How you like DEM apples

EGEE 520

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PennState

What is DEM

- Discrete Element Method
  - Particle Based
  - Explicit Time Steps

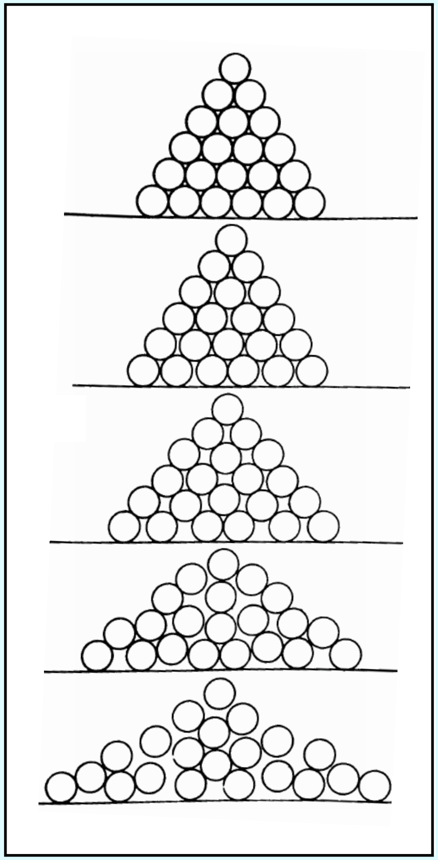
- Useful for:
  - Modeling Movement of Individual Particles
  - Rotation of Particles
  - Time Steps
  - Progressive Failure

- Not Useful for:
  - Complex Particle Geometries and Arrangements
  - Roughness, Texture
  - Grain Crushing, Particle Breakage
  - Non-Idealized Contacts

Historical perspective

- First developed by Cundall in his 1971 thesis- "A computer model for simulating progressive large-scale movements in blocky rock systems"
  - Modeled the movement of particles as a collapse of cylinders and toppling of blocks

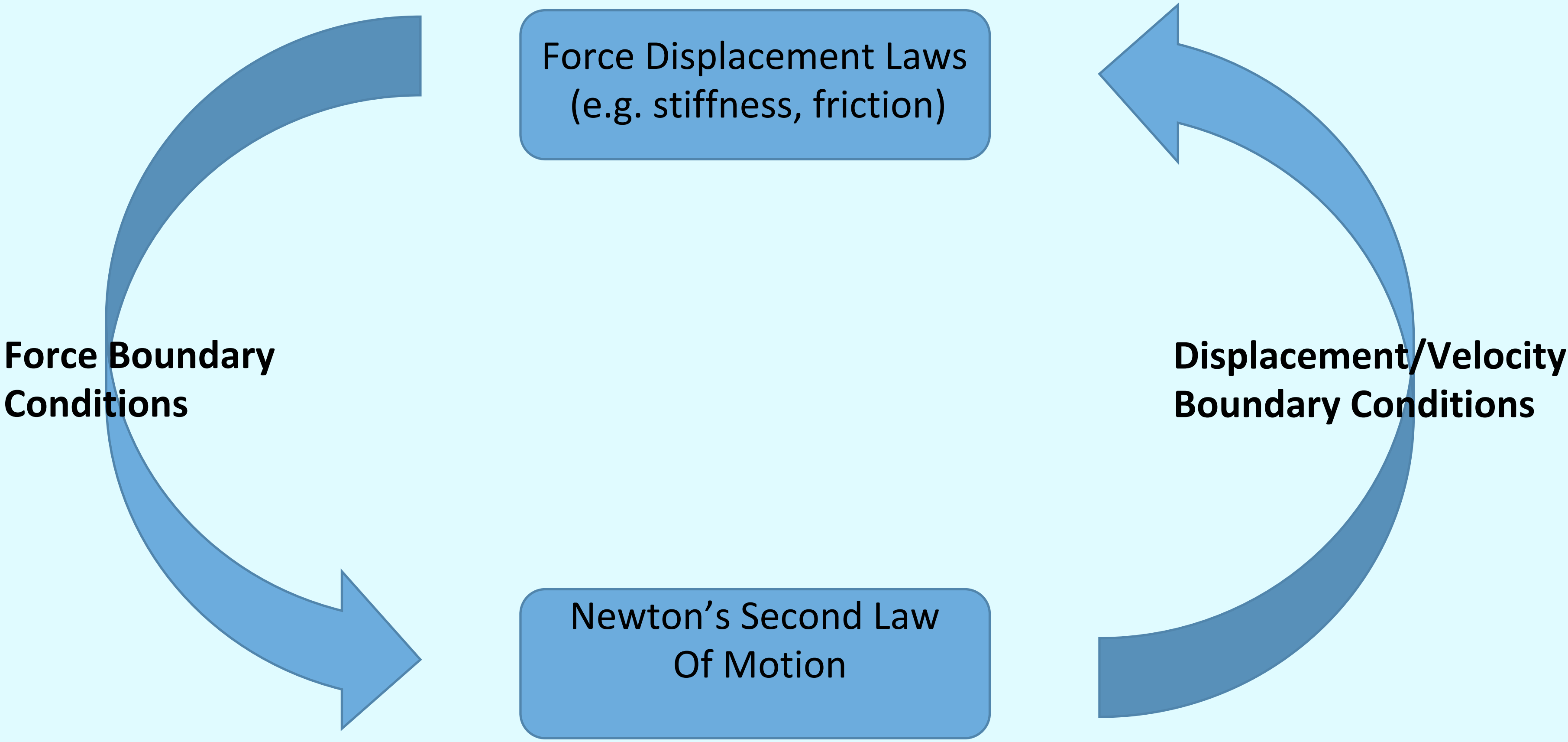
- Modified into a RBM (restricted Boltzmann machines) code (Cundall 1974), FORTRAN code (Cundall 1978), and a 3D model including fluid and pore pressure (Cundall and Hart 1985)



- Current Uses:
  - Agriculture
  - Food Transport
  - Pharmaceutical
  - Civil Engineering
  - Powder Metallurgy
  - Chemical Engineering

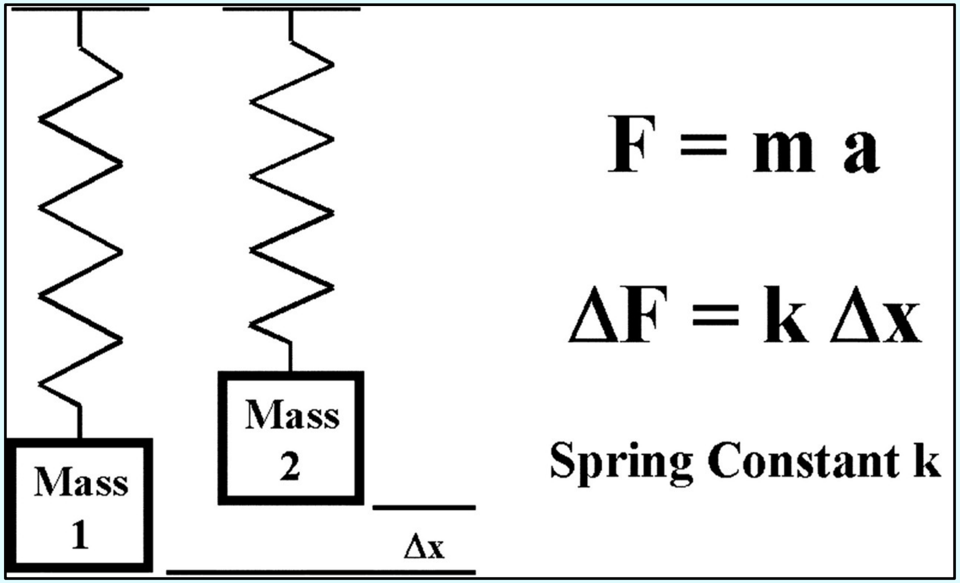
General Principles

- Newton’s Second Law of Motion
- Force Displacement Law

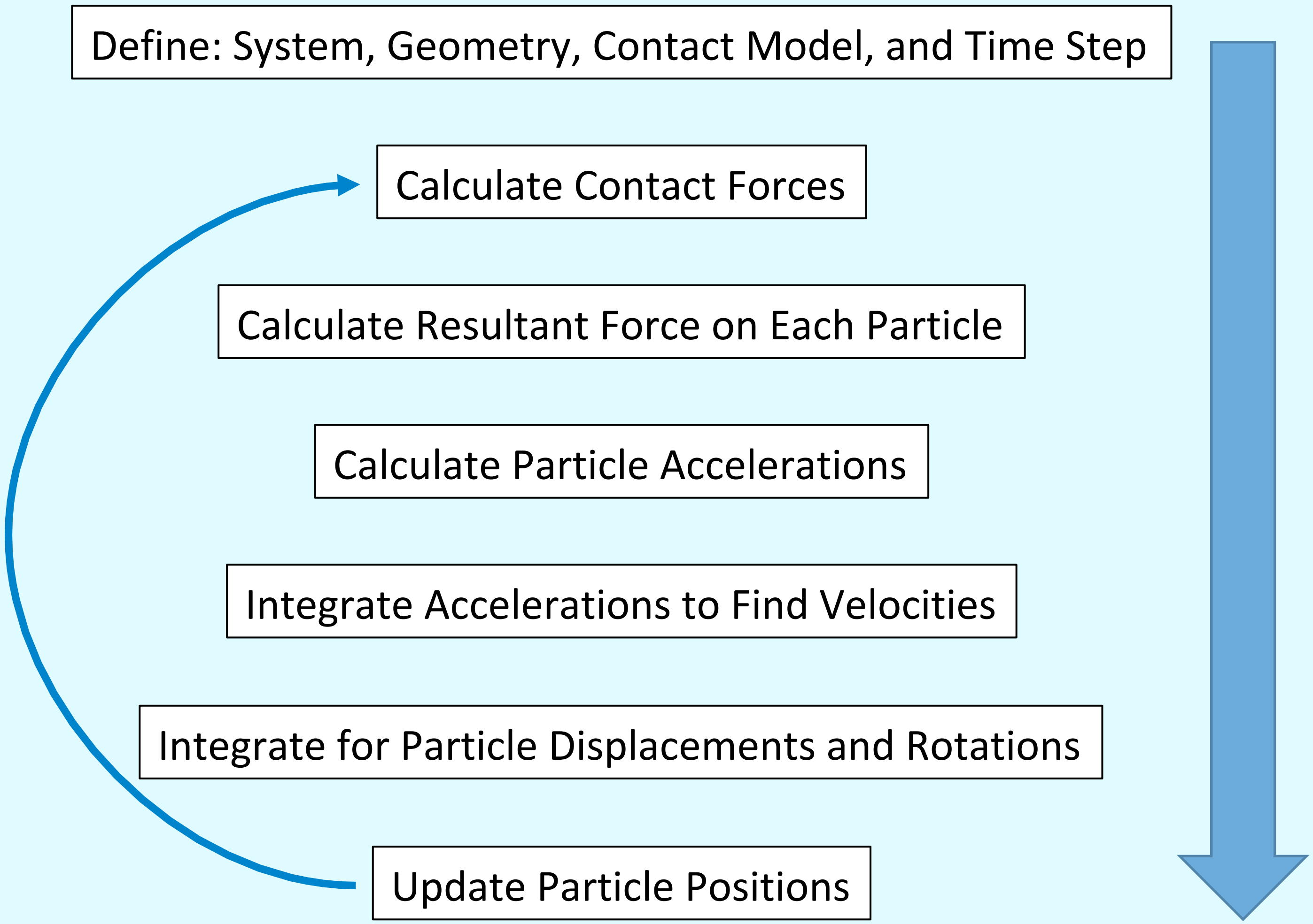


Governing Equations

- DEM uses two types of governing laws:
- Force-Displacement Law
  - Hooke's law, friction etc…
- Newton's Second Law of Motion
  - F=MA
- Time Step
  - Discrete
  - Critical Time Step



DEM Process Flow



Hand Calculation

Time Step

$\Delta T=\sqrt{(M/K)}$

Forces on Grains

$\Delta F_n = K_n(\Delta n)_{t1} = K_n(V)(\Delta t)$

Newton's Second Law

$F=ma$

$\ddot{X}=F_{(x)}/m$

Integrate to find velocity

$\dot{X}_{t2} = (F_x/m)\Delta t$

Integrate again to find relative displacements

$(\Delta n_{(A)})_{t2} = (v-[F_{(x)}/m]\Delta t)\Delta t$

$(\Delta n_{(B)})_{t2} = ([F_{(x)}/m_{(x)}]\Delta t - [F_{(y)}/m_{(y)}]\Delta t)\Delta t$

$(\Delta n_{(C)})_{t2} = ([F(y)/m(y)]\Delta t-[-v])\Delta t$

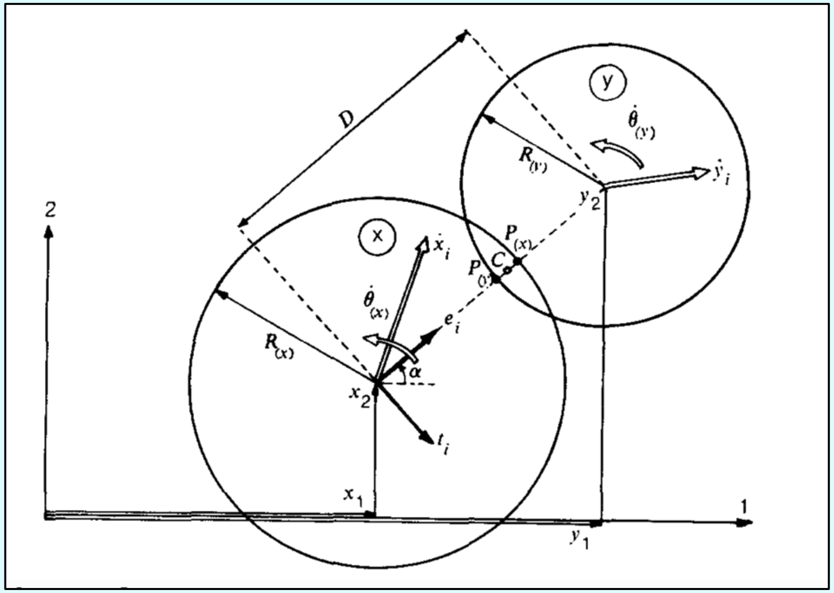
Realistic Grain Orientation

Unit Vector-Normal Direction

$e_i = (y_i - x_i)/D = (\cos\alpha, \sin\alpha)$

Shear Direction

$t_i = (e_2, -e_1)$



Velocity:

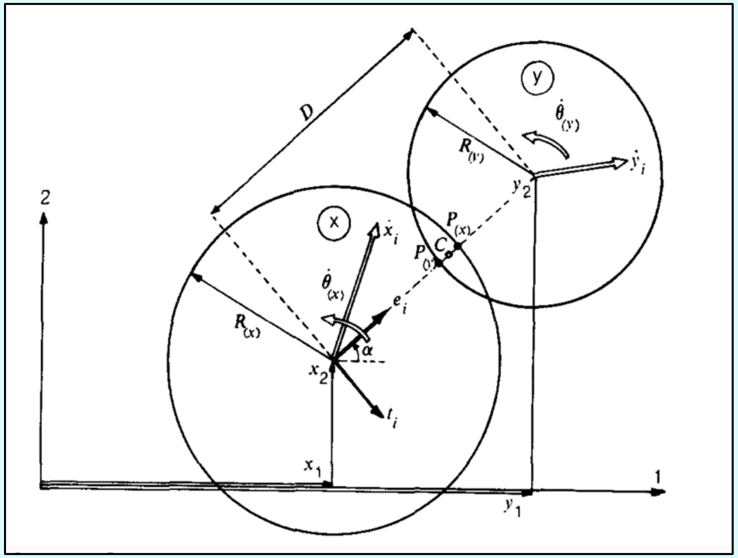
$\dot{X}_i = (\dot{x}_i - \dot{y}_i) - (\dot{\theta}_{(x)} R_{(x)} + \dot{\theta}_{(y)} R_{(y)}) t_i$

Velocity Components:

$\dot{n} = \dot{X}_i e_i = (\dot{x}_i - \dot{y}_i) e_i - (\dot{\theta}_{(x)} R_{(x)} + \dot{\theta}_{(y)} R_{(y)}) t_i$

$\dot{s} = \dot{X}_i t_i = (\dot{x}_i - \dot{y}_i) t_i - (\dot{\theta}_{(x)} R_{(x)} + \dot{\theta}_{(y)} R_{(y)}) t_i t_i$

Putting it all Together



Force-Displacement

$\Delta F_n = K_n(\Delta n)_{t1}$

$= K_n(V)(\Delta t)$

$= K_n[(\dot{x}_i - \dot{y}_i)e_i]\Delta t$

$\Delta F_s = K_s[(\dot{x}_i - \dot{y}_i)t_i - (\dot{\theta}_{(x)} R_{(x)} + \dot{\theta}_{(y)} R_{(y)})\Delta t$

Force Increment Sum

$(F_n)_N = (F_n)_{N-1} + \Delta F_n$; $(F_s)_N = (F_s)_{N-1} + \Delta F_s$

Failure

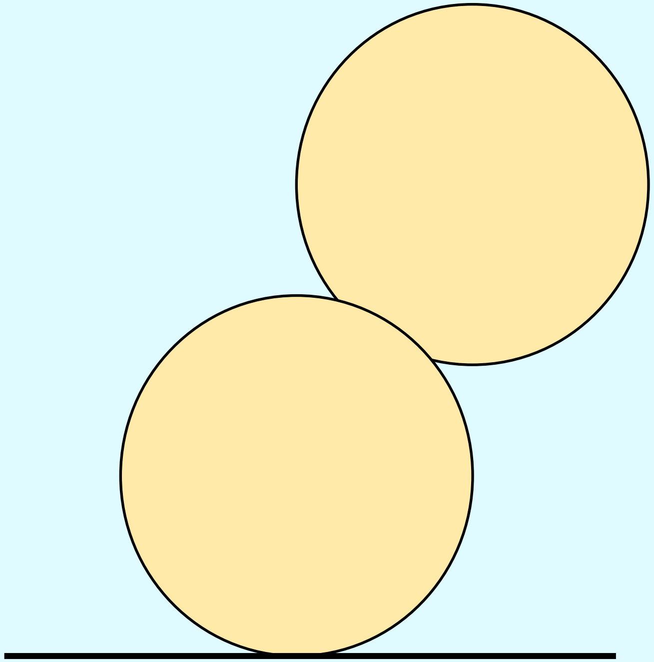
$(F_s)_{max} = F_n \tan\Phi_\mu + c$

Damping-Contact

$C_n = \beta K_n$; $C_s = \beta K_s$

Damping-Global

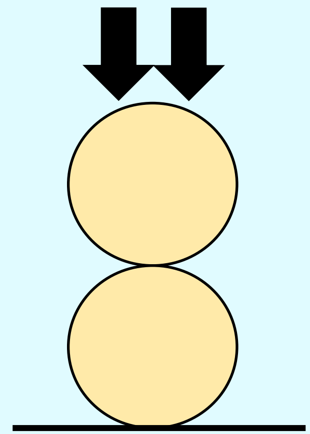
$C = \alpha m_{(x)}$; $C^* = \alpha I_{(x)}$

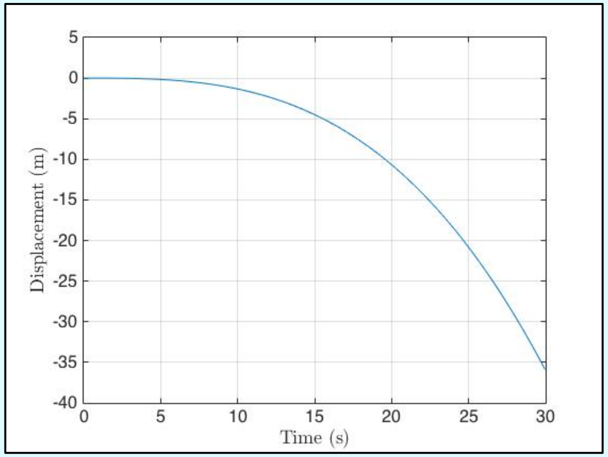


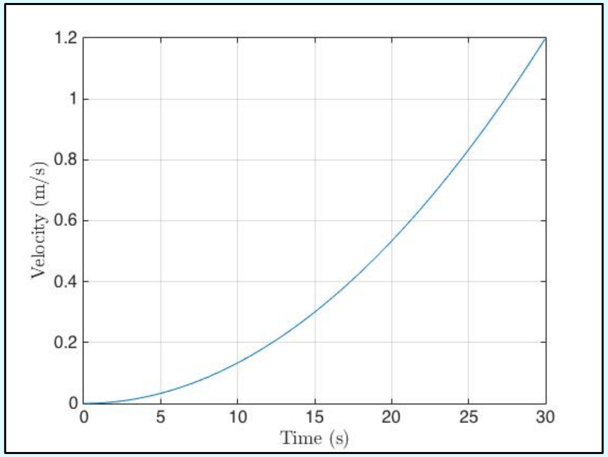
Numerical Model

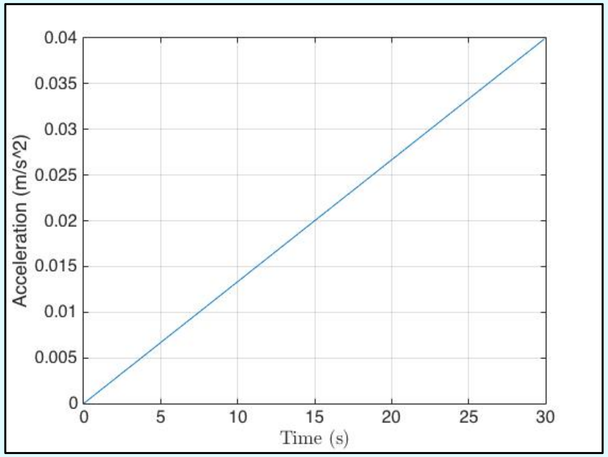
Input:

- Stiffness:
  - K=0.002N/m
- Mass
  - 1.5e-5kg
- Time Step
  - 0.08s
- Velocity-initial
  - 1e-5m/s
- Radius
  - 0.001m









Output:

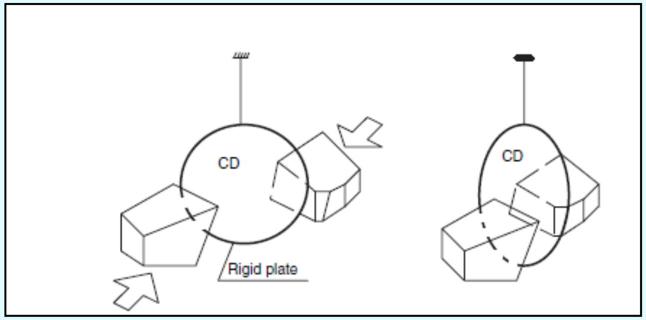
Time (s)	Displacement (m)	Velocity (m/s)	Acceleration (m/s^2)
0.1732	-5.20E-06	4.00E-05	2.31E-04
15.0688	-4.5621	0.3028	0.0201
29.7047	-34.947	1.1765	0.0396

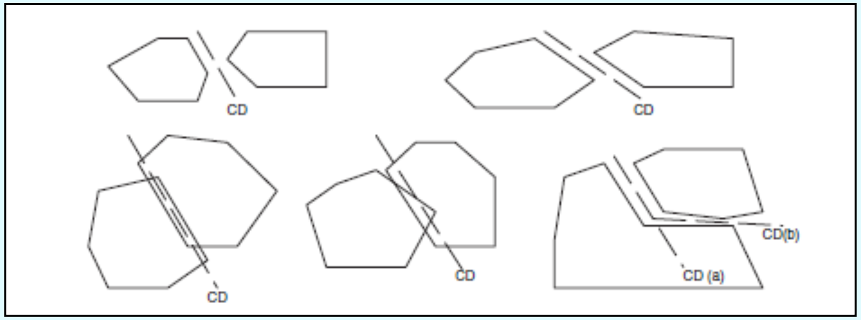
Other Approaches

- Varying Contact Types
- Utilize Thousands of Grains
- Propagation and Mechanics of Fractures

Table 8.2 Types of contacts for 2D polygons and 3D polyhedral blocks

Block shape	Contact type
General 2D polygons (convex or concave, singly or multiply connected)	Vertex-to-vertex Vertex-to-edge Edge-to-edge
Convex 3D polyhedra	Vertex-to-vertex Vertex-to-edge Vertex-to-face Edge-to-edge Edge-to-face Face-to-face





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Open Source DEM Programs

LIGGGHTS

ESyS-Particle

Newton

EDEM®

eLearning

Input Parameters

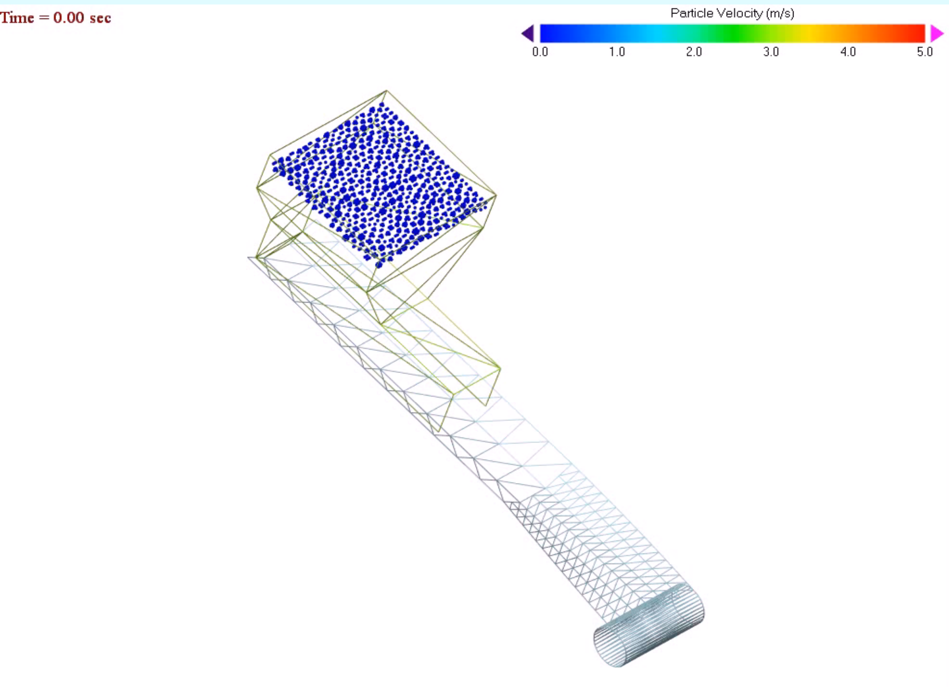
Wet Particles

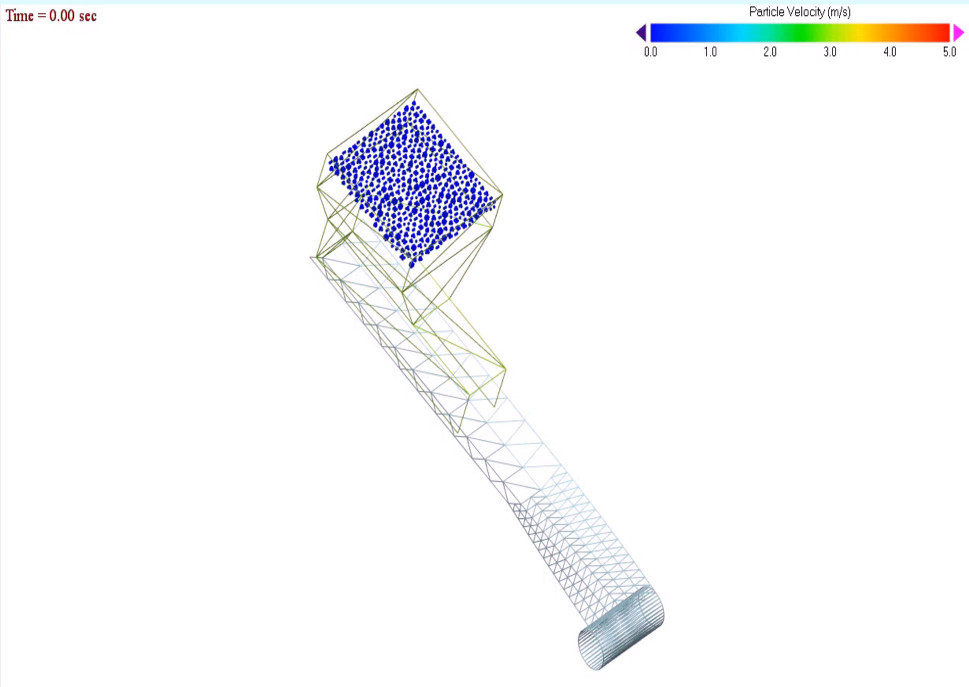
General Properties	A
Particle-Particle Friction Coefficient (0-1)	0.85
Particle-Boundary Friction Coefficient (0-1)	0.75
Coefficient of Restitution (0.075-1)	0.100
Rotational Damping (0-10)	1.00
Ratchet Effect	
Use Ratchet Effect	YES
Particle-Particle Cohesion Factor (0-0.25)	0.150
Particle-Boundary Cohesion Factor (0-0.25)	0.150
Liquid Bridge	
Use Liquid Bridge	YES
Surface Tensions (0.05 - 0.50 J/m²)	0.50
Water Content (%)	15.0
Boundary Surface Tension Multiplier (0-10)	2.00
Equivalent Sphere Size Ratio	15.00

Dry Particles

General Properties	A
Particle-Particle Friction Coefficient (0-1)	0.30
Particle-Boundary Friction Coefficient (0-1)	0.20
Coefficient of Restitution (0.075-1)	0.150
Rotational Damping (0-10)	2.00
Ratchet Effect	
Use Ratchet Effect	NO
Particle-Particle Cohesion Factor (0-0.25)	
Particle-Boundary Cohesion Factor (0-0.25)	
Liquid Bridge	
Use Liquid Bridge	NO
Surface Tensions (0.05 - 0.50 J/m²)	
Water Content (%)	
Boundary Surface Tension Multiplier (0-10)	
Equivalent Sphere Size Ratio	

Animation Results

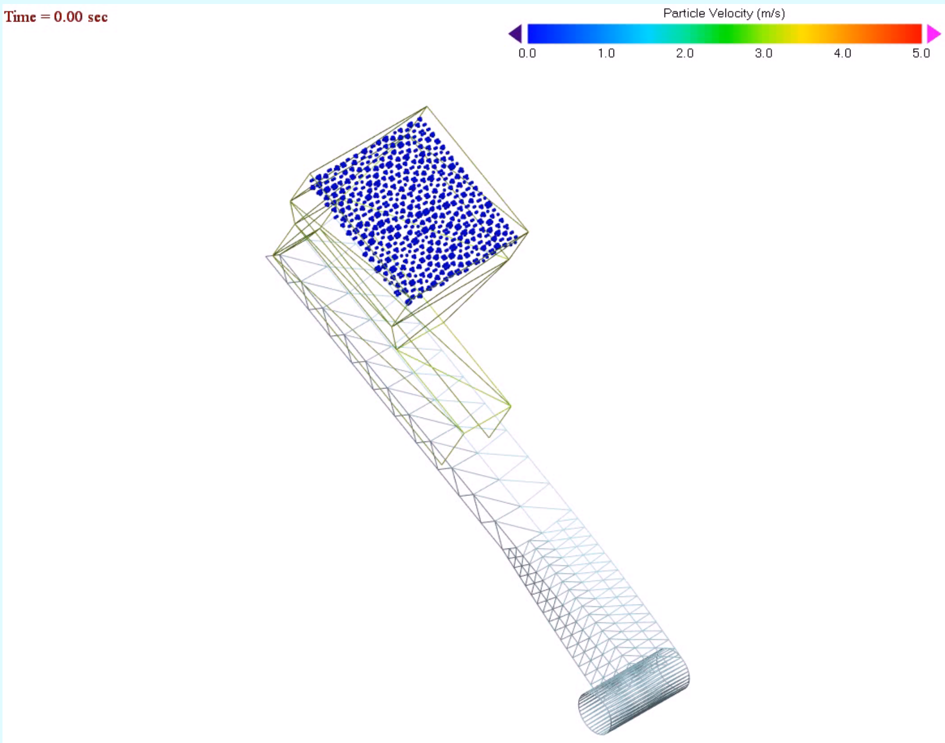




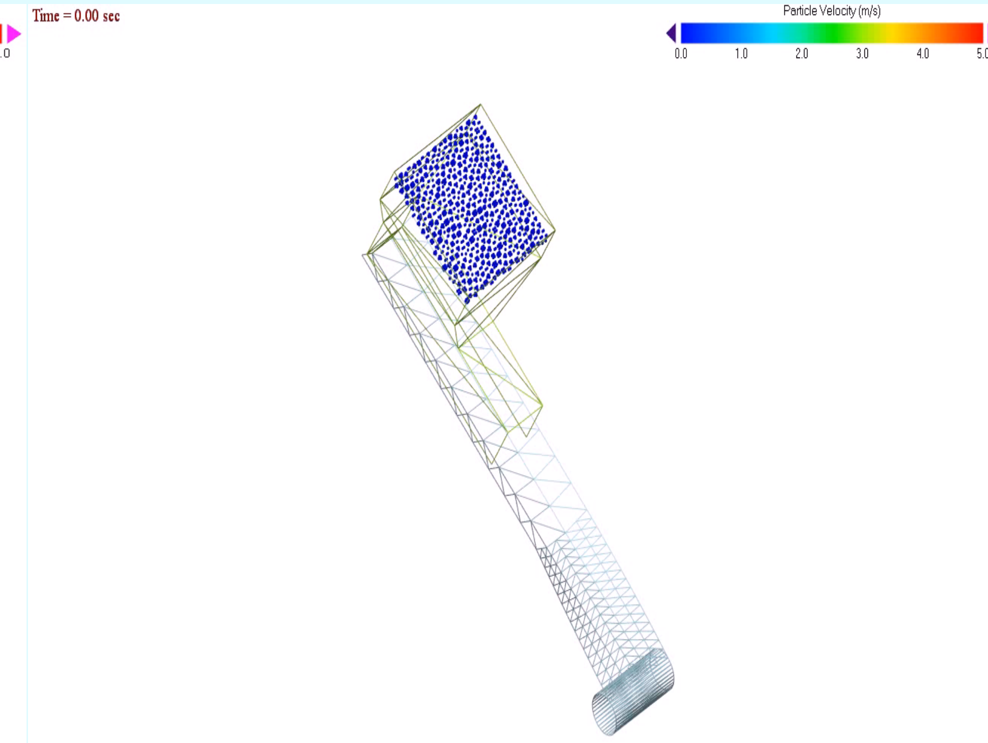
Dry particles on 20^{o} decline

Wet particles on 20^{o} decline

Animation Results



Dry particles on 30↑*o* decline



Wet particles on 30↑*o* decline

Example Animations

L-shaped box and Funnel

Bruising on Pears

Fault Motion

Thank You!