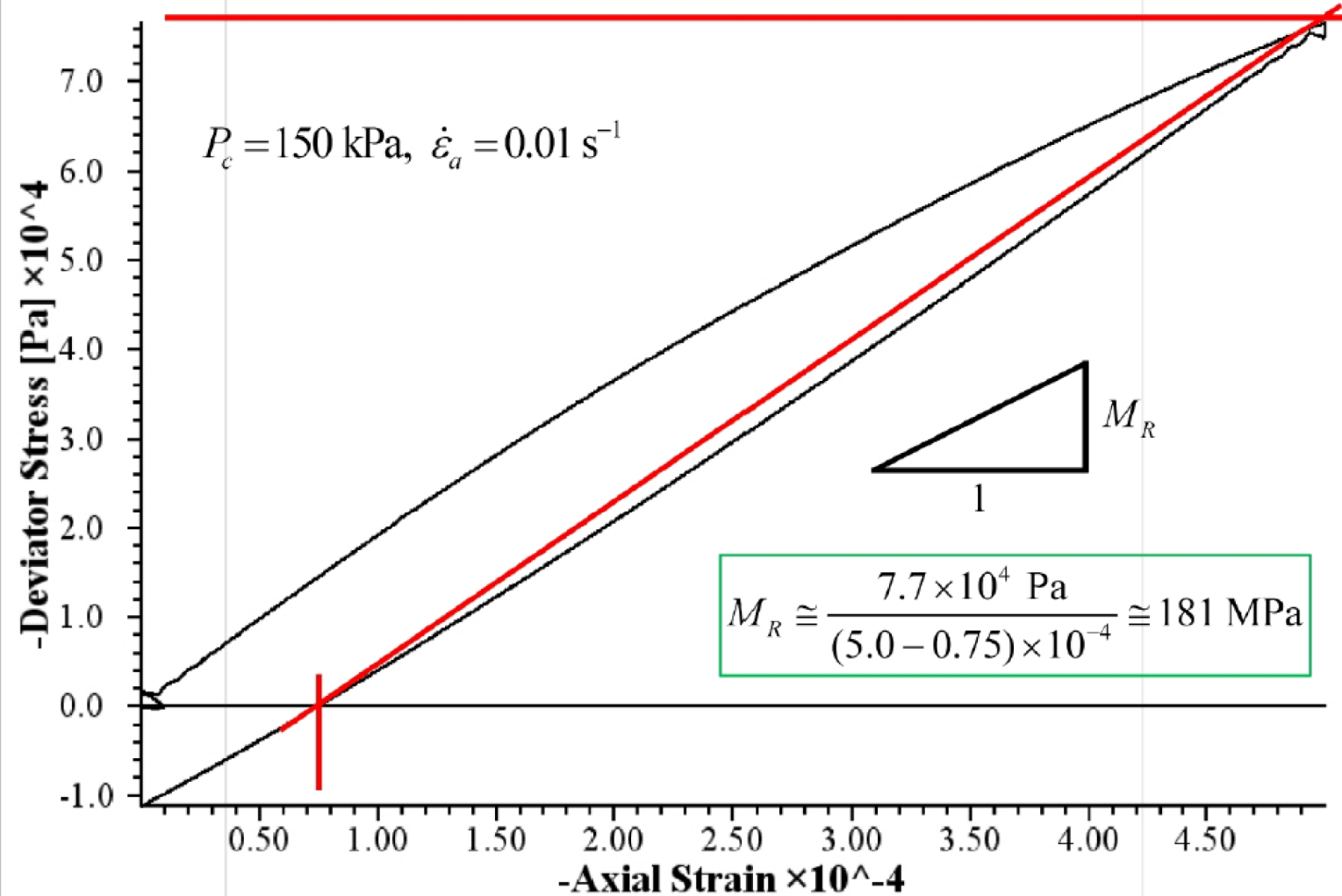
Figure 2   *Deviator stress versus axial strain for AG_Linear material tested at 150 kPa confinement, and measurement of resilient modulus.*

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.

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[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.

Example Materials (contact-bonded material)

Table 5 *Microproperties of SS_ContactBonded Material**

Property	Value
Common group:	
N_m	SS_ContactBonded
T_m, α, C_ρ, $\rho_v \left[\mathrm{kg/m^3} \right]$	1, 0.7, 1, 1960
S_g, T_{SD}, $\left\{ D_{\{l,u\}} \left[\mathrm{mm} \right], \phi \right\}$, D_{mult}	0, 0, {4.0, 6.0, 1.0}, 1.0
Packing group:	
S_{RN}, $P_m \left[\mathrm{MPa} \right]$, ε_P, ε_{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:	
$E^* \left[\mathrm{GPa} \right]$, κ^*, μ	3.0, 1.5, 0.4
Contact-bond group:	
$g_i \left[\mathrm{mm} \right]$	0
$\left(T_\sigma \right)_{\{m, sd\}} \left[\mathrm{MPa} \right]$, $\left(S_\sigma \right)_{\{m, sd\}} \left[\mathrm{MPa} \right]$	{1.0, 0}, {20.0, 0}
Linear material group:	
$E_n^* \left[\mathrm{GPa} \right]$, κ_n^*, μ_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)

$E_v^* = 3.0$ GPa

cube, s = 50 mm

cube, s = 20 mm

$P_m = 30$ MPa
$g_i = 0$

SS_ContactBonded
1276 grains, $c_b = 6.1$
$\tilde{D} = 4.8$ mm, $D_{50} = 5.1$ mm

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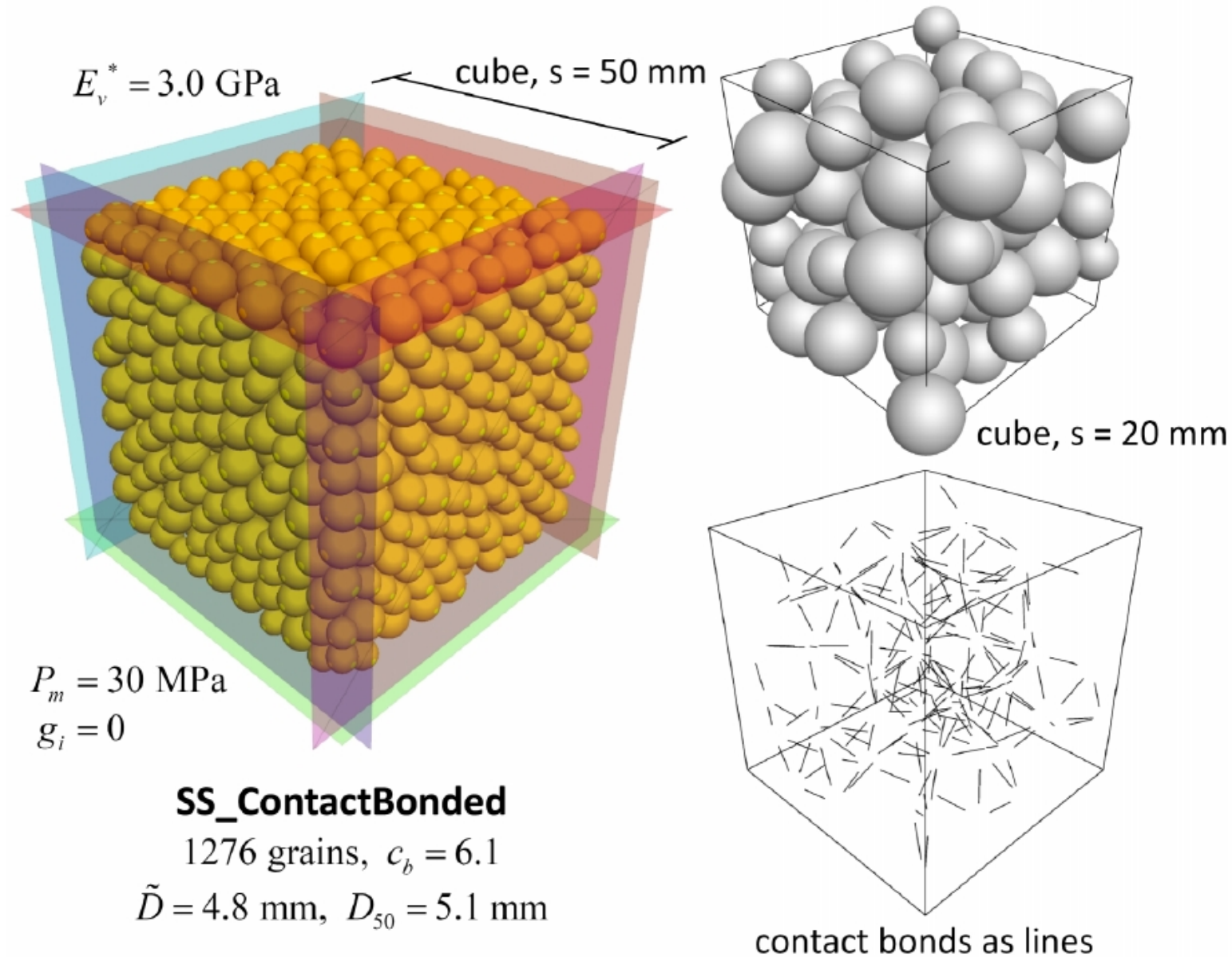
Figure 11   SS_ContactBonded material at the end of material genesis with grains and contact bonds in the microstructural box.

Example Materials (contact-bonded material)
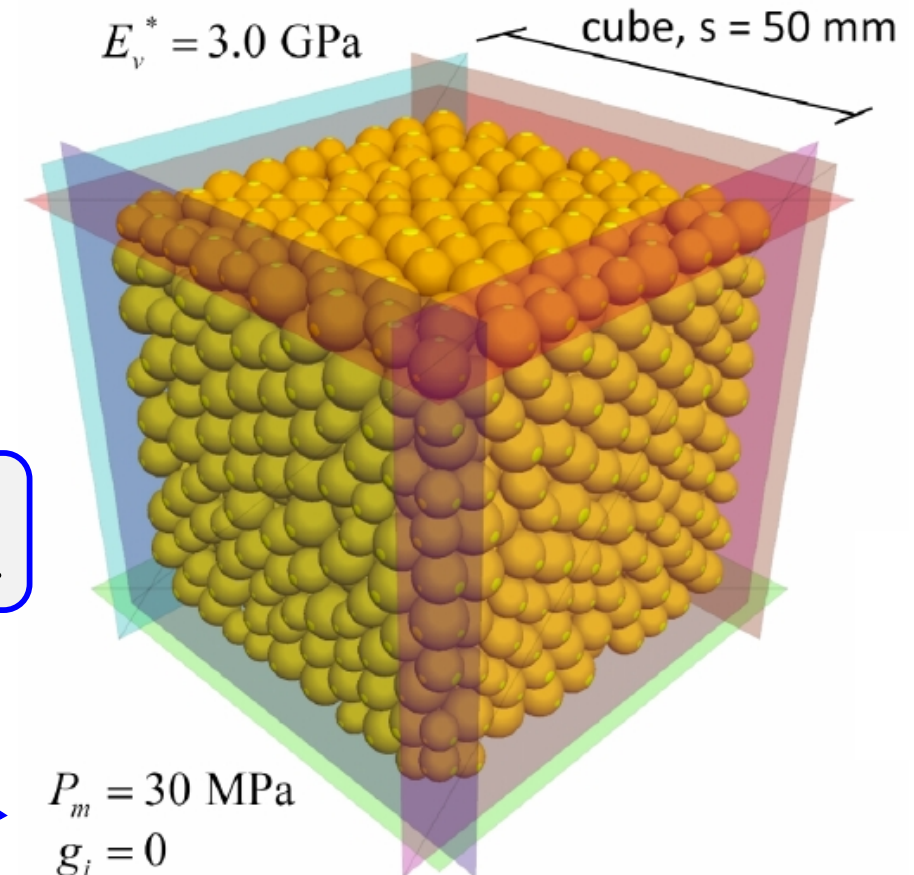
$E_v^* = 3.0 \text{ GPa}$

cube, s = 50 mm

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

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

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

Example Materials (contact-bonded material)

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Mechanical step : 41117

Wall name
Facets (12)
- mvBack
- mvBottom
- mvFront
- mvLeft
- mvRight
- mvTop

Ball
Balls (1276)
- ball

Fracture group 1
Fractures (469)
- CB-tenFail

SS_ContactBonded material, Compression test (unconfined, eRate = 0.05 s^-1), end of load stage 1.
Compression Test Cell

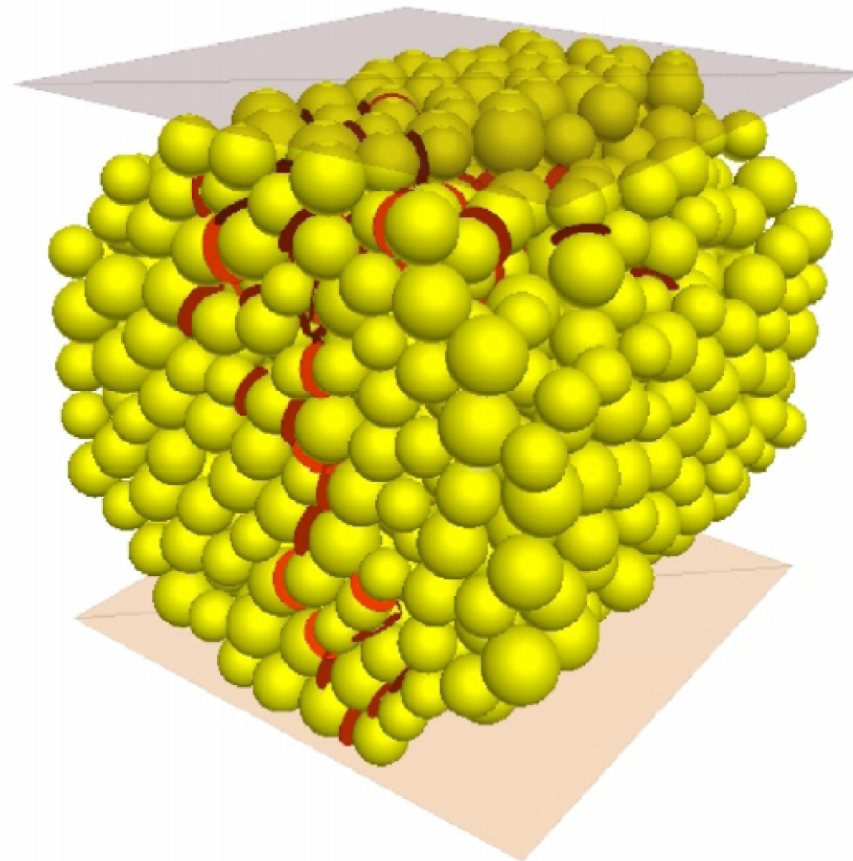$$P_c = 0, \quad \dot{\varepsilon}_a = 0.05 \text{ s}^{-1}$$
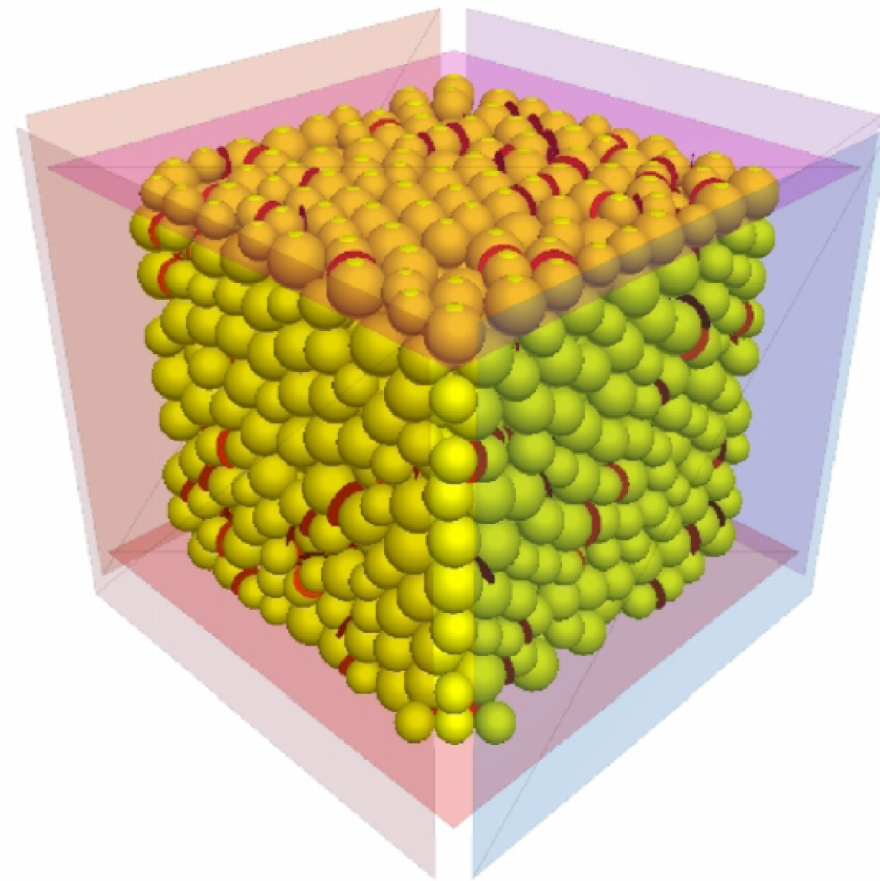
Figure 12   SS_ContactBonded material at the end of the fully unconfined test with grains and cracks.
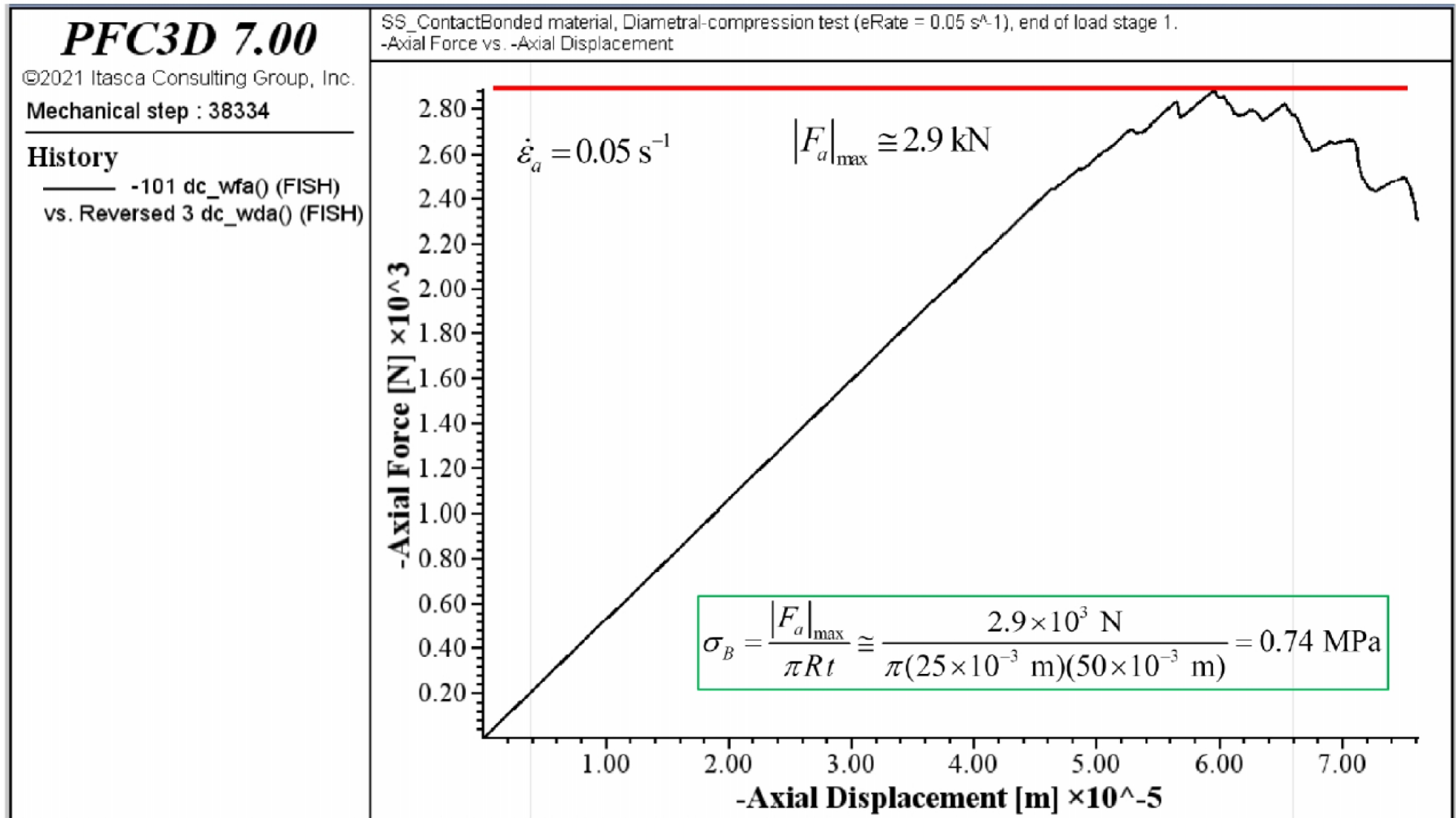
Example Materials (contact-bonded material)
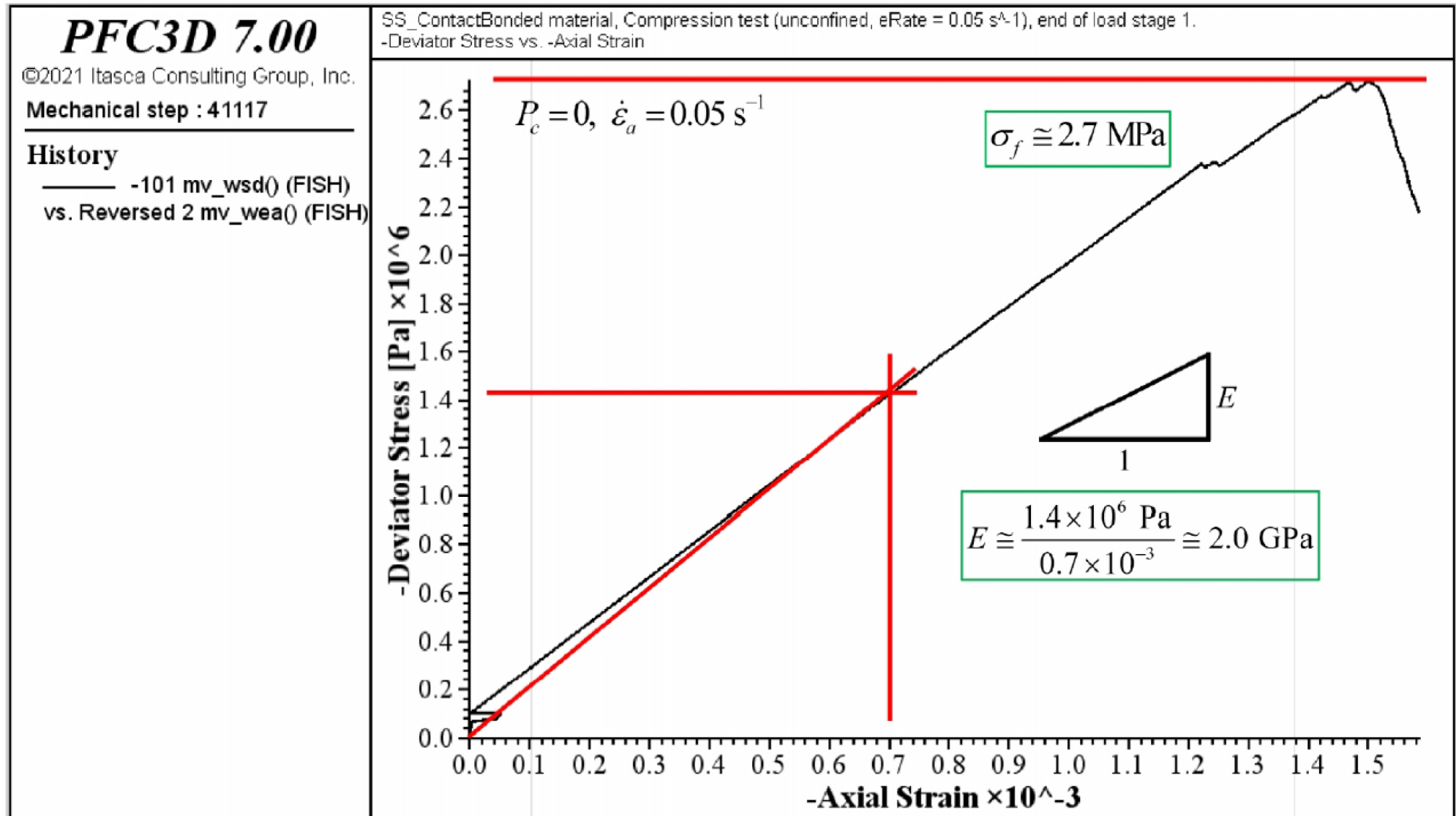
Figure 13   *Deviator stress versus axial strain for SS_ContactBonded material tested fully unconfined, and measurement of peak strength and Young's modulus.*

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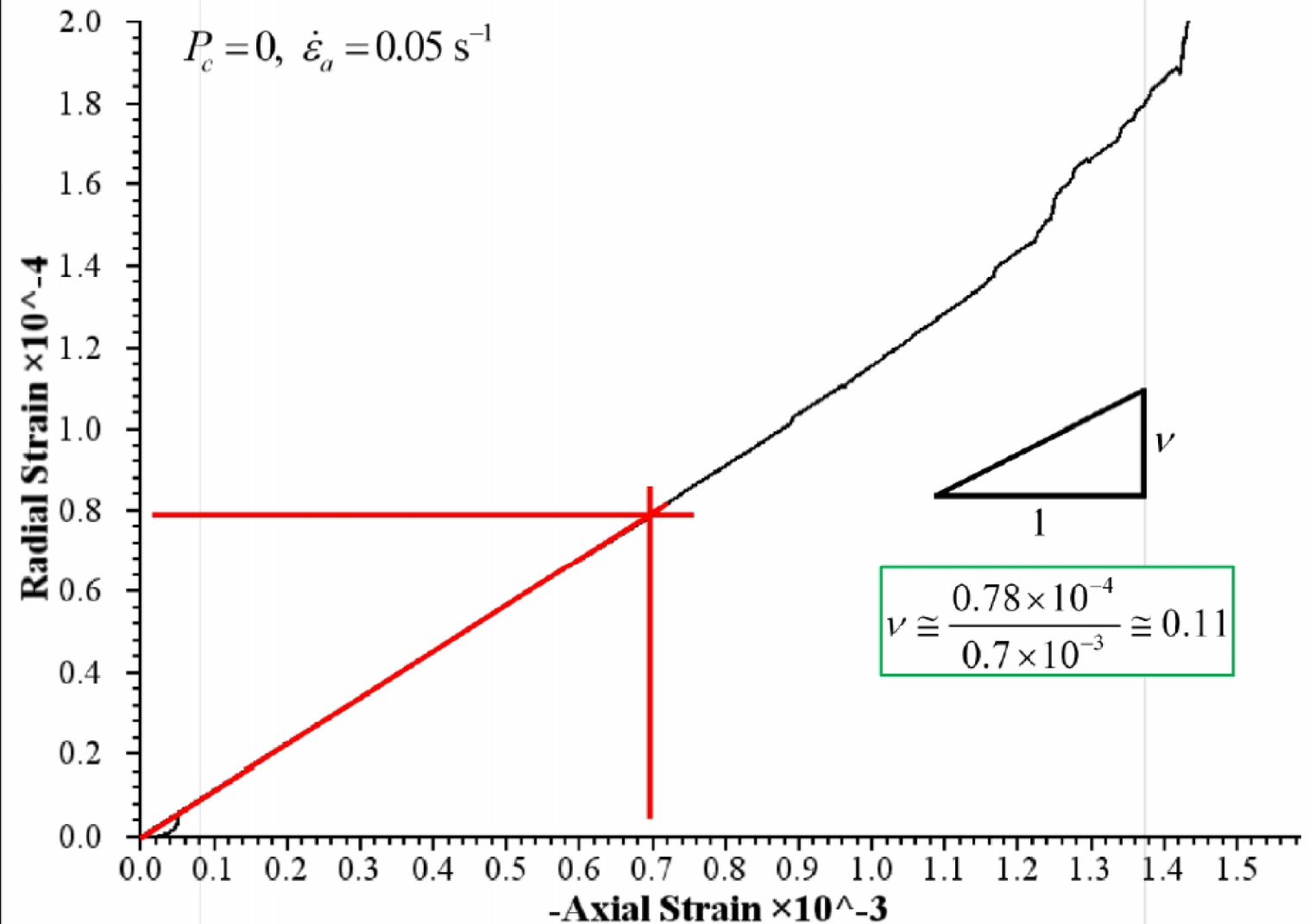
Figure 14 *Radial strain versus axial strain for SS_ContactBonded material tested fully unconfined, and measurement of Poisson's ratio.*

Example Materials (contact-bonded material)

PFC3D 7.00

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Mechanical step : 38334

SS_ContactBonded material, Diametral-compression test (eRate = 0.05 s^-1), end of load stage 1.
Diametral Compression Test Specimen

$$\dot{\varepsilon}_a = 0.05 \text{ s}^{-1}$$

Wall name
  Facets (4)
    ■ dcBottom
    ■ dcTop
Ball
  Balls (1044)
    ■ ball
Fracture group 1
  Fractures (439)
    ■ CB-tenFail

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.*
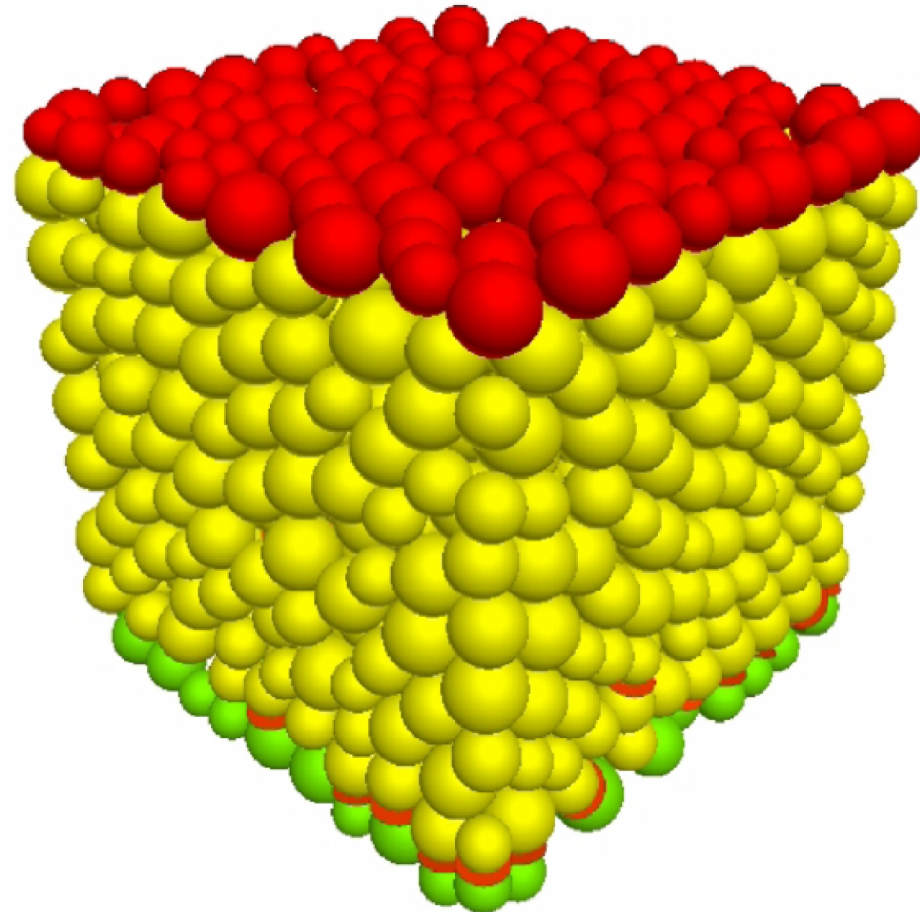
Example Materials (contact-bonded material)

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

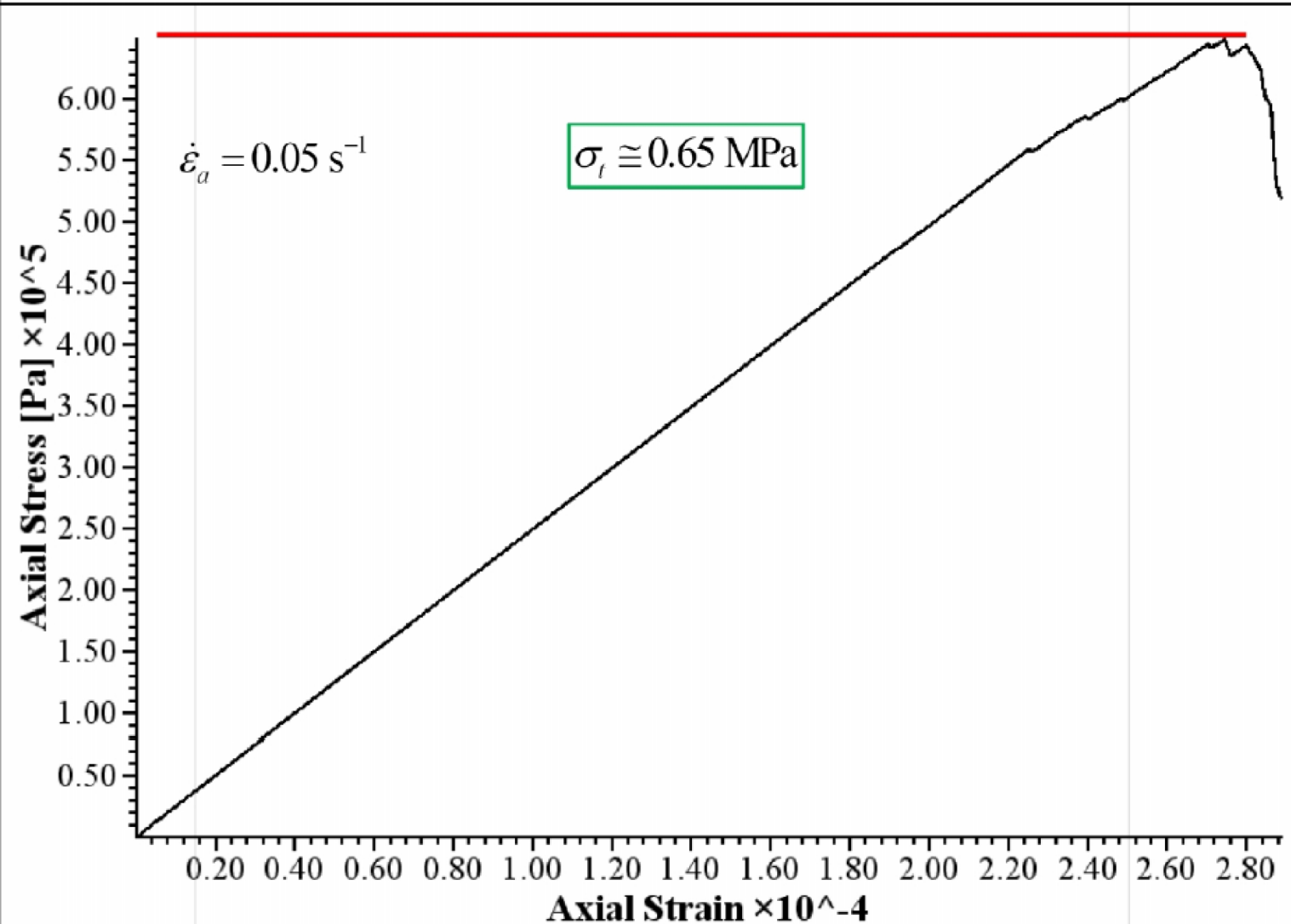# Example Materials (contact-bonded material)

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

Stay tuned for more. . .

For now, calibration notes and material behavior:

> Potyondy, D. (2018) "Calibration of the Flat-Jointed Material," PowerPoint Slide Set (April, 13, 2018).
> Potyondy, D. (2021) "Flat-Jointed Material Behavior," PowerPoint Slide Set (June 21, 2021).

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