Numerical Methods in Rock Engineering - Introduction to Discrete Element Method

(Week 8, 9, 10, 11) (26 April, 3, 10, 17 May 2021)





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Introduction Home Assignments (40%)



- #1 1 page summary of selected papers on numerical analysis
- #2 1D(or 2D) coding of FEM/FDM (use excel, matlab, or other codes)
- #3 Exercise with FEM code (comsol multiphysics)
- #4 Paper reading (DEM) classical paper of your choice
- #5 Exercise with UDEC/PFC



Introduction Term Project (20%)



- Select a subsurface engineering problem of your interest and conduct a numerical analysis using any available codes.
- Term paper must include;
 - $rac{}$ Clear objectives
 - $\ensuremath{\mathfrak{P}}$ One or two verification cases
 - ন্থ Thorough formulation of the chosen numerical method
 - $\ensuremath{\mathfrak{B}}$ Concise presentation and discussion on the results
- Timeline
 - a 31 MayProposal (1 page) & 10 minutes presentationa 7 JuneConsultation with instructora 14 JunePresentation and submission of Term Paper

Introduction Term Project



- A list of example topics
 - Reproduction of published landmark papers
 - Borehole Stability problem in Anisotropic Media (FEM or FDM)
 - Fracture propagation in petroleum/geothermal reservoir (BEM or DEM)
 - Calibration of micromechanical parameters for transversely isotropic rock rock (DEM)
 - Coupled (thermo) hydromechanical analysis in porous medium
 - CO2 injection in saline formation
 - Thermomechanical analysis for geological repository of nuclear waste
 - Slope Stability in fractured or continuum rock
 - Reinforcement of tunnel
 - Determination of equivalent properties of fractured rock mass (DEM)

Introduction Term Project



- Presentation
 - Presentation is an extremely important part of your professional life. Therefore, you have a good reason to be serious about this.
 - 10 minutes + 5 min (questions)

Introduction Term Project



• Your term papers will be published as proceedings.

 Your term papers may be developed into journal papers in the future.

Proceedings of
2011 SNU Student Conference - Numerical Analysis in Rock Engineering -

Editor : Ki-Bok Min

Department of Energy Resources Engineering

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Explicit Discrete Element Method Outline



- Introduction
- Solution techniques Governing Equations
- Implementation issues Numerical Stability, Damping, Contact Detection,
- Explicit DEM
 - Unbonded particulate system
 - Bonded particulate system
 - Blocky system
- Hydraulic processes fluid flow in fractured rock
- Examples



• Up to this point, we were able to model various physical problems using FEM and FDM. Essentially we solved a single or a coupled set of partial differential equation in *continuum*.

 Can we solve following problem using FEM or FDM? – a system of particles interacting each other.



Explicit Discrete Element Method Introduction – particulate system



Powder technology, chemical engineering

Powder or gravels in a hopper. Thickness of lines indicate forces.



And, of course, billiards...

Sodium chloride aqueous solution, each particle represent sodium, hydrogen, oxygen and chloride. http://www.ornl.gov/info/ornlreview/v34_2_01/p23b.jpg

Explicit Discrete Element Method Introduction – blocky system





Discontinuum

Discrete Element Method



- The name 'discrete element method' can be used only if it
 - Allows finite displacements and rotations of discrete bodies; including complete detachment
 - Recognizes new interactions (contact) automatically as calculation progresses
- A DEM code will embody an efficient algorithm for detecting and classifying contacts. It will maintain a data structure and memory allocation scheme that an handle many discontinuities or contacts.
- Two types of DEM
 - Explicit DEM (often called distinct element method): use explicit FDM for solution. Ex) PFC, UDEC, FLOBALL
 - Implicit DEM: similar to FEM solution technique. Matrix is formed.
 Ex) DDA

Explicit Discrete Element Method Introduction



- Explicit Discrete Element Method (DEM) solves a motion of interacting particles or blocks (in bonded or unbonded form).
 - DEM recognize new contacts within internal algorithm.
 - Applications rock mechanics, powder mechanics, granular materials.
 - Finite Difference Method is used to integrate the equation we replace the time derivative with difference equation in finite time interval.
- DEM is very similar to Molecular Dynamics (MD) which has applications in biophysics, material science and biochemistry atoms and molecule are used for particles. MD simulate material properties, for examples.
- This lecture is focused on DEM, however, large portions of DEM principle is directly applicable for MD.

Explicit Discrete Element Method Introduction – a seminal paper



Cundall, P.A. and O.D.L. Strack, Discrete Numerical Model for Granular Assemblies. Geotechnique. 1979. 29(1): p. 47-65



Explicit Discrete Element Method Introduction – a seminal paper

- POWDER TECHNOLOGY
 GRANULAR MATTER
 CHEMICAL ENGINEERING SCIENCE
 PHYSICAL REVIEW E
 computer and Geotechnics
 Int J Rock Mech Min Sci
- 16. Geotechnique



• Drastic increase of citations in the past 25 years

- Appreciation in various fields proves DEM is a truly interdisciplinary science!
- What is going to happen in the next 10-20 years???



citations (798) (353) (275) (272) (195) (80) (71)

Explicit DEM Introduction – a seminal paper



- ...rock mechanics has traditionally attempted to use procedures from other branches of mechanics; however, the developments by Dr Cundall and his colleagues in the modelling of the deformation behaviour of blocky or particulate systems are now attracting interest from these other branches. It appears that there are many fields of study where a discrete or discontinuum approach can provide illuminating insights into the mechanics of deformation--insights and behaviours that may be obscured by classical continuum analyses. (Charles Fairhurst, 1988, IJRMMS foreword)
- DEM is probably the first export product from rock mechanics community to other branches of science/engineering

Explicit DEM Introduction – overview





Explicit DEM Introduction



- Damage, and its evolution, is explicitly represented in the model; no empirical relations are needed to define damage or quantify its effect upon material behavior.
- Microcracks form and coalesce "automatically" without the need for grid reformulation.
- Complex nonlinear behaviors arise as emergent features, given simple behavior at particle level.
 - dependence of strength on confining stress
 - Dilatancy
 - evolution of material anisotropy
- Secondary phenomena, such as acoustic emission, occur in the DEM model without additional assumptions.





- How do we model this system?
 - Equation of motion and interacting force





Explicit Finite Difference Method (such as FLAC) and Explicit DEM (such as PFC and UDEC) essentially have the same calculation scheme – i.e., FDM

Hart R, IJRMMS 2003;40:1089-1097



- Let's now talk about the technique to integrate the equation of motions and calculate forces.
 - For integration two methods will be explained interlaced central difference method (leapfrog method) and Verlet algorithm.
 - For force calculation, spring model will be used







• From central difference scheme



the same as Leapfrog algorithm (Frenken & Smith, 2002)

Governing Equation Time integration of equation of motion (2) – Verlet algorithm SEOUL NATIONAL UNIVERSIT (Verlet, 1967*)

$$u(t + \Delta t) = u(t) + \dot{u}(t)\Delta t + \frac{\ddot{u}(t)}{2}\Delta t^{2} + \frac{\ddot{u}(t)}{3!}\Delta t^{3} + O(\Delta t^{4}) \longleftarrow \text{Taylor expansion}$$

$$u(t - \Delta t) = u(t) - \dot{u}(t)\Delta t + \frac{\ddot{u}(t)}{2}\Delta t^{2} - \frac{\ddot{u}(t)}{3!}\Delta t^{3} + O(\Delta t^{4})$$

$$u(t + \Delta t) + u(t - \Delta t) = 2u(t) + \ddot{u}(t)\Delta t^{2} + O(\Delta t^{4})$$

$$u(t + \Delta t) = 2u(t) - u(t - \Delta t) + \frac{f(t)}{m}\Delta t^{2}$$

Verlet does not use the velocity to compute the new position. However, velocity can be calculated as follows,

$$\dot{u}(t) = \frac{u(t + \Delta t) - u(t - \Delta t)}{2\Delta t}$$

Verlet algorithm is the most widely used in MD simulations

*Verlet L, 1967, Computer 'experiemtns' on classical fluids. I. Thermodynamical Properties of Lennard-Jones Molecules, Phys Rev 159(1), 98-103,

Governing Equation Contact Force





Directions of F in each particle

F can be defined differently depending on the nature of the problem (e.g., gradient of potential energy, Frenkel and Smit, 2002).

Governing Equation Contact Force





From HCItasca.com

Explicit DEM Calculation Cycle – rotation, angular velocity, acceleration





- θ :rotation, $\dot{\theta}$: angular velocity, $\ddot{\theta}$: angular acceleration M: moment, I: moment of inertia
- tangential force (F_s)

 $\theta^{(t+\Delta t)} = \theta^{(t)} + \dot{\theta}^{(t+\Delta t/2)} \Delta t$

 $\dot{\theta}^{(t+\Delta t/2)} = \dot{\theta}^{(t-\Delta t/2)} + \left(\frac{\sum M^{(t)}}{I}\right) \Delta t$

- $F_{s} = K_{s}\delta_{s}$ $K_{s}: shear \ stiffness$ $\delta_{s}: shear \ displacement(when \ overlapped)$
- Slip condition

$$F_s \leq \mu K_n$$

 μ : friction coefficient





Explicit DEM Calculation Cycles





Explicit DEM Implementing issues



- We covered the 1) solution method of equation of motion and 2) force calculation
- There are a couple of implementing issues
 - Stability of solution
 - Contact detection
 - Extension to 2D, 3D
 - Damping scheme



- There are two important considerations with dynamic relaxation:
 - Choice of time step
 - Effect of damping



 Explicit schemes are only conditionally stable – have to use small enough time step (Δt)

$$my'' = -ky$$

$$y(t) = A\cos w_0 t + B\sin w_0 t, \quad w_0 = \sqrt{k/m}$$

$$T = 2\pi \sqrt{m/k}$$

 Stable condition for explicit FDM for a single degree of freedom (Cundall and Strack, 1979),

$$\Delta t < \frac{2}{w} = 2\sqrt{m/k}$$



- •Time step must be lower than the period of the system by some amount
- •This Δt is called critical Δt
- •DEM code can automatically determine the Δt but this can also be specified.

$$t_{\rm crit} = \begin{cases} \sqrt{m/k^{\rm tran}}, & \text{(translational motion)} \\ \sqrt{I/k^{\rm rot}}, & \text{(rotational motion)} \end{cases}$$



•Time step must be lower than the period of the system by some amount.

$$\Delta t_c = \alpha \sqrt{\frac{m}{k}} \qquad \alpha = 0.1 \text{ usually gives a stable}$$
results

Implementation issues for explicit DEM Dynamic Relaxation – Effect of Damping



- Damping is necessary to dissipate the kinetic energy, e.g., static problem
- damping force acts opposite to current velocity
- damping force magnitude proportional to out-ofbalance force – there are other way of applying damping force, e.g., proportional to velocity magnitude

$$F + F_d = m\ddot{u}$$

$$F_d = -\alpha |F| \operatorname{sign} |\dot{u}|$$

Implementation issues for explicit DEM Dynamic Relaxation – Effect of Damping



- Velocity-proportional damping introduces body forces that can affect the solution.
- Local damping is used in FLAC --- The damping force at a gridpoint is proportional to the magnitude of the unbalanced force with the sign set to ensure that vibrational modes are damped:
- Damping forces are introduced to the equations of motion:

$$\Delta \dot{u}_i = \left[\Sigma F_i - \alpha \left|\Sigma F_i\right| \operatorname{sgn}(\dot{u}_i)\right] \frac{\Delta t}{m} \qquad F_d = -\alpha \left|\Sigma F_i\right| \operatorname{sgn}(\dot{u}_i)$$

- In *FLAC* the unbalanced force ratio (ratio of unbalanced force, F_i , to the applied force magnitude, F_m) is monitored to determine the static state.
- By default, when $F_i/F_m < 0.001$, then the model is considered to be in an equilibrium state.

Explicit DEM Examples (1) – Falling Ball under gravity





- Step-by-step calculation of velocity, displacement, Force and acceleration
- Implementation of gravity and damping
- Appreciation of the ability to model the dissipation of kinetic energy

Explicit DEM Examples (2) – Colliding two balls



V=0.5 m/sec



- Contact detection between two balls
Governing Equation Extension of model to 2D & 3D



• 2D, 3D extension and inclusion of gravity

$$\dot{u}_{i}^{(t+\Delta t/2)} = \dot{u}_{i}^{(t-\Delta t/2)} + \left(\frac{\left(\sum F^{(t)}\right)_{i}}{m} + g_{i}\right)\Delta t$$
$$u_{i}^{(t+\Delta t)} = u_{i}^{(t)} + \dot{u}_{i}^{(t+\Delta t/2)}\Delta t$$

Can be achieved straightforwardly

Explicit DEM Examples (3) – Cundall's nine disc test





- Static problem using dynamic formulations
- Biaxial loading with constant velocity, 0.001 m/s
- Loading stopped after 300 cycles
- Ball & Wall stiffness: 1e5 N/m
- Friction coefficient 0.5, damping coefficient 0.7

*Cundall PA, Strack ODL, discrete numerical model for granular assemblies, Geotechnique 29 (1):47-65, 1979

Explicit DEM Examples (3) – Cundall's nine disc test



Original presentation (Cundall & Strack, 1979)



*Cundall PA, Strack ODL, discrete numerical model for granular assemblies, Geotechnique 29 (1):47-65, 1979

Explicit DEM Examples (3) – Cundall's nine disc test



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 Static analysis possible by solving dynamic equations with damping

Implementation issues Contact detection - Cell-mapping



Why is this important? - Imagine we run simulation with 10,000 particles and try to check forces between them.



• Calculation time: Naïve calculation of all contacts, ${}_{n}C_{2} \sim n^{2}$

Mapping cell logic

Implementation issues Contact detection - Cell-mapping





Cell entries in main array



Explicit DEM Examples (4) – Granular flow in a hopper





Can complement expensive large scale physical test

Physical model for 2D DEM





- Conceptually, 2D DEM can be said to be 'plane stress' on 'rigid' 'cylindrical' particle with unit thickness (hence, disc) as shown here.
- Stress (actually force) is in 2D and there is no third directional deformation due to Poisson's effect.

Explicit DEM – Bonded Particulate system Motivation



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 Rock behaves like a cemented granular material of complexshaped grains in which both the grains and the cement are deformable and may break.



- Bonded-particle model
 - Fundamental particle is circular or spherical, but complex "grains" produced by bonding particles.
 - Damage occurs by bond breakages, material evolves from solid to granular.
 - Exhibits rich set of emergent behaviors similar to crystalline rock.

Explicit DEM – Bonded Particulate system Bonding logic



from www.HCltasca.com

This is definitely not for billiards balls!

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Explicit DEM – Bonded Particulate system Grain-cement microproperties





HCItasca.com

cement behavior

Explicit DEM – Bonded Particulate system Overall behavior of bonded system



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From HCItasca.com

- System behavior affected by:
 - grain shape
 - grain size distribution
 - grain packing
 - grain-cement microproperties
 - material-genesis procedure





Explicit DEM – Bonded Particulate system Overall behavior of bonded system



O29 m



- System behavior affected by:
 - grain shape
 - grain size distribution
 - grain packing
 - grain-cement microproperties
 - material-genesis procedure

circular disks in 2D uniform $\begin{bmatrix} D_{\min}, D_{\max} \end{bmatrix}$ arbitrary & isotropic deformability & strength material vessel

From Cltasca.com

Explicit DEM – Bonded Particulate system Calibration – determination of microparameter



HCItasca.com

Weaker and less stiff biotite bands within rock matrix

Explicit DEM – Bonded Particulate system Calibration – determination of microparameter COLL NATIONAL UNIVERSITY



Macroproperty characterization



Biaxial-test environment

- elastic constants E and ν
- unconfined compressive strength
- crack-initiation stress
- strength envelope: linearize by: friction angle cohesion

Brazilian tensile strength

HCItasca.com



material-genesis procedure



1. Compact initial assembly.



2. Install isotropic stress, sig0.



3. Remove "floating" particles.



4. Install parallel bonds.



5. Remove from material vessel.

Locked-in forces (red-tension, blue-compression).

Magnitude is small relative to UCS.

HCItasca.com

Example of initial packing





- Initial packing is an important issue for PFC type modeling
- In this example, radius of balls are fixed and random locations are selected via a method similar to Monte Carlo Method.

Explicit DEM Examples



- Implementation examples
 - 1) Falling ball under gravity
 - 2) Colliding two balls
 - 3) Static loading of a nine disc system
- Application examples
 - 4) Gravel or powder in a hopper
 - 5) Uniaxial strength test of a material
 - 6) Uniaxial strength test of a material with a crack
 - 7) Modeling of transversely isotropic rock

Explicit DEM Examples (5) – Uniaxial Strength Test





- Samples were generated through genesis scheme
- Stress and strain were monitored in the sample
- Elastic modulus, Poisson's ratio and strength can be measured by numerical experiment this needs to be compared with actual(real) measurement.
- Different resolution (av. # of balls/section)
- Min. ball D \approx 2 cm (L40) \sim 15 cm (L5), D_{max}/D_{min}=1.66

Explicit DEM Examples (5) – Uniaxial Strength Test





Displacement + cracking

Parallel bond force + cracking

Examples (5) – Uniaxial Strength Test Obtained σ-ε seoul NATIONAL UNIVERSITY (stress-strain) curve



Very similar observation to actual experiments can be obtained.

Hendersen Mine, 2006 (Min)

Hustrulid & Bullock, 2001

Explicit DEM Examples (6) - Rock Mass Strength - Uniaxial Strength Test (with a internal fracture)

- To understand the nature of fracturing around a cave
- Use numerically based analysis for caving prediction







Explicit DEM Examples (6) - Rock Mass Strength – Uniaxial Strength Test (with a internal fracture)





Ivars et al., 2011, IJRMMS

Explicit DEM Examples (6) - Rock Mass Strength – Uniaxial Strength Test (with a internal fracture)





Ivars et al., 2011, IJRMMS

Explicit DEM Examples (6) - Rock Mass Strength Motivation



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 $\sigma_{\rm c}$ of intact rock $\neq \sigma_{\rm c}$ of fractured rock mass.

 \rightarrow <u>Numerical experiment can be an alternative</u> To understand the nature of fracturing around a cave Use numerically based analysis for caving prediction

Explicit DEM Examples (6) - Rock Mass Strength Sliding Joint Model



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- Identify all contacts between balls that lie upon opposite side of a plane, remove bond
- Kn, Ks defined, Failure Coulomb failure
- Special command (fishcall in case of PFC) that automatically detect new contact lie in joint

Explicit DEM Examples (6) - Rock Mass Strength – Uniaxial Strength Test (with a internal fracture)



Job Title: sW 1mL40 f0 00 tAucs Job Title: sW_1mL40_f0_00_tAucs PFC2D 4.00 PFC2D 4.00 /iew Title: Step 30000 11:12:45 Wed Sep 28 2005 Step 30000 11:12:45 Wed Sep 28 2005 View Size: View Size: X: -1.038e+000 <=> 1.038e+000 X: -9.926e-001 <=> 9.926e-001 Y: -1.100e+000 <=> 1.100e+000 Y: -1.100e+000 <=> 1.100e+000 Wall Wall Sliding Joint Sliding joint Bond Force Crack Compression Tension Maximum = 1.001e+005 Scale to Max = 1.000e+006 Itasca Consulting Group, Inc. Itasca Consulting Group, Inc. Minneapolis, MN USA Minneapolis, MN_USA

Propagation of crack

Distribution of force











Strength Anisotropy with respect to Weak Planes



 σ_1 : axial strength, σ_3 : confining stress, C: cohesion, φ : friction angle, β : inclination

✓ Mechanical Behaviors
 -> Smoothly Change



(a) Step 1 (Intact Rock Part)

	Microproperties of Bonded Part	icle Model	
	Grain	Cement	
	Elastic modulus = 38 Gpa	Elastic modulus = 38 Gpa	
	Stiffness ratio = 3.5	Stiffness Ratio = 3.5	
	Friction coefficient = 0.839	Tensile stress = 75 Mpa	
(b)	Step 2 (Weak Plane Part)		
ı	Microproperties of Smooth Join		
1	Normal stiffness = 33700 Gpa/m	Dilation angle = 0°	
	Shear stiffness = 960 Gpa/m	Tensile strength = 3 Mpa	SJM
	Friction coefficient = 0.364 (20)	•) Cohesion = 15	



Boryeong Shale vs. Numerical Model



- Iso Experiments /
 Numerical Results
- ✓ E, UCS and BTS with respect to the smooth joints orientation
- Capture the overall trend of anisotropic mechanical behaviors









(Lab Results Obtained from Cho et al., 2012)

6158 Particles



Dominated by Intact Rock (BPM) Dominated by Layers (Smooth Joint Model)

Explicit DEM in Blocky System Introduction

 Explicit DEM in blocky system (such as UDEC) essentially have the same calculation scheme – i.e., FDM – for both contact and blocks




Identification of contact character between 2 blocks

We need to know:

- 1) type of contact (e.g. corner-to-corner, corner-to-edge, etc.)
- 2) direction of normal to sliding direction
- 3) gap between blocks, or contact overlap

Explicit DEM in Blocky System Contact





A contact is created at each corner interacting with a corner or edge of an opposing block.

Explicit DEM in Blocky System Corner handling





Corner rounding scheme with constant length d



Corner rounding scheme with constant radius r, showing that small angles in the corner leads to large distances d

Explicit DEM in blocky system Contact





Rounded corner-to-edge contact

Rounded corner-to-corner contact

Definition of contact normal



Contacts and Domains between Two Deformable Blocks



Explicit DEM in blocky system Blocks



- Two formulations for Solid body mechanics
 - Rigid body translation and rotation
 - Deformable body mechanics



(a) distinct element blocks



- Geometry
 - joint set assigned with orientation/length/spacing...
 - complete Discrete Fracture Network (DFN) not implemented but easily combined via FISH or separate program
 - dead-end joint cannot be generated
 - continuum model \rightarrow use of fictitious joint with high stiffness values (UDEC) or glue (3DEC)
- Constitutive model
 - Linear model

$$F = K_n \delta_n \qquad F = K_s \delta_s$$

- Nonlinear model

step-wise nonlinear continuously yielding model Barton-Bandis model

Explicit DEM in blocky system Joint Model (Barton-Bandis model)





- Normal nonlinear
- Shear Affected by the magnitude of normal stress and JRC

(Min & Jing, 2004)

Explicit DEM in blocky system Joint Model (Barton-Bandis model)





• More prominent peak with the increase of JRC

Explicit DEM in blocky system Fluid flow





Real rock fracture

Idealized rock fracture

$$p = p_0 + K_w Q \frac{\Delta t}{V} - K_w \frac{\Delta V}{V_m}$$

 p_0 : domain pressure in the preceding timestep Q: sum of flowrate into the domain K_w : bulk modulus of fluid $\Delta V = V - V_0$ $V_m = (V + V_0) / 2$

$$Q = -\frac{e^3}{12\mu} \frac{\partial p}{\partial x}$$

$$\Delta t_f = \min\left[\frac{V}{K_w \sum Q_i / \Delta p_i}\right]$$

For edge-to-edge contact

Explicit DEM in blocky system Fluid flow and coupled hydromechanical calculation





Explicit DEM in blocky system Fluid flow and coupled hydromechanical calculation



 Relation between hydraulic aperture, a, and joint normal stress in UDEC (from UDEC manual)



$$a = a_0 + u_n$$

Explicit DEM in blocky system Convective Heat Transfer





Explicit DEM in Blocky System Examples



- 2D Explicit DEM in blocky system

 Stability analysis of fractured rock for low and intermediate level nuclear waste underground repository
 determination of rock mass elastic properties (E, v) (Min & Jing, 2003), (Min et al., 2005)
- 3D Explicit DEM in blocky system
 effect of fracture zones on stress distribution (Min, 2009)
- Coupled Hydromechanical Analysis
 - effect of stress on permeability (Min et al., 2004)

Explicit DEM in Blocky System Example - Rock mass E and v (Min and Jing, 2003)





- In situ experiments is difficult scale, boundary condition, cost
- <u>Numerical Experiments</u> can be alternative and effective to handle all these difficult questions as long as.....
- DFN-DEM approach

Discrete Fracture Network (DFN) – geometry of fractured rock mass Distinct Element Method (DEM) – solution technique



Example - Rock Mass Determination Methodology





- Three linearly independent B.C.s and consider full anisotropy
- This overcomes the difficulty in Stietel at al (1996)

Example - Rock Mass Determination Methodology





6 Boundary conditions

$$\begin{pmatrix} \varepsilon_{xx}^{(1)} \varepsilon_{xx}^{(2)} \varepsilon_{xx}^{(3)} \varepsilon_{xx}^{(4)} \varepsilon_{xx}^{(5)} \varepsilon_{xx}^{(6)} \\ \varepsilon_{yy}^{(1)} \varepsilon_{yy}^{(2)} \varepsilon_{yy}^{(3)} \varepsilon_{yy}^{(4)} \varepsilon_{yy}^{(5)} \varepsilon_{yy}^{(6)} \\ \varepsilon_{zz}^{(1)} \varepsilon_{zz}^{(2)} \varepsilon_{zz}^{(3)} \varepsilon_{zz}^{(4)} \varepsilon_{zz}^{(5)} \varepsilon_{zz}^{(6)} \\ \gamma_{yz}^{(1)} \gamma_{yz}^{(2)} \gamma_{yz}^{(3)} \gamma_{yz}^{(4)} \gamma_{yz}^{(5)} \gamma_{yz}^{(6)} \\ \gamma_{zx}^{(1)} \gamma_{zx}^{(2)} \gamma_{zx}^{(3)} \gamma_{xy}^{(4)} \gamma_{yz}^{(5)} \gamma_{yz}^{(6)} \\ \gamma_{zz}^{(1)} \varepsilon_{zx}^{(2)} \varepsilon_{zz}^{(3)} \varepsilon_{zz}^{(4)} \varepsilon_{zz}^{(5)} \varepsilon_{zz}^{(6)} \\ \varepsilon_{31}^{(1)} S_{32}^{(2)} S_{33}^{(3)} S_{34}^{(4)} S_{35}^{(5)} S_{36}^{(6)} \\ S_{41}^{(1)} S_{42}^{(2)} S_{43}^{(3)} S_{44}^{(4)} S_{45}^{(5)} S_{46}^{(6)} \\ s_{51}^{(1)} S_{52}^{(2)} S_{53}^{(3)} S_{54}^{(4)} S_{55}^{(5)} S_{56}^{(6)} \\ s_{61}^{(1)} S_{62}^{(2)} S_{63}^{(3)} S_{64}^{(4)} S_{55}^{(5)} S_{66}^{(6)} \\ \varepsilon_{51}^{(1)} S_{52}^{(2)} S_{53}^{(3)} S_{54}^{(4)} S_{55}^{(5)} S_{56}^{(6)} \\ \varepsilon_{61}^{(1)} S_{62}^{(2)} S_{63}^{(3)} S_{64}^{(4)} S_{55}^{(5)} S_{66}^{(6)} \\ \varepsilon_{61}^{(1)} S_{62}^{(2)} S_{63}^{(3)} S_{64}^{(4)} S_{65}^{(5)} S_{66}^{(6)} \\ \varepsilon_{61}^{(1)} S_{61}^{(2)} S_{61}^{(3)} S_{61}^{(4)} S_{61}^{(5)} S_{61}^{(5)} S_{61}^{(5)} \\ \varepsilon_{61}^{(1)} S_{61}^{(2)} S_{61}^{(3)} S_{61}^{(4)} S_{61}^{(5)} S_{61}^{(5)} S_{61}^{(5)} \\ \varepsilon_{61}^{(1)} S_{61}^{(2)} S_{61}^{(3)} S_{61}^{(5)} S_{61}^{(5)} S_{61}^{(5)} S_{61}^{(5)} S_{61$$

- 6 linearly independent B.C. 3D
- 3 linearly independent B.C. 2D

Example - Rock Mass Determination Methodology









 $\begin{bmatrix} \varepsilon_{xx}^{(1)} & \varepsilon_{xx}^{(2)} & \varepsilon_{xx}^{(3)} \\ \varepsilon_{yy}^{(1)} & \varepsilon_{yy}^{(2)} & \varepsilon_{yy}^{(3)} \\ \gamma_{xy}^{(1)} & \gamma_{xy}^{(2)} & \gamma_{xy}^{(3)} \end{bmatrix}^{-} \begin{pmatrix} S_{13} \\ S_{23} \\ S_{63} \end{pmatrix} \begin{pmatrix} \sigma_{zz}^{(1)} & \sigma_{zz}^{(2)} & \sigma_{zz}^{(2)} \end{pmatrix}^{-} = \begin{pmatrix} S_{11} & S_{12} & S_{16} \\ S_{21} & S_{22} & S_{26} \\ S_{61} & S_{62} & S_{66} \end{pmatrix} \begin{pmatrix} \sigma_{xx}^{(1)} & \sigma_{xx}^{(2)} & \sigma_{xy}^{(3)} \\ \sigma_{yy}^{(1)} & \sigma_{yy}^{(2)} & \sigma_{yy}^{(3)} \\ \sigma_{xy}^{(1)} & \sigma_{xy}^{(2)} & \sigma_{xy}^{(3)} \end{pmatrix}$ $[\varepsilon] - [S_{z}] [\sigma_{z}] = [S] [\sigma]$ $[\varepsilon] [\sigma]^{-1} - [S_{z}] [\sigma_{z}] [\sigma]^{-1} = [S]$



In 2D plane strain condition, 6 elastic constants are determined.

Example - Rock Mass Determination Methodology - Verification





Example - Rock Mass Determination Data from Forsmark, Sweden





- Forsmark and Oskarshamn, two candidate sites for Swedish Program.
- 2002-2009: site investigation.
- 2009: Forsmark, as the final site
- 2011: License application
- 2014: decision (?)
- 2025: Operation (?)

Map of Sweden

Example - Rock Mass Determination E mass results (elastic modulus from Forsmark)





Elastic moduli ↑ with stress ↑ - highly stress-dependent

Stress induced anisotropy - $E_h 20\%$ higher than E_v in shallow depth

Effect of stress is more evident in low stress condition.

(Min, Jing & Stephansson, 2005)

Explicit DEM in Blocky System Example – Stress state modeling (Min, 2009)

•



500 -

deep repository

hedrock



Example – Stress state modeling Geometry





Example – Stress state modeling Boundary Condition





Example – Stress state modeling Mesh generation







Example – Stress state modeling Results - Predicted vs. Measured stress (KLX04)





Intermediate principal stress (MPa), KLX04 Measured x modeled X Depth (m) **Intermediate Principal Stress** X

Numerically predictions capture the dramatic change of in situ stress

(Min, 2009)

Example - Stress-dependent permeability (Min et al., 2004)



Example - Stress-dependent permeability (Min et al., 2004) - Results





- Deformation of aperture occur uniformly
- Normal closure is dominating the k_x,k_y change





Example - Stress-dependent permeability (Min et al., 20 Results - Implications



Enhanced Geothermal System Hydrofrac for shale gas reservoir

Increased hydraulic pressure → hydraulic stimulation →
bir HYDROSHEARING

A few words for application of DEM



- Start from very very simple model when you do complicated modeling try to gain insight into the implemented physics & constitutive equation of code
- Modeler should be able to explain every bit of observation numerical code is not a black box!
- There can be many many interesting applications you are encouraged to apply DEM to novel applications
- There are much rooms for improvement in DEM development

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