ITASCA
Consulting Group, Inc.

Material-Modeling Support in PFC

[via PFC 5.0 FISHTank (fistPkg25)]

David Potyondy

March 16, 2017

Preamble

- We describe material-modeling support in PFC 5 by summarizing the contents of the technical memo:

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

- This slide set also contains material from the bonded-particle modeling portion of the latest PFC Training Course.

Introduction

The PFC model provides a synthetic material consisting of an assembly of rigid grains that interact at contacts. . .

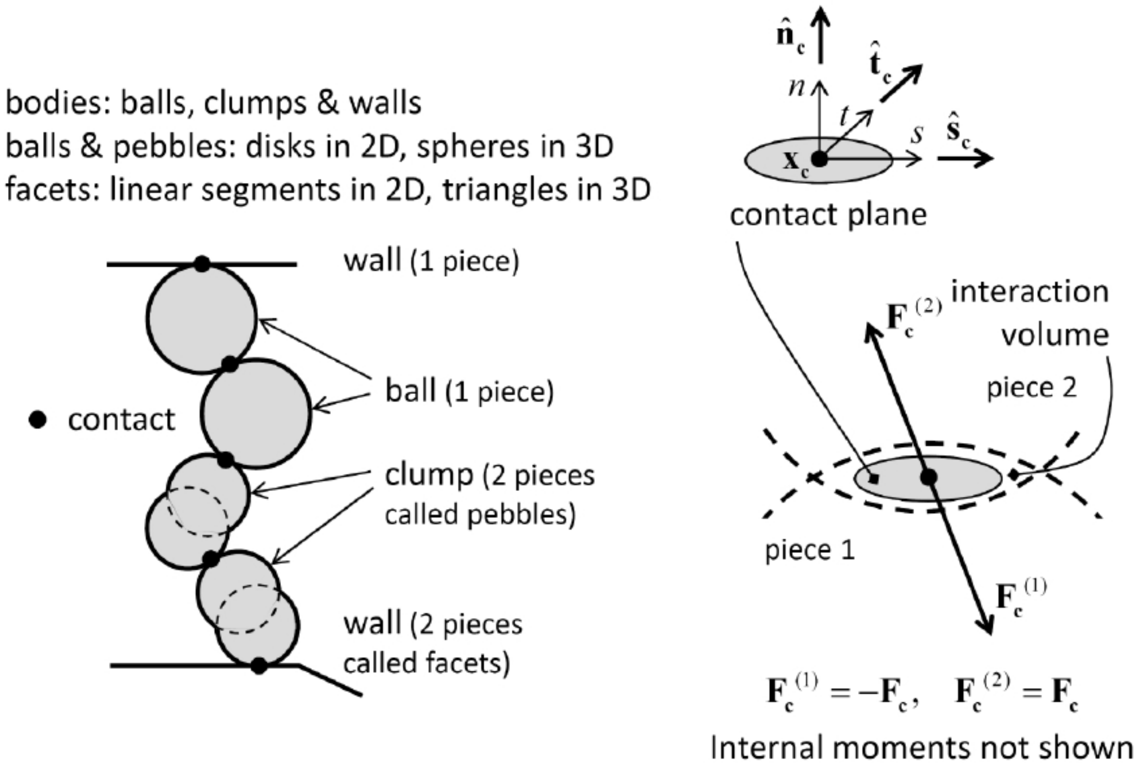


Figure 1 ***PFC model showing bodies and contacts (left) and contact plane with internal force (right).*** (From Fig. 1 of Itasca [2015, PFC Model Components: PFC Model Formulation: Model Components])

show cemented plastic pellets

Introduction

The PFC model provides a synthetic material consisting of an assembly of rigid grains that interact at contacts. . .

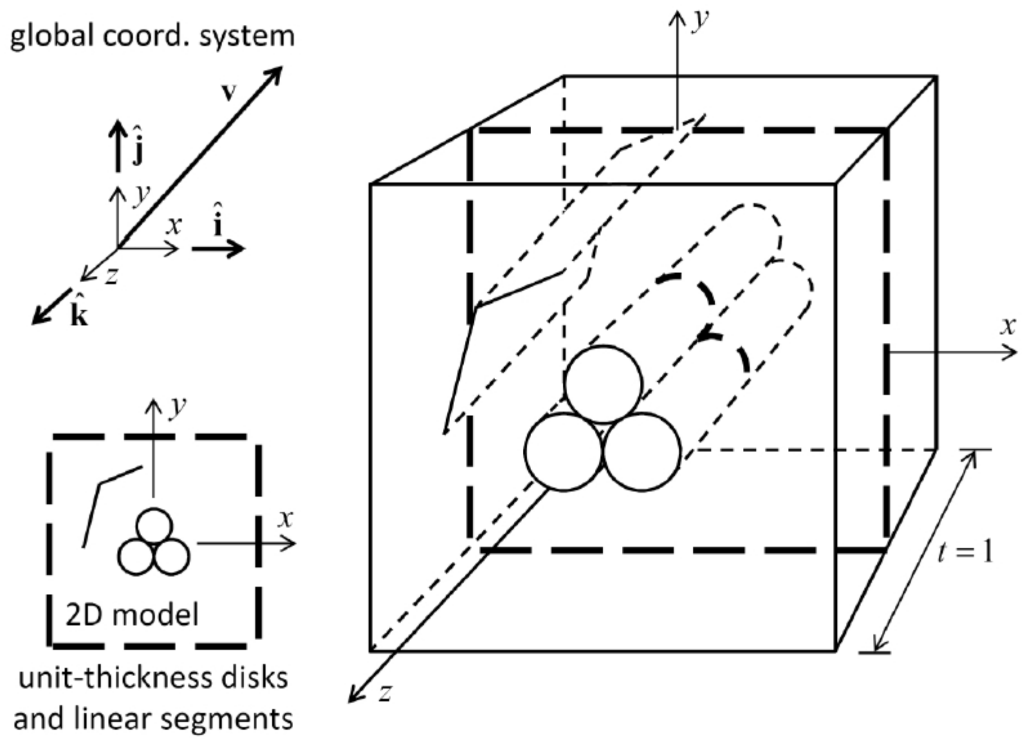


Figure 2 ***Global coordinate system and orientation of the 2D model, which consists of unit-thickness disks and linear segments centered in the xy plane.*** (From Fig. 1 of Itasca [2015, PFC Model Components: PFC Model Formulation: Conventions]

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).

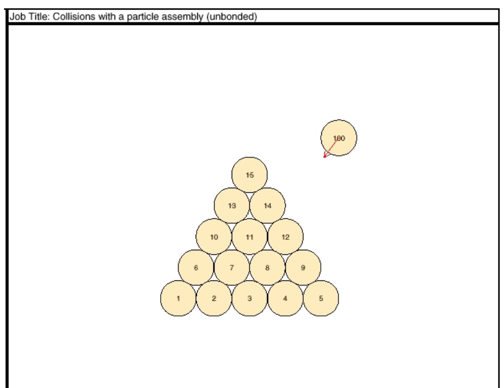
The support for material modeling provided by PFC 5.0 consists of a consistent set of FISH functions, which we call the PFC 5.0 FISHTank (or fistPkg).

Introduction

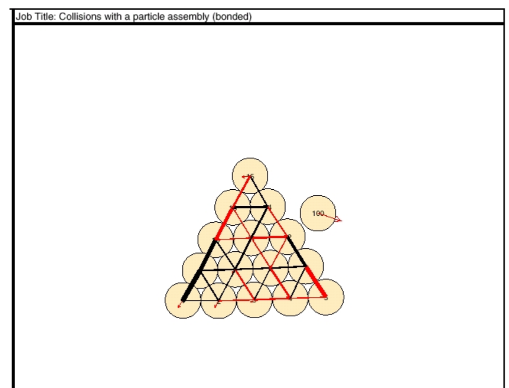
The grains of the PFC material can be either balls or clumps drawn from a general grain-size distribution. It is the type of contact model at the grain-grain contacts that defines the material as being:

linear, contact-bonded, parallel-bonded or flat-jointed.

The linear material is a granular material, and the other materials are bonded materials.

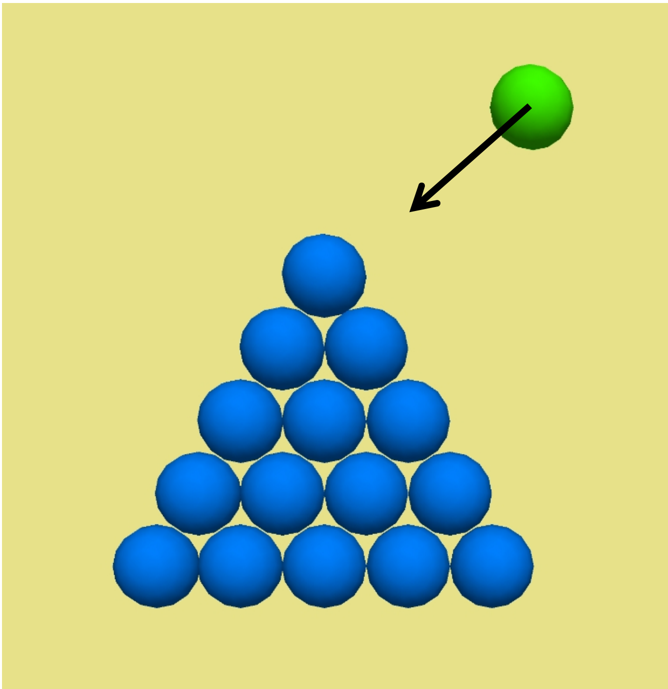


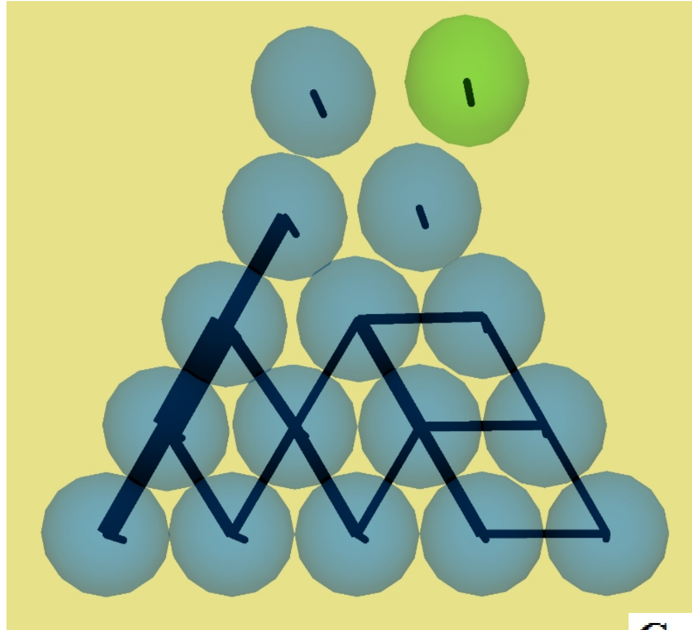
granular material



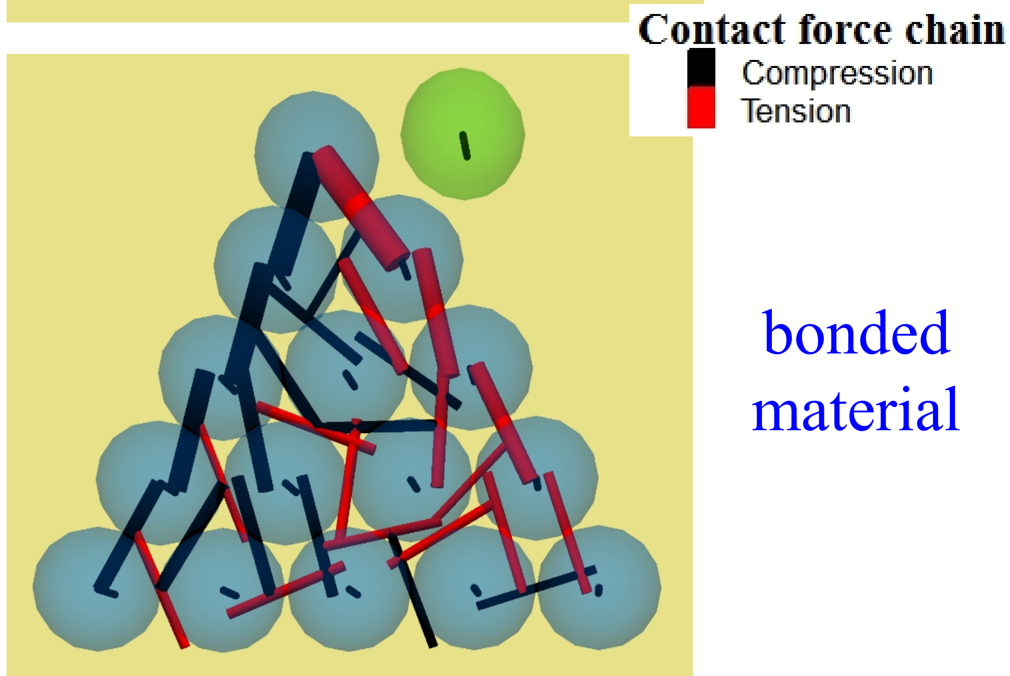
bonded material

Introduction





granular material



bonded material

Run myPoolTable.p3prj

One needs simpler models. . .

In order to comprehend that which is incomprehensible because it is too huge or too complex, one needs simpler models. Often, mathematics can provide the right starting point, which is why beautiful mathematical concepts are so pervasive in explanations of the phenomena of nature on the micro-level.

Hofstadter, D.R. (1985) *Metamagical Themas: Questing for the Essence of Mind and Pattern*, New York: Basic Books (page xxvii).

Why Model?

See the five papers referred to at end of ***Section 1.0 PFC MODEL*** of Potyondy (2017).

- 1. create synthetic material (& system)
- 2. subject to loading & boundary conditions
- 3. monitor response → predict behavior

VALIDATION *Is predicted behavior similar to that of actual physical material & system?*

- (a) parametric studies
- (b) what-if scenarios

→ applied mode

- (c) test mechanistic hypotheses research mode

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

Why Model?

Verification establishes that the formulation & implementation accurately represent a model (conceptual description) of material behavior.

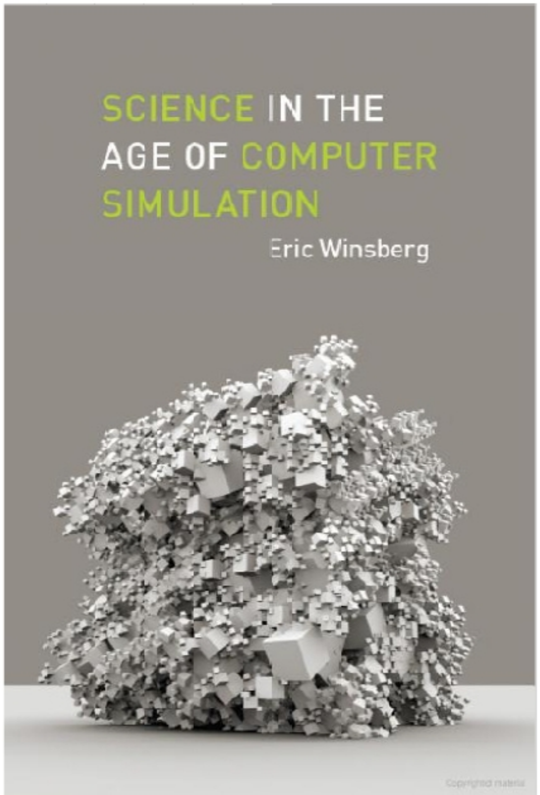
This is a mathematics issue. Is the model solved correctly?

Validation determines the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

This is a physics issue. Is the correct model solved?

Jeremic, B., Z. Cheng, M. Taiebat & Y. Dafalias. (2008) "Numerical Simulation of Fully Saturated Porous Materials," *Int. J. Num. Anal. Meth. Geomech.*, ***32***, 1635-1660.

Oreskes, N., K. Shrader-Frechette and K. Belitz. (1994) "Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences," *Science,* ***263***, 641–646.



Why Model?

Sanctioning gives us confidence in the results.
It is a tricky process.

19. Winsberg, E. (2010) ***Science in the Age of Computer Simulation***, Chicago: University of Chicago Press.

> The sanctioning of simulations does not cleanly divide into verification and validation. In fact, simulation results are sanctioned all at once: simulationists try to maximize fidelity to theory, to mathematical rigor, to physical intuition, and to known empirical results. But it is the *simultaneous confluence* of these efforts, rather than the establishment of each one separately, that ultimately gives us confidence in the results. [Winsberg (2010), p. 23]

Some thoughts on modeling. . .

In his analysis of a real system, a physicist constructs a well-defined model of the system and addresses the model. The system we address here is baseball. . . . We cannot calculate from first principles the character of the collision of an ash bat with a sphere made up of layers of different tightly wound yarns, nor do we have any precise understanding of the effect of the airstream on the flight of that sphere, with its curious yin-yang pattern of stitches. What we can do is construct plausible models of those interactions that play a part in baseball that do not violate basic principles of mechanics. Though these basic principles. . . severely constrain such models, they do not completely define them. It is necessary that the models touch the results of observations — or the results of the controlled observations called experiments — at some points so that the model can be more precisely defined and used to interpolate between known results, or to extrapolate from them . . . . If the model is well chosen, so as to represent the salient points of the real system adequately, conclusions derived from an analysis of the model can apply to the system to a useful degree. . . .

Adair, Robert K. (2002) ***The Physics of Baseball***, 3rd Ed., New York: HarperCollins.

The BPM provides a well-defined model of rock consisting of three microstructures:

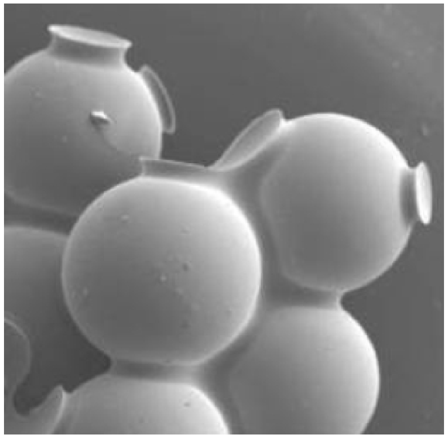
contact-bonded, parallel-bonded and flat-jointed.

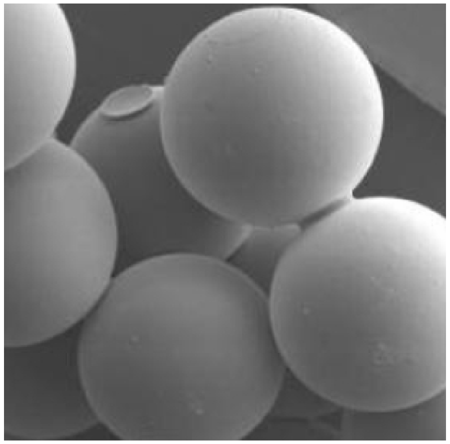
show the baseball

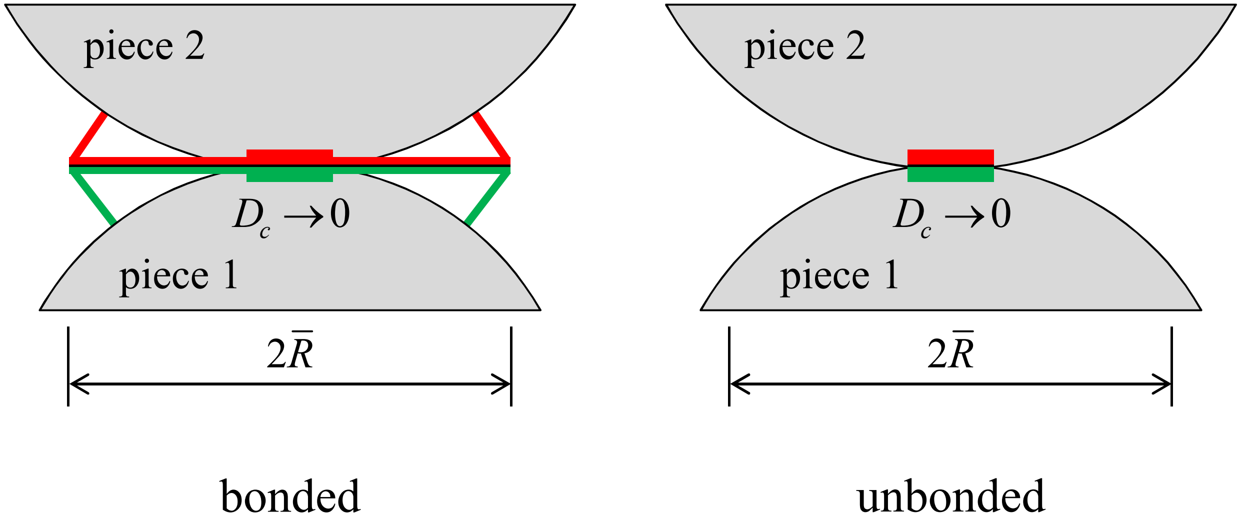
The contact and parallel-bonded microstructures approximate:

$$\text{contact bond} = \lim_{\bar{R} \to 0} \left(\text{parallel bond} \right)$$

Glass beads cemented with epoxy





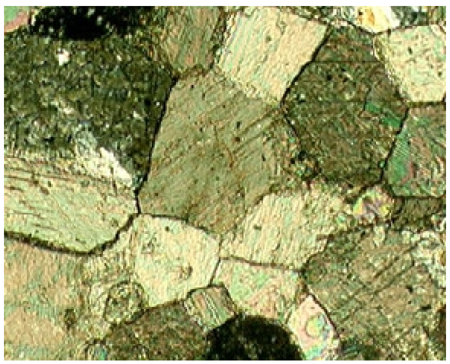


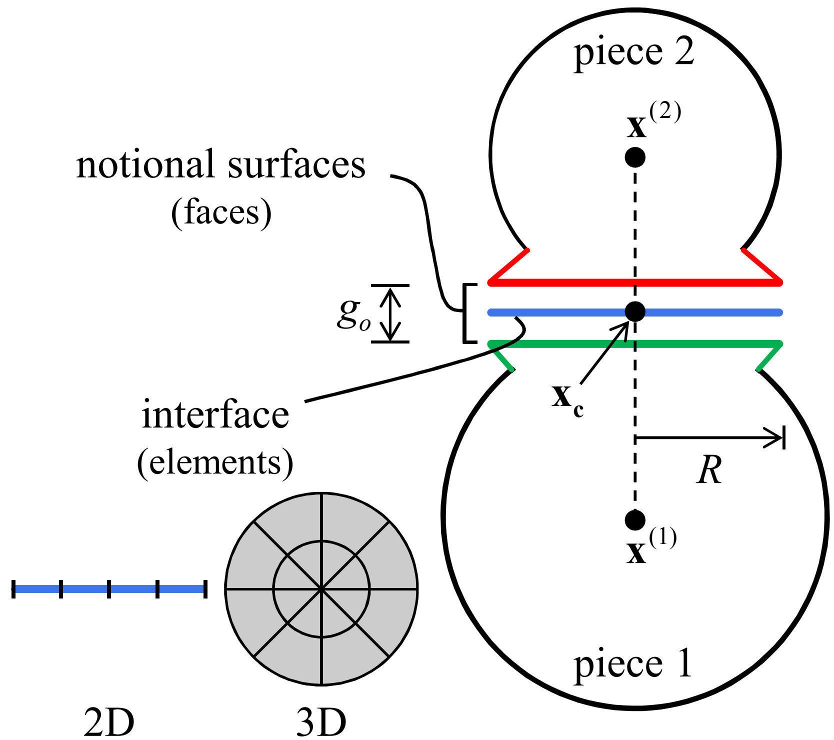
Bond breaks ➔ it is removed, no longer resists relative rotation.

Holt et al. (2005) “Comparison Between Controlled Laboratory Experiments and Discrete Particle Simulations of the Mechanical Behaviour of Rock,” *Int. J. Rock Mech. & Min. Sci.*, ***42***, 985-995.

The flat-jointed microstructure approximates:

Marble with angular, interlocked grains





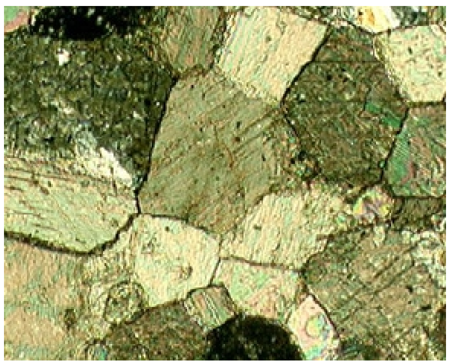
flat-joint contact

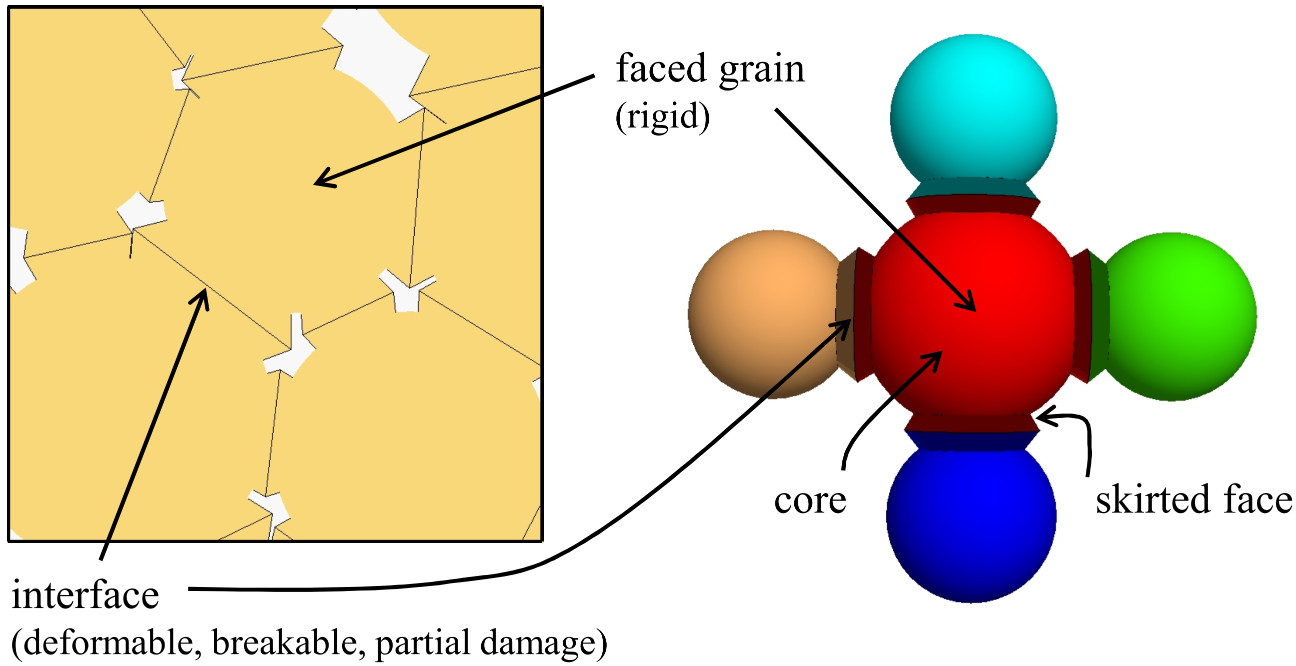
Each interface is discretized into elements that may be initially bonded, after breakage they are frictional.

Bandini et al. (2012) "Effects of Intra-Crystalline Microcracks on the Mechanical Behavior of a Marble Under Indentation," *Int. J. Rock Mech. & Min. Sci.*, ***54***, 47-55.

The flat-jointed microstructure approximates:

Marble with angular, interlocked grains

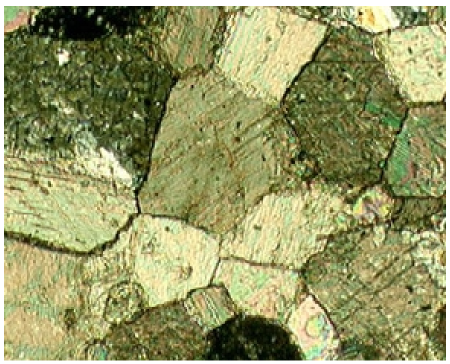




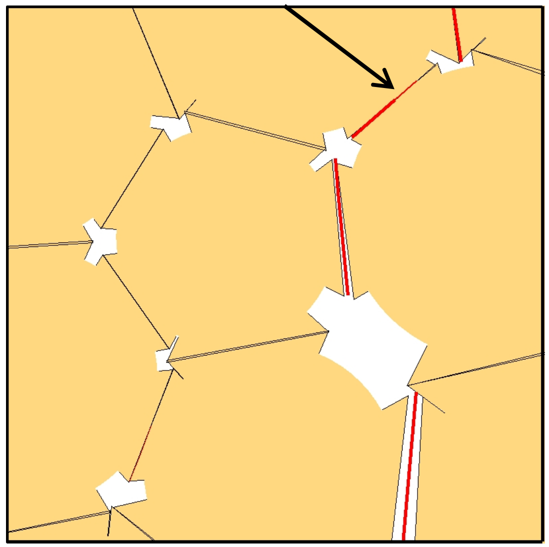
flat-jointed material consists of faced grains

The flat-jointed microstructure approximates:

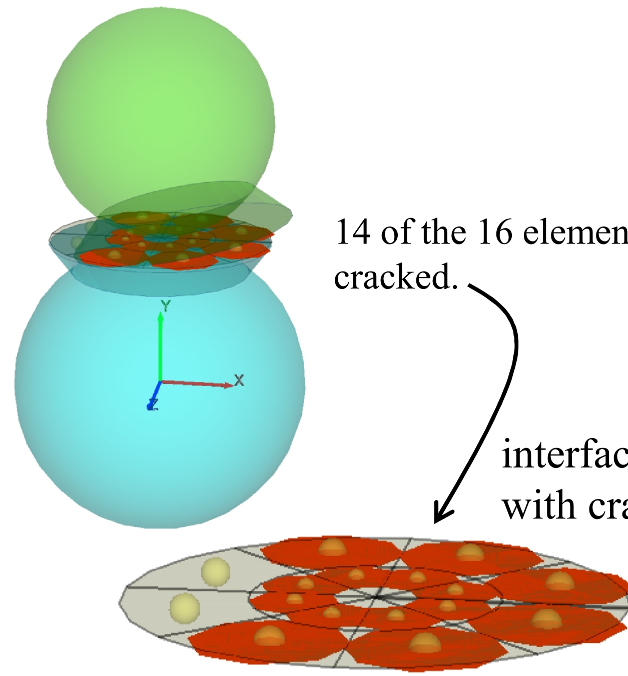
Marble with angular,
interlocked grains



Bending failure with 3 of the 4 elements cracked.



Crack thickness is proportional to gap.



14 of the 16 elements cracked.

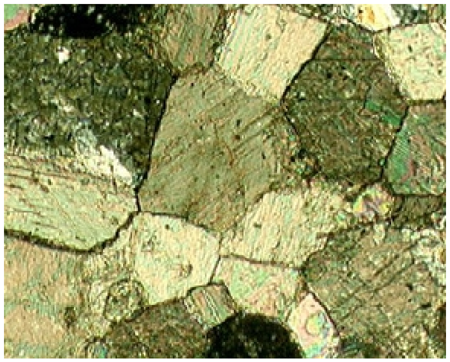
interface with cracks

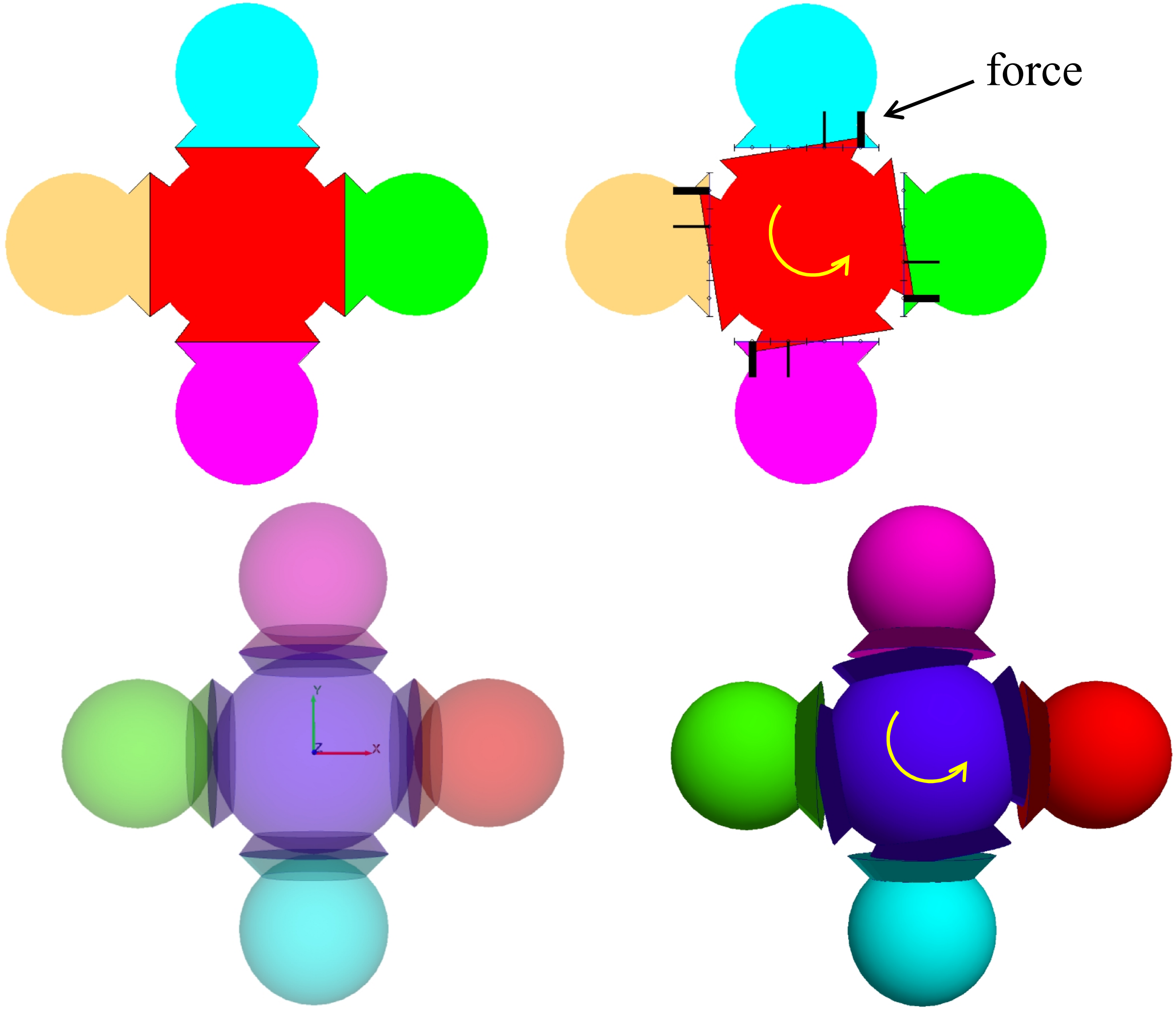
flat-jointed material
is partially damaged

The interface can sustain partial damage.

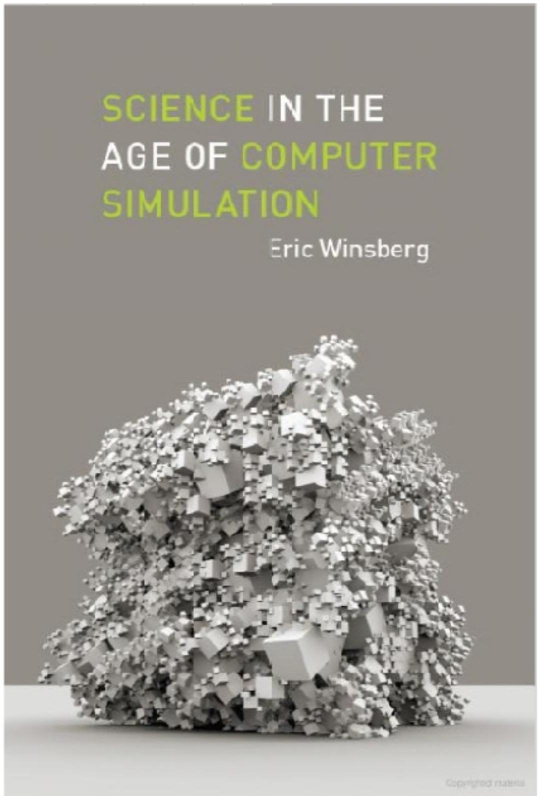
The flat-jointed microstructure approximates:

Marble with angular, interlocked grains





Even a fully broken interface continues to resist relative rotation.



Why Model?

Sanctioning gives us confidence in the results.
It is a tricky process.

The BPM provides a well-defined model of rock consisting of three microstructures:

contact-bonded, parallel-bonded and flat-jointed.

PFC models for intact rock have been sanctioned by demonstrating that they match the response obtained during tension and compression tests of typical compact rocks.

The complexity of early programming . . .

ENIAC (Electronic Numeric Integrator
And Calculator), ~1945

As one example of the complexity of early programming, a wiring diagram served as the program for the ENIAC, requiring two to three days to set up. A programmer in those days had to know the interior of the machine in order to function.

Slater, R. (1987) *Portraits in Silicon*, Cambridge, Mass.: MIT Press.

And you think that it is hard to program with FISH.

Well-designed objects are good things. . .

"You would need an engineering degree from MIT to work this," someone once told me, shaking his head in puzzlement over his brand new digital watch. Well, I have an engineering degree from MIT. Give me a few hours and I can figure out the watch. But why should it take hours?

Norman, D.A. (1988) *The Design of Everyday Things*, New York: Doubleday (from Chapter 1: The Psychopathology of Everyday Things).

Poorly designed objects can be difficult and frustrating to use. They provide no clues --- or sometimes false clues.

Norman, D. A. (2002) *Emotion and design: Attractive things work better,* Interactions Magazine, ix (4), 36-42.

Well-designed objects are easy to interpret and understand. They contain visible clues to their operation.

Well-designed objects are easy to interpret and understand. They contain visible clues to their operation.

The fistPkg is a well-designed object. Let’s run it together. . .

Aggregate Base (triaxial test to obtain properties)

ChalkTalk

Use fistPkg20.

Begin with the User-Defined Material Example.

Before we run it, let's talk about what we want. . .

> Grain size ranges from 4.75-25 mm, use all spheres. Make cylindrical specimen large enough to get representative response. . .
>
> How will we measure stress and strain?
>
> What are relevant response plots?

Aggregate Base (triaxial test to obtain properties)

ChalkTalk

Play with the model. . .

Increase material friction coefficient from 0.4 to 1.0.

Increase triaxial-test confinement from 150 to 750 kPa.

. . .

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, servomechanism
  - 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).

What is effective modulus?
(see the TwoBaseballs lecture)

Material Vessels

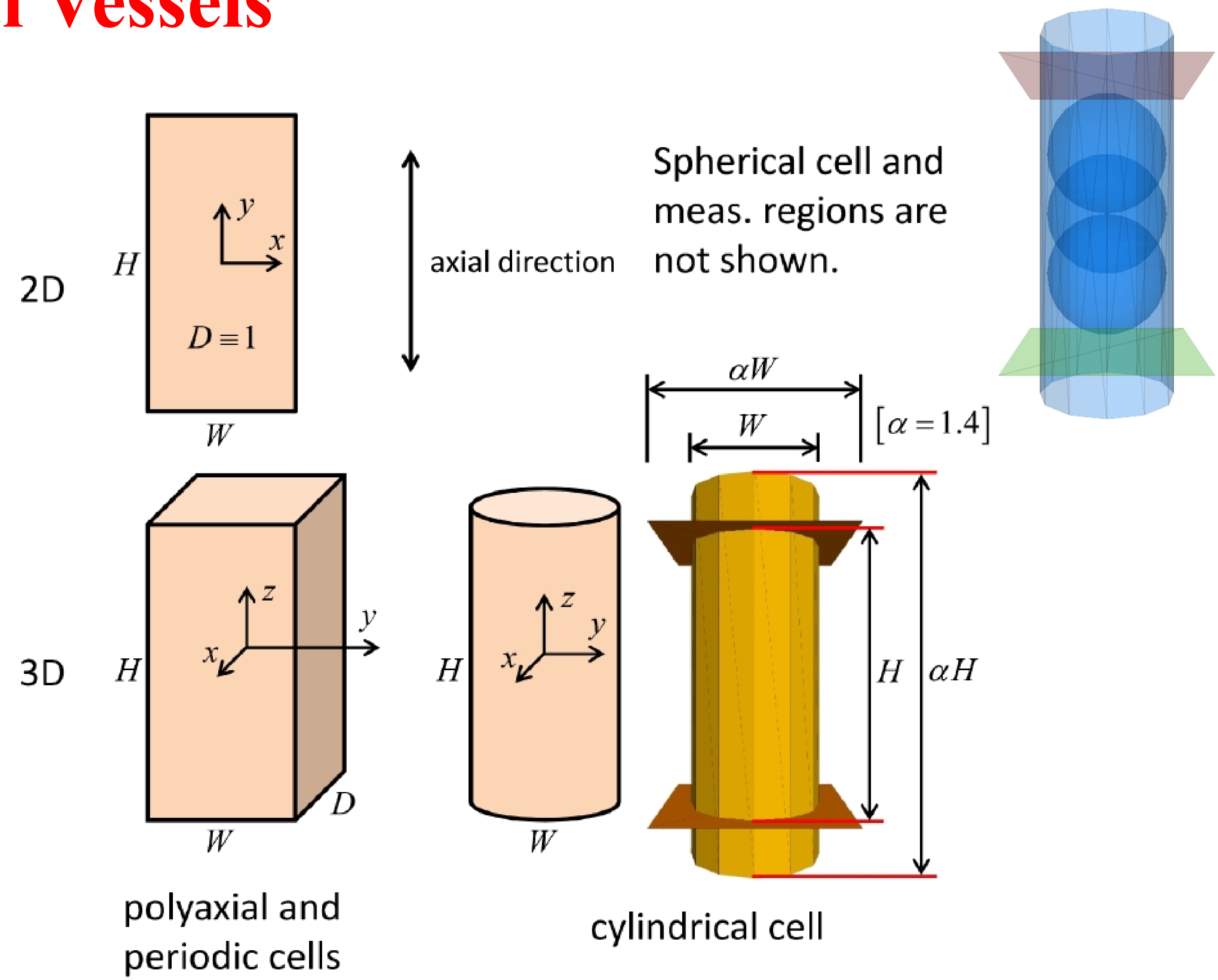
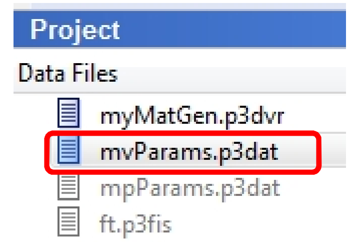


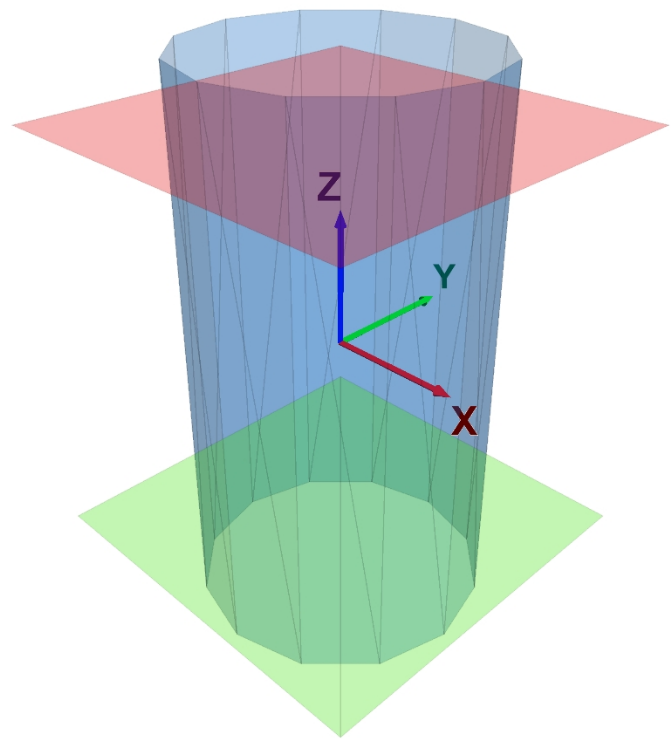
Figure 17 Material vessels with global coordinate system centered in each cell and associated axial direction.

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

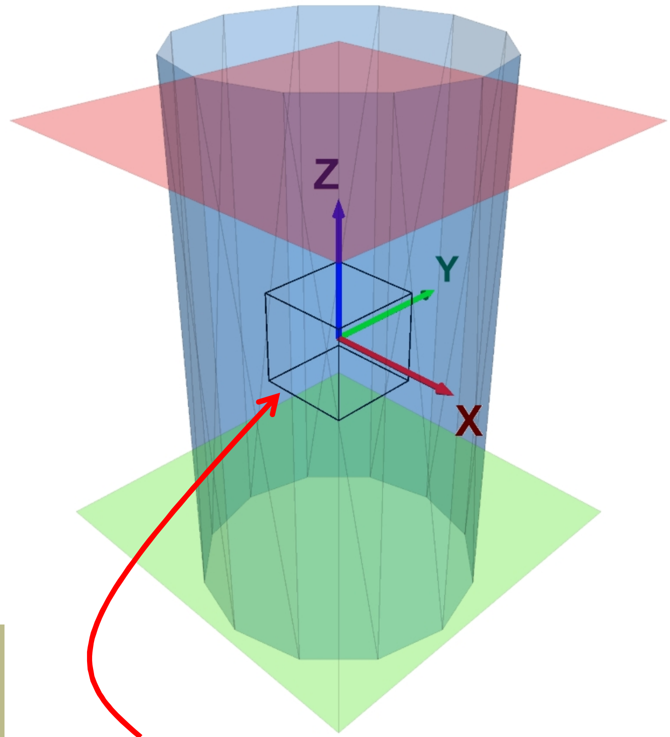
```
Edit mvParams.p3dat*
;fname: mvParams.p3dat

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
```



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]

Material-Genesis Procedure (packing phase)

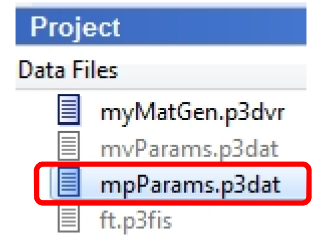


Table 7 Packing Parameters

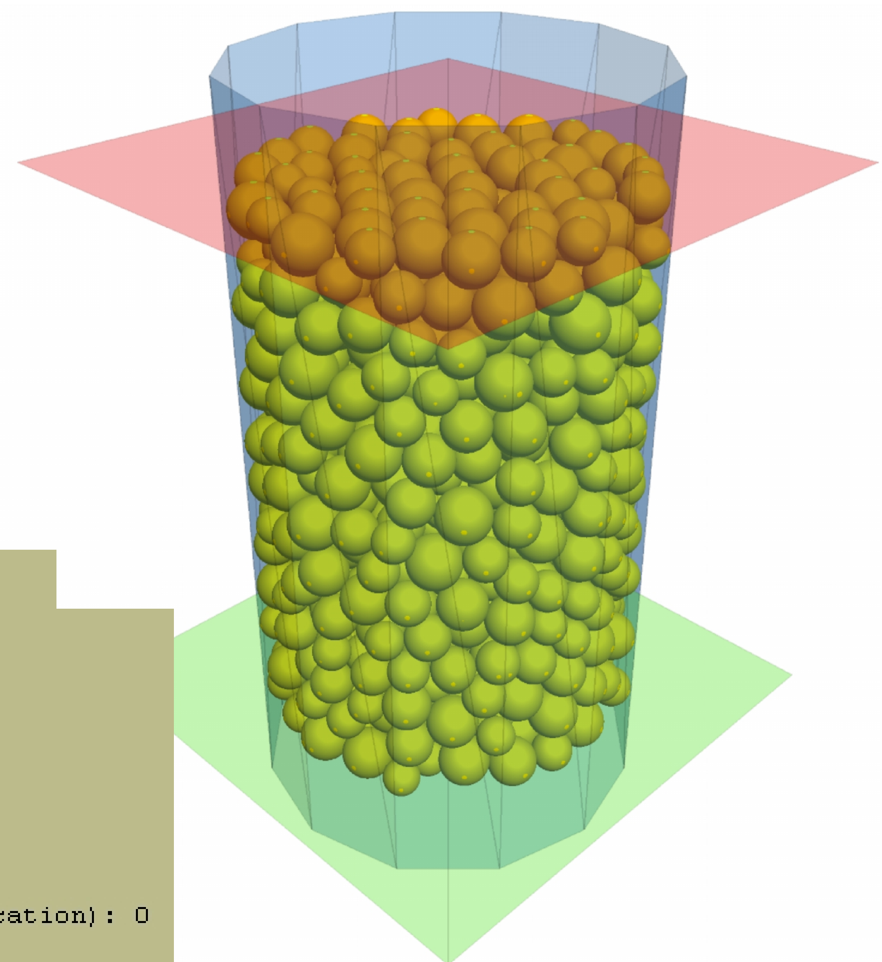
Parameter	Type	Range	Default	Description
S_{RN}, **pk_seed**	INT	$S_{RN} \ge 10{,}000$	$10{,}000$	seed of random-number generator (affects packing)
P_m, **pk_Pm**	FLT	$(0.0, \infty)$	NA	material pressure
ε_P, **pk_PTol**	FLT	$(0.0, \infty)$	1×10^{-2}	pressure tolerance $\left(\frac{\lvert P - P_m \rvert}{P_m} \le \varepsilon_P \right)$ 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)

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
```



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.				
A	**Parallel-bonded material group:**				
A	**Linear group:**				
A	• • •				
A	**Parallel-bond group:**				
A	• • •				
B	**Linear material group** (for grain-grain contacts that may form subsequent to material finalization):				

Material-Genesis Procedure (finalization phase)

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

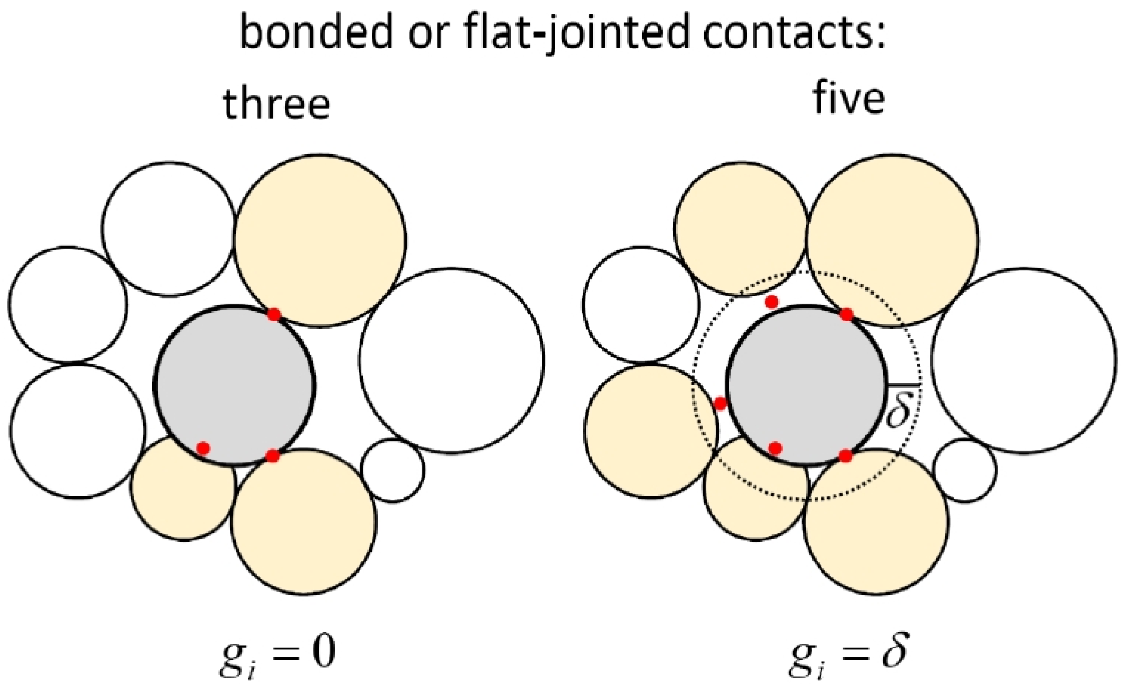


Figure 12 ***Grain assembly at end of packing phase with the bonded or flat-jointed contacts of a typical grain when the installation gap is zero (left) and greater than zero (right). Increasing the installation gap increases the grain connectivity.***

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.

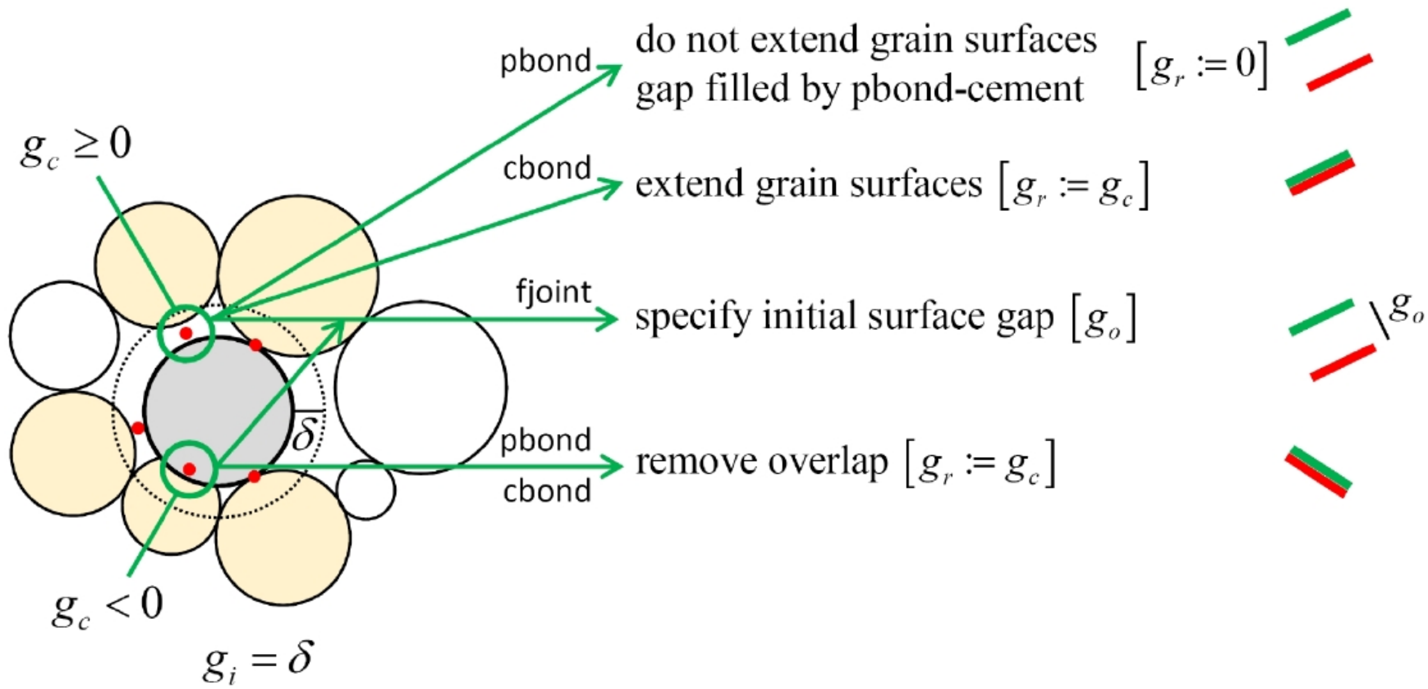


Figure 15 Setting final material properties of bonded materials to establish reference surfaces that do not overlap (contact-bonded, parallel-bonded and flat-jointed materials denoted by cbond, pbond and fjoint, respectively).

Material-Genesis Procedure (finalization phase)

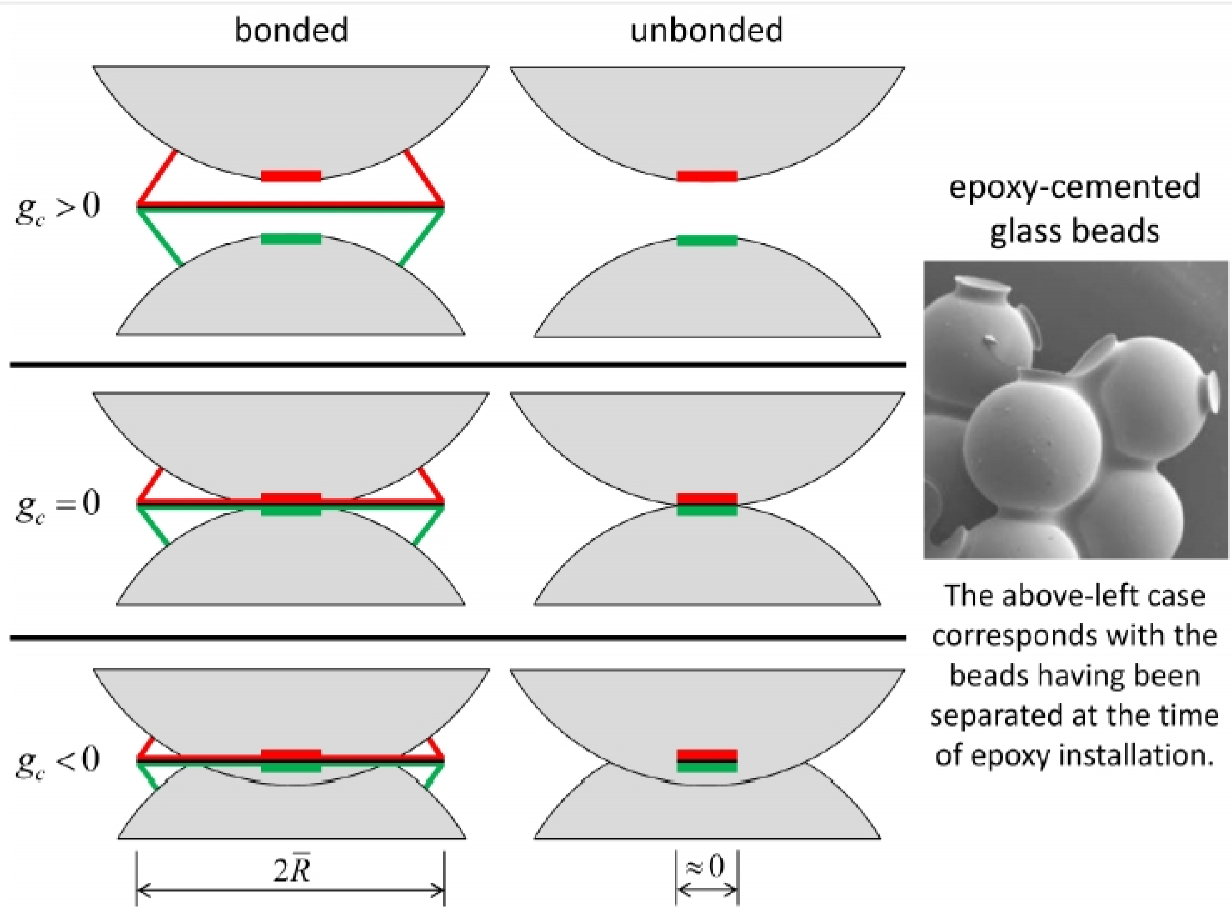


Figure 6 *Parallel-bonded contact before (left) and after (middle) bond breakage. After the bond breaks, it is removed and the contact no longer resists relative rotation. The image of epoxy-cemented glass beads is from Fig. 4 of Holt et al. (2005). The reference surfaces are depicted in red and green for the three cases of contact gap at the end of the material-finalization phase being positive, zero and negative.*

Material-Genesis Procedure (finalization phase)

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

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

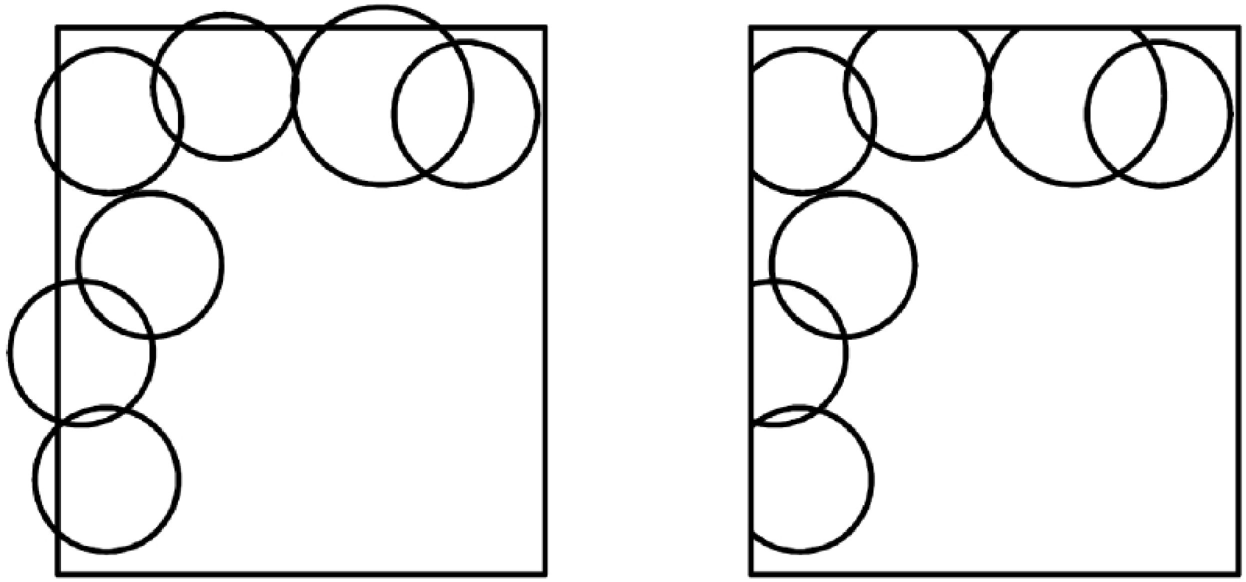
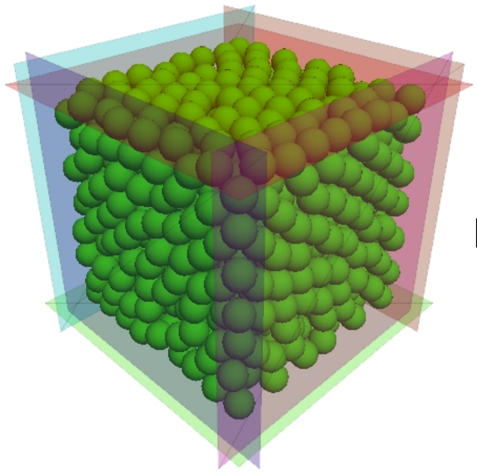


Figure 13 The effective grain-vessel interface before (left) and after (right) the smoothing operation, which effectively cuts off the part of each ball or pebble that protrudes from the material vessel.

Material-Genesis Procedure

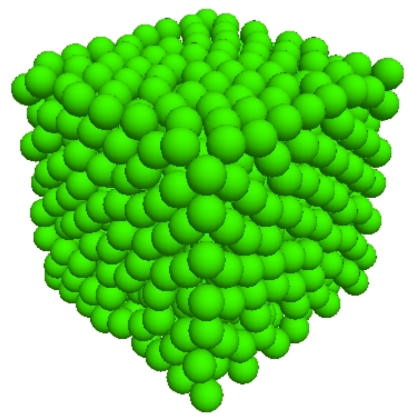
The specimen remains within the material vessel, and the model state is saved.



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,[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).
- **User-Defined Material Information.** A user-defined material may provide this information via **`udm_{compute,list}MicroStrucProps`**.

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
   User-Defined Material Information:
     mp_nHLc  (# active hill contacts, all are grain-grain): 2037
     The function hlm_makeWet has not been called.
     Moisture state of active hill contacts:
       mp_nHLms0 (# dry):             2037
       mp_nHLms1 (# dry & ruptured): 0
       mp_nHLms2 (# wet):             0
```

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
```

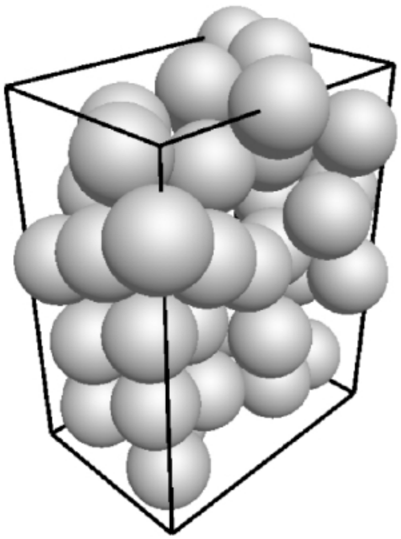
Material-Genesis (microstructural plot sets)

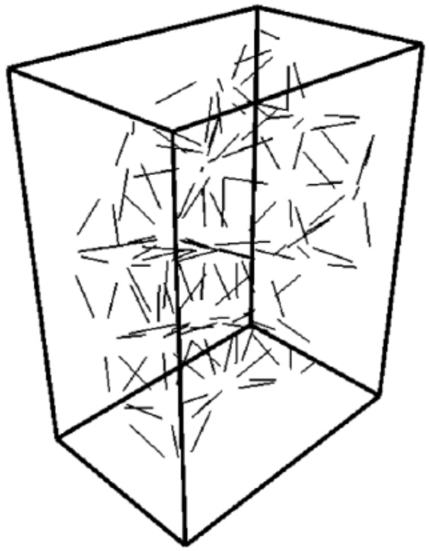
Microstructural plot sets are provided for the bonded materials to display the material microstructure and thereby reveal how the evolution of the microstructure influences the macroscopic behavior. The microstructural plot sets include depictions of the grains and the grain-grain interfaces, and when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

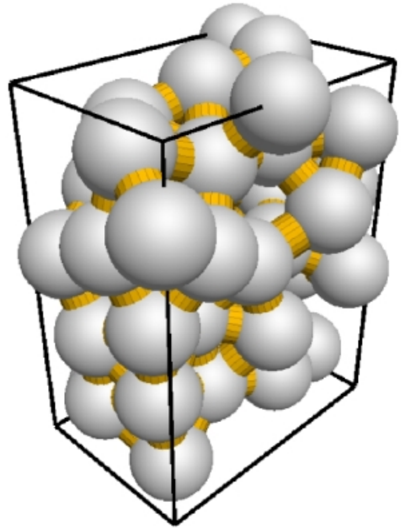
Figure image on next slide.

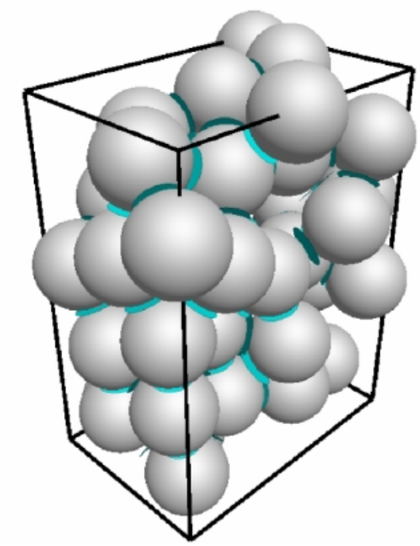
Figure 15 Microstructural plot sets for bonded materials with the same initial packing showing (clockwise from upper left): microstructural box and grains in the box (grey); contact-bonded material with contact bonds in the box; parallel-bonded material with parallel-bond cement (gold, 50% size) and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

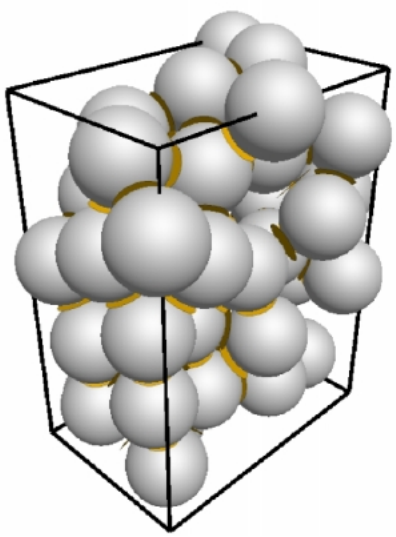
Material-Genesis (microstructural plot sets)



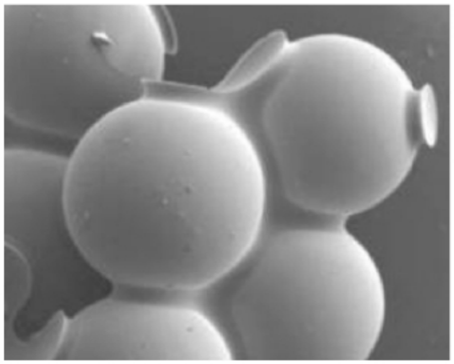




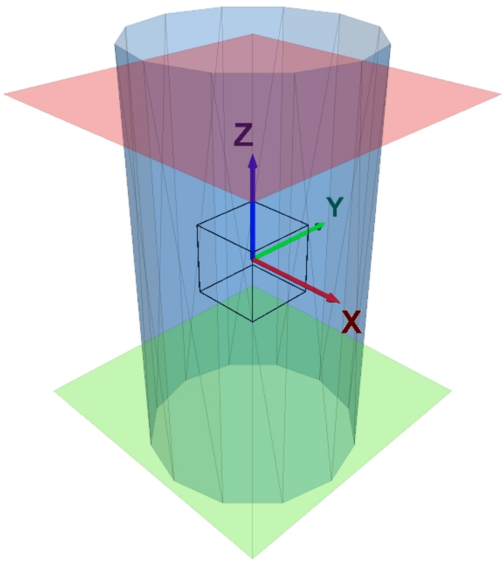




Glass beads cemented with epoxy



Holt et al. (2005)

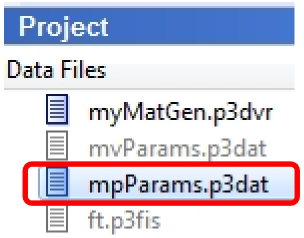


microstructural box

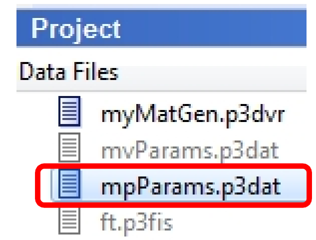
Materials (common material properties)

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_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)



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
```

Materials (common material properties)

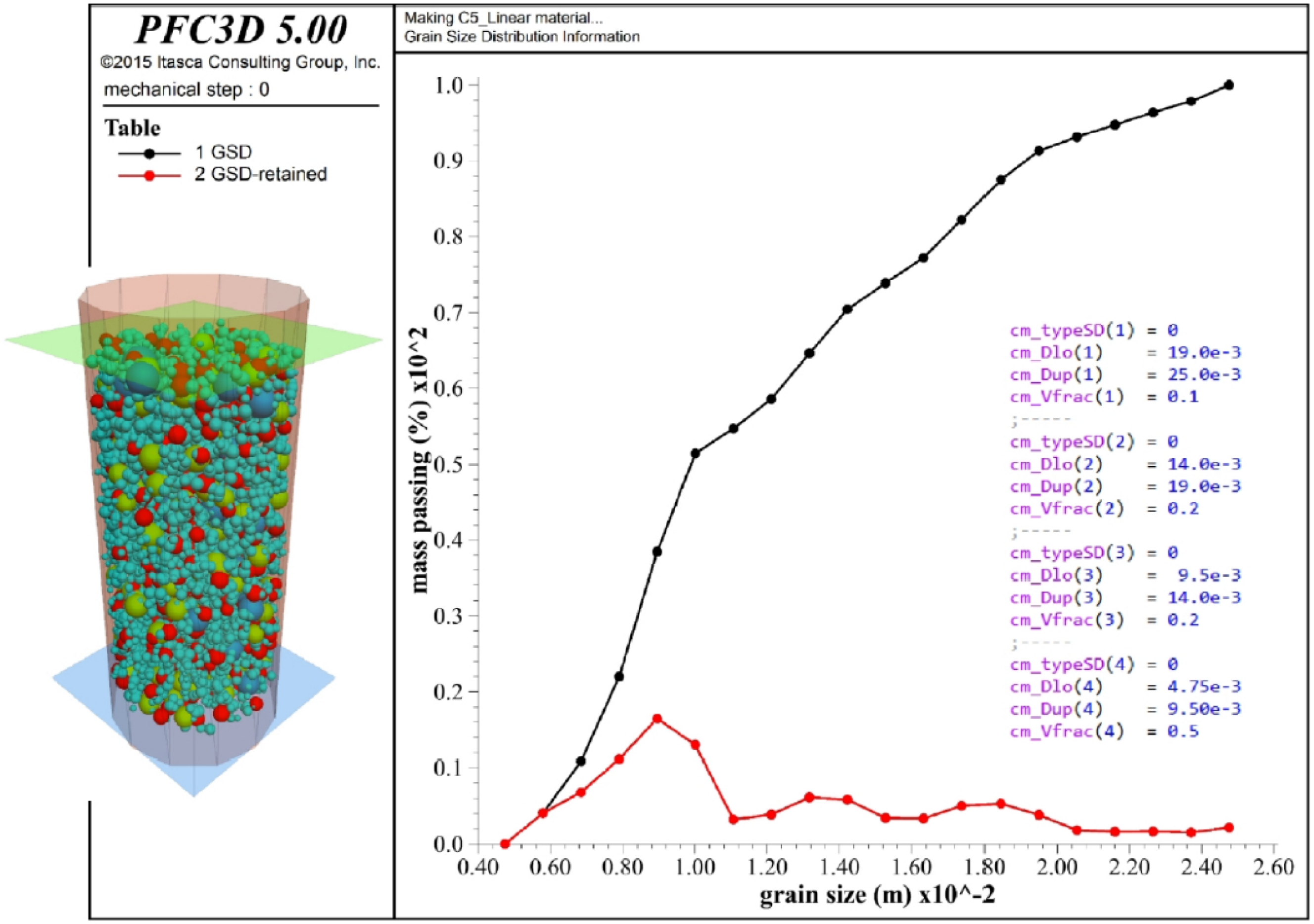


Figure 14 ***Grain size distribution information produced by the FISH function sdMeasure(19) showing cumulative mass percent passing (in black) and incremental mass percent retained (in red).***

[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).

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:
```

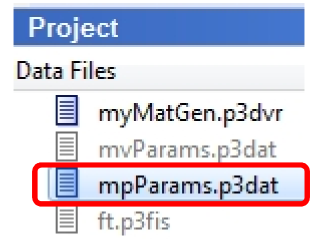
• • •

```
  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



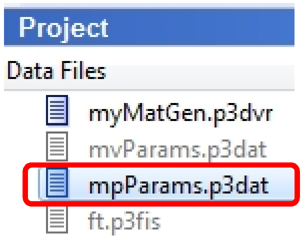
Materials (contact-bonded material)

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
$(\bar{\sigma}_c)_{\{m,sd\}}$ **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)
$\bar{\phi}$, **pbm_fa**	FLT	$[0.0, 90.0)$	0.0	friction angle [degrees]

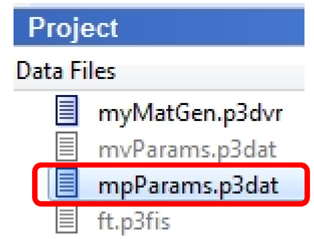
Linear material group (for grain-grain contacts that may form subsequent to material finalization):

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, `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
$(g_o)_{\{\text{msd}\}}$, `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 $\begin{cases} 0, & \text{fixed} \\ 1, & \text{varying} \end{cases}$



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: $\phi_S = 1 - \phi_B - \phi_G \quad (0 \le \phi_S \le 1)$.

Materials (flat-jointed material microstructure)

```
pfc3d>@mpListMicroStrucProps
## Material Microstructural Properties [# is "number of"]:
     mp_Dg (average grain diameter): 0.00433872
       [Get grain-size distribution via measurement logic.]
     mp_ng                 (# grains): 753
     mp_PhiV     (vessel resolution): 8.7814
     mv_mn (measure-based porosity): 0.37113
     mp_nLNc (# active linear-based contacts): 0
     mp_nFJc (#         flat-jointed contacts): 2867
     mp_nFJe (# flat-jointed elements): 8601
     mp_nFJb (# flat-jointed    bonds): 8601
     mp_nCBb (# contact-bonded  bonds): 0
     mp_nPBb (# parallel-bonded bonds): 0
   Initial microstructural types of flat-jointed material:
     mp_nFJiB (# FJs initially bonded): 2867
     mp_nFJiG (# FJs initially gapped): 0
     mp_nFJiS (# FJs initially   slit): 0
     mp_nFJiU (# FJs initially undef.): 0
```

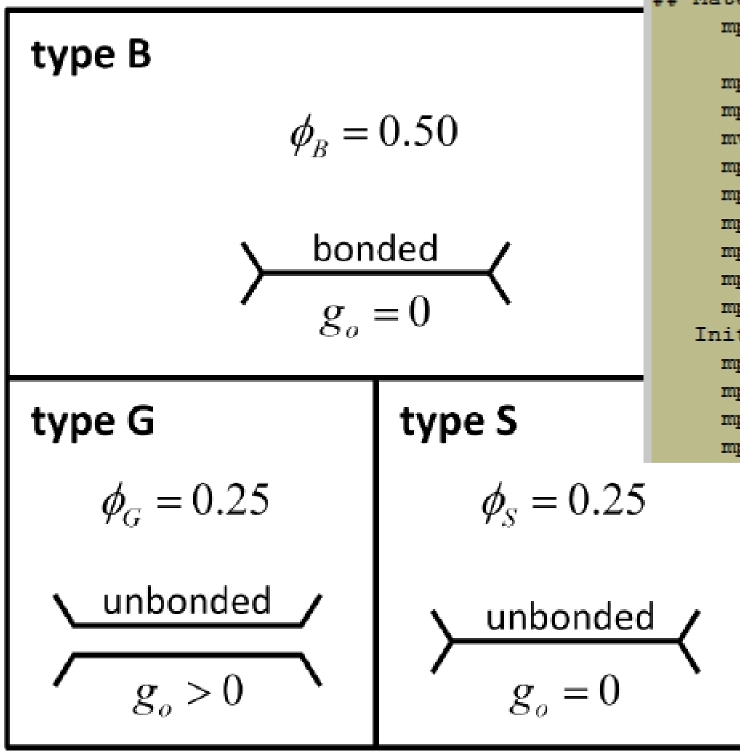


Figure 9 Initial microstructure of flat-jointed material: each flat-joint contact is bonded (type B), gapped (type G) or slit (type S).

$$\phi_B = \frac{n_B}{n_{\mathrm{FJ}}}, \quad \phi_G = \frac{n_G}{n_{\mathrm{FJ}}}, \quad \phi_S = \frac{n_S}{n_{\mathrm{FJ}}}$$

$$\phi_B + \phi_G + \phi_S = 1 \quad \text{and} \quad n_{\mathrm{FJ}} = n_B + n_G + n_S .$$

Materials (flat-jointed material microstructure)

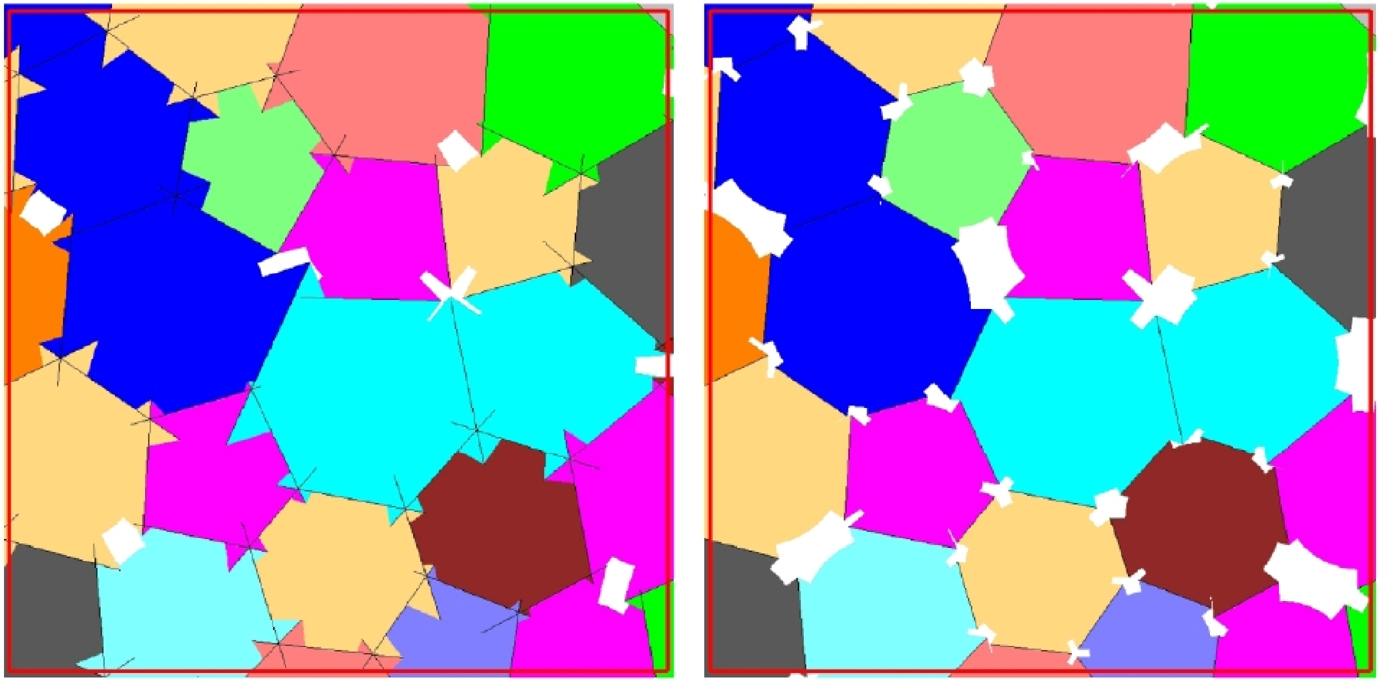
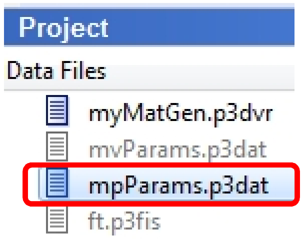


Figure 12 Initial radius multipliers of flat-jointed material: each flat-joint radius multiplier is fixed, which may produce an invalid microstructure (left) or each flat-joint radius may be reduced from an initial maximum value to obtain a valid microstructure (right). {DP: This image was produced by PFC2D 4.0; it will be reproduced using the faced-grain plotting capability in PFC2D 5.0.}

Materials (user-defined material, 3D hill material)

Table 2 Hill Material Parameters

Parameter	Type	Range	Default	Description
Material microproperties are listed via **@mpListMicroProps**.				
Common material parameters are listed in Table 1 of Potyondy (2016).				
Packing parameters are listed in Table 7 of Potyondy (2016).				
Add moisture via **@hlm_makeWet(**ψ**,** g_m**)**, where ψ is suction and g_m is moisture gap. Remove moisture via **@hlm_makeDry**.				
Set and modify the following properties via **@hlm_setMatBehavior**.				
Hill material group:				
E_g, **hlm_youngMod**	FLT	$[0.0, \infty)$	0.0	Young's modulus of grains
ν_g, **hlm_poisRatio**	FLT	$(-1.0, 0.5]$	0.0	Poisson's ratio of grains
μ, **hlm_fricCoef**	FLT	$[0.0, \infty)$	0.0	friction coefficient
α_h, **hlm_dampCon**	FLT	$[0.0, 1.0]$	0.0	damping constant
ψ, **hlm_suction**	FLT	$[0.0, \infty)$	0.0	suction



* Potyondy, D. (2016) "Hill Contact Model [version 4]," Itasca Consulting Group, Inc., Minneapolis, MN, Technical Memorandum ICG7795-L (October 12, 2016).

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.

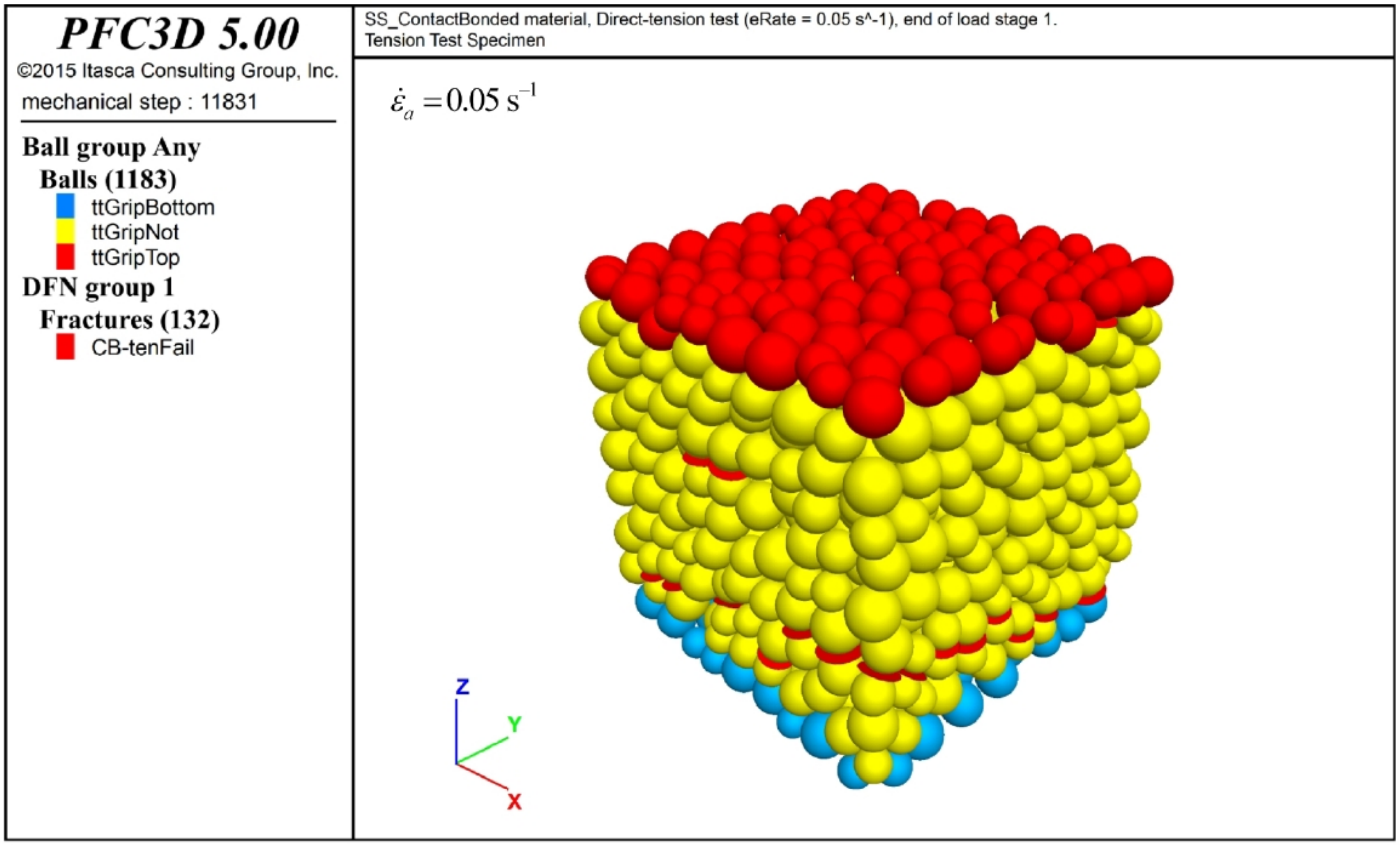
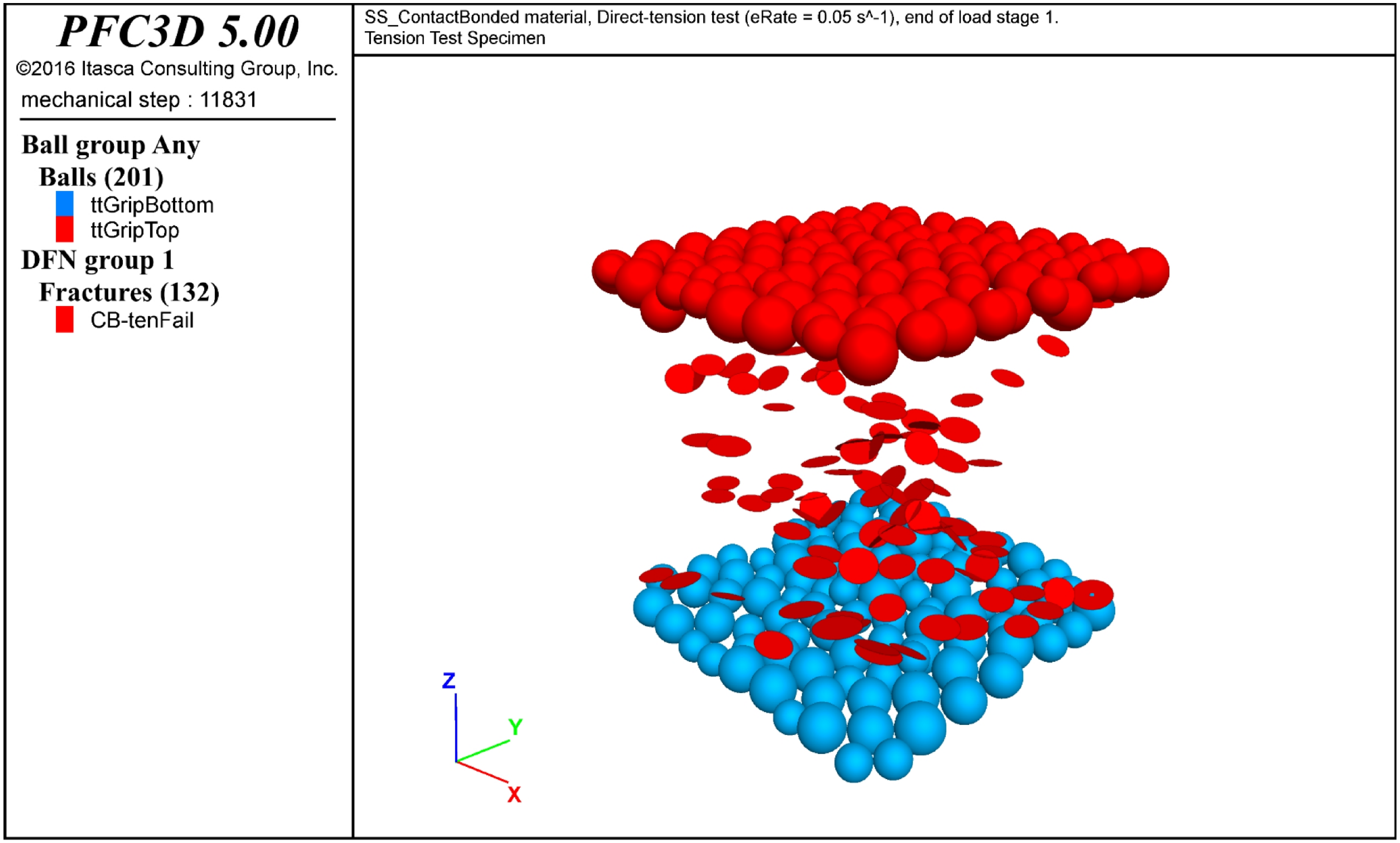


Figure 12 SS_ContactBonded material at the end of the direct-tension test with grains and cracks.

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.

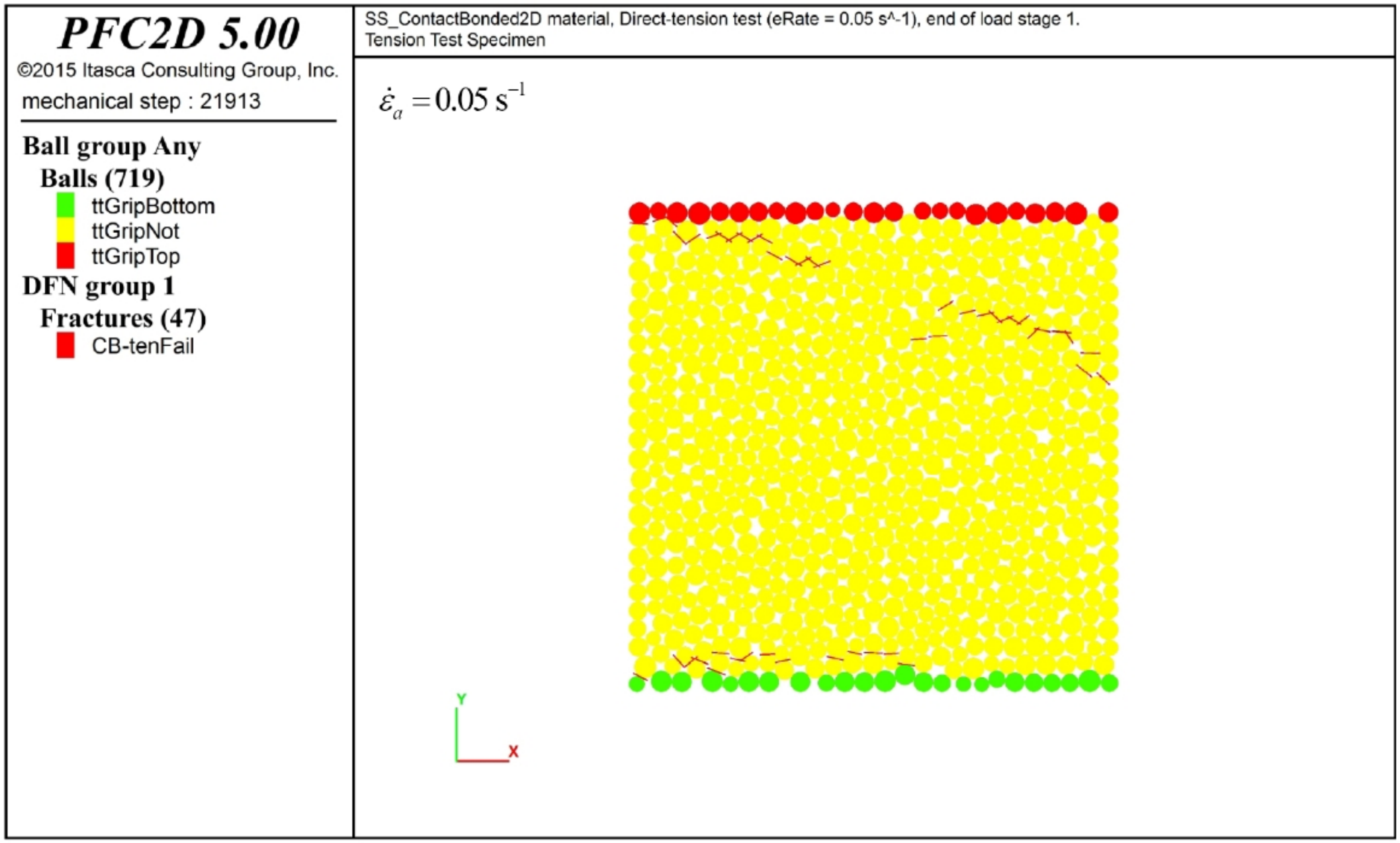
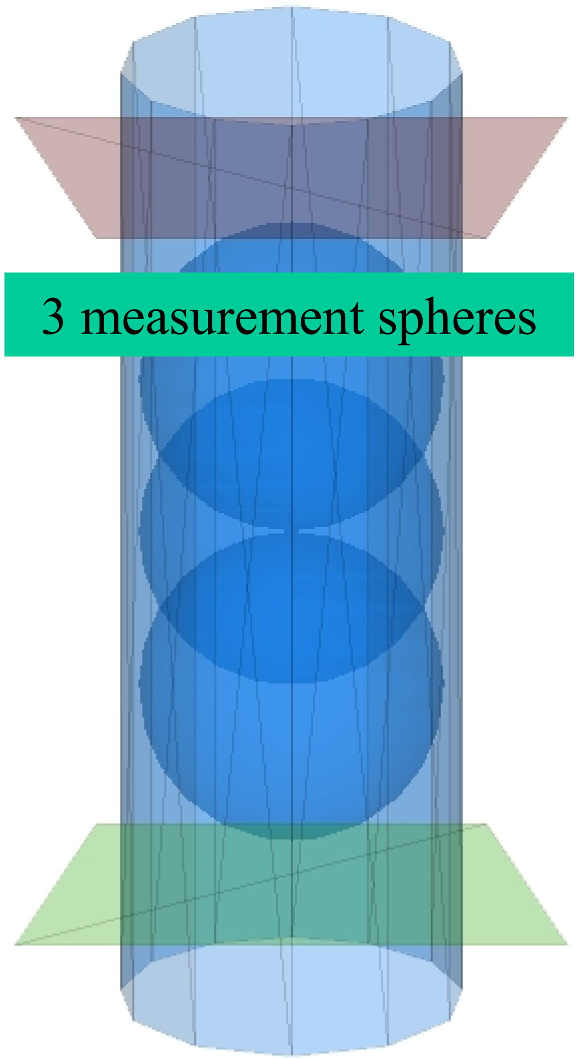


Figure 20 SS_ContactBonded2D material at the end of the direct-tension test with grains and cracks.

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

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

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

The three measurement techniques measure the following quantities:

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

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

ε_{k}^{g} guage-based (3 terms)

$i, j = \{x, y, z\}$, $k = \{x, y, z, r\}$

Lab-Testing Procedures (servomechanism)

The velocities of the walls of the polyaxial and cylindrical cells are controlled by a servomechanism. The boundary condition for each pair of walls and the cylindrical wall can be either velocity or pressure. The servomechanism controls the velocities to maintain the specified pressure.

Table 9 Servomechanism Parameters

Parameter	Type	Range	Def.	Description
$(B_c)_k$, `mvs_BC{x,y,z,r}`	INT	$\{0,1\}$	NA	boundary-condition code $\begin{cases} 0, & \text{velocity} \\ 1, & \text{pressure} \end{cases}$, $k = \{x,y,z\}$ or $\{z,r\}$
$(B_v)_k$, `mvs_BC{x,y,z,r}Val`	FLT	$\{0,1\}$	NA	boundary-condition value $\begin{cases} v_k, & \text{velocity } ((B_c)_k = 0) \\ P_k^t, & \text{pressure } ((B_c)_k = 1) \end{cases}$, $k = \{x,y,z\}$ or $\{z,r\}$
n_{gain}, `mvs_gainUpdateRate`	FLT	$[1,\infty)$	25	servo gain update rate
$v_{\lim}$, `mvs_vLimit`	FLT	$\mathbb{R}$	NA	velocity limit $(\lvert v_k \rvert \le v_{\lim},\ v_{\lim} > 0)$

Lab-Testing Procedures (summary)

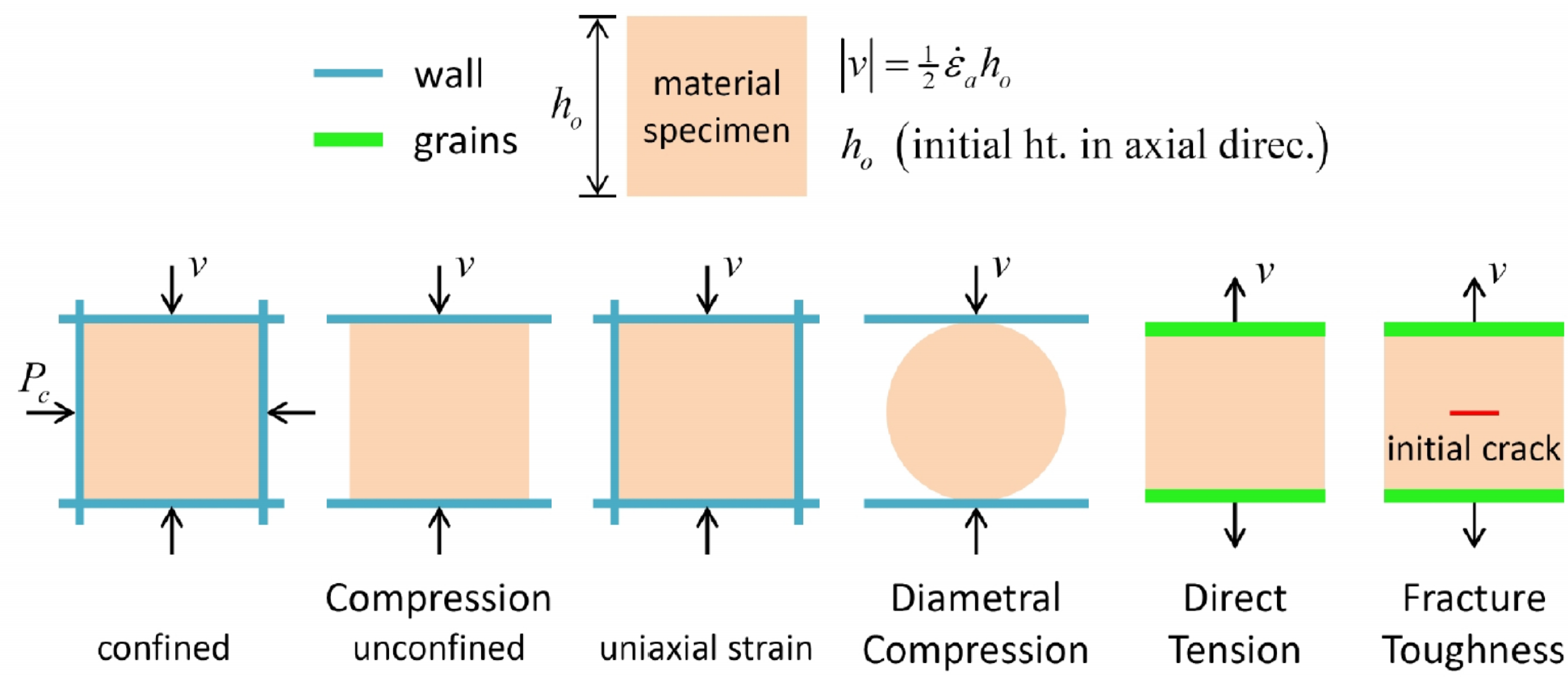
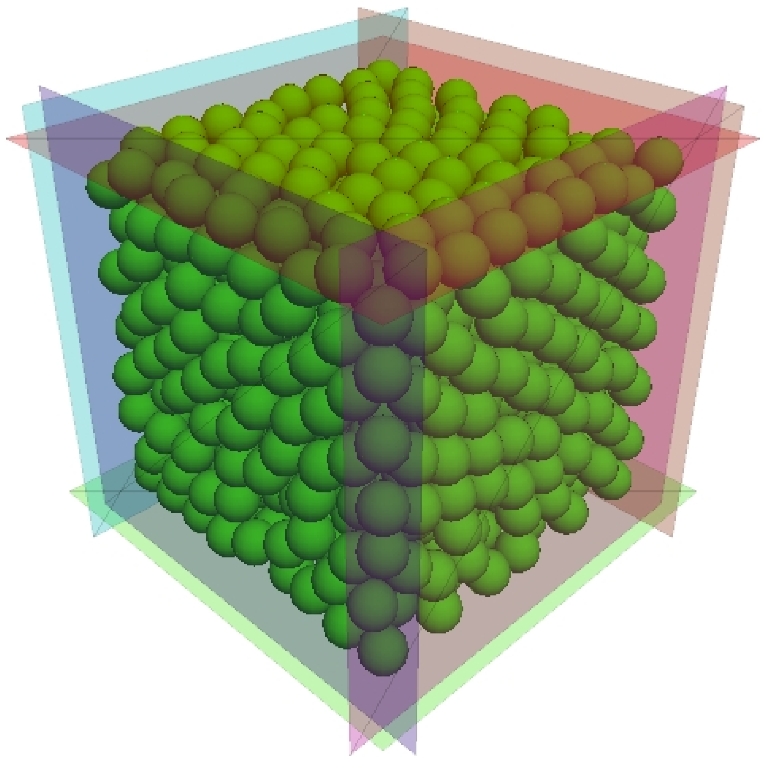


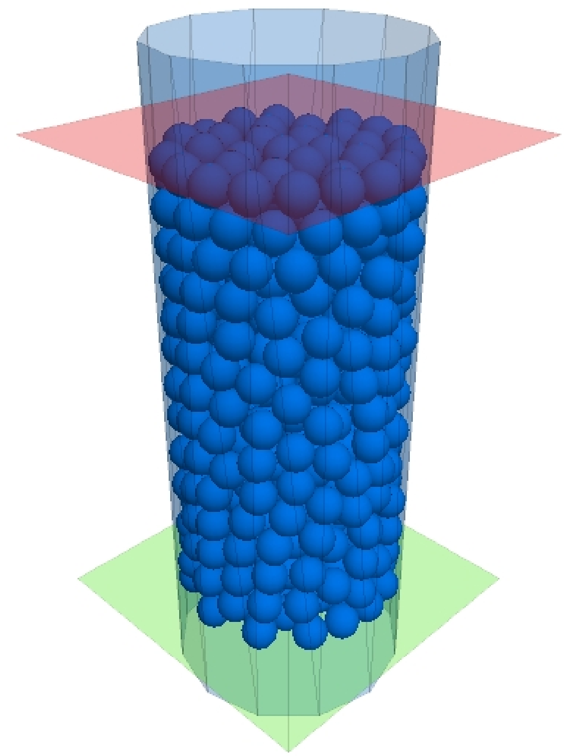
Figure 23 Loading conditions of laboratory-testing procedures.

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

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.

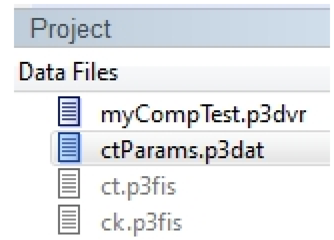
The loading phase may consist either of a single stage that ends when the applied deviatoric stress falls below a specified fraction of its peak value or multiple stages during which the axial-strain increments are specified.

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 ($\lvert v \rvert = \frac{1}{2}\dot{\varepsilon}_a h_o$, $\dot{\varepsilon}_a > 0$, see Figure 23 and Section 5.4)
C_l, **ct_loadCode**	INT	$\{0,1\}$	0	loading-phase code $\begin{cases} 0, \text{ single stage} \\ 1, \text{ multiple stages} \end{cases}$
α , **ct_loadFac**	FLT	$(0.0,1.0)$	0.9	load-termination factor ($C_l = 0$) for termination criterion: $\lvert\sigma_d^w\rvert \le \alpha \lvert\sigma_d^w\rvert_{max}$
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)

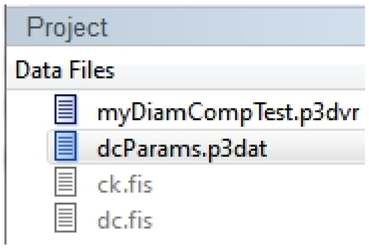


Lab-Testing Procs. (diametral-compression test)

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`)



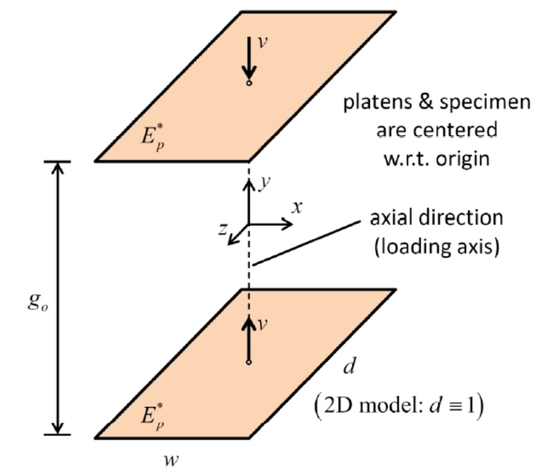


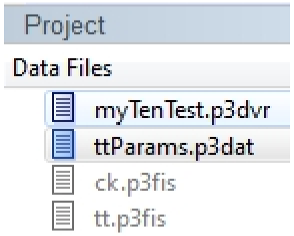
Figure 18 Loading configuration of diametral-compression test.

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: $\lvert\sigma_a^m\rvert \le \alpha \lvert\sigma_a^m\rvert_{max}$



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)

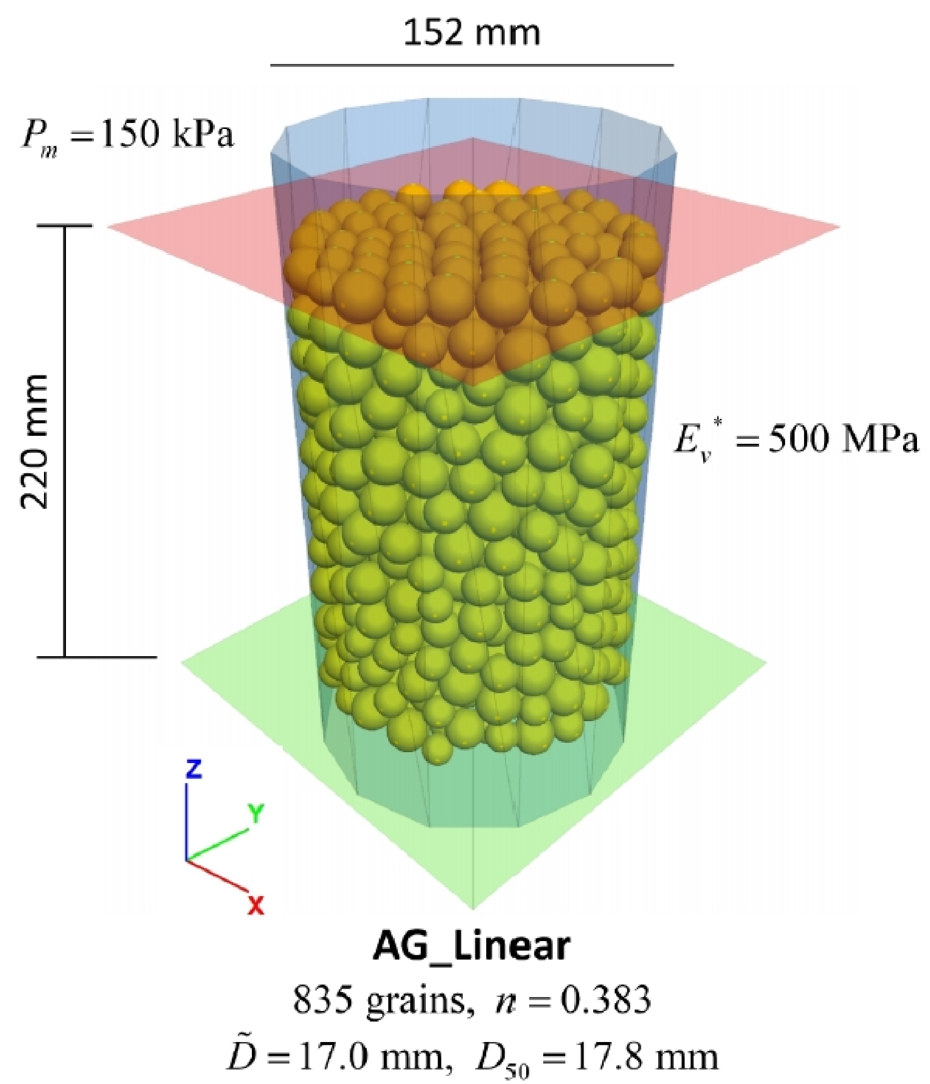


Figure 1 AG_Linear material packed at 150 kPa material pressure at the end of material genesis.

Example Materials (linear material)

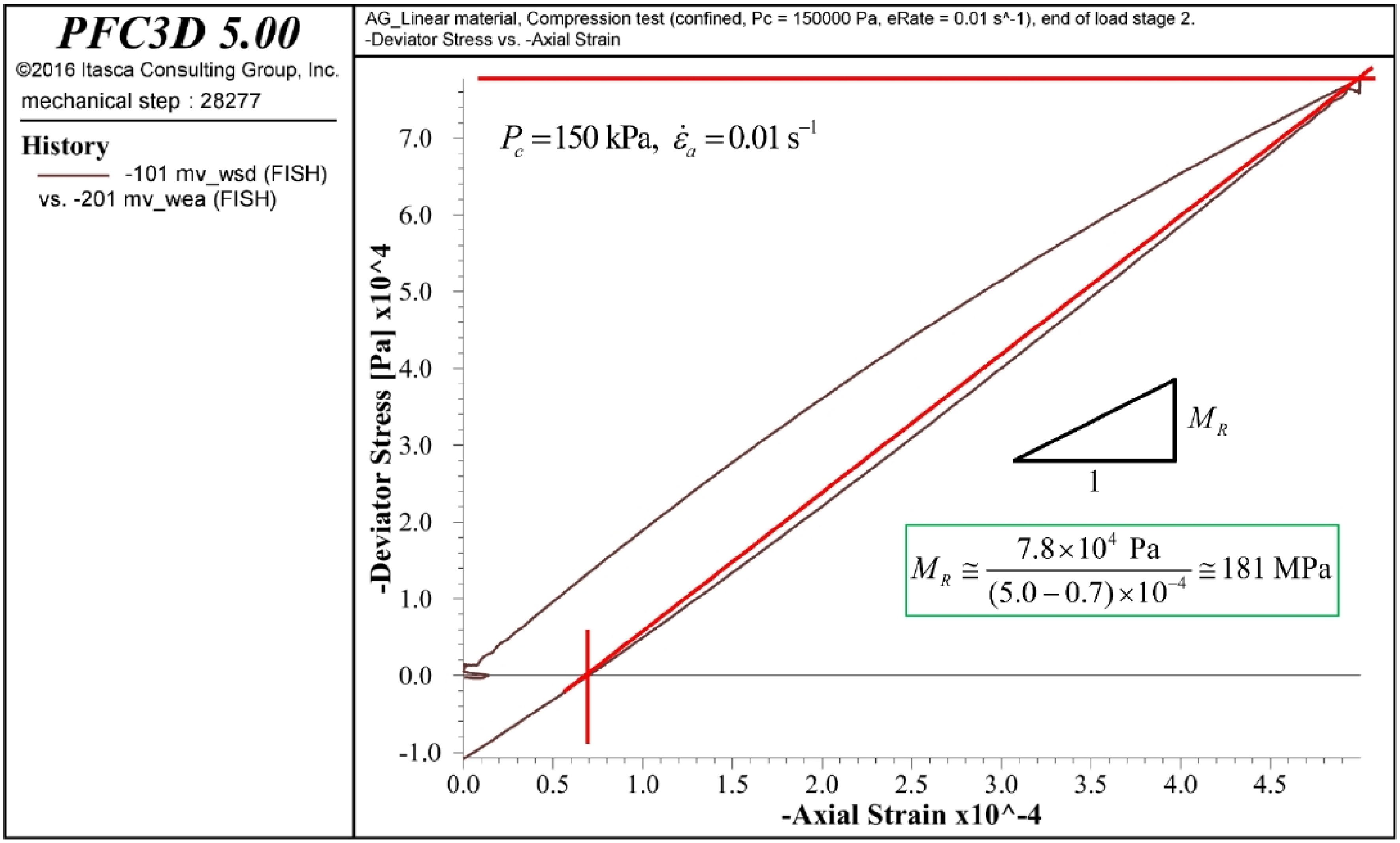


Figure 2 ***Deviator stress versus axial strain for AG_Linear material tested at 150 kPa confinement, and measurement of resilient modulus.***

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
$T_m,\ \alpha,\ C_\rho,\ \rho_v\ [\mathrm{kg/m^3}]$	1, 0.7, 1, 1960
$S_g,\ T_{SD},\ \{D_{\{l,u\}}\ [\mathrm{mm}],\ \phi\},\ D_{mult}$	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
$(T_\sigma)_{\{m,sd\}}\ [\mathrm{MPa}],\ (S_\sigma)_{\{m,sd\}}\ [\mathrm{MPa}]$	$\{1.0, 0\}$, $\{20.0, 0\}$
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)

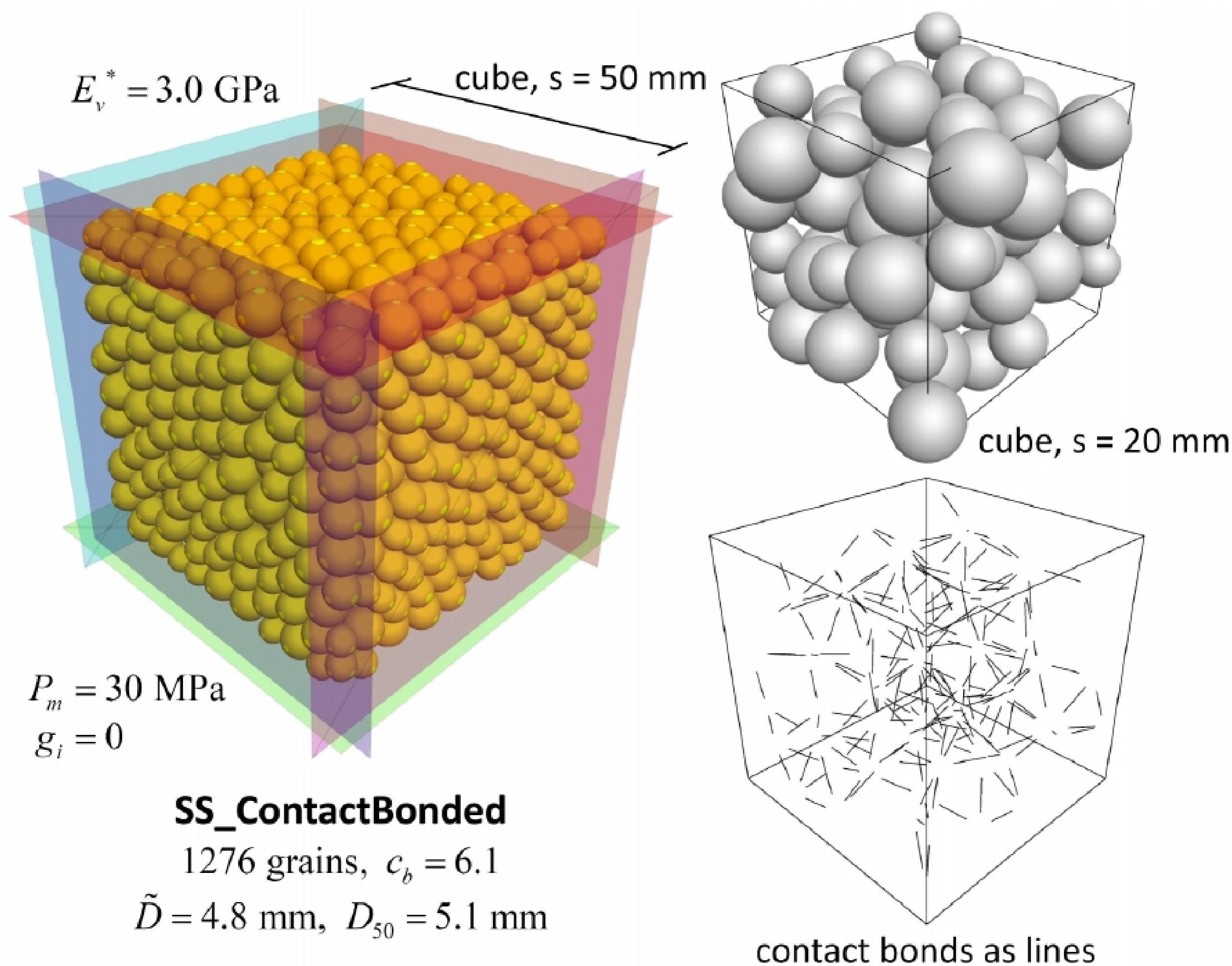


Figure 11 SS_ContactBonded material at the end of material genesis with grains and contact bonds in the microstructural box.

Example Materials (contact-bonded material)

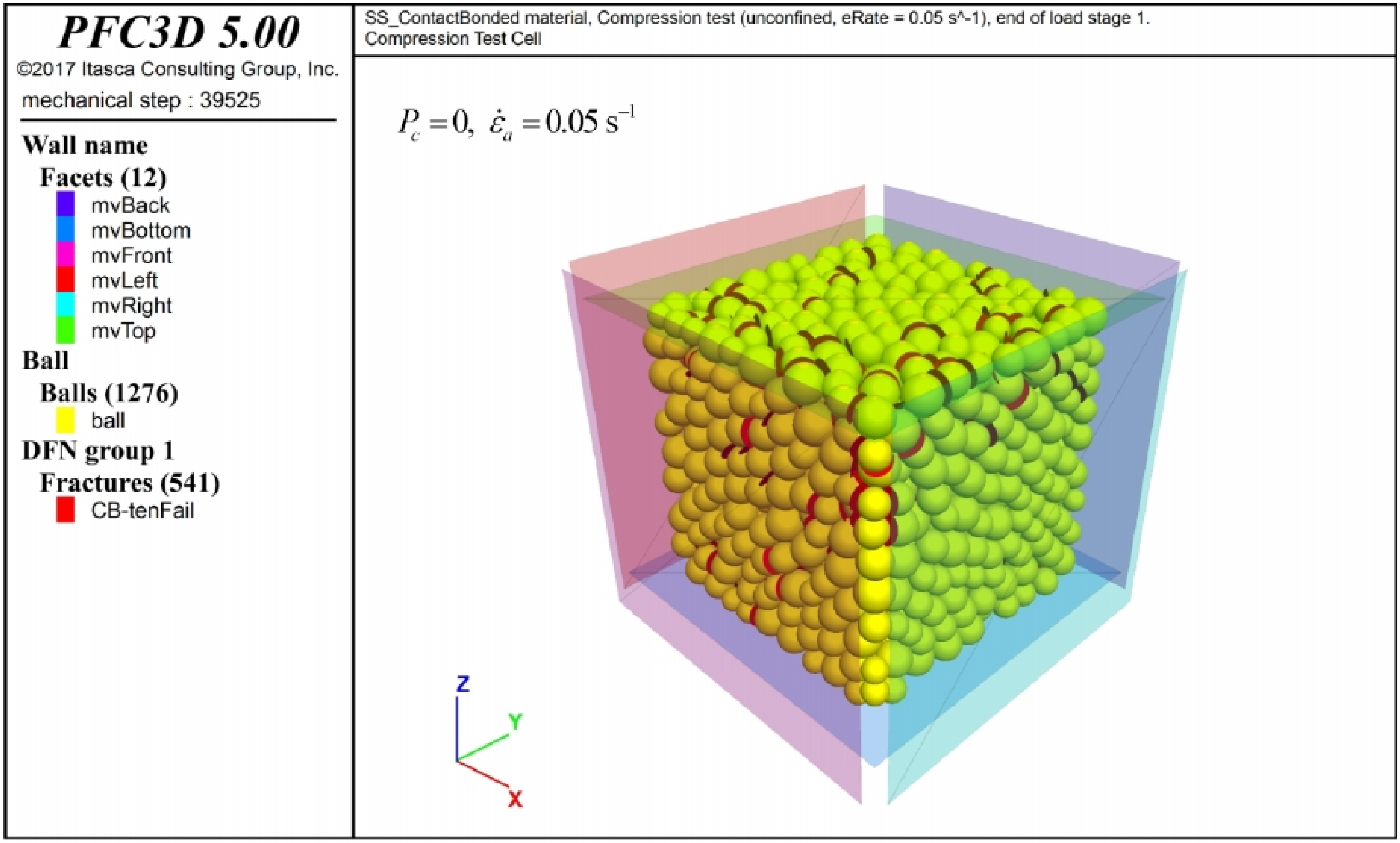


Figure 12 SS_ContactBonded material at the end of the fully unconfined test with grains and cracks.

Example Materials (contact-bonded material)

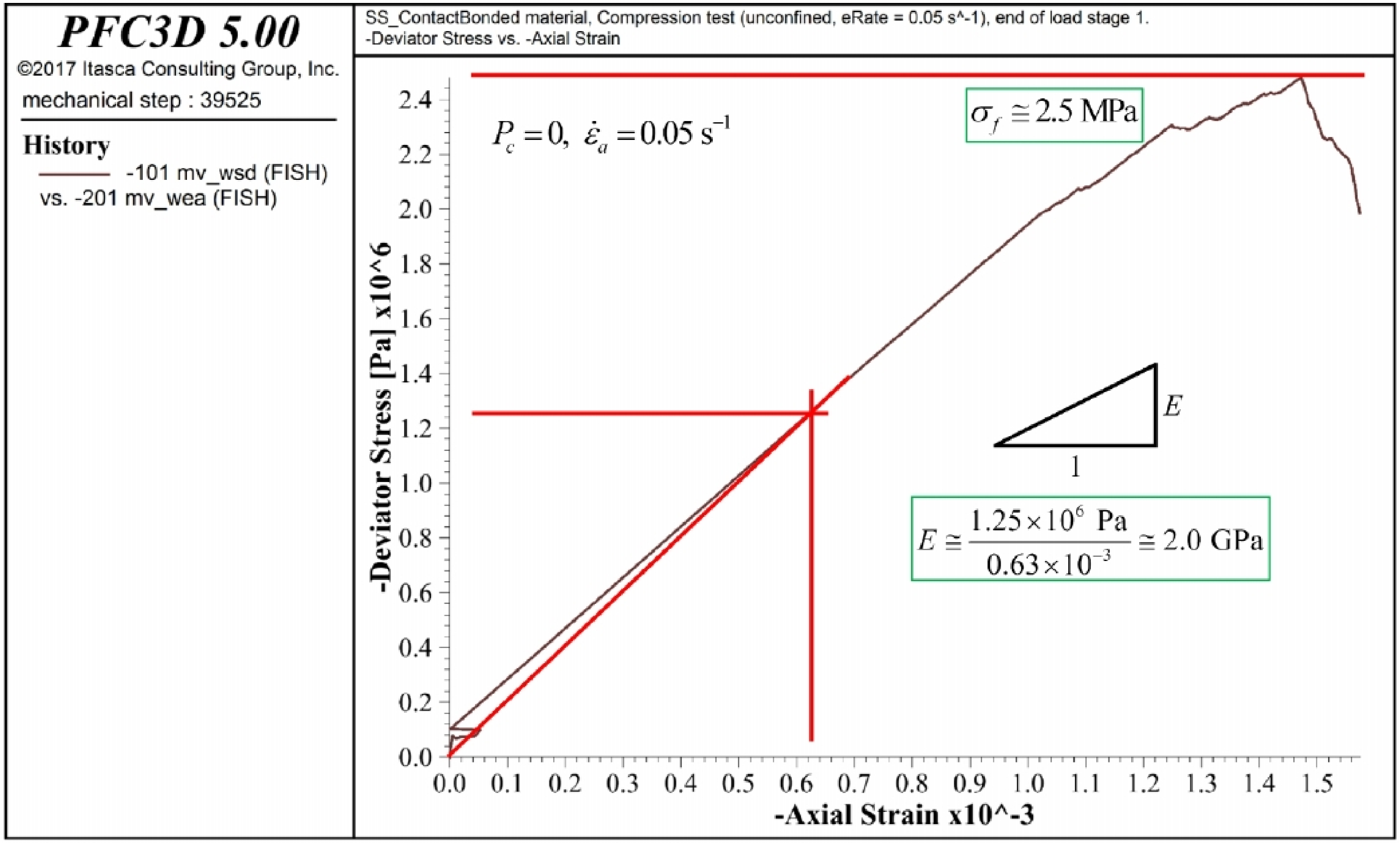


Figure 13 Deviator stress versus axial strain for SS_ContactBonded material tested fully unconfined, and measurement of peak strength and Young's modulus.

Example Materials (contact-bonded material)

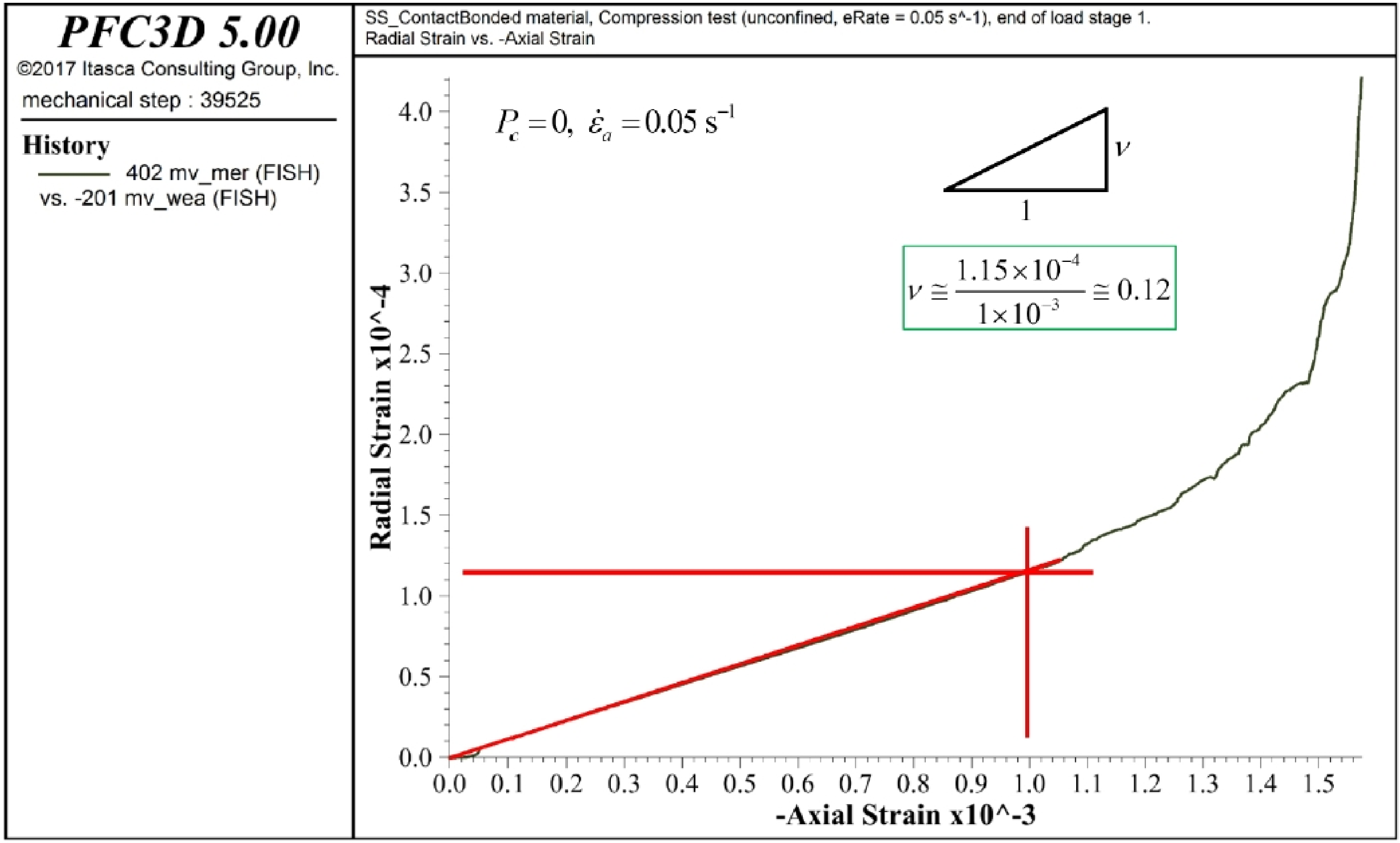


Figure 14 ***Radial strain versus axial strain for SS_ContactBonded material tested fully unconfined, and measurement of Poisson's ratio.***

Example Materials (contact-bonded material)

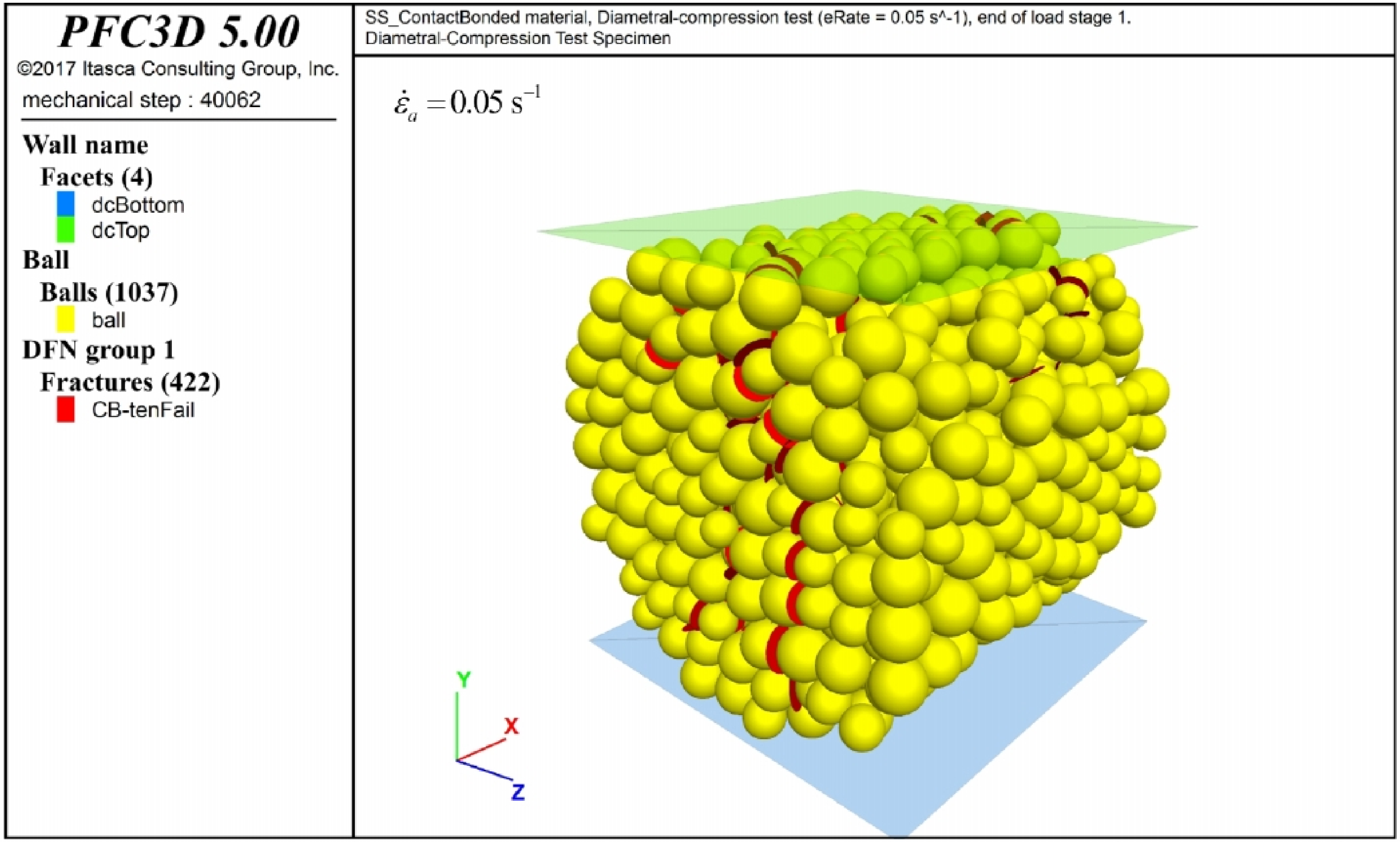


Figure 15 SS_ContactBonded material at the end of diametral-compression test with grains and cracks.

Example Materials (contact-bonded material)

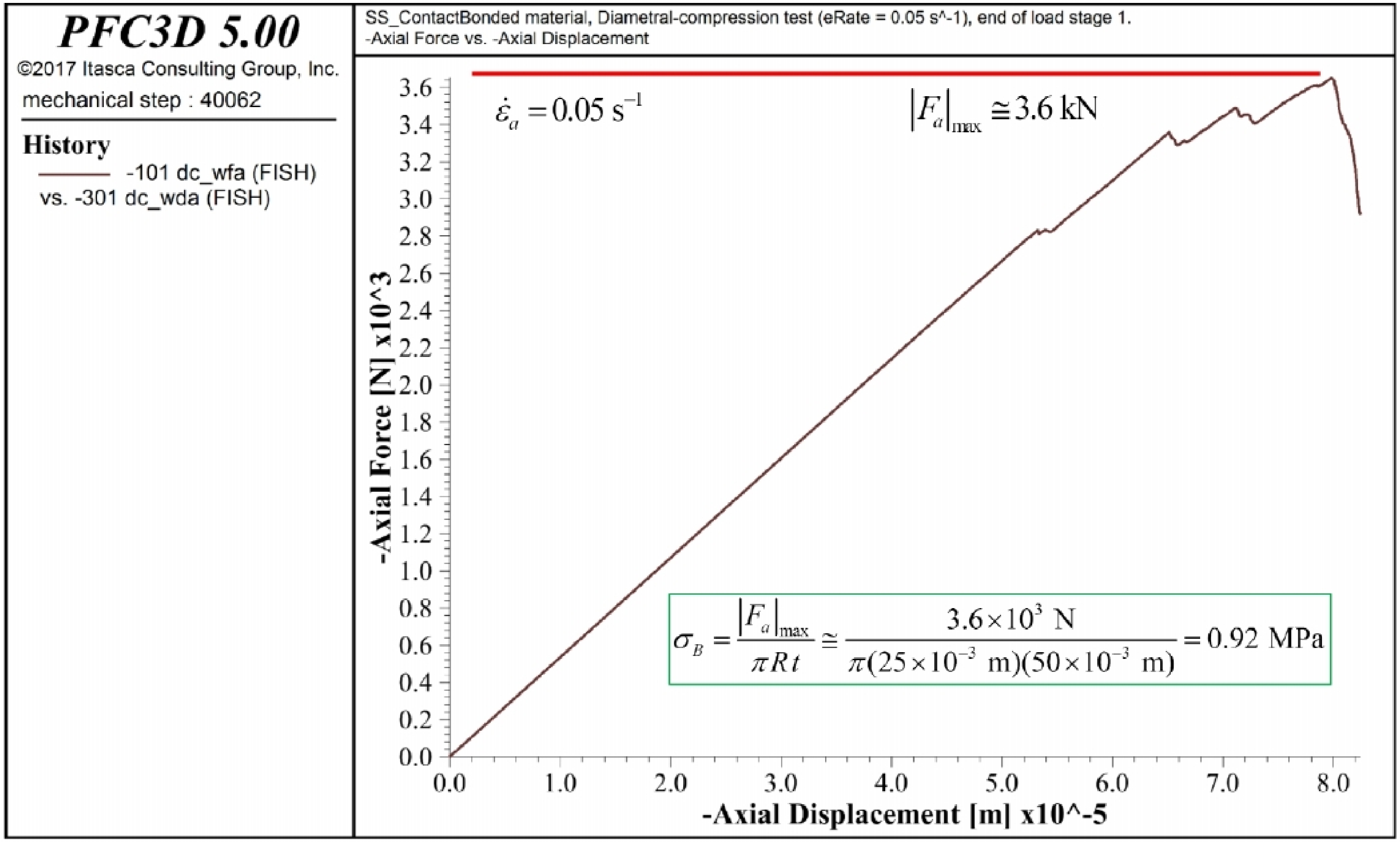


Figure 16 Axial force versus axial displacement for SS_ContactBonded material during the diametral-compression test, and measurement of Brazilian tensile strength.

Example Materials (contact-bonded material)

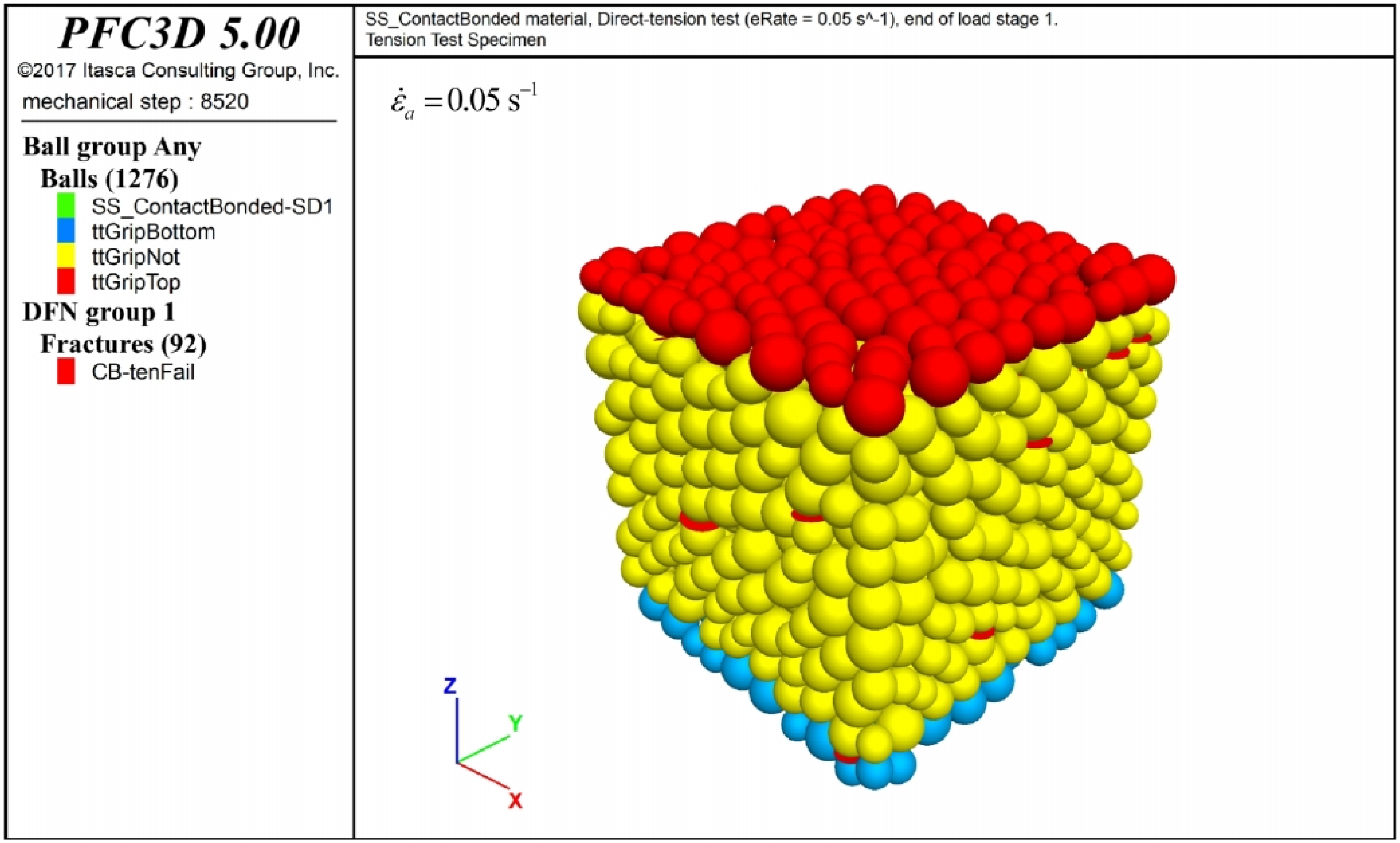


Figure 17 SS_ContactBonded material at the end of the direct-tension test with grains and cracks.

Example Materials (contact-bonded material)

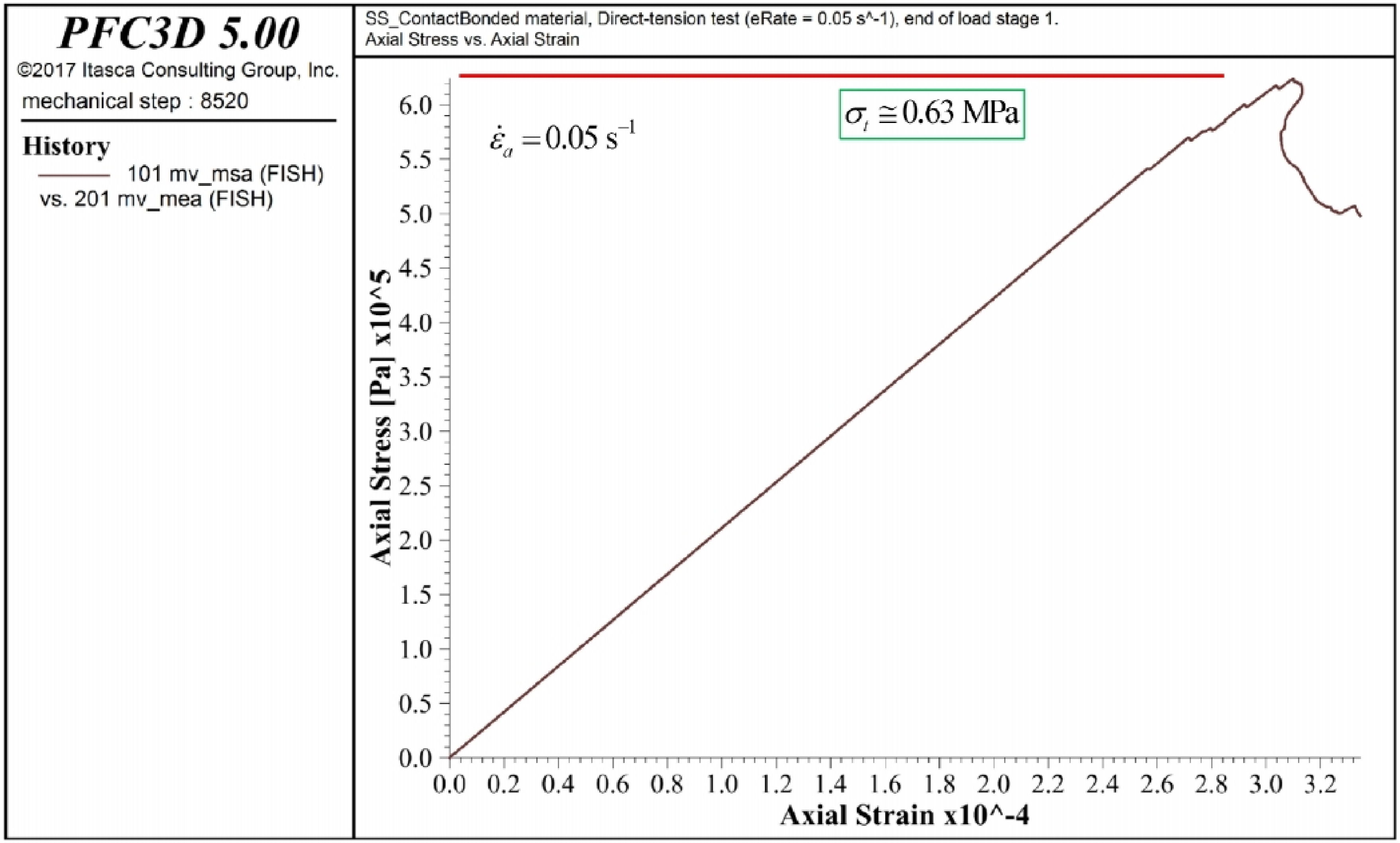


Figure 18 Axial stress versus axial strain for SS_ContactBonded material during the direct-tension test, and measurement of tensile strength.

Example Materials (2D contact-bonded clumped material)

Clumped materials are created by calling **`mpParams-Clumped.p{2,3}dat`**.

The effect of grain shape is illustrated by the 2D contact-bonded example.

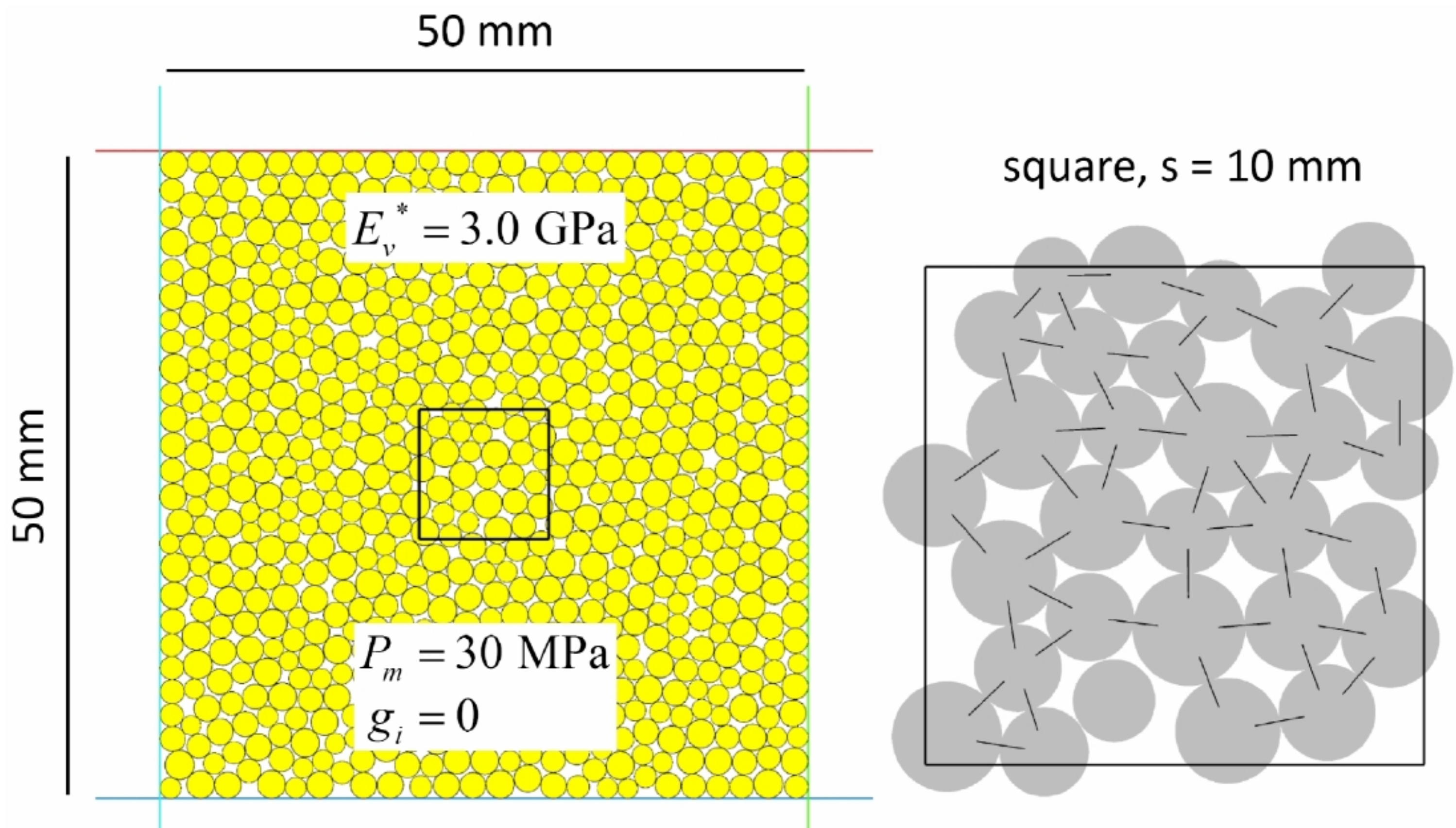
Two grain shapes: dyads (75%) and peanuts (25%).

The dyads and peanuts pack to a denser state than the disks.

For a UCS test, clumped material is stronger and stiffer.

Example Materials (2D contact-bonded clumped material)

Disk-only material:



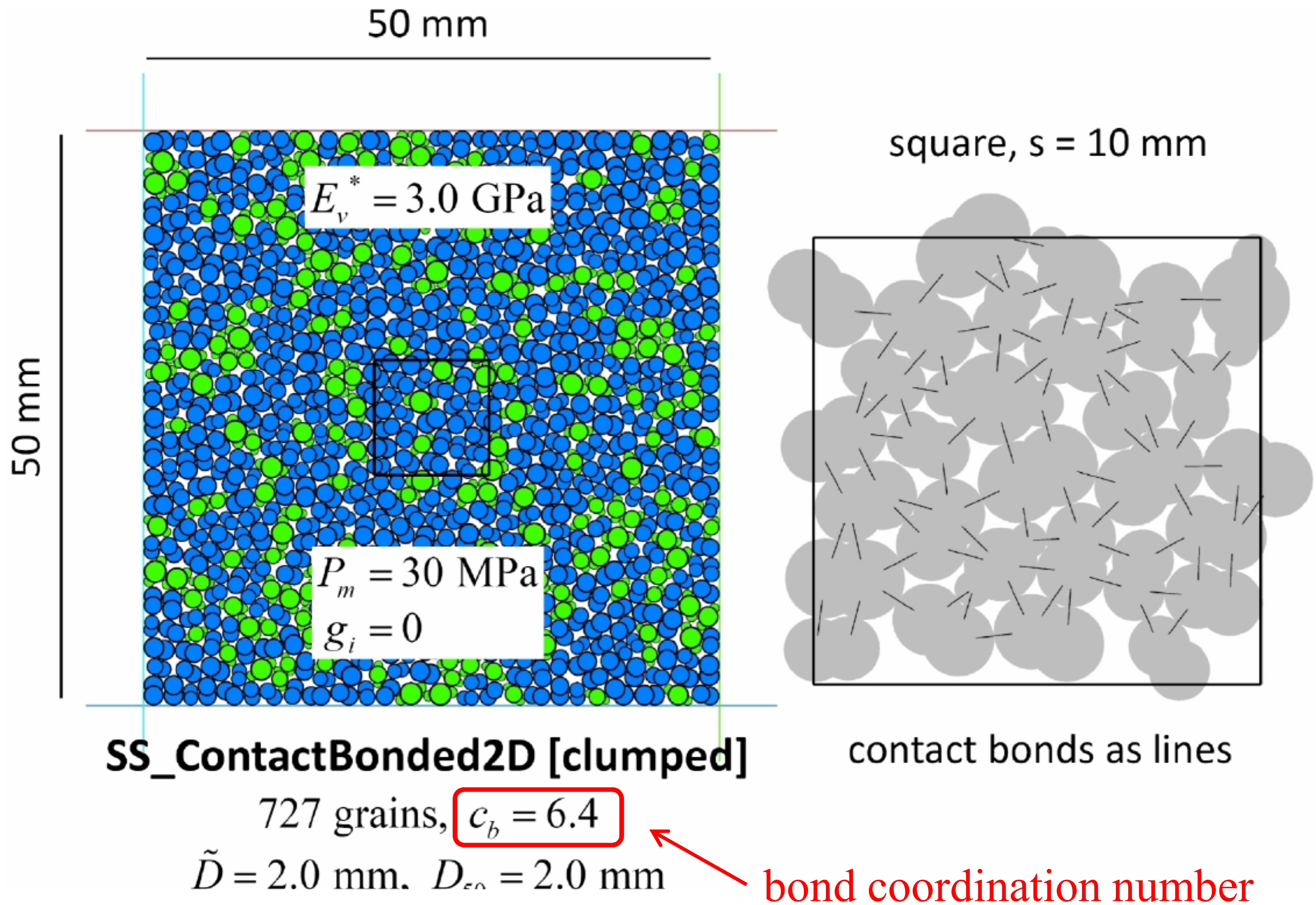
SS_ContactBonded2D

719 grains, $c_b = 4.0$ ← bond coordination number

$\tilde{D} = 1.9$ mm, $D_{50} = 2.0$ mm

Example Materials (2D contact-bonded clumped material)

Clumped material:



bond coordination number

Example Materials (parallel-bonded material)

1.1 Parallel-Bonded Material Example

The parallel-bonded material example is in the **`MatGen-ParallelBonded`** example-project directory. A parallel-bonded material is created to represent a typical sandstone, which we take to be Castlegate sandstone.[2] We denote our sandstone material as the SS_ParallelBonded material with microproperties listed in Table 1. The material is created in a cubic material vessel (of 50 mm side length, with a 3 GPa effective modulus).[3] The grain-scaling packing procedure is used to pack the grains to a 30 MPa material pressure, and then parallel bonds are added between all grains that are in contact with one another (see Figure 1). The material is then subjected to compression, diametral-compression and direct-tension tests. The test results can be displayed and interpreted in the same way as for the contact-bonded material example in the Example Materials 1 memo.

---

[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 (parallel-bonded material)

*Table 1 Microproperties of CG_ParallelBonded Material**

Property	Value
Common group:	
N_m	SS_ParallelBonded
$T_m,\ \alpha,\ C_\rho,\ \rho_v\ \left[\mathrm{kg/m^3}\right]$	2, 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
Parallel-bonded material group:	
Linear group:	
$E^*\ [\mathrm{GPa}],\ \kappa^*,\ \mu$	1.5, 1.5, 0.4
Parallel-bond group:	
$g_i\ [\mathrm{mm}],\ \bar{\lambda},\ \bar{E}^*\ [\mathrm{GPa}],\ \bar{\kappa}^*,\ \bar{\beta}$	0, 1.0, 1.5, 1.5, 1.0
$(\bar{\sigma}_c)_{\{m,sd\}}\ [\mathrm{MPa}],\ (\bar{c})_{\{m,sd\}}\ [\mathrm{MPa}],\ \bar{\phi}\ [\mathrm{degrees}]$	$\{1.0, 0\}$, $\{20.0, 0\}$, 0
Linear material group:	
$E_n^*\ [\mathrm{GPa}],\ \kappa_n^*,\ \mu_n$	1.5, 1.5, 0.4

* Parallel-bonded material parameters are defined in Table 4 of the base memo.

Example Materials (parallel-bonded material)

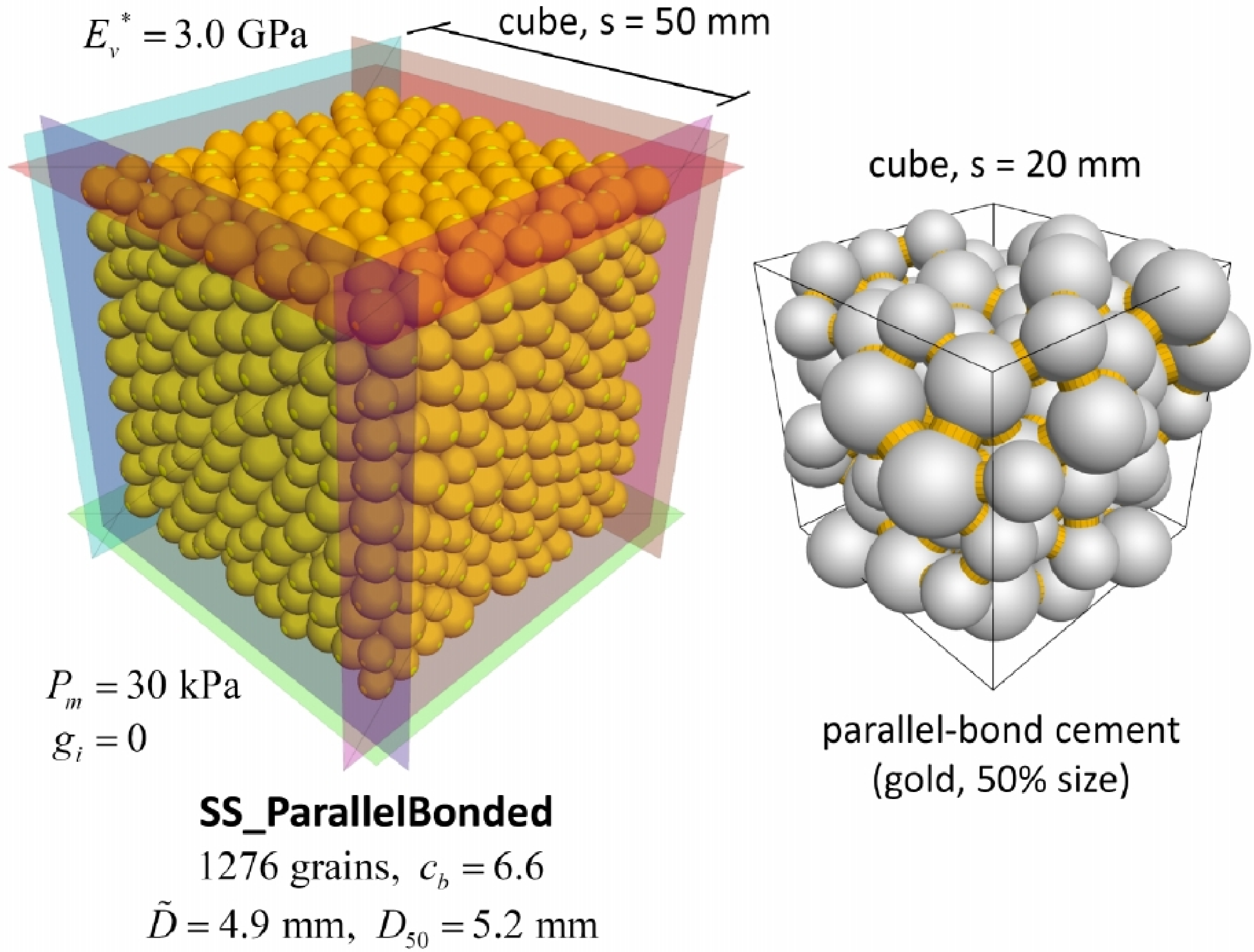


Figure 1 *SS_ParallelBonded material at the end of material genesis with grains and intact parallel bonds in the microstructural box.*

Example Materials (flat-jointed material)

1.3 Flat-Jointed Material Example

The flat-jointed material example is in the **`MatGen-FlatJointed`** example-project directory. A flat-jointed material is created to represent a typical sandstone, which we take to be Castlegate sandstone.[6] We denote our sandstone material as the SS_FlatJointed material with microproperties listed in Table 3. The material is created in a cubic material vessel (of 50 mm side length, with a 3 GPa effective modulus).[7] The grain-scaling packing procedure is used to pack the grains to a 30 MPa material pressure, and then the flat-joint contact model is installed between all grains that are in contact with one another and the flat-jointed material properties are assigned to those flat-jointed contacts (see Figure 3). The material is then subjected to compression, diametral-compression and direct-tension tests. The test results can be displayed and interpreted in the same way as for the contact-bonded material example in the Example Materials 1 memo.

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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 (flat-jointed material)

*Table 3 Microproperties of CG_FlatJointed Material**

Property	Value
Common group:	
N_m	SS_FlatJointed
$T_m,\ \alpha,\ C_\rho,\ \rho_v\left[\mathrm{kg/m^3}\right]$	3, 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:	
$S_{RN},\ P_m\,[\mathrm{MPa}],\ \varepsilon_P,\ \varepsilon_{\lim},\ n_{\lim}$ $C_p,\ n_c$	10000, 30, 1×10^{-2}, 8×10^{-3}, 2×10^{6} 1, 0.30
Flat-jointed material group:	
$C_{MS},\ g_i\,[\mathrm{mm}],\ \phi_B,\ \phi_G,\ (g_o)_{\{\mathrm{m,sd}\}}\,[\mathrm{mm}],\ \{N_r, N_\alpha\}$	false, 0, 1, 0, $\{0,0\}$, $\{1,3\}$
$\{C_\lambda,\ \lambda_v\},\ E^*\,[\mathrm{GPa}],\ \kappa^*,\ \mu$	$\{0,\ 1.0\}$, 3.0, 1.5, 0.4
$(\sigma_c)_{\{\mathrm{m,sd}\}}\,[\mathrm{MPa}],\ (c)_{\{\mathrm{m,sd}\}}\,[\mathrm{MPa}],\ \phi\,[\mathrm{degrees}]$	$\{1.0, 0\}$, $\{20.0, 0\}$, 0
Linear material group:	
$E_n^*\,[\mathrm{GPa}],\ \kappa_n^*,\ \mu_n$	1.5, 1.5, 0.4

* Flat-jointed material parameters are defined in Table 5 of the base memo.

Example Materials (flat-jointed material)

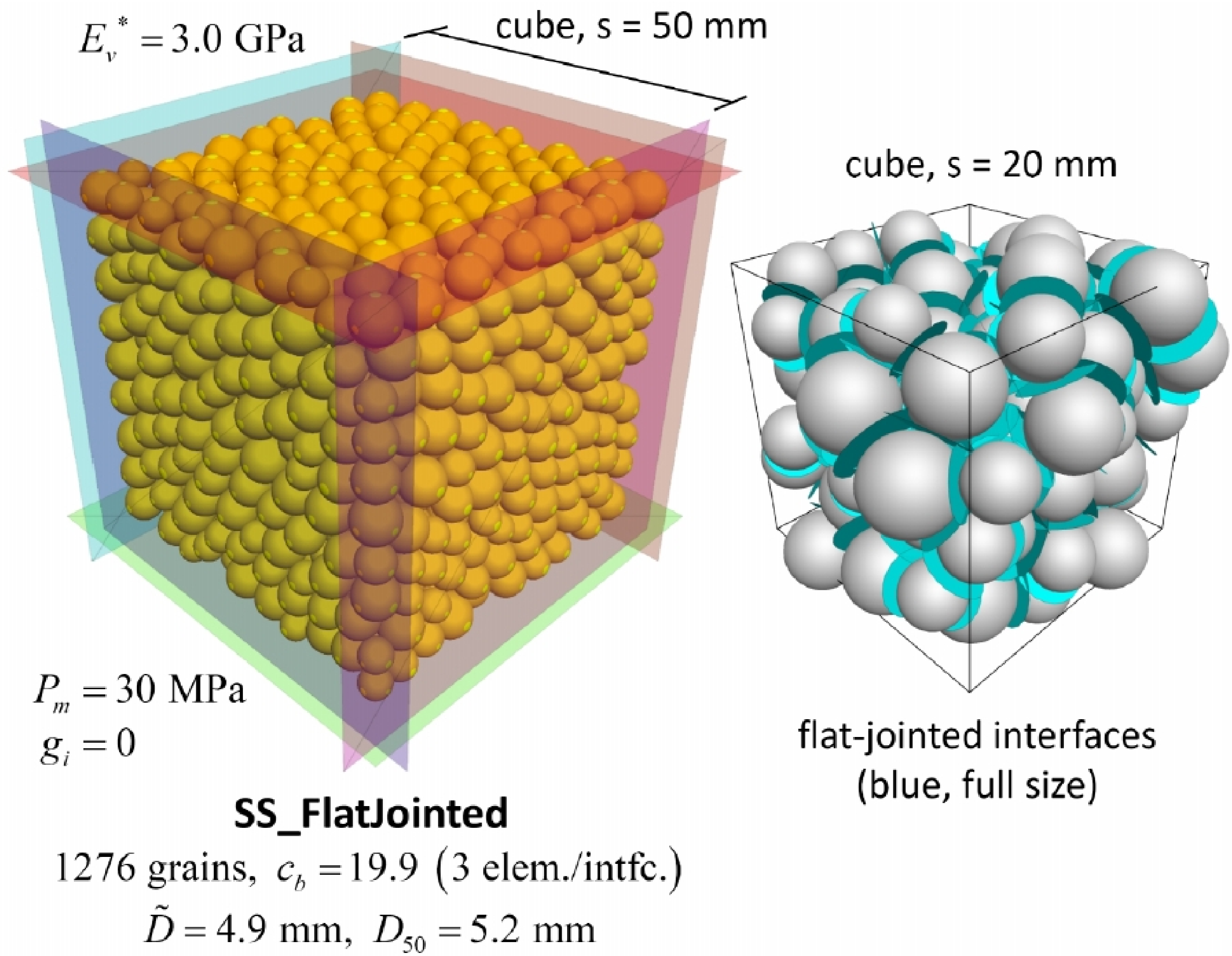

Figure 3 *SS_FlatJointed material at the end of material genesis with grains and flat-jointed interfaces in the microstructural box.*

Example Materials (user-defined, hill material)

1.1 User-Defined Material Example

The user-defined material example is in the **`MatGen-Hill`** example-project directory. A hill material is created to represent a typical aggregate base layer of an asphalt-surface roadway (Potyondy et al., 2016).[2] We denote our aggregate material as the AG_Hill material with microproperties listed in Table 1. The material is dry while being created in a cylindrical material vessel (of 240-mm height and 170-mm diameter, with a 500 MPa effective modulus) and packed at a 150 kPa material pressure as shown in Figure 1. The material is then subjected to triaxial testing. The material is tested dry and wet. The wet material has a 20 kPa suction added between all grains that are within 3 mm of one another at the end of material genesis.[3] During each 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 moduli of the dry and wet materials (see Figures 2 and 3).[4] The hysteretic response is the expected behavior, and the resilient modulus is increased for the wet material.

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[3] The suction is typical for aggregates with gravimetric moisture content ranging from 5 to 10 percent.
[4] The confinement is similar to that defined in resilient modulus laboratory protocols, and axial strains correspond with vertical strains in the aggregate base layer for typical traffic loads.

Example Materials (user-defined, hill material)

*Table 1 Microproperties of AG_Hill Material**

Property	Value
Common group:	
N_m	AG_Hill
$\{T_m, N_{cm}\}$, α, C_ρ, ρ_v $\left[\mathrm{kg/m^3}\right]$	$\{4, \mathrm{hill}\}$, 0.7, 0, 2650
S_g, T_{SD}, $\{D_{\{l,u\}}$ [mm], $\phi\}$, D_{mult}	0, 0, $\{14, 20, 1.0\}$, 1.0
Packing group:	
S_{RN}, P_m [kPa], ε_P, $\varepsilon_{\lim}$, $n_{\lim}$	10000, 150, 1×10^{-2}, 8×10^{-3}, 2×10^{6}
C_p, n_c, μ_{CA}, $v_{\lim}$ [m/s]	0, 0.58, 0, 1.0
Hill material group:	
E_g [GPa], ν_g, μ, α_h, ψ [kPa]	29, 0.15, 0.4, 0, 20

* Hill material parameters are defined in Table 2 of Potyondy (2016).

Example Materials (user-defined, hill material)

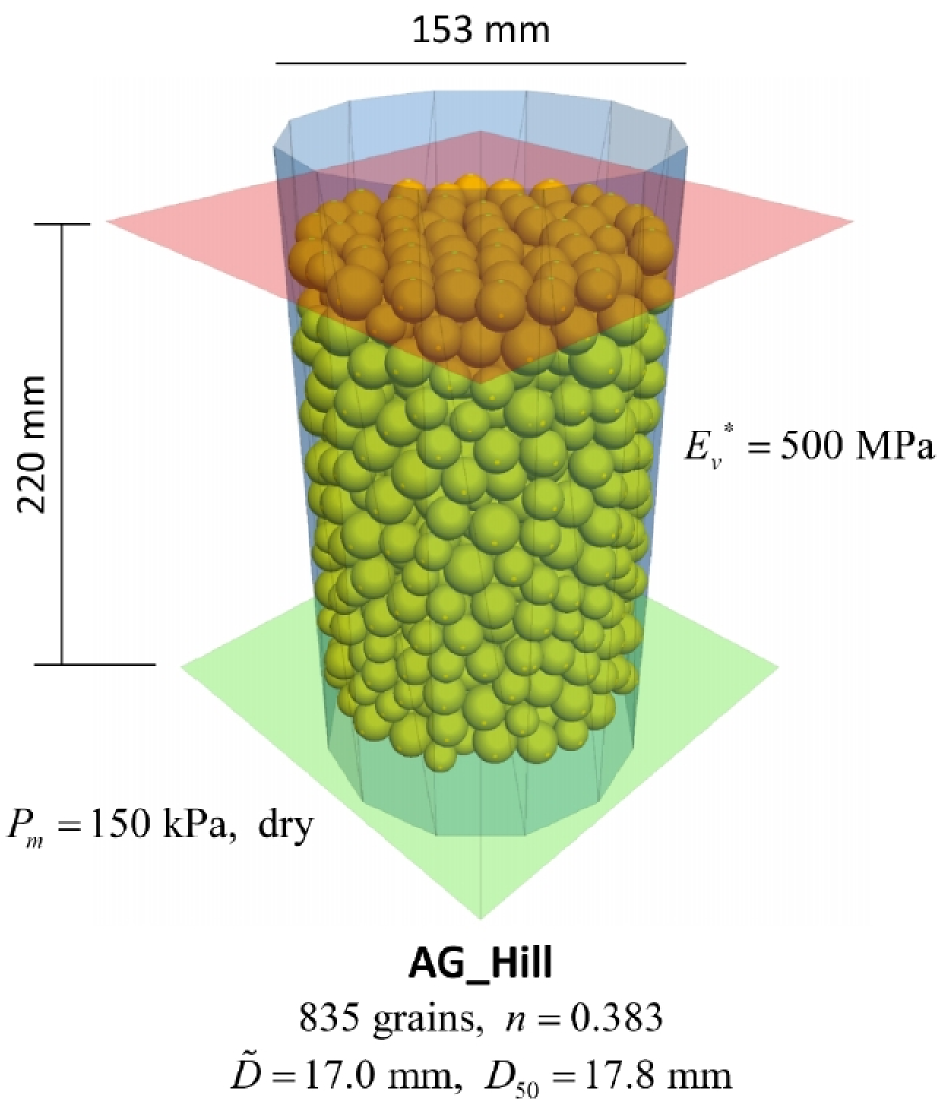

Figure 1 ***Dry AG_Hill material packed at 150 kPa material pressure at the end of material genesis.***

Example Materials (user-defined, hill material)

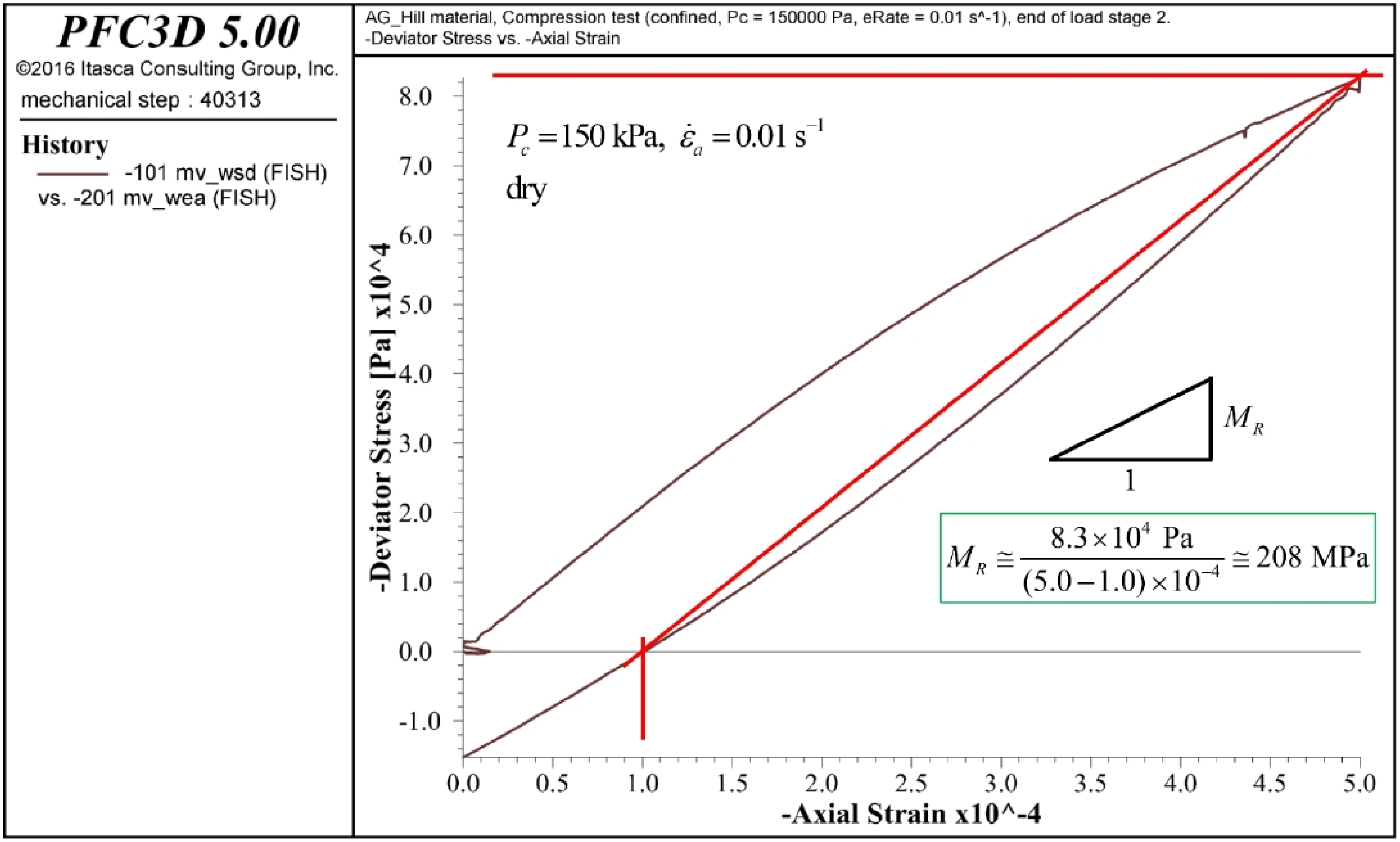

Figure 2 Deviator stress versus axial strain for dry AG_Hill material tested at 150 kPa confinement, and measurement of resilient modulus.

Example Materials (user-defined, hill material)

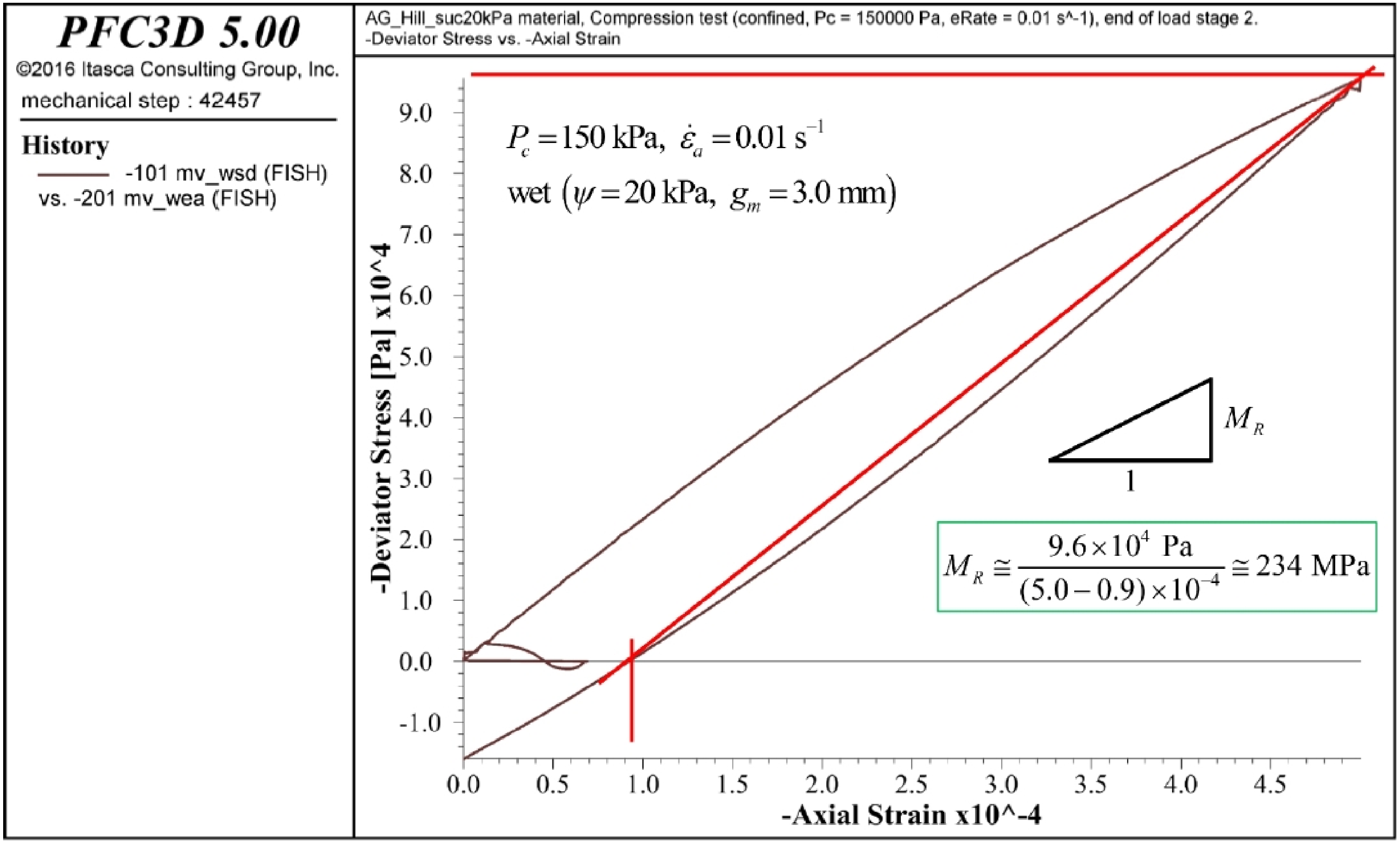

Figure 3 *Deviator stress versus axial strain for wet AG_Hill material tested at 150 kPa confinement, and measurement of resilient modulus.*

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 5.0 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).