

The Bonded-Particle Model as a Tool for Rock Mechanics Research and Application

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Preamble

• We provide an overview of Bonded-Particle Modeling, and suggest avenues for further research by summarizing & expanding on the contents of:

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

Potyondy, D.O, and P.A. Cundall (2004) "A Bonded-Particle Model for Rock," *Int. J. Rock Mech. & Min. Sci.*, *41*(8), 1329–1364.

• You need not be a rock-mechanics practitioner to understand this talk. So, let's get started. . .



Overview

- Bonded-Particle Modeling
 - Basic idea & essential features
- Microstructural Physics of intact rock
 - Micromechanical processes that control brittle fracture
 - Nature of pore space: compact or porous
 - Two complimentary idealizations of rock (BPM & LEFM)



Overview

- Bonded-Particle Modeling Methodology
 - PFC model (distinct-element model of *synthetic material*: rigid grains that interact at contacts, vast microstructural space)
 - BPM (*bonded materials* & interface)
 - Microstructural models provided by BPM



Overview

- Bonded-Particle Modeling Methodology
 - PFC model (distinct-element model of *synthetic material*: rigid grains that interact at contacts, vast microstructural space)
 - BPM (bonded materials & interface)
 - Microstructural models provided by BPM
- Examples
 - Ceramic bead and undercut cemented backfill
 - Two intact BPMs that match both uniaxial & tensile strength of compact rock
 - Embed BPM in larger continuum model
 - Sandstone perforation damage
- Conclusions & Future Directions



Poem: "What's In My Journal" by William Stafford *Clues that lead nowhere, that never connected anyway. Deliberate obfuscation,* The action of making something obscure, *unclear or unintelligible. the kind that takes genius.*

This talk: "What's In My Lecture" by David Potyondy *Clues that spawn understanding, arrived at by modeling. Deliberate simplification, the kind that gives clarity.*



There is a need for simplification in rock-mechanics modeling.

We build models because the real world is too complex for our understanding; it does not help if we build models that are also too complex.

The art of modeling lies in determining what aspects of the geology are essential for the model.

Starfield & Cundall (1988)



Starfield, A.M., and P.A. Cundall (1988) "Towards a Methodology for Rock Mechanics Modeling," Int. J. Rock Mech. & Min. Sci., 25, 99–106.



Mechanical behavior arises from interactions:

- microstructure (grain scale) of intact rock
- orientations & properties of joints





emergent phenomena

Mechanical behavior arises from interactions:

- microstructure (grain scale) of intact rock \rightarrow fracture & flow

Bonded-Particle Models mimic intact rock & joints

Closer match to microstructural & structural features \rightarrow Closer match to macroscopic behavior



BPM consists of a base material (intact rock) to which larger-scale joints can be added.

- base material : bonded rigid grains
- joints : interfaces



Damage consists of bond breakages.

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Damage consists of bond breakages.



broken bonds



heterogeneous force transmission induces microtension

1 m (100 grains)



blue: compression between grainsblack/red: compression/tension in cement



Microstructural mechanisms in cemented granular material to induce microtension and bond breakage.





1 m (100 grains)



Intact rock can be viewed as an aggregate of crystals & amorphous particles joined by varying amounts of cementing materials.

Intact rock can be represented as...

Heterogeneous material comprised of cemented grains.

Much disorder in system: grain size, shape & packing grain & cement properties degree of cementation locked-in stresses



sandstone Dittes & Labuz (2002)

Each item influences mechanical behavior, and may evolve under load application.



Dittes, M., and J.F. Labuz (2002) "Field and Laboratory Testing of St. Peter Sandstone," J. Geotech. Engr., 128(5), 372-380, May.

Brittle mechanical properties measured:

uniaxial & triaxial compression tests tension tests

Two principal modes of brittle failure: shear fracture extension fracture





Brittle mechanical properties are controlled by nature of pore space → classify intact rock as compact or porous



Bandini et al. (2012)

marble with interlocking grains





Haimson (2007)

sandstone with broad grain sutures



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.

Haimson, B. (2007) "Micromechanisms of Borehole Instability Leading to Breakouts in Rocks," Int. J. Rock Mech. & Min. Sci., 44, 157-173.

Compression-induced damage manifests itself as inelastic volume change (dilation or compaction) resulting from microstructural changes that are precursors to macroscopic failure.

granular aggregate

Deviatoric loading → dilatancy, repacking of grains



Brzesowsky et al. (2014)

quartz sand



Brzesowsky et al. (2014) "Time-Independent Compaction Behavior of Sands," J. Geophys. Res. Solid Earth, 119, doi:10.1002/2013JB010444..

Compression-induced damage manifests itself as inelastic volume change (dilation or compaction) resulting from microstructural changes that are precursors to macroscopic failure.

compact rock

Deviatoric loading → dilatancy, microcracking



marble



Compression-induced damage manifests itself as inelastic volume change (dilation or compaction) resulting from microstructural changes that are precursors to macroscopic failure.

porous rock

Hydrostatic loading → compactancy, grain crushing

Deviatoric loading → dilatancy, microcracking OR

compactancy, brittle grain crushing or plastic collapse of pores (shear-enhanced compaction)



sandstone



Compressive behavior is described by stress-strain curves:



Four stages:

- 1. crack closure
- 2. elastic region
- 3. stable crack growth
- 4. unstable crack growth



Martin, C.D., and N.A. Chandler (1994) "The Progressive Fracture of Lac du Bonnet Granite," Int. J. Rock Mech. & Min. Sci., 31, 643-659.

Compressive behavior is explained in terms of flaws & heterogeneities in the rock material on the microscopic scale in which brittle fracture is viewed as a localization in the proliferation of microcracking.

It is essential to have a realistic structural description of the rock as a basis for...theoretical developments, and to consider the evolution of the structure during the progression of the failure.

BPMs provide a micromechanical theory of brittle failure

- various physical models of the brittle-fracture process
- discern the effects of microstructure on macroscopic behavior



BPM material

(cemented granular material)



Microstructural mechanisms to induce microtension and bond breakage



BPM material

(cemented granular material)

LEFM material

(linear-elastic body with initial population of cracks)



 γ

Microstructural mechanisms to induce microtension and bond breakage

Microstructural mechanism to induce microtension and crack extension via sliding crack & wing cracks



Why does axial splitting occur?

It originates from local transverse tensile stresses at flaws or heterogeneities in the rock.

For both materials, the axial splits nucleate

- as wing cracks in LEFM material
- as broken bonds in BPM material



Why does axial splitting occur?

It originates from local transverse tensile stresses at flaws or heterogeneities in the rock.

For both materials, the axial splits nucleate

- as wing cracks in LEFM material
- as broken bonds in BPM material

and then grow into an orientation parallel to direction of compression

- as lengthening cracks in LEFM material
- as additional broken bonds that coalesce into extension fractures in BPM material



BPM material

- Supports microcrack nucleation as well as growth and eventual interaction
- Provides rich set of grain-scale discontinuities that can be related to microstructural features



marble with interlocking grains

sandstone with broad grain sutures

• Grain-scale discontinuities need not be mapped into initial population of cracks



Two Complementary Idealizations of Rock BPM material

• Provides rich set of grain-scale discontinuities that can be related to microstructural features



marble with interlocking grains



sandstone with broad grain sutures

Closer match to microstructural & structural features \rightarrow Closer match to macroscopic behavior



Bonded-Particle Modeling Methodology (PFC model)

PFC programs (PFC2D & PFC3D) provide a general-purpose, distinct-element modeling framework that includes a computational engine and a graphical user interface.

Simulate movement & interaction of many finite-sized particles via distinct-element method, which provides an explicit dynamic solution to Newton's laws of motion.





Bonded-Particle Modeling Methodology (PFC model)

Particles are rigid bodies with finite mass that move independently of one another and can both translate and rotate. Particles interact at pair-wise contacts by means of internal force and moment.

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





soft-contact approach

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





soft-contact approach

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





DEM model employs a "soft contact" approach:

all deformation occurs at the contacts between the rigid bodies.

Bonded-Particle Modeling (PFC model)

PFC model provides four basic entities:

balls, clumps & rigid blocks

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







What is a clump?

- Group of pebbles that behaves as rigid body with deformable boundary.
- Provides generalized particle shapes.



made of *pebbles*





What is a rigid block?

- Convex polyhedron with rounded edges.
- Granular: angular shapes, good interlock
- Solid: zero-porosity intact rock (BBM)





Bonded-Particle Modeling (PFC model)

PFC model provides four basic entities:

balls, clumps & rigid blocks

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

walls

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

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






Rich variety of models, described and classified

- base material itself (intact rock)
- overlay joints, voids & material regions



Provide wide range of rock behaviors that encompass

• compact & porous rock at both an intact and rock-mass scale



Base material itself can serve as model of intact rock

• rigid grains joined by deformable & breakable cement



grains can be balls, clumps or rigid blocks

cement can be

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- contact-bonded contact
- parallel-bonded contact

Also soft-bonded contact

• flat-joint contact

When bond breaks, behaves as linear contact.

grains can be balls, clumps. . .



circular grains (balls) mixed-shape grains (balls & clumps)

Bonded material consisting of grains (with balls in yellow and clumps in blue and red) and cement (drawn as pairs of black lines).



grains can be balls, clumps or rigid blocks

Bonded Tetrahedral Grains



Bonded-block model consisting of grains (tetrahedrons) and cement between grain faces subjected to unconfined-compression test.

Lorig, L., D. Potyondy and Varun. (2020) "Quantifying Excavation-Induced Rock Mass Damage in Large Open Pits," in *Proceedings, 2020 International Symposium* on *Slope Stability in Open Pit Mining and Civil Engineering (Virtual Conference, May 2020)*, 969–982. Perth: Australian Centre for Geomechanics.

grains can be balls, clumps or rigid blocks

Bonded Voronoi Grains





Bonded-block model consisting of grains (Voronoi cells) and cement between grain faces subjected to unconfined-compression test.

Potyondy, D., J. Vatcher, and S. Emam (2020) "Modeling of Spalling with PFC3D: A Quantitative Assessment," Itasca Consulting Group, Inc., Report to Svensk Kärnbränslehantering AB (SKB), Stockholm, Sweden, 2-5732-02:20R50, October 22, 2020, Minneapolis, Minnesota.

cement can be

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

When bond breaks, behaves as linear contact.

It is the type of contact model at the grain-grain contacts that defines the PFC material as being linear, contact-bonded, parallel-bonded, soft-bonded or flat-jointed.

Also soft-bonded contact

Let's examine each contact model:

Linear Model Linear Contact Bond Model Linear Parallel Bond Model Soft-Bond Model Flat-Joint Model



Potyondy, D. (2018) "Material-Modeling Support for PFC [fistPkg6.4]," Itasca Consulting Group, Inc., Technical Memorandum ICG7766-L (December 26, 2018), Minneapolis, Minnesota.

linear contact (behavior summary)

The linear model with a reference gap of zero corresponds with the model of Cundall & Strack (1979).





Cundall, P.A, and O.D.L. Strack. (1979) "A Discrete Numerical Model for Granular Assemblies," Géotechnique, 29, 47-65.

contact-bonded contact (behavior summary)

Add a spot of glue to the linear contact model, no slip while bond is intact.





parallel-bonded contact (behavior summary)

Two interfaces.

First interface is same as linear model. Second interface is finite-sized.





parallel-bonded contact (behavior summary 2)





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

parallel-bonded contact (behavior summary 3)

Glass beads cemented with epoxy



Holt et al. (2005)



resists relative rotation.



soft-bonded contact (behavior summary)

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Like parallel bond with tensile softening. When unbonded, has rolling resistance.



soft-bonded contact (behavior summary 2)



- σ : maximum normal stress at bond periphery
- *l*: elongation at bond periphery $(l \ge 0)$
- l_c : critical bond elongation at peak strength

 $\sigma_{c} : \text{tensile strength [stress]}$ $k_{n} : \text{normal stiffness [stress/displacement]}$ $\zeta : \text{softening factor } (\zeta \ge 0, \ \zeta = 0 \text{ is no softening})$ $\gamma : \text{strength-reduction factor } \begin{pmatrix} 0 \le \gamma \le 1 \\ \gamma = 0 \text{ is full softening} \\ \gamma = 1 \text{ is no softening} \end{pmatrix}$



flat-joint contact (behavior summary)



notional-surface element bonded bond σ_c k_s { c,ϕ } k_n

unbonded





flat-joint contact (behavior summary 2)

Marble with angular, interlocked grains



Bandini et al. (2012)



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.

flat-joint contact (behavior summary 3)





flat-joint contact (behavior summary 4)

Bending failure with. . .



Crack thickness is proportional to gap.

The interface can sustain partial damage.



flat-joint contact (behavior summary 5)





Joints can be overlaid on base material

• joint behaves as **interface**

interface is collection of smooth-joint contacts



Smooth-joint contacts may be initially bonded. When bond breaks, they behave as linear contact.



smooth-joint contact (behavior summary)





smooth-joint contact (behavior summary)

Joint friction coefficient equals one. . .





smooth-joint contact (behavior summary)

Joint friction coefficient equals zero. . .





fixed bottom



Void regions are identified...

• grains within these regions are removed





Potyondy (2007) "The Effect of Voids on the Mechanical Properties of Rock," in Proc. 4th Int. Conf. on Discrete Element Methods, Brisbane, Australia, Cleary, Ed., MEI Conferences, CD.

Material regions are identified...

• grains & contacts within these regions are assigned properties





Katsaga, T. (2010) "Geophysical Imaging and Numerical Modelling of Fractures in Concrete," Ph.D. Thesis, University of Toronto.

Joints are identified...

• contacts that lie along these joints are assigned properties

Synthetic Rock Mass (SRM)



SRMs are used to represent a rock mass. The BPMs are remarkably complex, and used to study impact of joint fabric on rock mass strength, brittleness and fragmentation.



Mas Ivars et al. (2011) "The Synthetic Rock Mass Approach for Jointed Rock Mass Modelling," Int. J. Rock Mech. & Min. Sci., 48, 219–244.

Microstructural Models Provided by BPM Synthetic Rock Mass (SRM)





Microstructural Models Provided by BPM Synthetic Rock Mass (SRM)





Material regions & joints are identified...



GBMs are used to represent intact compact rock, allow partial interface damage and grain breakage.

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Potyondy (2010) "A Grain-Based Model for Rock: Approaching the True Microstructure," in *Rock Mechanics in the Nordic Countries 2010*, pp. 225–234, C.C. Li, et al., Eds., ISBN: 978-82-8208-017-0, Kongsberg: Norwegian Group for Rock Mechanics.

Examples

Ceramic bead & Undercut cemented backfill

Matching uniaxial & tensile strengths of compact rock

• two alternative intact BPMs

Embed BPM within larger continuum model

• study fracturing around advancing stope in quartzite

Sandstone Perforation Failure



Examples (ceramic bead PFC3D, parallel-bonded material)

These models:

- * Matched Hertzian response
- * Computed breakage stress (solid & hollow beads)





Varun, and D.O. Potyondy (2015) "Mechanical Modeling of Ceramic Beads," Itasca Consulting Group, Inc., Report to JPL: Thermal Energy Conversion Technologies Group, Pasadena, CA, 15-2929-40, May 18, 2015.

Examples (undercut cemented backfill PFC2D, flat-jointed material)

Fill UCS = 1.0 MPa, Panel = 15.0 m

Fill UCS = 2.0 MPa, Panel = 15.0 m



Examples (undercut cemented backfill PFC2D, flat-jointed material)

Fill UCS = 1.0 MPa, Panel = 15.0 m





Undercut movies:



Alex Turichshev (Itasca Canada)

Examples

Ceramic bead & Undercut cemented backfill

Matching uniaxial & tensile strengths of compact rock

• two alternative intact BPMs

Embed BPM within larger continuum model

• study fracturing around advancing stope in quartzite

Sandstone Perforation Failure



Examples (match uniaxial & tensile strengths)

BPM of parallel-bonded disks or spheres cannot match both tensile and compressive strengths of typical compact rock.

This limitation is overcome by introducing intergranular interlock in the form of a well-connected grain structure with interfaces that are deformable, breakable and can sustain partial damage.

Partial interface damage with continued moment-resisting ability is an important microstructural feature of a BPM.



Flat-jointed material (Differs from parallel bond)





Examples (match uniaxial & tensile strengths)

Two alternative intact BPMs:



grain-based material f

flat-jointed material


Examples (grain-based material)

axial splitting

50 mm (200 disks, 20 grains)





Potyondy (2010) "A Grain-Based Model for Rock: Approaching the True Microstructure," in *Rock Mechanics in the Nordic Countries 2010*, pp. 225–234, C.C. Li, et al., Eds., ISBN: 978-82-8208-017-0, Kongsberg: Norwegian Group for Rock Mechanics.

Examples (flat-jointed material)



Castlegate sandstone



CG material

Potyondy, D.O. (2017) "Simulating Perforation Damage with a Flat-Jointed Bonded-Particle Material," paper ARMA 17-223 in Proceedings of 51st U.S. Rock Mechanics/Geomechanics Symposium, San Francisco, USA, 25–28 June 2017. [2D flat-jointed sandstone material --- described here.]



Potyondy, D.O. (2018) "A Flat-Jointed Bonded-Particle Model for Rock," paper ARMA 18-1208 in Proceedings of 52nd U.S. Rock Mechanics/Geomechanics Symposium, Seattle, USA, 17–20 June 2018. [3D flat-jointed granite material]

Material Behavior (compression tests)



Stress-strain response during triaxial testing



Material Behavior (tension & compression tests)

- The mechanisms that are exhibited during tension & compression tests are like the brittle failure behavior of compact rock, with the exception that transgranular cracking occurring within and across grains during compression tests is absent.
 - The following mechanisms are exhibited during these tests and shown on the next 5 slides.



Direct-tension (& fracture-toughness) tests

• Peak stress coincides with formation of a few tensile fractures aligned perpendicular to specimen axis.



Damaged microstructure at post-peak state of tension tests.



Compression test (unconfined)

• Peak stress coincides with axial splitting in which the material breaks apart into multiple interlocking columns.



Damaged microstructure at post-peak state of UCS test.



Compression test (unconfined)

• Peak stress coincides with axial splitting in which the material breaks apart into multiple interlocking columns.



bonded Voronoi grains

Damaged microstructure at post-peak state of UCS test.



Compression test (confined)

• Peak stress coincides with formation of a few diagonally aligned shear fractures.

3.81 mm

max disp. = 0.5 mm

Damaged microstructure at post-peak state of confined-compression test.



Compression tests (fragmentation)





Fragmentation at post-peak (top) and residual (bottom) states of compression tests.





Ceramic bead & Undercut cemented backfill

Matching uniaxial & tensile strengths of compact rock

• two alternative intact BPMs

Embed BPM within larger continuum model

• study fracturing around advancing stope in quartzite

Sandstone Perforation Failure



Examples (embed BPM in continuum model)

quartzite modeled (continuum) as strain-hardening/softening material *ad hoc* strength reduction (intact → in-situ)



roller BCs

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Katsaga, T., and D. O. Potyondy (2012) "A Generic Stope Model for Investigation of Fracturing Mechanisms in Deep Gold Mines," paper ARMA 12-541 in Proceedings of 46th U.S. Rock Mechanics/Geomechanics Symposium, Chicago, USA, 24–27 June 2012.

Examples (embed BPM in continuum model)

Fracture pattern compares well with expected pattern.



Could benefit by comparing responses of these two different material idealizations (e.g., damage processes in shear fractures).





Ceramic bead & Undercut cemented backfill

Matching uniaxial & tensile strengths of compact rock

• two alternative intact BPMs

Embed BPM within larger continuum model

• study fracturing around advancing stope in quartzite

Sandstone Perforation Failure





Damage begins as swarm of intra-granular microcracks, that first extend transgranularly, loosening grains and grain fragments...

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Potyondy, D.O. (2017) "Simulating Perforation Damage with a Flat-Jointed Bonded-Particle Material," paper ARMA 17-223 in Proceedings of 51st U.S. Rock Mechanics/Geomechanics Symposium, San Francisco, USA, 25–28 June 2017.



...and then extend inter-granularly toward borehole wall, where a thin layer of grains & fragments begins to separate (ready to spall or be removed by drilling fluid).







This episodic process produces wide-angle, dog-eared breakouts.





Model of a Thick-Walled Cylinder test showing pressure-application procedure



We now describe the formation of a stable notch above the borehole when the external pressure reaches 30.5 MPa. • damage

damage & forces



 $P_o = 30.5$ MPa (stable)



 $P_o = 30.5$ MPa (stable)

Bonded-particle modeling is in early phase of development

- have generic models for 2D & 3D intact compact rock
- Next step: generic model of intact porous rock



marble with interlocking grains



Haimson (2007)

sandstone with broad grain sutures



All BPM modeling benefits from increased computational speed via

- multi-threading capability in *PFC2D* and *PFC3D* 5.0 & above!
- support for MPI under development



With continuing increases in computational speed, BPM modeling will be increasingly applied to boundary-value problems

• How to incorporate scale effects that make in-situ strength less than intact strength?



Future BPMs should be constructed to match particular types of rock

• granite, sandstone, limestone,...





Granite (minerals)

Basalt (minerals & matrix)



Images from Enes Zengin

Challenge is to keep models as simple as possible

• include features to allow relevant micromechanisms to occur

Closer match to microstructural & structural features → Closer match to macroscopic behavior

