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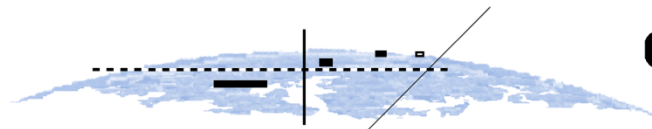
A new method of microparameter determination for PFC^{2D} synthetic rock model generation



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GFZ

GEOFORSCHUNGSZENTRUM POTSDAM

STIFTUNG DES ÖFFENTLICHEN RECHTS

Ove STEPHANSSON

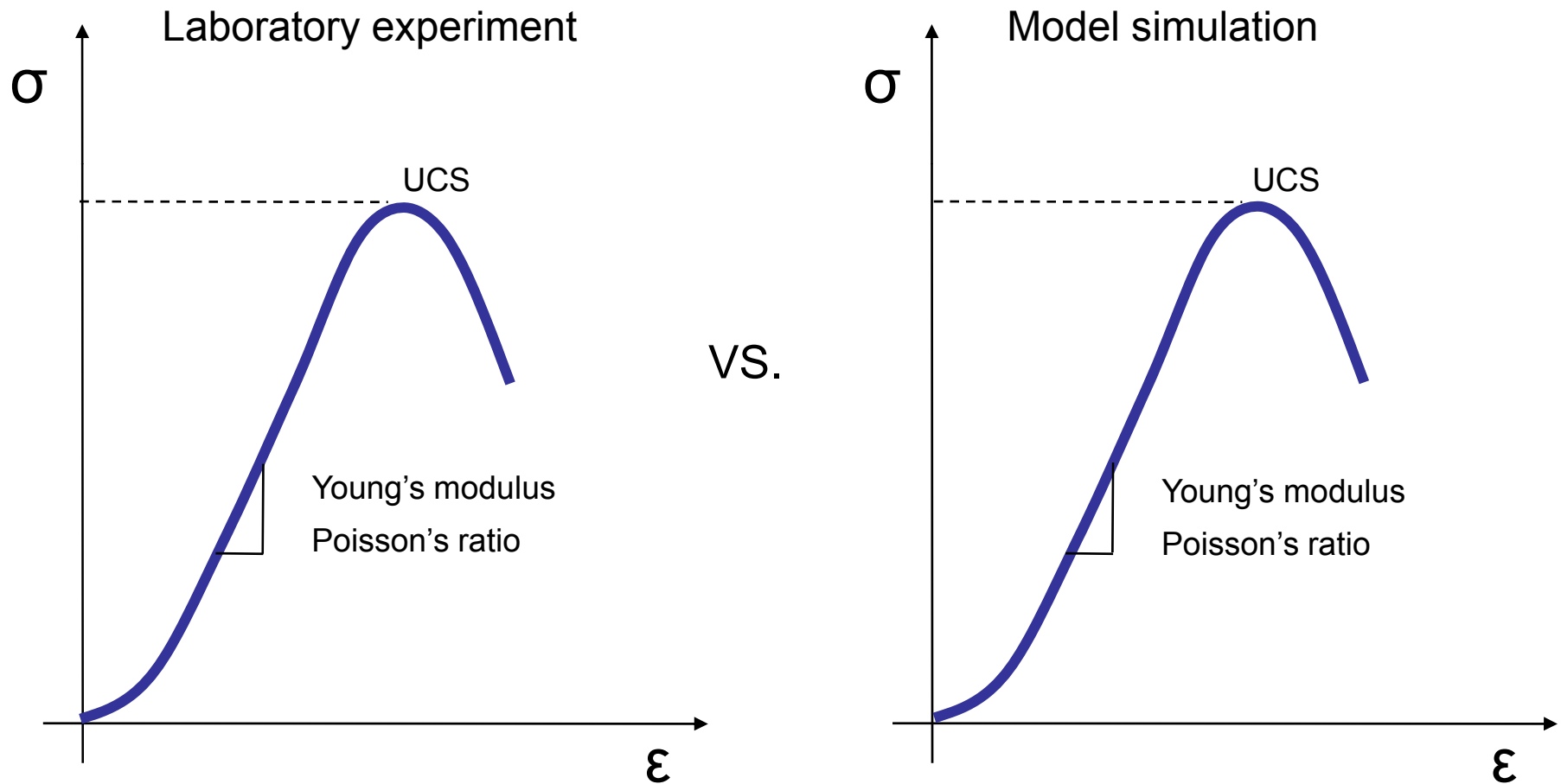
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Background

- Objective : To develop a method of model parameter calibration for a contact-bonded model in uniaxial compression test



Parameters of contact-bonded model

Parameters required in the Augmented FISHTANK*

Parameter and Description	FISH name
Ball-ball contact modulus [Pa]	md_Ec
Ball stiffness ratio [-]	md_knoverks
Ball friction coefficient [-]	md_fric
Contact-bond normal strength, mean [Pa]	cb_sn_mean
Contact-bond normal strength, std. dev. [Pa]	cb_sn_sdev
Contact-bond shear strength, mean [Pa]	cb_ss_mean
Contact bond shear strength, std. dev. [Pa]	cb_ss_sdev

* FISHTANK is provided in the PFC2D manual FISH volume.

Parameters in the present study

Factor	Description
BCM [Pa]	Ball-ball contact modulus
KNKS [-]	Ball stiffness ratio
FRIC [-]	Ball friction coefficient
NBS [Pa]	Contact-bond normal strength, mean
NBS*ROSD [Pa]	Contact-bond normal strength, std. dev.
SBS [Pa]	Contact-bond shear strength, mean
SBS*ROSD [Pa]	Contact-bond shear strength, std. dev.
BRAD [mm]	Minimum ball radius

* Factor ROSD is a ratio of standard deviation to mean of bond strength., i.e. $ROSD = \text{std.dev.} / \text{mean}$

Method

Methods

Expected outcomes

Factorial analysis
Plackett-Burman analysis

Response Surface analysis
Central Composite analysis

Optimization
Constrained non-linear
optimization programming

$$\text{UCS} = a_0 + \sum_{i=1}^7 a_i x_i$$

$$\text{Young's modulus} = b_0 + \sum_{i=1}^7 b_i x_i$$

$$\text{Poisson's ratio} = c_0 + \sum_{i=1}^7 c_i x_i$$

$$\text{Brazilian tensile strength} = d_0 + \sum_{i=1}^7 d_i x_i$$

Linear relations between macro-properties and model parameters are established.

Two most influencing model parameters are selected for UCS, Young's modulus, Poisson's ratio, and Brazilian tensile strength.

Method

Methods

Expected outcomes

Factorial analysis
Plackett-Burman analysis

Response Surface analysis
Central Composite analysis

Optimization
Constrained non-linear
optimization programming

$$\text{UCS} = a + \sum_{i=1}^2 b_i x_i + \sum_{i=1}^2 c_i x_i^2 + dx_1 x_2$$

$$\text{Young's modulus} = a + \sum_{i=1}^2 b_i x_i + \sum_{i=1}^2 c_i x_i^2 + dx_1 x_2$$

$$\text{Poisson's ratio} = a + \sum_{i=1}^2 b_i x_i + \sum_{i=1}^2 c_i x_i^2 + dx_1 x_2$$

$$\text{Brazilian tensile strength} = a + \sum_{i=1}^2 b_i x_i + \sum_{i=1}^2 c_i x_i^2 + dx_1 x_2$$

Non-linear relations between macro-properties and the most influencing model parameters are established.

Method

Methods

Expected outcomes

Factorial analysis
Plackett-Burman analysis

$$\begin{aligned}
 \text{UCS} &= a_0 + \sum_{i=1}^7 a_i x_i & \text{Young's modulus} &= b_0 + \sum_{i=1}^7 b_i x_i \\
 \text{Poisson's ratio} &= c_0 + \sum_{i=1}^7 c_i x_i & \text{Brazilian tensile strength} &= d_0 + \sum_{i=1}^7 d_i x_i \\
 \text{UCS} &= a + \sum_{i=1}^2 b_i x_i + \sum_{i=1}^2 c_i x_i^2 + dx_1 x_2 & \text{Young's modulus} &= a + \sum_{i=1}^2 b_i x_i + \sum_{i=1}^2 c_i x_i^2 + dx_1 x_2 \\
 \text{Poisson's ratio} &= a + \sum_{i=1}^2 b_i x_i + \sum_{i=1}^2 c_i x_i^2 + dx_1 x_2 & & \\
 \text{Brazilian tensile strength} &= a + \sum_{i=1}^2 b_i x_i + \sum_{i=1}^2 c_i x_i^2 + dx_1 x_2 & &
 \end{aligned}$$

Response Surface analysis
Central Composite analysis

Choosing model parameters

-> Constrained non-linear optimization problem

Optimization
Constrained non-linear
optimization programming

Optimized
model
parameters



Model
generation
&
Uniaxial test



Model
UCS
Young's
modulus
Poisson's
ratio

VS.

Rock
UCS
Young's
modulus
Poisson's
ratio

Method 1 – Factorial analysis

Model parameter	Description	-1 level	Avg	+1 level
BCM	Ball-ball contact modulus	40 GPa	70 GPa	100 GPa
KNKS	Ball stiffness ratio	1.0	2.5	4.0
FRIC	Ball friction coefficient	0.25	0.50	0.75
NBS	Normal bond strength (avg.)	50 MPa	125 MPa	200 MPa
SBS	Shear bond strength (avg.)	50 MPa	125 MPa	200 MPa
ROSD	Ratio of std. dev. to avg. bond strength	0.24	0.32	0.40
BRAD	Minimum ball radius	0.24 mm	0.36 mm	0.48 mm

Macro-property	Range
UCS	70 ~250 [MPa]
Young's modulus	25 ~ 70 [GPa]
Poisson's ratio	0.1 ~ 0.3

Yoon J. 2007. Application of experimental design and optimization to PFC model calibration in uniaxial compression simulation. Int. J. Rock Mech. & Min. Sci 44.: 871-889.

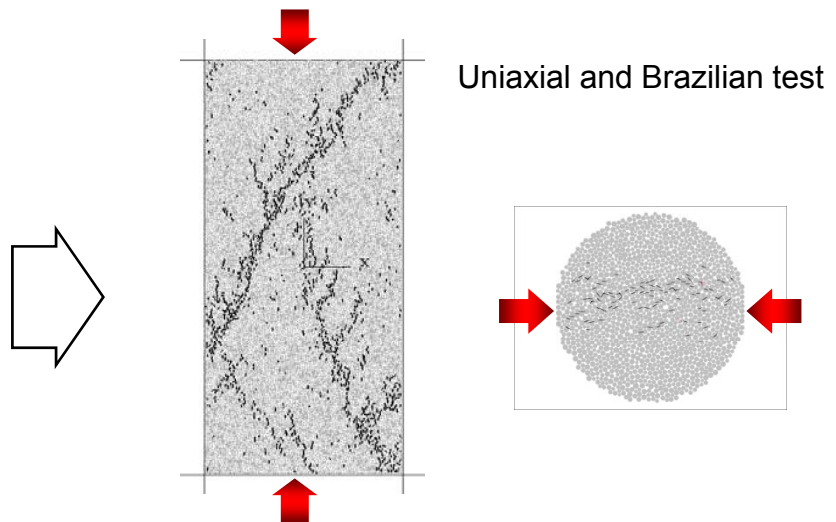
Design matrix for Plackett-Burman design and test results

Plackett RL, Burman JP. 1946. The design of multifactorial experiments. Biometrika; 33: 305-325.

Run no.	BCM	KN KS	FRIC	NBS	SBS	RO SD	BR AD	UCS (MPa)	Young's Modulus (GPa)	Poisson's Ratio (---)	Tensile Strength (MPa)
1	-1	+1	+1	+1	-1	-1	-1	86.56	23.16	0.234	22.02
2	-1	-1	-1	+1	-1	-1	+1	58.96	33.75	0.122	15.49
3	-1	+1	-1	-1	+1	-1	+1	77.98	22.40	0.266	19.45
4	+1	-1	-1	-1	+1	-1	-1	91.47	86.92	0.100	18.37
5	+1	+1	+1	+1	+1	+1	+1	196.27	55.37	0.273	51.55
6	+1	-1	+1	+1	+1	-1	-1	225.02	87.01	0.097	50.26
7	+1	+1	+1	-1	-1	-1	+1	58.23	55.70	0.265	12.36
8	+1	+1	-1	-1	-1	+1	-1	45.59	55.81	0.268	9.55
9	+1	-1	-1	+1	-1	+1	+1	45.74	83.18	0.113	18.93
10	-1	+1	-1	+1	+1	+1	-1	199.81	23.00	0.247	38.56
11	-1	-1	+1	-1	-1	+1	-1	46.67	33.64	0.103	10.12
12	-1	-1	+1	-1	+1	+1	+1	86.37	33.62	0.130	16.70

For example)

Factor	Setting	Value
BCM	-1	40 GPa
KNKS	-1	1.0
FRIC	+1	0.75
NBS	-1	50 MPa
SBS	+1	200 MPa
ROSD	+1	0.40
BRAD	+1	0.48 mm



Linear relations resulted from Plackett-Burman design analysis

Uniaxial compressive strength

$$= 101.56 + 8.83 \text{ BCM} + 9.18 \text{ KNKS} + 14.96 \text{ FRIC} \\ + 33.84 \text{ NBS} + 44.60 \text{ SBS} + 1.85 \text{ ROSD} - 14.30 \text{ BRAD}$$

Young's modulus

$$= 49.54 + 21.28 \text{ BCM} - 10.30 \text{ KNKS} - 1.31 \text{ FRIC} \\ + 1.52 \text{ NBS} + 2.00 \text{ SBS} - 2.10 \text{ ROSD} - 2.20 \text{ BRAD}$$

Poisson's ratio

$$= 0.1848 + 0.0012 \text{ BCM} + 0.0740 \text{ KNKS} - 0.0012 \text{ FRIC} \\ - 0.0038 \text{ NBS} + 0.0006 \text{ SBS} + 0.0042 \text{ ROSD} + 0.1000 \text{ BRAD}$$

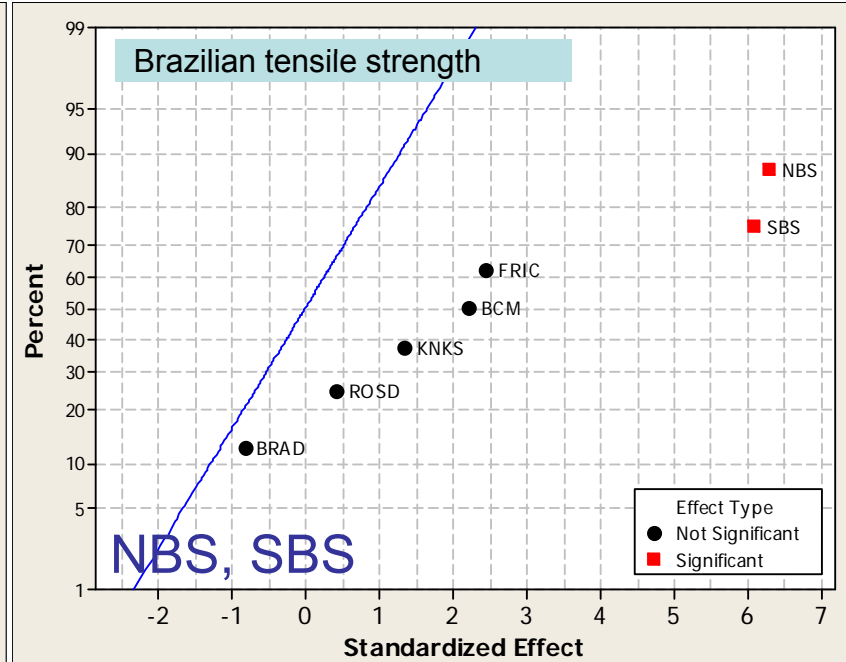
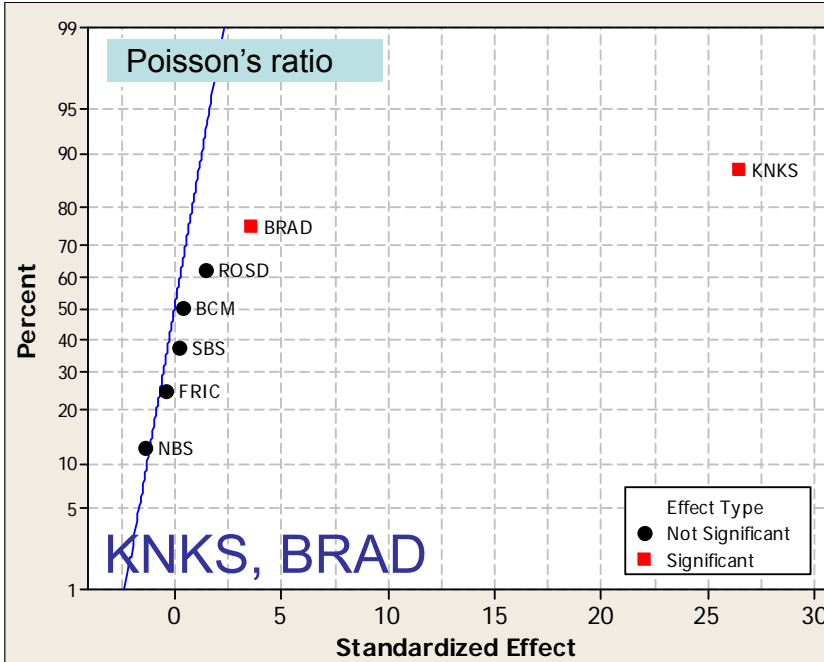
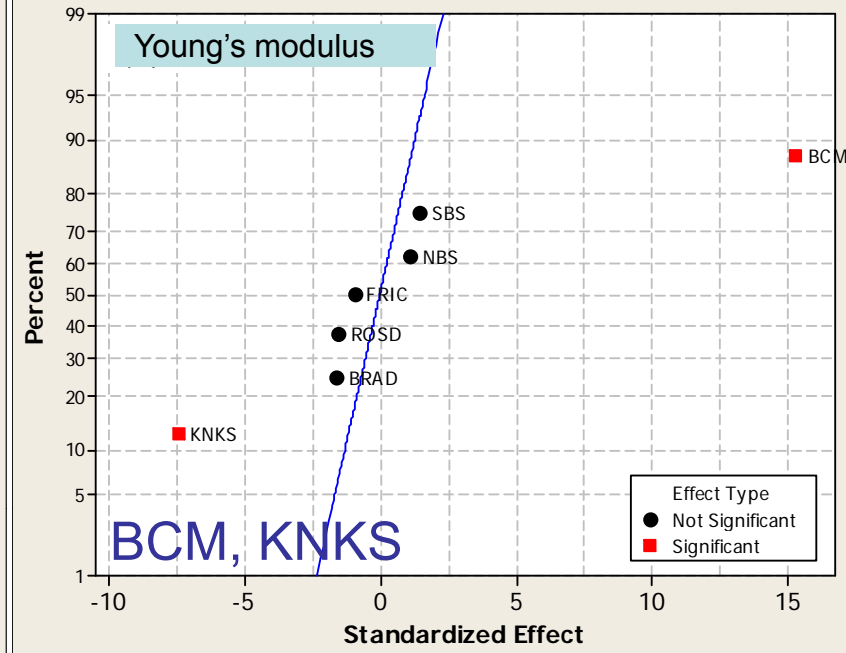
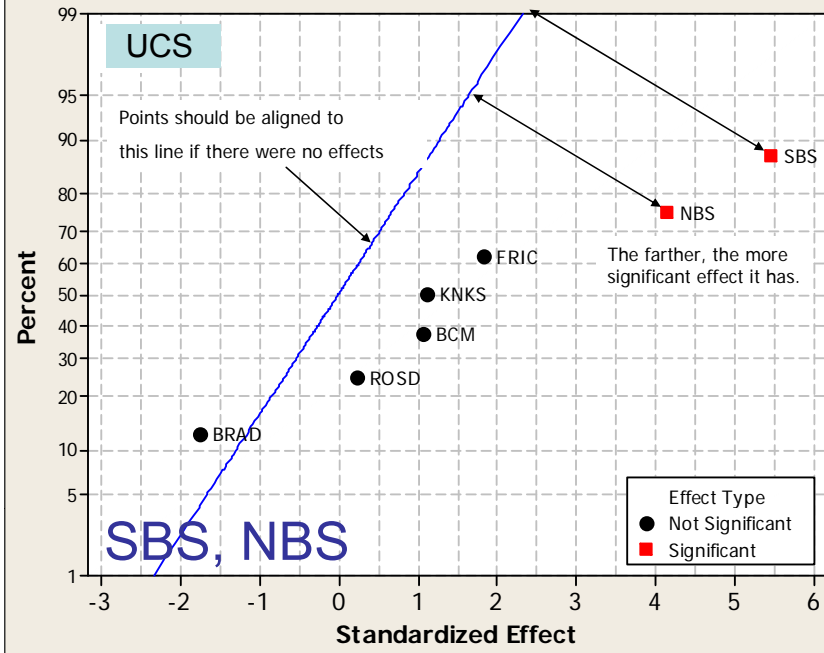
Brazilian tensile strength

$$= 23.613 + 3.223 \text{ BCM} + 1.968 \text{ KNKS} + 3.555 \text{ FRIC} \\ + 9.188 \text{ NBS} + 8.868 \text{ SBS} + 0.622 \text{ ROSD} - 1.200 \text{ BRAD}$$

Matrix form)

$$\begin{pmatrix} 101.56 & 8.83 & 9.18 & 14.96 & 33.84 & 44.60 & 1.85 & -14.30 \\ 49.54 & 21.28 & -10.30 & -1.31 & 1.52 & 2.00 & -2.10 & -2.20 \\ 0.1848 & 0.0012 & 0.0740 & -0.0012 & -0.0038 & 0.0006 & 0.0042 & 0.0100 \\ 23.613 & 3.223 & 1.968 & 3.555 & 9.188 & 8.868 & 0.622 & -1.200 \end{pmatrix} \times \begin{pmatrix} 1 \\ \text{BCM} \\ \text{KNKS} \\ \text{FRIC} \\ \text{NBS} \\ \text{SBS} \\ \text{ROSD} \\ \text{BRAD} \end{pmatrix} = \begin{pmatrix} \text{UCS} \\ \text{Young's modulus} \\ \text{Poisson's ratio} \\ \text{Tensile strength} \end{pmatrix}$$

The most influencing parameters for macro-property



Method 2 – Response Surface analysis

- Macro-properties are expressed by the most influencing parameters.

Macro-property	Two most influential parameters
UCS	SBS, NBS
Young's modulus	BCM, KNKS
Poisson's ratio	KNKS, BRAD
Brazilian tensile strength	NBS, SBS

$$\text{UCS} = f(\text{SBS}, \text{NBS})$$

$$\text{Young's modulus} = f(\text{BCM}, \text{KNKS})$$

$$\text{Poisson's ratio} = f(\text{KNKS}, \text{BRAD})$$

$$\text{Brazilian tensile strength} = f(\text{NBS}, \text{SBS})$$

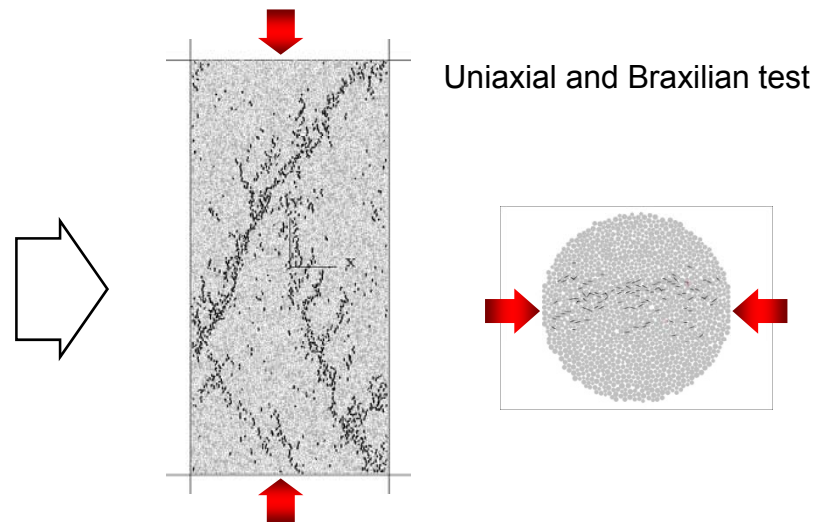
Design matrix of Central Composite design and test results

No.	NBS	SBS	UCS (MPa)	Tensile strength (MPa)	BCM	KNKS	Young's Modulus (GPa)	KNKS	BRAD	Poisson's ratio
1	-√2	Avg	32.81	6.58	Avg	Avg	45.92	+√2	Avg	0.255
2	-1	+1	75.04	16.48	Avg	+√2	36.79	Avg	Avg	0.194
3	-1	-1	50.39	11.22	Avg	Avg	45.92	-1	+1	0.114
4	+1	-1	69.08	16.68	Avg	Avg	45.92	Avg	Avg	0.194
5	+1	+1	215.42	47.63	-1	+1	22.48	-√2	Avg	0.019
6	Avg	Avg	128.79	30.29	+1	+1	55.78	-1	-1	0.093
7	Avg	Avg	128.79	30.29	-√2	Avg	18.55	Avg	-√2	0.178
8	Avg	Avg	128.79	30.29	Avg	-√2	70.92	Avg	+√2	0.202
9	Avg	Avg	128.79	30.29	Avg	Avg	45.92	Avg	Avg	0.194
10	Avg	Avg	128.79	30.29	+√2	Avg	72.98	+1	+1	0.250
11	+√2	Avg	157.12	38.87	Avg	Avg	45.92	Avg	Avg	0.194
12	Avg	+√2	154.54	40.89	-1	-1	34.68	Avg	Avg	0.194
13	Avg	-√2	26.69	6.59	+1	-1	85.79	+1	-1	0.252

The values of the rest of model parameters are set to avg. value.

For example)

Factor	Setting	Value
BCM		70 GPa
KNKS		2.5
FRIC		0.50
NBS	+√2	231 MPa
SBS	Avg	125 MPa
ROSD		0.32
BRAD		0.36 mm



Non-linear relations resulted from Central Composite design analysis

UCS

$$= 128.79 + 41.86 \text{ NBS} + 43.97 \text{ SBS} - 14.49 \text{ NBS}^2 - 16.66 \text{ SBS}^2 + 30.42 \text{ NBS*SBS}$$

Young's modulus

$$= 45.92 + 20.17 \text{ BCM} - 11.31 \text{ KNKS} - 0.11 \text{ BCM}^2 + 3.93 \text{ KNKS}^2 - 4.45 \text{ BCM*KNKS}$$

Poisson's ratio

$$= 0.194 + 0.078 \text{ KNKS} + 0.006 \text{ BRAD} - 0.025 \text{ KNKS}^2 + 0.001 \text{ BRAD}^2 - 0.006 \text{ KNKS*BRAD}$$

Brazilian tensile strength

$$= 30.29 + 10.28 \text{ NBS} + 10.59 \text{ SBS} - 3.84 \text{ NBS}^2 - 3.32 \text{ SBS}^2 + 6.42 \text{ NBS*SBS}$$

Matrix form)

$$\begin{pmatrix}
 128.79 & 41.86 & 43.97 & -14.49 & -16.66 & 30.42 \\
 45.92 & 20.17 & -11.31 & -0.11 & 3.93 & -4.45 \\
 0.194 & 0.078 & 0.006 & -0.025 & 0.001 & -0.006 \\
 30.29 & 10.28 & 10.59 & -3.84 & -3.32 & 6.42
 \end{pmatrix}
 \times
 \begin{pmatrix}
 1 & 1 & 1 & 1 \\
 \text{NBS} & \text{BCM} & \text{KNKS} & \text{NBS} \\
 \text{SBS} & \text{KNKS} & \text{BRAD} & \text{SBS} \\
 \text{NBS}^2 & \text{BCM}^2 & \text{KNKS}^2 & \text{NBS}^2 \\
 \text{SBS}^2 & \text{KNKS}^2 & \text{BRAD}^2 & \text{SBS}^2 \\
 \text{NBS} & \text{BCM} & \text{KNKS} & \text{NBS} \\
 \text{*SBS} & \text{*KNKS} & \text{*BRAD} & \text{*SBS}
 \end{pmatrix}
 =
 \begin{pmatrix}
 \text{UCS} & 0 & 0 & 0 \\
 0 & \text{Young's modulus} & 0 & 0 \\
 0 & 0 & \text{Poisson's ratio} & 0 \\
 0 & 0 & 0 & \text{Tensile strength}
 \end{pmatrix}$$

Results of PB design and CCD

PB

UCS

$$= 101.56 + 8.83 \text{ BCM} + 9.18 \text{ KNKS} + 14.96 \text{ FRIC} \\ + 33.84 \text{ NBS} + 44.60 \text{ SBS} + 1.85 \text{ ROSD} - 14.30 \text{ BRAD}$$

Young's modulus

$$= 49.54 + 21.28 \text{ BCM} - 10.30 \text{ KNKS} - 1.31 \text{ FRIC} \\ + 1.52 \text{ NBS} + 2.00 \text{ SBS} - 2.10 \text{ ROSD} - 2.20 \text{ BRAD}$$

Poisson's ratio

$$= 0.1848 + 0.0012 \text{ BCM} + 0.0740 \text{ KNKS} - 0.0012 \text{ FRIC} \\ - 0.0038 \text{ NBS} + 0.0006 \text{ SBS} + 0.0042 \text{ ROSD} + 0.1000 \text{ BRAD}$$

Brazilian tensile strength

$$= 23.613 + 3.223 \text{ BCM} + 1.968 \text{ KNKS} + 3.555 \text{ FRIC} \\ + 9.188 \text{ NBS} + 8.868 \text{ SBS} + 0.622 \text{ ROSD} - 1.200 \text{ BRAD}$$

CCD

UCS

$$= 128.79 + 41.86 \text{ NBS} + 43.97 \text{ SBS} - 14.49 \text{ NBS}^2 - 16.66 \text{ SBS}^2 + 30.42 \text{ NBS*SBS}$$

Young's modulus

$$= 45.92 + 20.17 \text{ BCM} - 11.31 \text{ KNKS} - 0.11 \text{ BCM}^2 + 3.93 \text{ KNKS}^2 - 4.45 \text{ BCM*KNKS}$$

Poisson's ratio

$$= 0.194 + 0.078 \text{ KNKS} + 0.006 \text{ BRAD} - 0.025 \text{ KNKS}^2 + 0.001 \text{ BRAD}^2 - 0.006 \text{ KNKS*BRAD}$$

Brazilian tensile strength

$$= 30.29 + 10.28 \text{ NBS} + 10.59 \text{ SBS} - 3.84 \text{ NBS}^2 - 3.32 \text{ SBS}^2 + 6.42 \text{ NBS*SBS}$$

Method 3 - Optimization

- Objective function, $f(x)$:

Minimize $|\text{UCS (simulated)} - \text{UCS (tested)}|$

- Constraints :

Young's modulus (simulated) = Young's modulus (tested)

Poisson's ratio (simulated) = Poisson's ratio (tested)

$$3 \leq \frac{\text{UCS}}{\text{Tensile strength}} \leq 10$$

$$2 \leq \frac{\text{Shear bond strength}}{\text{Normal bond strength}} \leq 3$$

Mathematical formulation

Standardized format of
constrained non-linear
optimization problem

min $f(x)$
; subject to
 $C(x) \leq 0$ (non-linear inequality constraint)
 $C_{eq} = 0$ (non-linear equality constraint)
 $A \cdot x \leq b$ (linear inequality constraint)
 $A_{eq} \cdot x = b_{eq}$ (linear equality constraint)
 $lb \leq x \leq ub$ (side constraint)

Mathematical formulation

Objective

$$\text{Minimize } |128.79 + 41.86x_4 + 43.97x_5 - 14.49x_4^2 - 16.66x_5^2 + 30.42x_4x_5 - UCS^*|$$

Linear equality constraints

$$101.56 + 8.83x_1 + 9.18x_2 + 14.96x_3 + 33.84x_4 + 44.60x_5 + 1.85x_6 - 14.30x_7 - UCS^* = 0$$

$$49.54 + 21.28x_1 - 10.30x_2 - 1.31x_3 + 1.52x_4 + 2.00x_5 - 2.10x_6 - 2.20x_7 - \text{Young's modulus}^* = 0$$

$$0.1848 + 0.0012x_1 + 0.0740x_2 - 0.0012x_3 - 0.0038x_4 + 0.0006x_5 + 0.0042x_6 + 0.0100x_7 - \text{Poisson's ratio}^* = 0$$

Linear inequality constraints

$$-30.721 + 0.839x_1 - 3.276x_2 - 4.295x_3 - 6.276x_4 - 17.996x_5 + 0.016x_6 + 10.700x_7 \leq 0$$

$$-134.57 - 23.40x_1 - 10.50x_2 - 20.59x_3 - 58.04x_4 - 44.08x_5 - 4.37x_6 - 2.30x_7 \leq 0$$

$$0x_1 + 0x_2 + 0x_3 + 6x_4 - 3x_5 + 0x_6 + 0x_7 \leq -5$$

$$0x_1 + 0x_2 + 0x_3 - 9x_4 + 3x_5 + 0x_6 + 0x_7 \leq 10$$

Non-linear inequality constraints

$$-37.92 - 11.01x_4 - 12.20x_5 + 2.97x_4^2 + 6.66x_5^2 - 11.15x_4x_5 \leq 0$$

$$-174.11 - 60.98x_4 - 61.93x_5 + 23.91x_4^2 + 16.66x_5^2 - 33.81x_4x_5 \leq 0$$

Side constraints

$$-1 \leq x_i \leq 1, \quad i=1, 2, \dots, 7;$$

where, x_1 =BCM, x_2 =KNKS, x_3 =FRIC, x_4 =NBS, x_5 =SBS, x_6 =ROSD, x_7 =BRAD.

UCS*, Young's modulus*, Poisson's ratio* (Laboratory test results)

MATLAB programming

```
MATLAB Command Window
File Edit View Window Help
[Icons]
?doeopti
=====
PLEASE NOTE! YOU MUST CHANGE THE UCS VALUE
IN THE objfun.m FILE TO WHAT YOU ARE GOING
TO INPUT ON THE NEXT LINE (PROCEED WITH CARE)
=====
Programmed by Yoon 1st ed. 22/10/2005 GFZ
Programmed by Yoon 2nd ed. 15/10/2007 SNU
=====
Uniaxial compressive strength [MPa] : 134
Youngs modulus [GPa] : 48
Poissons ratio [---] : 0.25
=====
1496 14171 0.00129274 1.332e-015 0.0625 -0.00136
1497 14180 7.08828e-005 2.776e-017 1 -0.000682
1498 14191 9.95697e-005 2.776e-017 0.25 -8.52e-005
Optimization terminated successfully:
Search direction less than 2*options.TolX and
maximum constraint violation is less than options.TolCon
Active Constraints:
1
2
15
uncoded_x = Optimized parameters
( 83.2753 3.6728 0.6092 118.4210 143.0916 0.4000 0.3916 )
?
Ready NUM
```

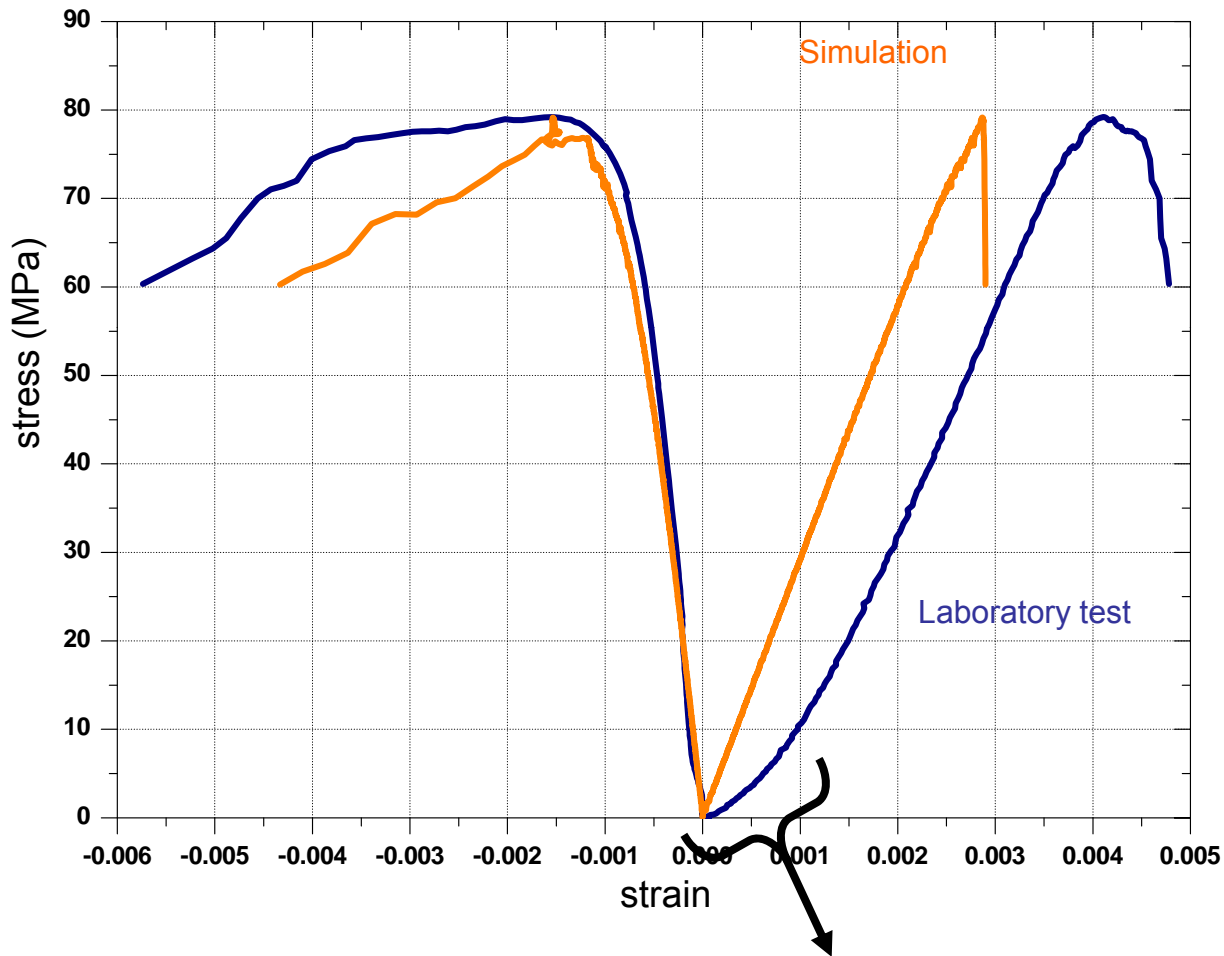
UCS
Young's modulus
Poisson's ratio

(Uniaxial compressive strength [MPa] : 134
Youngs modulus [GPa] : 48
Poissons ratio [---] : 0.25)

Do these optimized parameter ???

*** Optimization function: fmincon (Matlab ver 5.3 Optimization)

Verification of solution – Quantitative matching



(*) Non-linear portion due to grain boundary sliding and closure of pre-existing flaws and micro-cracks

Macro-properties
UCS : 79.0 MPa
Young's modulus: 25 GPa
Poisson's ratio : 0.21

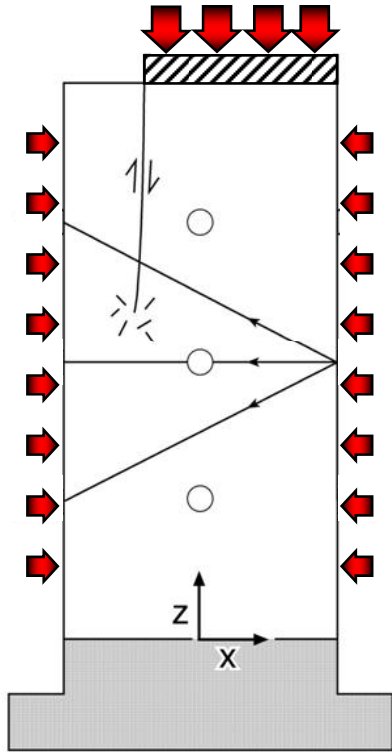


Optimized parameters
BCM : 45 GPa
KNKS : 3.1
FRIC : 0.75
NBS : 81 MPa
SBS : 82 MPa
ROSD : 0.35
BRAD : 0.27 mm



Simulation
UCS : 76 MPa
Young's modulus : 28 GPa
Poisson's ratio : 0.23

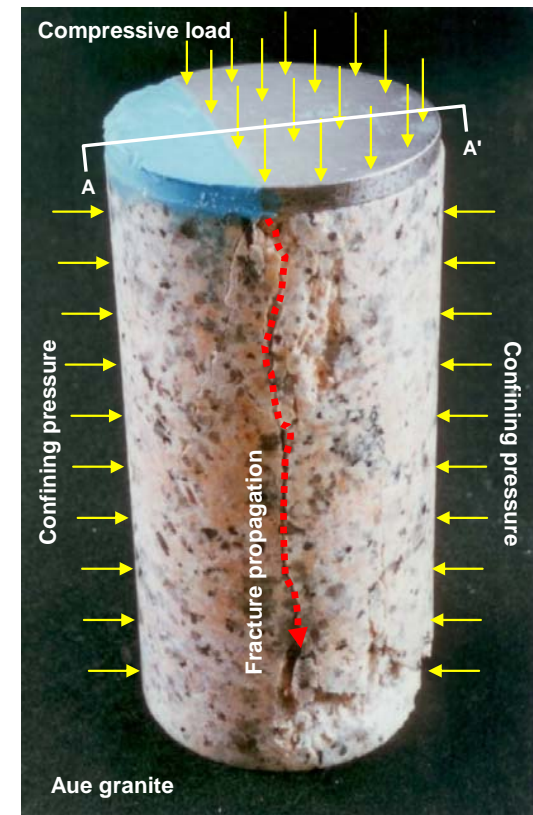
Verification of solution – Qualitative matching



Fracture and friction triaxial compression test
(Zang et al., 1998; 2000; 2002)

- Starting point of fracturing/cracking is pre-determined.
- Pure rock fracture and friction properties are tested in one test configuration

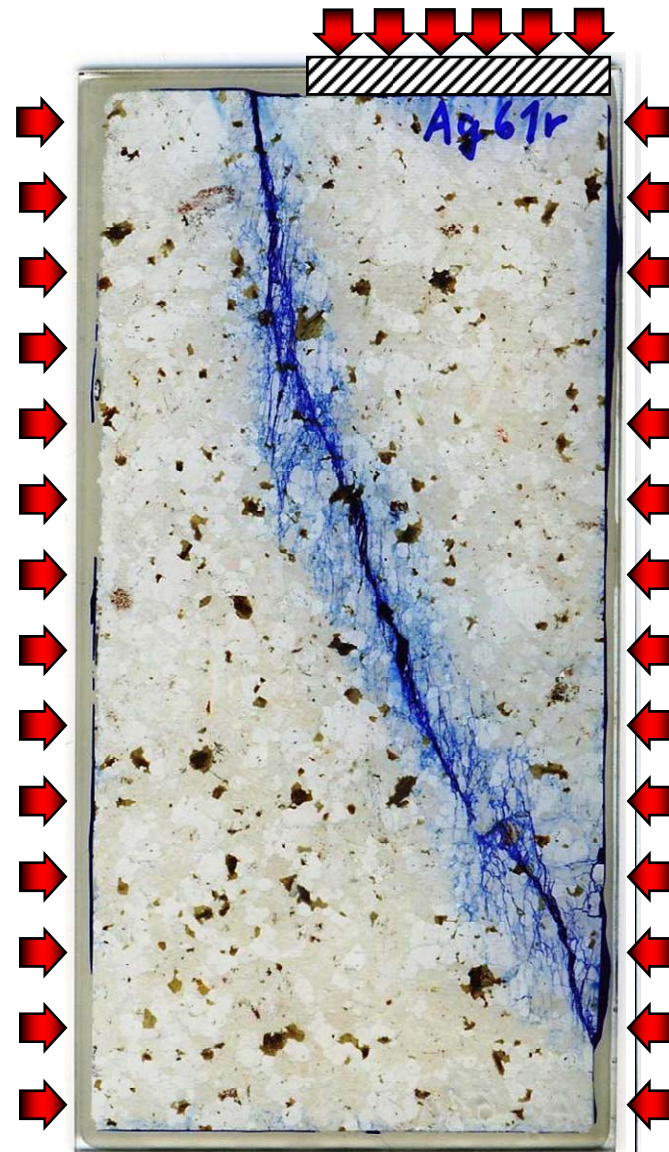
Aue granite, Germany
UCS : 137 MPa
Young's modulus : 70 GPa
Poisson's ratio : 0.19



Cracking and fracturing patterns



$P_{con} = 0 \text{ MPa}$



$P_{con} = 10 \text{ MPa}$

With $2 \leq \frac{SBS}{NBS} \leq 3$ constraint

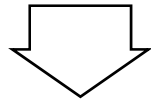
Without $2 \leq \frac{SBS}{NBS} \leq 3$ constraint

Target macro-properties
UCS : 137 MPa
Young's modulus : 70 GPa
Poisson's ratio : 0.19

Model #1

Parameters	Optimum value
BCM	96.6460 GPa
KNKS	2.5167
FRIC	0.4395
NBS	100.0025 MPa
SBS	200.0000 MPa
ROSD	0.3132
BRAD	0.2500 mm

Model generation & Uniaxial
compression



Simulated results

UCS : 145 MPa (5.8%)

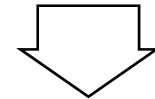
Young's modulus : 65 GPa (7.1%)

Poisson's ratio : 0.20 (5.3%)

Model #2

Parameters	Optimum value
BCM	98.8960 GPa
KNKS	2.7744
FRIC	0.7461
NBS	139.2425 MPa
SBS	126.1850 MPa
ROSD	0.3123
BRAD	0.2500 mm

Model generation & Uniaxial
compression



Simulated results

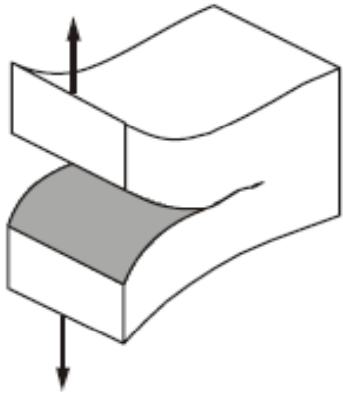
UCS : 129 MPa (5.8%)

Young's modulus : 64 GPa (8.6%)

Poisson's ratio : 0.21 (11%)

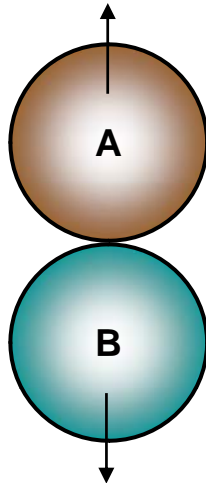
Physical interpretation of the imposed constraint

Rock material



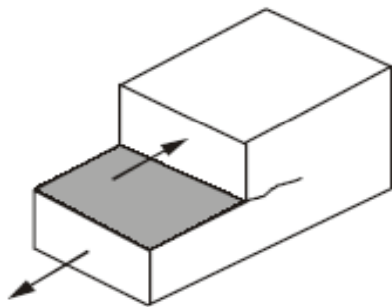
K_{Ic}

PFC model

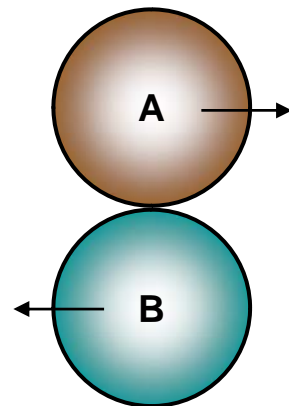


Contact-bond normal strength
(NBS)

$$K_{Ic} = NBS$$



K_{IIc}

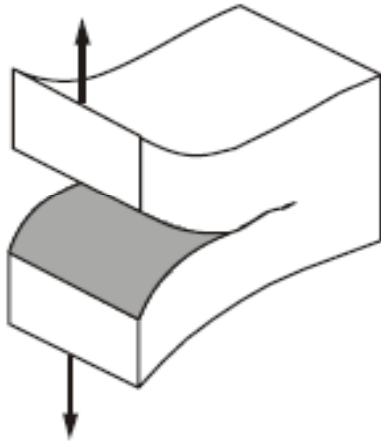


Contact-bond shear strength
(SBS)

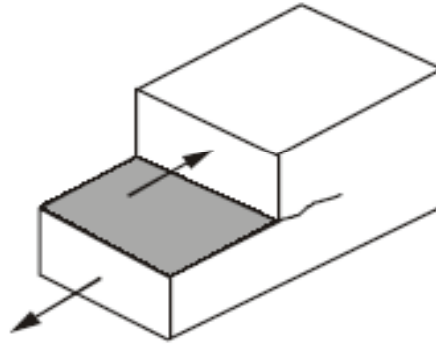
$$K_{IIc} = SBS$$

Physical interpretation of the imposed constraint

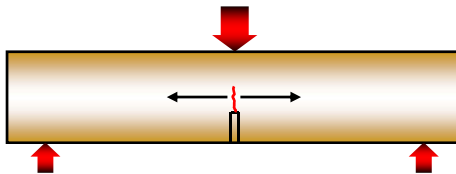
Rock material



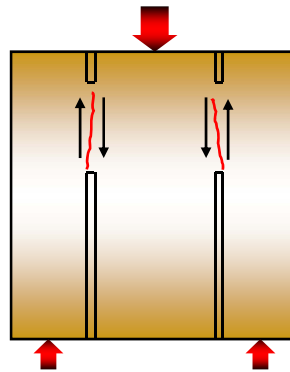
K_{Ic}
Chevron Bend method



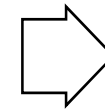
K_{IIc}
Punch Through Shear method*



K_{Ic} of Aue granite
= 1.2 MPa√m



K_{IIc} of Aue granite
= 3.1 MPa√m

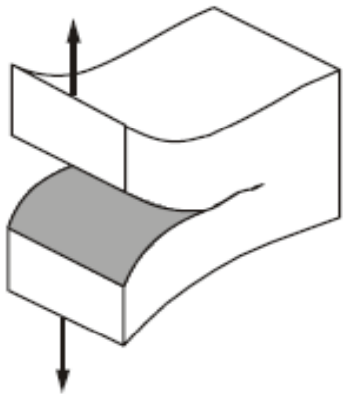


$$\frac{K_{IIc}}{K_{Ic}} = \frac{3.1}{1.2} = 2.6$$

* Backers T. 2005. Fracture toughness determination and micromechanics of rock under mode I and mode II loading. Doctoral Thesis. University of Potsdam. Germany.

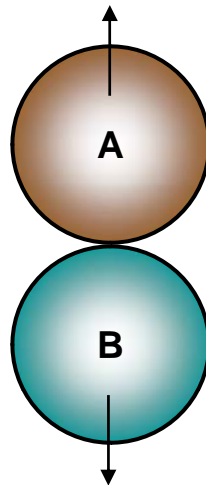
Physical interpretation of the imposed constraint

Rock material

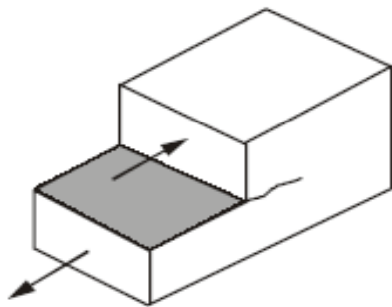


K_{Ic}

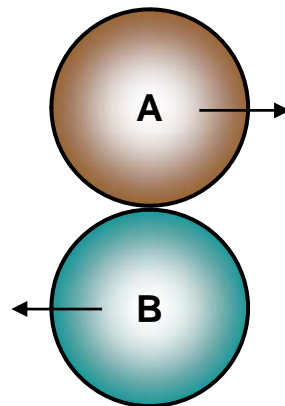
PFC model



Contact-bond normal strength (NBS)



K_{IIc}



Contact-bond shear strength (SBS)

Experiment $\frac{K_{IIc}}{K_{Ic}} = 2.6$

Assumption $2 \leq \frac{SBS}{NBS} \leq 3$

$$2 \leq \frac{SBS}{NBS} \leq 3 \Rightarrow \begin{cases} 2*NBS - SBS \leq 0 \\ -3*NBS + SBS \leq 0 \end{cases}$$

Mathematical formulation

$$\begin{aligned} NBS &= 75*x_4 + 125 \\ SBS &= 75*x_5 + 125 \end{aligned}$$

Constraints to be used

$$6x_4 - 3x_5 \leq -5$$

$$-9x_4 + 3x_5 \leq 10$$

Mathematical formulation

Standardized format of
constrained non-linear
optimization problem

min $f(x)$
; subject to
 $C(x) \leq 0$ (non-linear inequality constraint)
 $C_{eq} = 0$ (non-linear equality constraint)
 $A*x \leq b$ (linear inequality constraint)
 $A_{eq}*x = b_{eq}$ (linear equality constraint)
 $lb \leq x \leq ub$ (side constraint)

Mathematical formulation

Objective

$$\text{Minimize } |128.79+41.86x_4+43.97x_5-14.49x_4^2-16.66x_5^2+30.42x_4x_5-UCS^*|$$

Linear equality constraints

$$101.56+8.83x_1+9.18x_2+14.96x_3+33.84x_4+44.60x_5+1.85x_6-14.30x_7-UCS^*=0$$

$$49.54+21.28x_1-10.30x_2-1.31x_3+1.52x_4+2.00x_5-2.10x_6-2.20x_7-\text{Young's modulus}^*=0$$

$$0.1848+0.0012x_1+0.0740x_2-0.0012x_3-0.0038x_4+0.0006x_5+0.0042x_6+0.0100x_7-\text{Poisson's ratio}^*=0$$

Linear inequality constraints

$$-30.721+0.839x_1-3.276x_2-4.295x_3-6.276x_4-17.996x_5+0.016x_6+10.700x_7 \leq 0$$

$$-134.57-23.40x_1-10.50x_2-20.59x_3-58.04x_4-44.08x_5-4.37x_6-2.30x_7 \leq 0$$

$$\left(\begin{array}{l} 0x_1+0x_2+0x_3+6x_4-3x_5+0x_6+0x_7 \leq -5 \\ 0x_1+0x_2+0x_3-9x_4+3x_5+0x_6+0x_7 \leq 10 \end{array} \right)$$

Non-linear inequality constraints

$$-37.92-11.01x_4-12.20x_5+2.97x_4^2+6.66x_5^2-11.15x_4x_5 \leq 0$$

$$-174.11-60.98x_4-61.93x_5+23.91x_4^2+16.66x_5^2-33.81x_4x_5 \leq 0$$

Side constraints

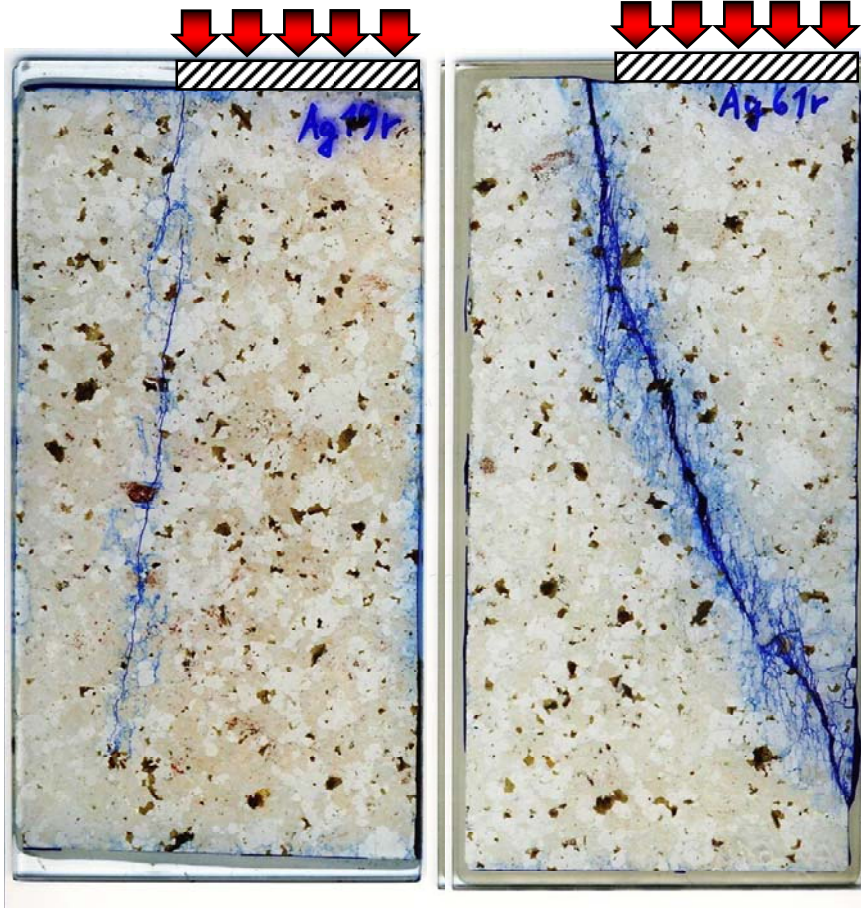
$$-1 \leq x_i \leq 1, \quad i=1,2,\dots,7;$$

where, x_1 =BCM, x_2 =KNKS, x_3 =FRIC, x_4 =NBS, x_5 =SBS, x_6 =ROSD, x_7 =BRAD.

UCS*, Young's modulus*, Poisson's ratio* (Laboratory test results)

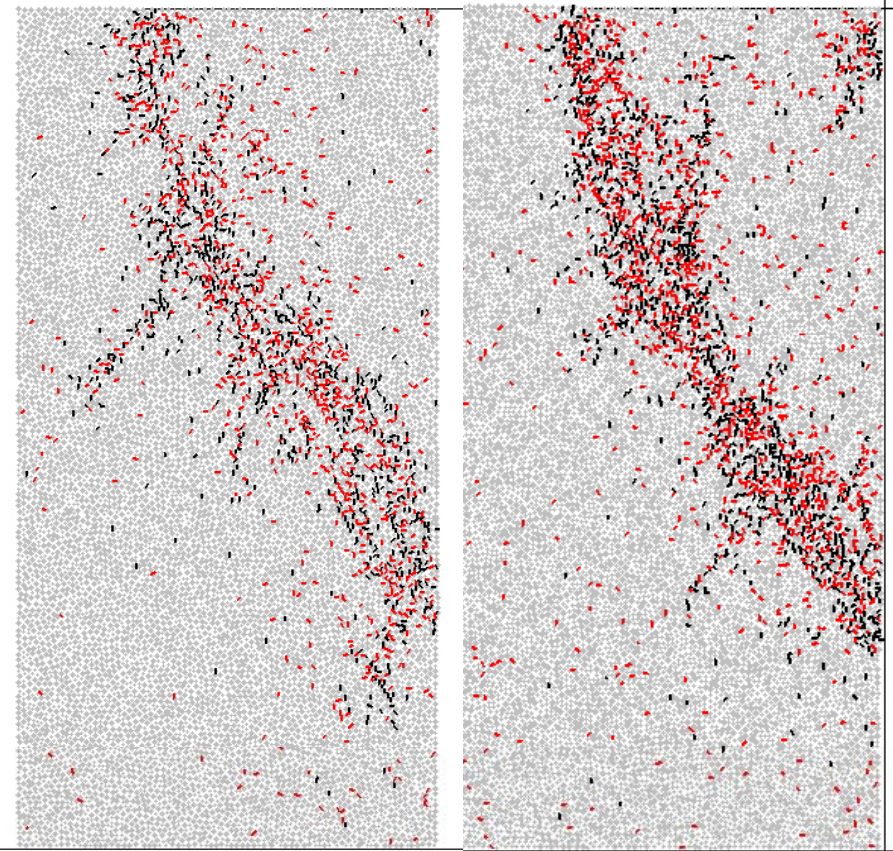
Without $2 \leq \frac{\text{SBS}}{\text{NBS}} \leq 3$ constraint

Black : tensile crack Red : shear crack



Pcon= 0 MPa

Pcon= 10 MPa

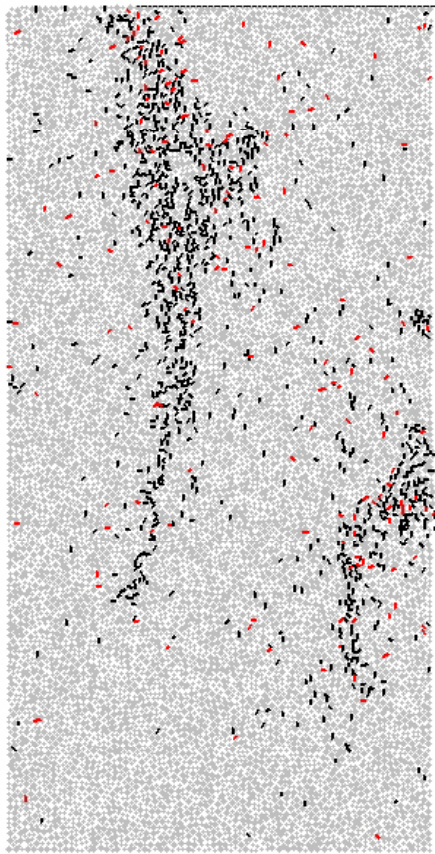


Pcon= 0 MPa

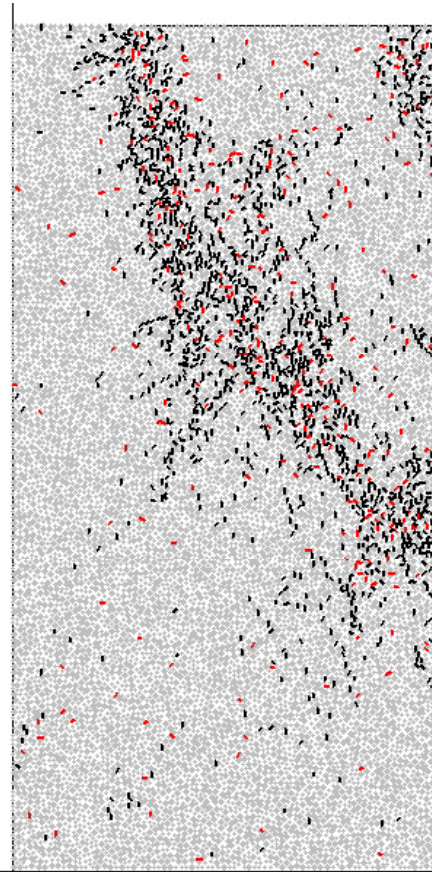
Pcon= 10 MPa

With $2 \leq \frac{SBS}{NBS} \leq 3$ constraint

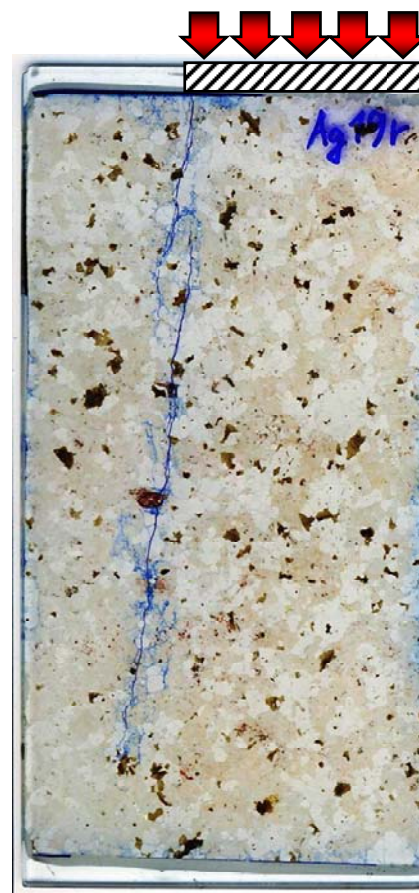
Black : tensile crack Red : shear crack



Pcon= 0 MPa



Pcon= 10 MPa



Pcon= 0 MPa



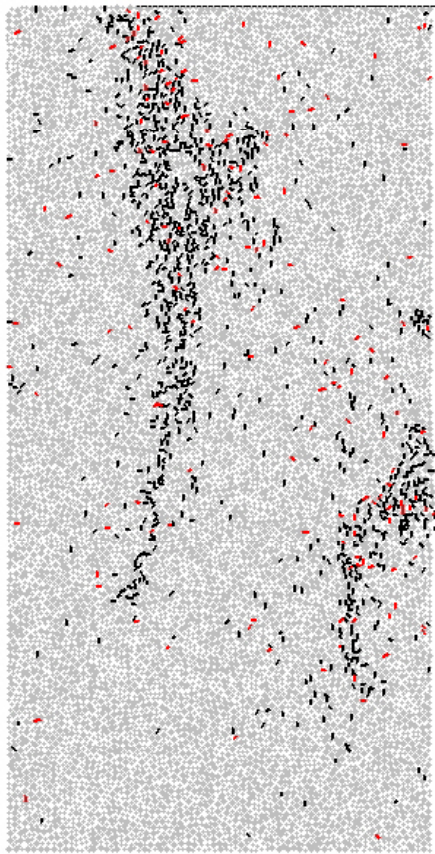
Pcon= 10 MPa

With $2 \leq \frac{SBS}{NBS} \leq 3$ constraint

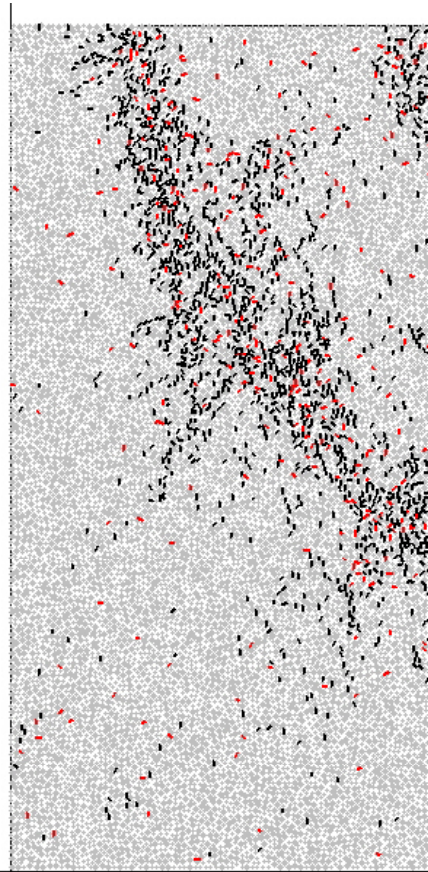
Without $2 \leq \frac{SBS}{NBS} \leq 3$ constraint

Black : tensile crack Red : shear crack

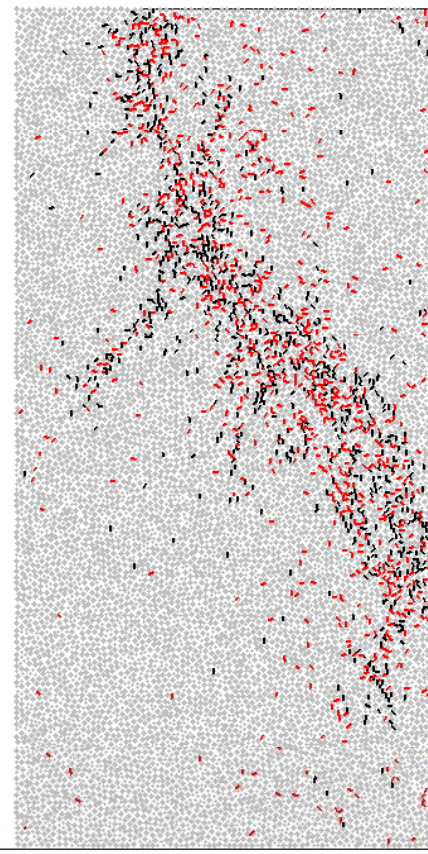
Black : tensile crack Red : shear crack



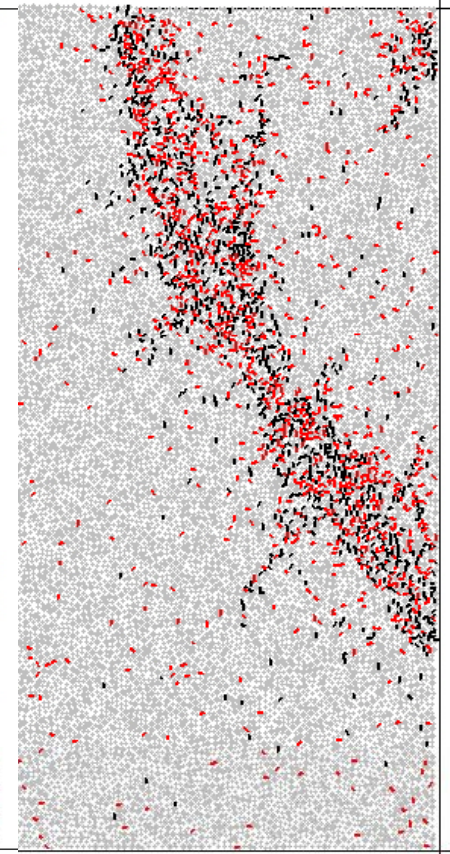
Pcon= 0 MPa



Pcon= 10 MPa



Pcon= 0 MPa



Pcon= 10 MPa

Intrinsic mechanical property of target material is converted to a constraint, so that an optimized set of model parameters is obtained.

Conclusions

- A new method of model parameter determination is introduced.
- Intrinsic mechanical properties of rock material were considered in the process of model parameter determination.
- Optimized model parameters provide not only quantitative match, but also qualitative match to the target rock material.

Thank you

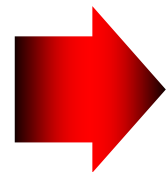
Possible modification

$$K_{IC} = NBS$$

Brazilian tensile strength & Mode I fracture toughness

$$\sigma_t = 6.88 K_{IC} \quad (\text{Zhang ZX, 2002})$$

$$\sigma_t \propto \frac{K_{IC}}{\sqrt{D}} \quad K_{IC} \propto \frac{\phi_n}{2Rt} \sqrt{\pi\alpha R} \quad (\text{Potyondy \& Cundall, 2004})$$


$$\sigma_t \propto \frac{NBS}{2Rt} \sqrt{\frac{\pi\alpha R}{D}}$$

Brazilian tensile strength & Contact-bond normal strength

* Zhang ZX. 2002. An empirical relation between mode I fracture toughness and the tensile strength of rock. Int J Rock Mech Min Sci Geomech Abstr; 39: 401-406.

** Potyondy DO, Cundall PA. 2004. A bonded-particle model for rock. Int J Rock Mech Min Sci; 41: 1329-1364.

Results of Plackett-Burman design analysis

Run no.	UCS Y1	Young's modulus Y2	Poisson's ratio Y3	Brazilian tensile strength Y4	Comp./Tens. Y1/Y4
1	86.56	23.16	0.234	22.02	3.93
2	58.96	33.75	0.122	15.49	3.80
3	77.98	22.40	0.266	19.45	4.01
4	91.47	86.92	0.100	18.37	4.98
5	196.27	55.37	0.273	51.55	3.81
6	225.02	87.01	0.097	50.26	4.48
7	58.23	55.70	0.265	12.36	4.71
8	45.59	55.81	0.268	9.55	4.77
9	45.74	83.18	0.113	18.93	2.42
10	199.81	23.00	0.247	38.56	5.18
11	46.67	33.64	0.103	10.12	4.61
12	86.37	33.62	0.130	16.70	5.17

Ratio : 2.5~5.2

Ratio of compressive strength to tensile strength

Bruno & Nelson (1991)

Discrete Element Modeling on Berea sandstone

Tensile strength : 2.4 MPa (both from DEM and Lab experiment)

Uniaxial compressive strength : 10 Mpa
(DEM simulation) -> ratio (4.16)

Uniaxial compressive strength : 30 Mpa
(Lab experiment) -> ratio (12.5)

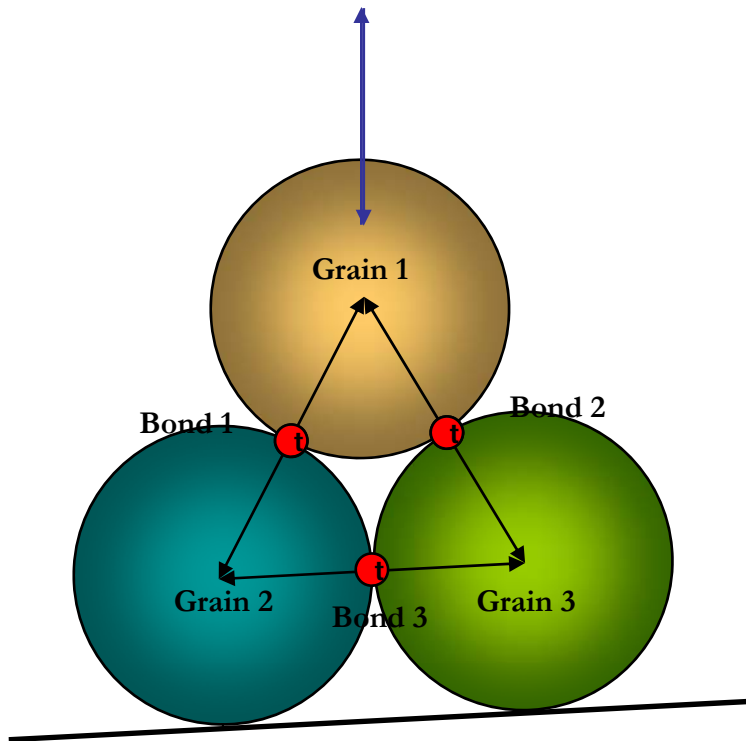
Reason 1) 2D representation of 3D structure

Reason 2) Missing physical characteristics

“the circular grains are more efficient wedges, and the use of circular particles tends to underestimate the load required to produce compressive failure compared to the load required for tensile failure”

Ratio of compressive strength to tensile strength

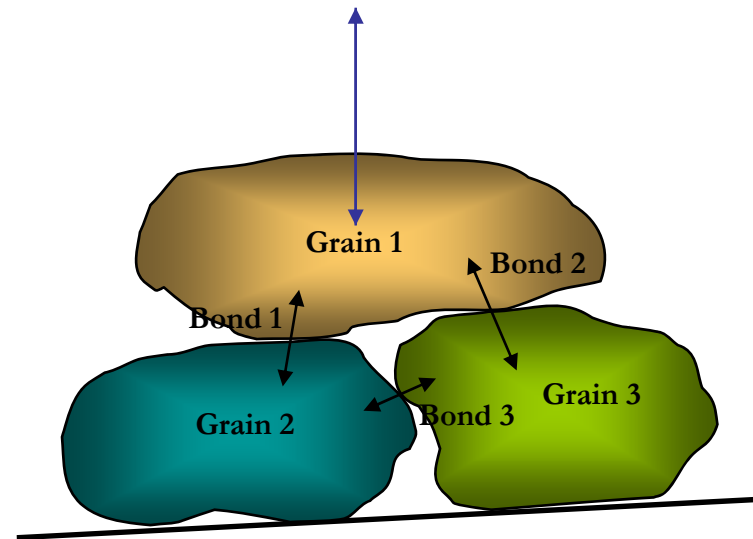
Uniform tensile load F_t F_c



Assembly failure in tension : $T/\sqrt{3}$
 Assembly failure in compression : $2*T/\sqrt{3}$
 Ratio (compressive/tensile) : 2

Maximum tension limit in all bonds : T

Uniform tensile load F_t F_c



Ratio (compressive/tensile) > 2