Memorandum

ITASCA Consulting Group, Inc.

Date: June 29, 2023

To: PFC 7 Documentation Set

From: David Potyondy

Re: Material-Modeling Support for PFC [fistPkg7.3] (Example Materials 2)

Ref: ICG7766-L

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1.0 EXAMPLE MATERIALS

The PFC FISHTank produces linear, contact-bonded, parallel-bonded, soft-bonded, flat-jointed and user-defined (3D hill) materials. Examples for each material are provided in the Example Materials memos. 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 **`fistPkg7.N/ExampleProjects/MatGen-M`** directory, where **`N`** is the version number of the PFC FISHTank, and **`M`** is the material type. There are separate 2D and 3D projects for each material, and both projects are contained within the same example-project directory. Examples for the parallel-bonded, soft-bonded and flat-jointed materials are provided in the following subsections.[1]

[1] The microstructural arrangement and stress-strain curves obtained with the current FISHTank may vary slightly from those shown here, which may have been generated by an earlier version of the FISHTank.

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.

Table 1 Microproperties of SS_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:	
$S_{RN},\ P_m\ [\mathrm{MPa}],\ \varepsilon_P,\ \varepsilon_{\lim},\ n_{\lim}$	$10000,\ 30,\ 1\times10^{-2},\ 8\times10^{-3},\ 2\times10^{6}$
$C_p,\ n_c$	$1,\ 0.30$
Parallel-bonded material group:	
Linear group:	
$E^*\ [\mathrm{GPa}],\ \kappa^*,\ \mu$	$1.5,\ 1.5,\ 0.4$
Parallel-bond group:	
$g_i\ [\mathrm{mm}],\ \bar{\lambda},\ \bar{E}^*\ [\mathrm{GPa}],\ \bar{\kappa}^*,\ \bar{\beta}$	$0,\ 1.0,\ 1.5,\ 1.5,\ 1.0$
$(\bar{\sigma}_c)_{\{\mathrm{m,\ sd}\}}\ [\mathrm{MPa}],\ (\bar{c})_{\{\mathrm{m,\ sd}\}}\ [\mathrm{MPa}],\ \bar{\gamma},\ \bar{\phi}\ [\mathrm{degrees}]$	$\{1.0, 0\},\ \mathrm{NA},\ 20,\ 0$
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.

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[2] Typical properties of Castlegate sandstone are listed in footnote 4 of the Example Materials 1 memo.
[3] A parallel-bonded clumped material can be created in the same way as for the contact-bonded material example.

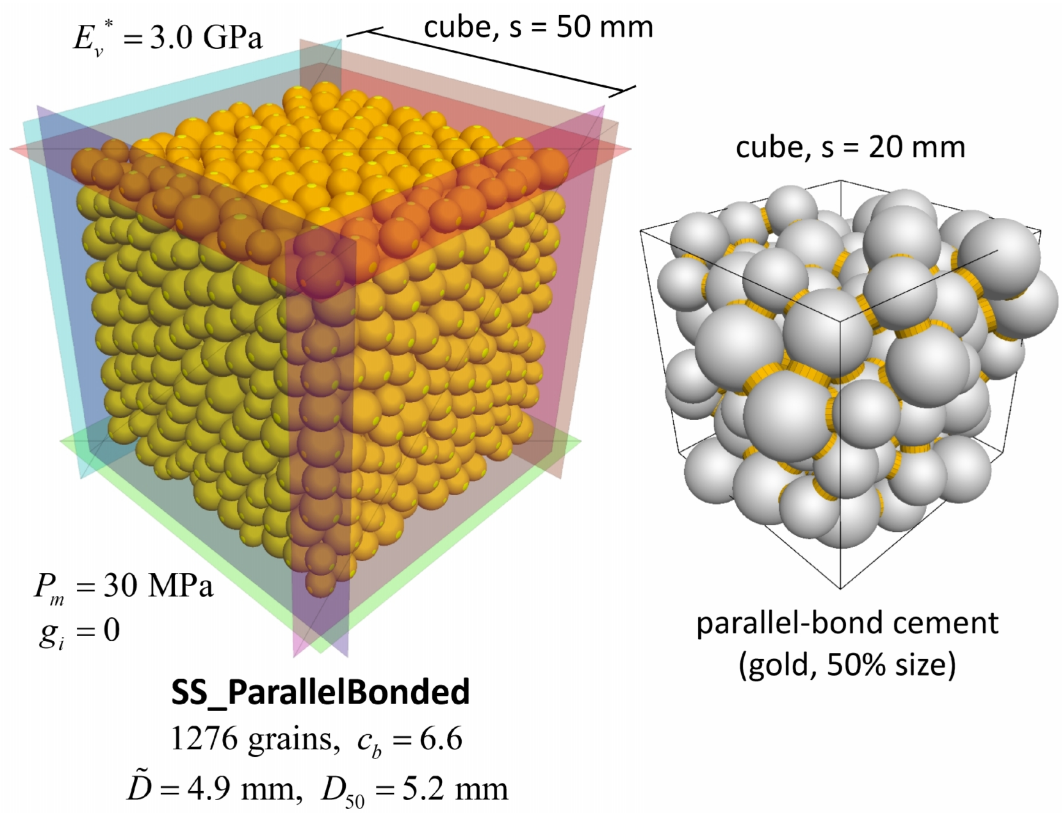

Figure 1 ***SS_ParallelBonded material at the end of material genesis with grains and intact parallel bonds in the microstructural box.***

1.2 Parallel-Bonded Material Example (2D model)

The parallel-bonded material example for the 2D model is in the **`MatGen-ParallelBonded`** example-project directory. The files for the 2D model contain the **`p2*`** extension (e.g., **`MatGen.p2prj`** and **`mpParams.p2dat`**). A 2D parallel-bonded material (consisting of rigid unit-thickness disks) is created to represent a typical sandstone, which we take to be Castlegate sandstone.[4] We denote our sandstone material as the SS_ParallelBonded2D material with microproperties listed in Table 2. The material is created in a square-cuboid material vessel (of 50 mm side length and unit depth, with a 3 GPa effective modulus).[5] 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 2). 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.

Table 2 Microproperties of SS_ParallelBonded2D Material*

Property	Value
Common group:	
N_m	SS_ParallelBonded2D
$T_m,\ \alpha,\ C_\rho,\ \rho_v\ [\text{kg/m}^3]$	2, 0.7, 1, 1960
$S_g,\ T_{SD},\ \{D_{\{l,u\}}\ [\text{mm}],\ \phi\},\ D_{mult}$	0, 0, $\{1.6, 2.4, 1.0\}$, 1.0
Packing group:	
$S_{RN},\ P_m\ [\text{MPa}],\ \varepsilon_P,\ \varepsilon_{\text{lim}},\ n_{\text{lim}}$	10000, 30, 1×10^{-2}, 8×10^{-3}, 2×10^{6}
$C_p,\ n_c$	1, 0.08
Parallel-bonded material group:	
Linear group:	
$E^*\ [\text{GPa}],\ \kappa^*,\ \mu$	1.5, 1.5, 0.4
Parallel-bond group:	
$g_i\ [\text{mm}],\ \bar{\lambda},\ \bar{E}^*\ [\text{GPa}],\ \bar{\kappa}^*,\ \bar{\beta}$	0, 1.0, 1.5, 1.5, 1.0
$(\bar{\sigma}_c)_{\{\text{m, sd}\}}\ [\text{MPa}],\ (\bar{c})_{\{\text{m, sd}\}}\ [\text{MPa}],\ \bar{\phi}\ [\text{degrees}]$	$\{1.0, 0\}$, $\{20.0, 0\}$, 0
Linear material group:	
$E_n^*\ [\text{GPa}],\ \kappa_n^*,\ \mu_n$	1.5, 1.5, 0.4

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

[4] Typical properties of Castlegate sandstone are listed in footnote 4 of the Example Materials 1 memo.
[5] A 2D parallel-bonded clumped material can be created in the same way as for the 2D contact-bonded material example.

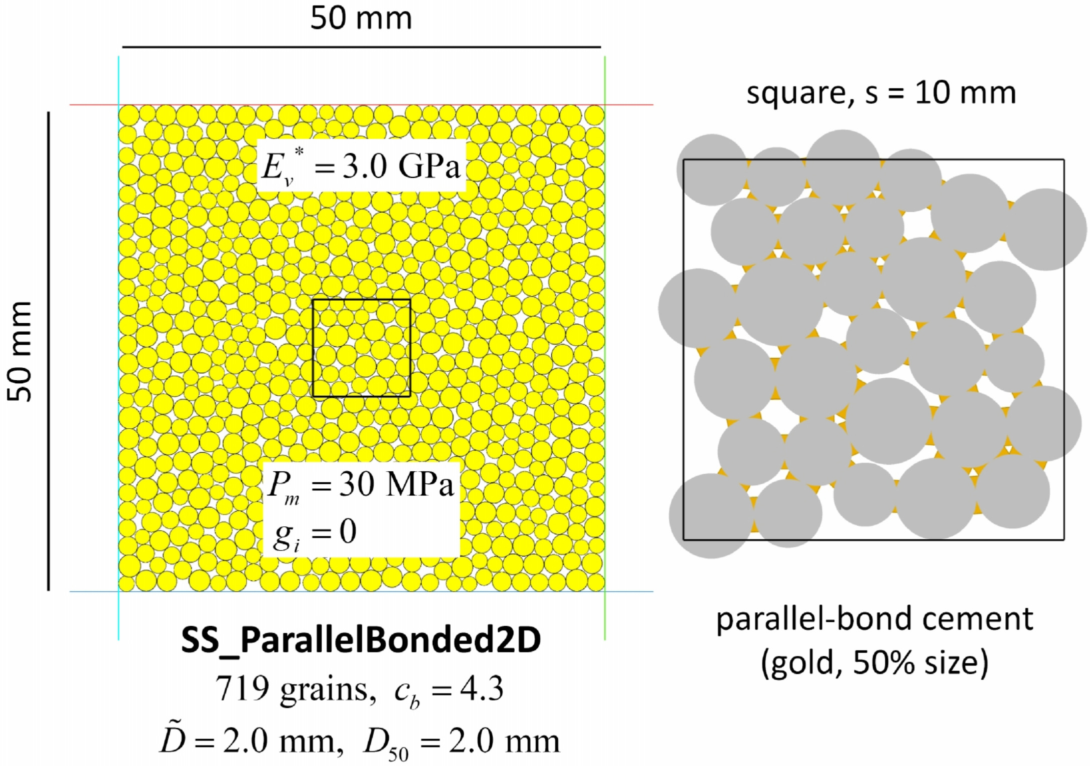

***Figure 2** SS_ParallelBonded2D material at the end of material genesis with grains and intact parallel bonds in the microstructural box.*

1.3 Soft-Bonded Material Example

The soft-bonded material example is in the `MatGen-SoftBonded` example-project directory. A soft-bonded material is created to represent a typical sandstone, which we take to be Castlegate sandstone.[6] We denote our sandstone material as the SS_SoftBonded material with microproperties listed in Figure 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 soft 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.

Table 3 Microproperties of SS_SoftBonded Material*

Property	Value
Common group:	
N_m	SS_SoftBonded
$T_m,\ \alpha,\ C_\rho,\ \rho_v\ \left[\text{kg/m}^3\right]$	$3,\ 0.7,\ 1,\ 1960$
$S_g,\ T_{SD},\ \left\{D_{\{l,u\}}\ [\text{mm}],\ \phi\right\},\ D_{mult}$	$0,\ 0,\ \{4.0, 6.0, 1.0\},\ 1.0$
Packing group:	
$S_{RN},\ P_m\ [\text{MPa}],\ \varepsilon_P,\ \varepsilon_{\lim},\ n_{\lim}$ $C_p,\ n_c$	$10000,\ 30,\ 1\times10^{-2},\ 8\times10^{-3},\ 2\times10^{6}$ $1,\ 0.30$
Soft-bonded material group:	
$g_i\ [\text{mm}],\ \lambda,\ E^*\ [\text{GPa}],\ \kappa^*,\ \beta$	$0,\ 1.0,\ 1.5,\ 1.5,\ 1.0$
$(\sigma_c)_{\{\text{m, sd}\}}\ [\text{MPa}],\ (c)_{\{\text{m, sd}\}}\ [\text{MPa}],\ \gamma,\ \phi\,[\text{degrees}]$	$\{1.0, 0\},\ \text{NA},\ 20,\ 0.0$
$\zeta,\ \gamma,\ \mu\ \lambda_b\ \lambda_t$	$0.0,\ 0.0,\ 0.4,\ 0.0,\ 0.0$
Linear material group:	
$E_n^*\ [\text{GPa}],\ \kappa_n^*,\ \mu_n$	$1.5,\ 1.5,\ 0.4$

* Soft-bonded material parameters are defined in Table 5 of the base memo.

[6] Typical properties of Castlegate sandstone are listed in footnote 4 of the Example Materials 1 memo.
[7] A soft-bonded clumped material can be created in the same way as for the contact-bonded material example.

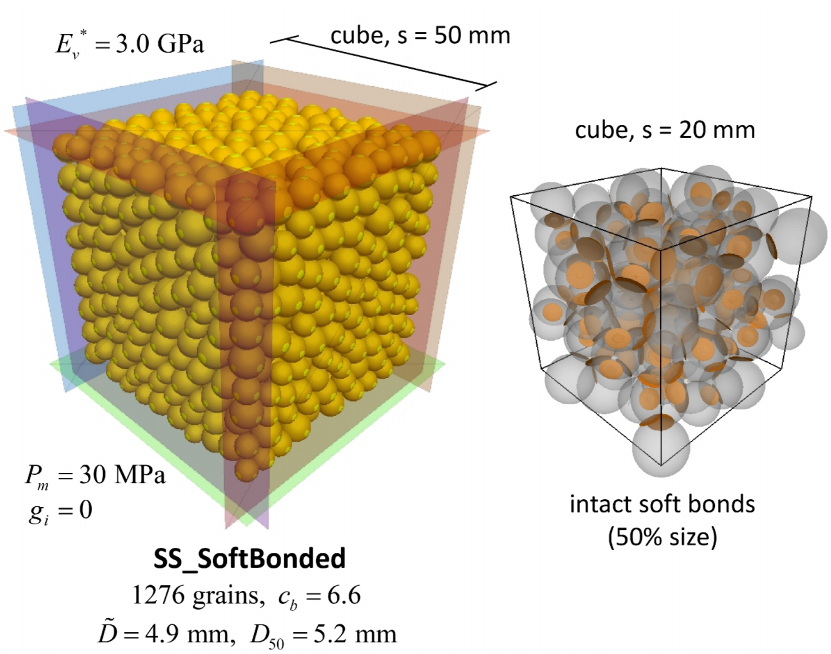

Figure 3 ***SS_SoftBonded material at the end of material genesis with grains and intact soft bonds in the microstructural box.***

1.4 Soft-Bonded Material Example (2D model)

The soft-bonded material example for the 2D model is in the **`MatGen-SoftBonded`** example-project directory. The files for the 2D model contain the **`p2*`** extension (e.g., **`MatGen.p2prj`** and **`mpParams.p2dat`**). A 2D soft-bonded material (consisting of rigid unit-thickness disks) is created to represent a typical sandstone, which we take to be Castlegate sandstone.[8] We denote our sandstone material as the SS_SoftBonded2D material with microproperties listed in Table 4. The material is created in a square-cuboid material vessel (of 50 mm side length and unit depth, with a 3 GPa effective modulus).[9] The grain-scaling packing procedure is used to pack the grains to a 30 MPa material pressure, and then soft bonds are added between all grains that are in contact with one another (see Figure 2). 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.

Table 4 Microproperties of SS_SoftBonded2D Material*

Property	Value
Common group:	
N_m	SS_SoftBonded2D
$T_m,\ \alpha,\ C_\rho,\ \rho_v\ [\text{kg/m}^3]$	$3,\ 0.7,\ 1,\ 1960$
$S_g,\ T_{SD},\ \{D_{\{l,u\}}\ [\text{mm}],\ \phi\},\ D_{mult}$	$0,\ 0,\ \{4.0, 6.0, 1.0\},\ 1.0$
Packing group:	
$S_{RN},\ P_m\ [\text{MPa}],\ \varepsilon_P,\ \varepsilon_{\lim},\ n_{\lim}$	$10000,\ 30,\ 1\times10^{-2},\ 8\times10^{-3},\ 2\times10^{6}$
$C_p,\ n_c$	$1,\ 0.08$
Soft-bonded material group:	
$g_i\ [\text{mm}],\ \lambda,\ E^*\ [\text{GPa}],\ \kappa^*,\ \beta$	$0,\ 1.0,\ 1.5,\ 1.5,\ 1.0$
$(\sigma_c)_{\{\text{m, sd}\}}\ [\text{MPa}],\ (c)_{\{\text{m, sd}\}}\ [\text{MPa}],\ \gamma,\ \phi\ [\text{degrees}]$	$\{1.0, 0\},\ \text{NA},\ 20,\ 0.0$
$\zeta,\ \gamma,\ \mu\ \lambda_b,\ \lambda_t$	$0.0,\ 0.0,\ 0.4,\ 0.0,\ 0.0$
Linear material group:	
$E_n^*\ [\text{GPa}],\ \kappa_n^*,\ \mu_n$	$1.5,\ 1.5,\ 0.4$

* Soft-bonded material parameters are defined in Table 5 of the base memo.

[8] Typical properties of Castlegate sandstone are listed in footnote 4 of the Example Materials 1 memo.
[9] A 2D soft-bonded clumped material can be created in the same way as for the 2D contact-bonded material example.

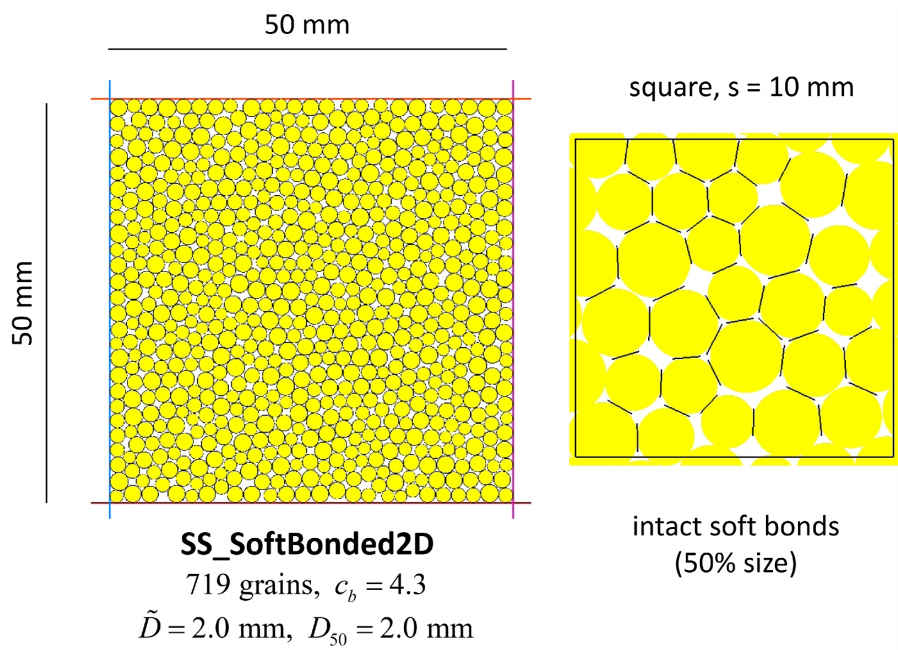

Figure 4 ***SS_SoftBonded2D material at the end of material genesis with grains and intact soft bonds in the microstructural box.***

1.5 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.[10] We denote our sandstone material as the SS_FlatJointed 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).[11] 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 5). 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.

Table 5 Microproperties of SS_FlatJointed Material*

Property	Value
Common group:	
N_m	SS_FlatJointed
$T_m,\ C_r,\ \varepsilon_s,\ \varepsilon_a,\ \alpha,\ C_\rho,\ \rho_v\left[\mathrm{kg/m^3}\right]$	4, NA, NA, NA, 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
$(\sigma_c)_{\{\mathrm{m,\,sd}\}}\,[\mathrm{MPa}],\ (c)_{\{\mathrm{m,\,sd}\}}\,[\mathrm{MPa}],\ \gamma,\ c_r,\ M_r,\ \phi\,[\mathrm{degrees}]$	$\{1.0,0\}$, NA, 20, 0.0, 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.

[10] Typical properties of Castlegate sandstone are listed in footnote 4 of the Example Materials 1 memo.
[11] A flat-jointed clumped material can be created in the same way as for the contact-bonded material example.

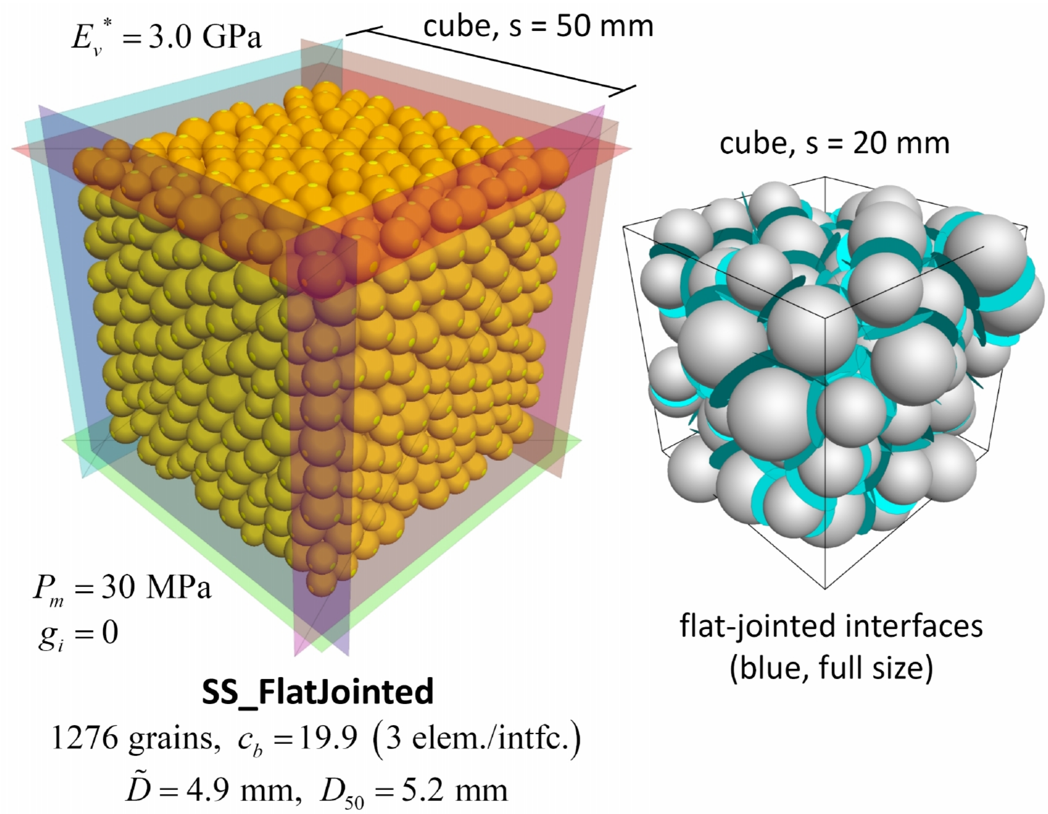

Figure 5 ***SS_FlatJointed material at the end of material genesis with grains and flat-jointed interfaces in the microstructural box.***

1.6 Flat-Jointed Material Example (2D model)

The flat-jointed material example for the 2D model is in the **`MatGen-FlatJointed`** example-project directory. The files for the 2D model contain the **`p2*`** extension (e.g., **`MatGen.p2prj`** and **`mpParams.p2dat`**). A 2D flat-jointed material (consisting of rigid unit-thickness disks) is created to represent a typical sandstone, which we take to be Castlegate sandstone.[12] We denote our sandstone material as the SS_FlatJointed2D material with microproperties listed in Table 6. The material is created in a square-cuboid material vessel (of 50 mm side length and unit depth, with a 3 GPa effective modulus).[13] 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 6). 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.

Table 6 Microproperties of SS_FlatJointed2D Material*

Property	Value
Common group:	
N_m	SS_FlatJointed2D
$T_m,\ \alpha,\ C_\rho,\ \rho_v\ [\mathrm{kg/m^3}]$	4, 0.7, 1, 1960
$S_g,\ T_{SD},\ \{D_{\{l,u\}}\ [\mathrm{mm}],\ \phi\},\ D_{mult}$	0, 0, $\{1.6, 2.4, 1.0\}$, 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, 0.08
Flat-jointed material group:	
$C_{MS},\ g_i\ [\mathrm{mm}],\ \phi_B,\ \phi_G,\ (g_o)_{\{\mathrm{m,sd}\}}\ [\mathrm{mm}],\ N_r$	false, 0, 1, 0, $\{0,0\}$, 2
$\{C_\lambda,\ \lambda_v\},\ E^*\ [\mathrm{GPa}],\ \kappa^*,\ \mu$	$\{0,\ 1.0\}$, 3.0, 1.5, 0.4
$(\sigma_c)_{\{\mathrm{m,sd}\}}\ [\mathrm{MPa}],\ (c)_{\{\mathrm{m,sd}\}}\ [\mathrm{MPa}],\ \gamma,\ c_r,\ M_r,\ \phi\,[\mathrm{degrees}]$	$\{1.0, 0\}$, NA, 20, 0.0, 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.

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[12] Typical properties of Castlegate sandstone are listed in footnote 4 of the Example Materials 1 memo.
[13] A 2D flat-jointed clumped material can be created in the same way as for the 2D contact-bonded material example.

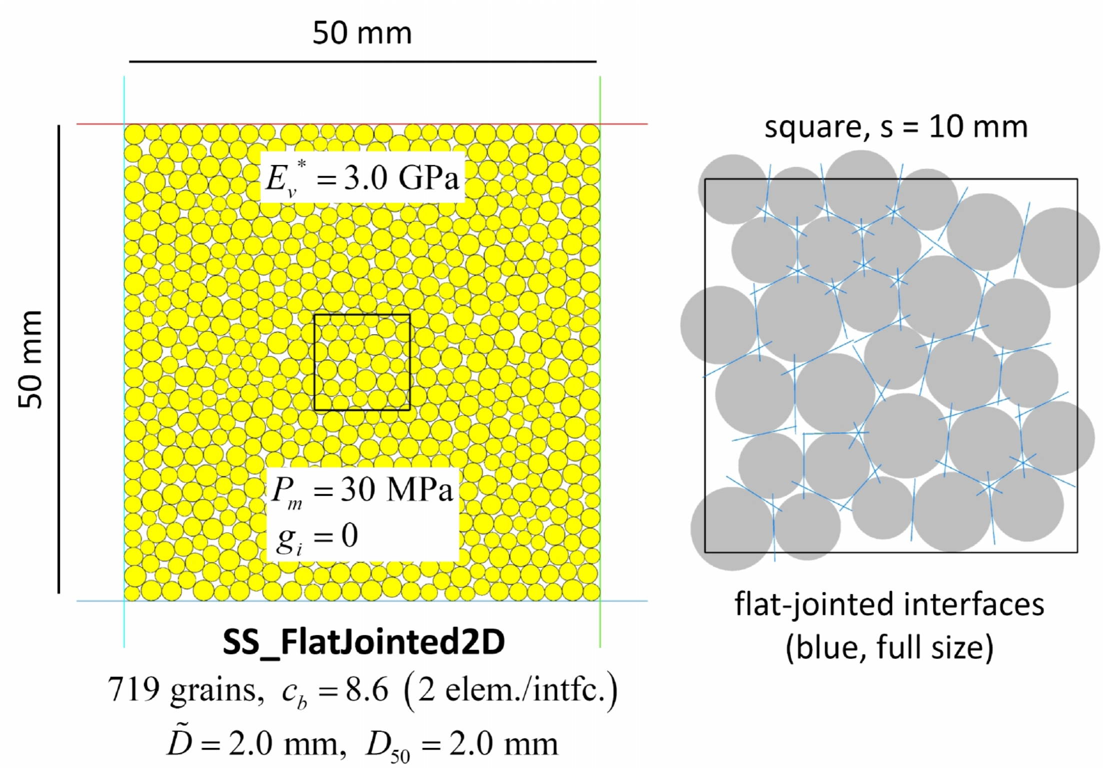

Figure 6 ***SS_FlatJointed2D material at the end of material genesis with grains and flat-jointed interfaces in the microstructural box.***

1.7 Flat-Jointed Voronoi and Tetrahedral Grain Material Examples

The flat-jointed Voronoi- and tetrahedral-grain material examples are in the **MatGen-FJ3DVoronoi** and **MatGen-FJ3DTet** example-project directories, respectively. These materials represent Lac du Bonnet granite and are denoted as LdB_FJvorC and LdB_FJtetC, respectively. Their microproperties are listed in Tables 7 and 8. The material-creation procedure and behavior during compression and tension tests are described in Potyondy et al. (2020), and the materials (including a spherical-grain material) are shown in Figure 7. The microproperties are listed here to show the relevant parameters.

Table 7 Microproperties of LdB_FJvorC Material (Voronoi grains)*

Property	Value
Common group:	
N_m	LdB_FJvorC
$T_m,\ C_r,\ \varepsilon_s,\ \varepsilon_a,\ \alpha,\ C_\rho,\ \rho_v\left[\text{kg/m}^3\right]$	4, 1, 0.01, 6, 0.7, 1, 2630
$S_g,\ T_{SD},\ \left\{D_{\{l,u\}}\,[\text{mm}],\ \phi\right\},\ D_{mult},\ f_s$	0, 0, {1.5,2.25,1.0}, 1.0, NA
Packing group:	
$S_{RN},\ P_m\,[\text{MPa}],\ \varepsilon_P,\ \varepsilon_{\lim},\ n_{\lim}$ $C_p,\ n_c$	$10001,\ 30,\ 1\times10^{-2},\ 8\times10^{-3},\ 2\times10^{6}$ 1, 0.30
Flat-jointed material group:	
$C_{MS},\ g_i\,[\text{mm}],\ \phi_B,\ \phi_G,\ (g_o)_{\{\text{m,sd}\}}\,[\text{m}],\ \{N_r, N_\alpha\}$	NA, NA, 1, 0, {0,0}, {1,3}
$\{C_\lambda,\ \lambda_v\},\ E^*\,[\text{GPa}],\ \kappa^*,\ \mu$	NA, 60, 1.5, 0.6
$(\sigma_c)_{\{\text{m, sd}\}}\,[\text{MPa}],\ (c)_{\{\text{m, sd}\}}\,[\text{MPa}],\ \gamma,\ c_r,\ M_r,\ \phi\,[\text{degrees}]$	{9.4,1.13}, {73,8.76}, 0, 0, 0, 53
Linear material group:	
$E_n^*\,[\text{GPa}],\ \kappa_n^*,\ \mu_n$	60, 1.5, 0.6

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

Table 8 Microproperties of LdB_FJtetC Material (tetrahedral grains)*

Property	Value
Common group:	
N_m	LdB_FJtetC
$T_m,\ C_r,\ \varepsilon_s,\ \varepsilon_a,\ \alpha,\ C_\rho,\ \rho_v\left[\mathrm{kg/m^3}\right]$	4, 2, 0.01, 6, 0.7, 1, 2630
$S_g,\ T_{SD},\ \left\{D_{\{l,u\}}\,[\mathrm{mm}],\ \phi\right\},\ D_{mult},\ f_s$	0, 0, {1.5,2.25,1.0}, 1.0, NA
Packing group:	
$S_{RN},\ P_m\,[\mathrm{MPa}],\ \varepsilon_P,\ \varepsilon_{\lim},\ n_{\lim}$ $C_p,\ n_c$	$10001,\ 30,\ 1\times10^{-2},\ 8\times10^{-3},\ 2\times10^{6}$ 1, 0.30
Flat-jointed material group:	
$C_{MS},\ g_i\,[\mathrm{mm}],\ \phi_B,\ \phi_G,\ (g_o)_{\{\mathrm{m,sd}\}}\,[\mathrm{m}],\ \{N_r,N_\alpha\}$	NA, NA, 1, 0, {0,0}, {1,3}
$\{C_\lambda,\ \lambda_v\},\ E^*\,[\mathrm{GPa}],\ \kappa^*,\ \mu$	NA, 80, 1.5, 0.2
$(\sigma_c)_{\{\mathrm{m,sd}\}}\,[\mathrm{MPa}],\ (c)_{\{\mathrm{m,sd}\}}\,[\mathrm{MPa}],\ \gamma,\ c_r,\ M_r,\ \phi\,[\mathrm{degrees}]$	{12,1.4}, {240,28.8}, 0, 0, 0, 0
Linear material group:	
$E_n^*\,[\mathrm{GPa}],\ \kappa_n^*,\ \mu_n$	180, 1.5, 0.2

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

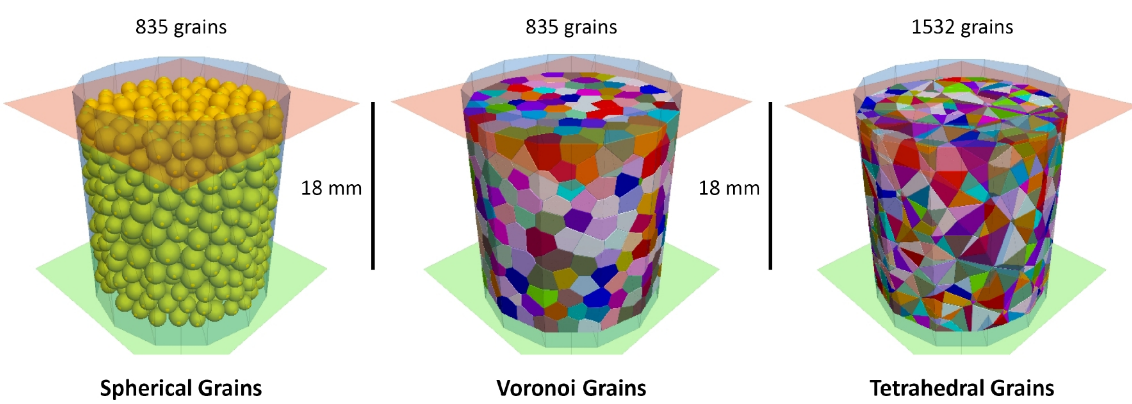

Figure 7 The three flat-jointed materials with spherical, Voronoi and tetrahedral grains at specimen resolutions of 10. (From Fig. 9 of Potyondy et al. [2020])